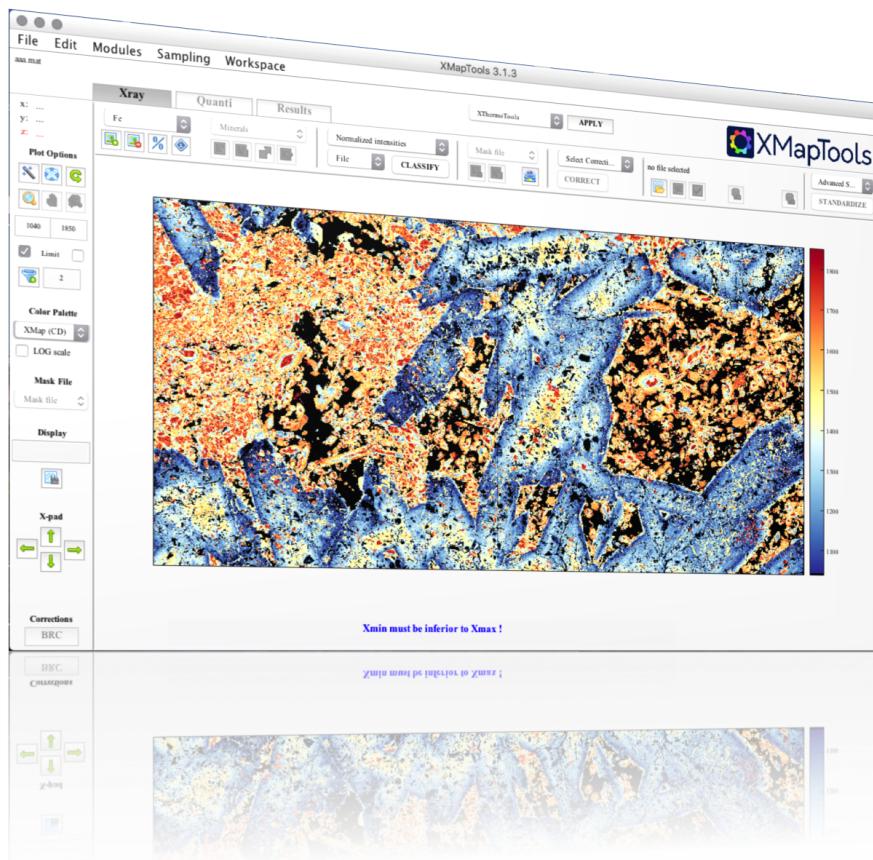


Prof. Dr. Pierre Lanari

An introduction to XMapTools 3.4

numerical tools for quantitative petrology ¹



INSTITUTE OF GEOLOGICAL SCIENCES
UNIVERSITY OF BERN

¹ Lanari, P. (2020) An introduction to XMapTools. *User-guide*, version 2020-6-10

Bern, Wednesday 10th June, 2020

Dear user,

It is a pleasure to introduce XMAPTOOLS 3.4, a sophisticated software solution providing advanced numerical tools in a guided environment to explore and visualize compositional maps. I initiated the XMAPTOOLS project in 2009 and the first public version was released in October 2012. In the past height years, XMAPTOOLS has evolved continuously. It now incorporates a large variety of options for data processing, data calibration and data visualization via single and multi-channel maps or via binary, ternary and spider diagrams and add-ons. The extension XTHERMOTOOLS for example implement the program BINGO-ANTIDOTE and allows iterative thermodynamic models to be computed based on compositional maps. XMAPTOOLS is an on-going product of research that I develop on a weekly basis. These are collected and provided to you via public updates twice a year.

This user guide aims to assist you and to give you the better experience possible with XMAPTOOLS. However, before to dive deeper into the details and see how each part of the program works, it is important to acknowledge those who actively participated in testing XMAPTOOLS; The software developments were and are still largely inspired by users, thank you!

Pierre Lanari

XMAPTOOLS HISTORY

XMAPTOOLS 3.X (2019-present) has been developed by Pierre Lanari at the University of Bern (Institute of Geological Sciences).

XMAPTOOLS add-ons:

- XTHERMOTOOLS (2015-present) has been developed by Pierre Lanari and Erik Duesterhoeft
- STACKMAPS (2019-present) has been developed by Julien Reynes and Pierre Lanari

XMAPTOOLS 2.X (2014-2019) was developed by Pierre Lanari at the University of Bern (Institute of Geological Sciences). The reduction schemes for LA-ICP-MS data were developed in collaboration with Tom Raimondo.

XMAPTOOLS 1.X (2009-2014) was developed by Pierre Lanari at the University of Grenoble (IS-Terre) with support from Olivier Vidal and Éric Lewin and largely inspired by previous work made by Vincent de Andrade and Benoit Dubacq.

ACKNOWLEDGEMENTS

I would like to thank M. Engi, J. Hermann, D. Rubatto, M. Burn, J. Reynes, A. Vho, M. Tedeschi, E. Kempf, T. Bovay, F. Giuntoli and A. Berger (University of Bern) O. Vidal, A.-M. Boullier, A. Verly, B. Gardonio, F. Bernier, L. Airaghi, E., Lewin, S. Guillot, S. Schwartz, M. Munoz, E. Janots, K. Malamoud, J. Braun, (ISTerre Grenoble) N. Riel (University of Mainz) C. Loury, Y. Rolland (GeoAzur Nice) T. Raimondo (University of South Australia) E. Duesterhoeft and R. Bousquet (Kiel University) C. Martin (American Museum of Natural History) E. Grosch (University of Bergen) C. de Capitani, L. Frantz (University of Basel) A. Pourteau, R. Oberhänsli (University of Potsdam) S. Centrella (University of Münster) F. Guillot, M. Dupuis (Université de Lille) A. Robert (Université de Toulouse) B. Dubacq, P. Agard, M. jentzer (ISTEP Paris) V. De Andrade (NSLS II Brookhaven) M. Zucali (University of Milano) D. Waters (University of Oxford) G. Ortolano (Catania University) C. R. Cioffi (University of São Paulo) and all participants of the PETROCHRO workshops for help, suggestions, comments, data and/or collaborations to develop and test XMAPTOOLS.

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INTRODUCTION

1

1.1 XMAPTOOLS PROGRAM

XMAPTOOLS is a MATLAB®-based graphic user interface (GUI) software for processing of compositional maps such as X-ray maps from electron microprobe or element concentration maps from LA-ICP-MS. XMAPTOOLS aims to make the treatment of such data easy with a large set of general functions that import and standardize the semi-quantitative data, calculate structural formulae as well as metamorphic and magmatic pressure and temperature estimates.

Many additional processing tools have been developed over the years and the software has frequently been updated. XMAPTOOLS' website (<https://www.xmaptools.com>) is available and provides the latest version of the software including online updates with additional tools, add-ons, user guide and a tutorial.

XMAPTOOLS software ([Lanari et al. 2014b](#)) uses a Castaing-like approach ([De Andrade et al. 2006](#), [Lanari et al. 2019](#)) to standardize semi-quantitative X-ray map data from electron microprobe analyses into maps of mineral oxide composition. High precision spot analyses are used as internal standards. Chemical groups corresponding to the mineral phases and other entities are separated using a K-means statistical approach (automated classification). From maps of element oxide composition, it is possible to estimate local bulk compositions of the mapped area or of a selected local micro-domain. One of the main advantages of XMAPTOOLS is that it can calculate mineral compositions, structural formulae and phase equilibrium conditions, such as pressure and temperature, at each pixel. This permits a detailed textural interpretation of recorded physico-chemical conditions on a micro-scale. Various geothermometers or geobarometers are provided in the program (about 50 functions are available) and it is straightforward to add his own calibrations into the software using the external function module. In addition, binary and ternary chemical diagrams can be plotted using the modules BINARY and TRIPLOT3D. These modules may be used to identify chemical variations and to define groups of composition. XMAPTOOLS can also be used to obtain local bulk compositions to be used for thermodynamic modelling ([Lanari and Engi 2017](#), [Lanari and Duesterhoeft 2019](#)).

1.2 CITATION GUIDELINES

Please use the following citations in your publications when you refer to XMAPTOOLS. The version of the program must be specified after the name. Example: *Mapping data were processed using XMAPTOOLS 3.3.1 (Lanari et al. 2014; 2019)*

Please use at least one of the official XMAPTOOLS logo ([available here](#)) in your talk / poster along with the references while figures have been generated using XMAPTOOLS.

Main software references:

- LANARI, P., VHO, A., BOVAY, T., AIRAGHI, L., CENTRELLA, S., (2019). Quantitative compositional mapping of mineral phases by electron probe micro-analyser. *Geological Society of London, Special Publication*, 478, 39-63
- LANARI, P., VIDAL, O., DE ANDRADE, V., DUBACQ, B., LEWIN, E., GROSCH, E., SCHWARTZ, S., 2014. XMAPTOOLS: a MATLAB®-based program for electron microprobe X-ray image processing and geothermobarometry. *Computers and Geosciences*, 62, 227-240

Local bulk compositions; density correction; applications for thermodynamic modeling:

- LANARI, P., ENGI, M., 2017. Local bulk composition effects on metamorphic mineral assemblages. *Reviews in Mineralogy and Geochemistry*, 83, 55-102
- LANARI, P. & DUESTERHOF, E. 2019. Modelling metamorphic rocks using equilibrium thermodynamics and internally consistent databases: past achievements, problems and perspectives. *Journal of Petrology*, 60, 19-56

Trace element mapping:

- RAIMONDO, T., PAYNE, J., WADE, B., LANARI, P., CLARK, C., HAND, M., 2017. Trace element mapping by LA-ICP-MS: assessing geochemical mobility in garnet. *Contributions to Mineralogy and Petrology*, 172, 17

Density maps:

- CENTRELLA, S., PUTNIS, A., LANARI, P., AUSTRHEIM, H. 2018. (2018). Textural and chemical evolution of pyroxene during hydration and deformation: a consequence of retrograde metamorphism. *Lithos*, 296-199, 245-264

Mapping technique:

- LANARI, P., VHO, A., BOVAY, T., AIRAGHI, L., CENTRELLA, S., (2018). Quantitative compositional mapping of mineral phases by electron probe micro-analyser. *Geological Society of London Special Publication*, DOI:10.1144/SP478.4
- DE ANDRADE, V., VIDAL, O., LEWIN, E., O'BRIEN, P., AGARD, P., 2006. Quantification of electron microprobe compositional maps of rock thin sections: an optimized method and examples. *Journal of Metamorphic Geology*, 24, 655-668.

Selected application examples: [Lanari et al. \(2012\)](#), [Pourteau et al. \(2013\)](#), [Martin et al. \(2013\)](#), [Lanari et al. \(2013; 2014b;a\)](#), [Trincal et al. \(2015\)](#), [Loury et al. \(2016\)](#), [Mészáros et al. \(2016\)](#), [Scheffer et al. \(2016\)](#), [Elmola et al. \(2017\)](#), [Airaghi et al. \(2017b;a\)](#), [Lanari and Engi \(2017\)](#), [Lanari et al. \(2017\)](#), [Raimondo et al. \(2017\)](#), [Engi et al. \(2018\)](#), [Laurent et al. \(2018\)](#), [Leydier et al. \(2019\)](#), [Santamaría-López et al. \(2019\)](#), [Airaghi et al. \(2019\)](#)

Note: XMAPTOOLS is a free software for scientists working in Universities and Public Research Agencies worldwide (see [1.3](#)). Software has become a critical part of modern research and yet there is little support across the Academic ecosystem for its acknowledgement and citation. We believe that scientific software developed by academics should be considered a legitimate and citable product of research. The developments of XMAPTOOLS are part of a research effort that includes costs not supported by the users. Users of XMAPTOOLS need to understand that citations are the only form of reward that directly support the software development. Please, cite XMAPTOOLS in your publications and mention his use in your presentations.

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Please, if you are a commercial institution, take the time to read at least the [Scientific Software Open Source Academic For Free License](#). And you will realise that this is exactly the policy and the philosophy that can work to conciliate your way of functioning and the normal behaviour of academic research. Such as everybody can profit of the exchange between the two worlds.

1.4 SPECIAL LICENSE FOR ADD-ONS

XMAPTOOLS' add-ons are generally distributed under MIT LICENSE (see the license file provided with each add-on).

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1.5 WHAT TUTORIAL SHOULD I FOLLOW FIRST?

Well, it mostly depends what you want to learn!

There are three guided tutorials provided with XMAPTOOLS:

1. **Tutorial 1: EPMA data processing (Central Alps - 2013)** (see chapter [7](#)) is designed for users who want to learn more about the main functionalities and features of XMAPTOOLS. This tutorial introduces most of the basic tools and gives you several examples of classification and standardization (for both in automated and manual modes). The mapping data of this *complicated case* allows some limits of the program to be discussed along with alternative strategies.
2. **Tutorial 2: EPMA data processing (Himalaya - 2020)** (see chapter [8](#)) is designed for new users who want to briefly discover the data reduction procedure for EPMA data implemented in XMAPTOOLS. This tutorial will guide you through the main steps for a *simple case*.
3. **Tutorial 3: Iterative thermodynamic modeling using XThermoTools and Bingo-Antidote (Himalaya - 2020)** (see chapter [9](#)) is designed to introduce the modeling extension XTHERMOTOOLS containing the program BINGO-ANTIDOTE. This tutorial is a continuation of Tutorial 2.

1.6 ANALYTICAL PROCEDURE (ELECTRON MICROPROBE)

If you want to acquire high-quality X-ray maps for quantitative analysis, we recommend you to follow the procedure given in [Lanari et al. \(2019\)](#). The analytical session is classically divided into two parts: (1) semi-quantitative compositional mapping via X-ray maps and (2) in-situ spot analyses of mineral compositions used to calibrate the X-ray maps. The section below briefly outlines some important aspects of this analytical procedure along with recommended electron microprobe operating conditions.

The following sections briefly outline some important aspects of this analytical procedure along with recommended electron microprobe operating conditions.

1.6.1 Micro-mapping

The acquisition of X-ray images must be performed using wavelength dispersive spectrometers (WDS) at specific wavelength of the considered elements. As there are only four or five WDS in modern electron microprobes, the acquisition is typically realized in two passes that can include at least 8-10 elements. The order of the acquisition is of first importance. The electron beam may cause local diffusion of light elements such as Na, K and Ca, therefore, these elements must be measured during the first pass.

The acceleration voltage is fixed at 15 KeV for major elements and 20 KeV for trace elements measurements. Beam current is typically fixed at 100 nA for major element analysis and can be increased up to 900 nA for some low concentration element analyses such as Pb, Th or U. Of course high values of current can be used only if the microprobe is able to reach and stabilize such high currents. For major element analysis and common silicates minerals, the optimal conditions for a good precision are 15 KeV accelerating voltage, 100 nA beam current and 200 ms dwell time ([Lanari et al. 2014b](#)).

Diffusion and volatilization of light elements: Light elements such as K or Na might volatilize or diffuse when working with a high-intensity electronic beam. [De Andrade et al. \(2006\)](#) showed that 100 nA current with dwell times of 50 ms do not affect the compositions of common K-bearing silicate minerals such as white mica. The effect of the high-intensity electronic beam in mapping condition may be easily tested by mapping a couple of times a small area with the same analytical conditions and by comparing the results with XMAPTOOLS. This test has been done using a JEOL-8200 microprobe at the Institute of Geological Sciences (University of Bern) on a meta-quartzite from the Western Alps (Marco Burn's thesis). A small area of $80 \times 120 \mu\text{m}^2$ containing plagioclase (albite), quartz and K-white mica (phengite) was analyzed using 15 KeV accelerating voltage, 200 nA specimen current and dwell time of 200 ms.

Si maps do not show any difference, excepted for some grain boundaries between quartz and phengite (white arrows in Fig. 1.1, top). Such small and localized differences can be explained by slight changes of the position of the mapped area of about $1\mu\text{m}$. The same feature is visible in the Al maps (white arrows in Fig. 1.1, bottom). This effect caused by the low precision (of about $1\mu\text{m}$) of the position of the sample holder.

In contrast, maps of Na and K show strong variations of their number of counts with time (Fig. 1.2). Na and K intensity variations are shown by pixels of plagioclase and phengite respectively. The volatilization of Na in plagioclase is quite visible in the second map. The pixels of this map show between 30 and 40% less counts than those of the first map. During the third pass Na in plagioclase is almost gone. Maps of K show the same effect of volatilization with a decrease of the number of counts with the successive maps. However in the case of K the decrease is smaller with only 50-60% of counts lost after 5 passes.

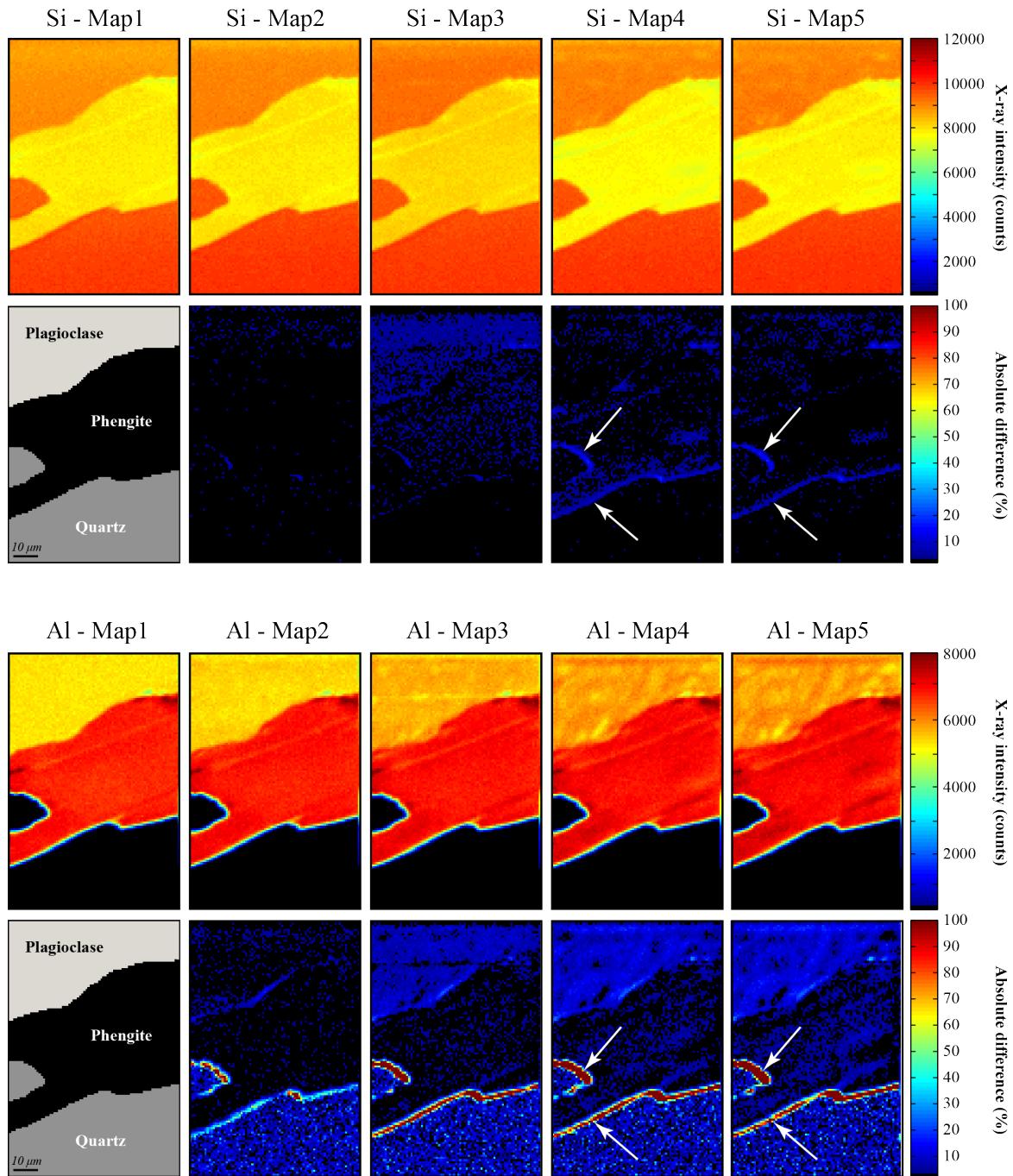


Figure 1.1 – X-ray maps Si (top) and Al (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating voltage was 15 KeV, specimen current 200 nA, dwell time 200 ms and the beam size 1 μm . The studied sample is a meta-quartzite coming from the Glacier-Rafray Klippe (Western Alps) sampled by Marco Burn (PhD Thesis).

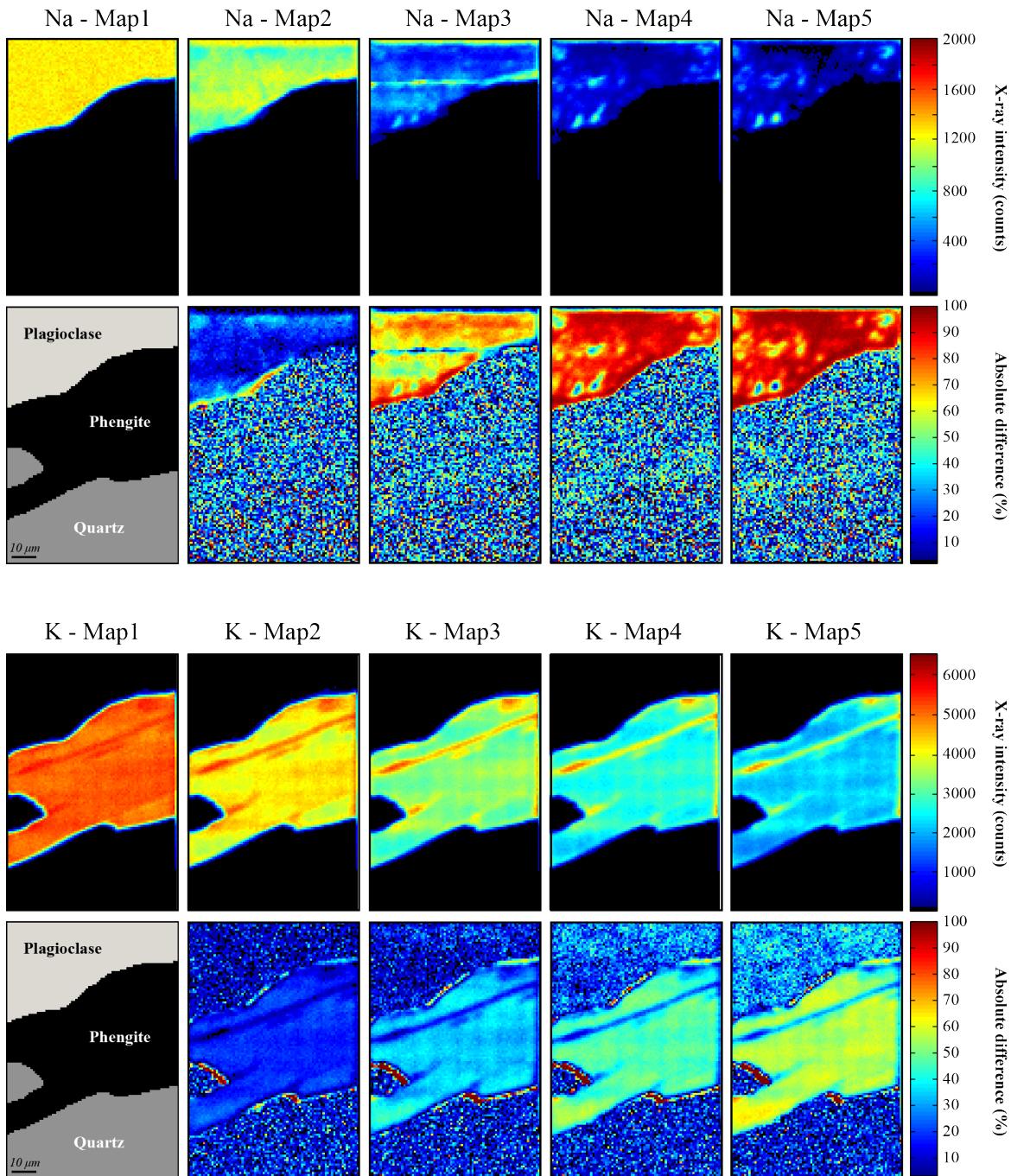


Figure 1.2 – X-ray maps Na (top) and K (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating voltage was 15 KeV, specimen current 200 nA, dwell time 200 ms and the beam size 1 μm . The studied sample is a meta-quartzite coming from the Glacier-Rafray Klippe (Western Alps) sampled by Marco Burn (PhD Thesis).

Precision of X-ray maps & total time of an analytical session: The precision of X-ray images is a fundamental question that must be discussed in details. However, we have first to estimate how long it take to measured X-ray maps in order to discuss the different parameters that will affect the precision of measurement. The total acquisition time (T_a) in mapping condition can be expressed as:

$$T_a(h) = \frac{Nb_{pixels} \times Td(s) \times Np}{3600} \quad (1.1)$$

with $Td(s)$ the dwell time, Np the number of passes and Nb_{pixels} , the number of pixels of the final image. Both spatial (i.e. size of the image and number of pixels) and chemical resolution (dwell time) of the X-ray images are very important and will strongly affect the total time of a mapping session (Eq. 1.1).

1.6.1.1 Spatial resolution

The size of an image is defined as $Nb_{pixels} = Nb_{rows} \times Nb_{cols}$. The surface of the mapped area is thus depending on the size of the pixel. The size of the pixel correspond to the distance between two analyses during mapping. It is recommended to use a beam size lower or equal to the pixel size in order to avoid overlapping (Fig. 1.3).

An example of the effect of different spatial resolutions on X-ray images is reported in Fig. 1.3. A virtual area with three phases was generated using fixed compositions of SiO_2 for the three phases (Fig. 1.3a). Phase 1 (45 wt.% of SiO_2) is an inclusion of $8 \times 16 \mu m^2$ in phase 2 (30 wt.% of SiO_2). The contact between phases 2 and 3 (60 wt.% of SiO_2) is oblique. The size of this area is $36 \times 35 \mu m^2$. Pixel sizes of 1, 2, 3 and 4 μm will generates images of 36×35 , 18×17 , 12×11 and 9×8 pixels respectively. For a given surface to be analyzed, the size of the image (in pixels) strongly affects the measurement time. In this example, estimated measurement times are 756 s, 184 s, 79 s and 43 s for 1, 2, 3 and 4 μm spot size respectively with dwell time of 300 ms and two passes.

The size of the pixel used for mapping does affect the measurement time, but also the visual quality of the X-ray image. In the example displayed in Fig. 1.3, the size of the inclusion of phase 1 is $8 \times 16 \mu m^2$. As in natural rocks this kind of inclusion can have chemical zoning, it is very important to have the higher number of pixels with individual measurements of the composition of this inclusion. For a beam size of 1 μm (first row in Fig. 1.3b), the number of pixels showing the true composition of the inclusion (i.e. 45 wt.% of SiO_2) changes with the pixel size used. 90 pixels of phase 1 have the correct composition with 1 μm spot size, 24 with 2 μm , 10 with 3 μm and 4 with 4 μm . This example demonstrates that a smaller pixel size provides better constrains for the chemical variations of the smallest object of the area of interest. A general rule proposed by Lanari and Riel (in prep) is that "*the pixel size must be at least 5 times smaller than the size of the smallest object*".

An other characteristic feature of X-ray images is that at the contact between two phases, mixing compositions are analyzed. It is important to remember that the compositions of the pixels at the contact between two phases are not the true composition of the phases. These pixels will be removed during the processing. The beam size used will strongly affect the size of this mixing area. In the example discussed above, for a given pixel size of 3 μm (third column), the size of the mixing area will increase with the beam size. This can be easily evidenced by comparing the contour of the inclusion of phase 1 between these three images ([3,1], [3,2] and [3,3] that correspond to [rows,column] coordinates). This result suggests that the smaller beam size must be used in order to reduce the number of mixing pixels at phase boundaries.

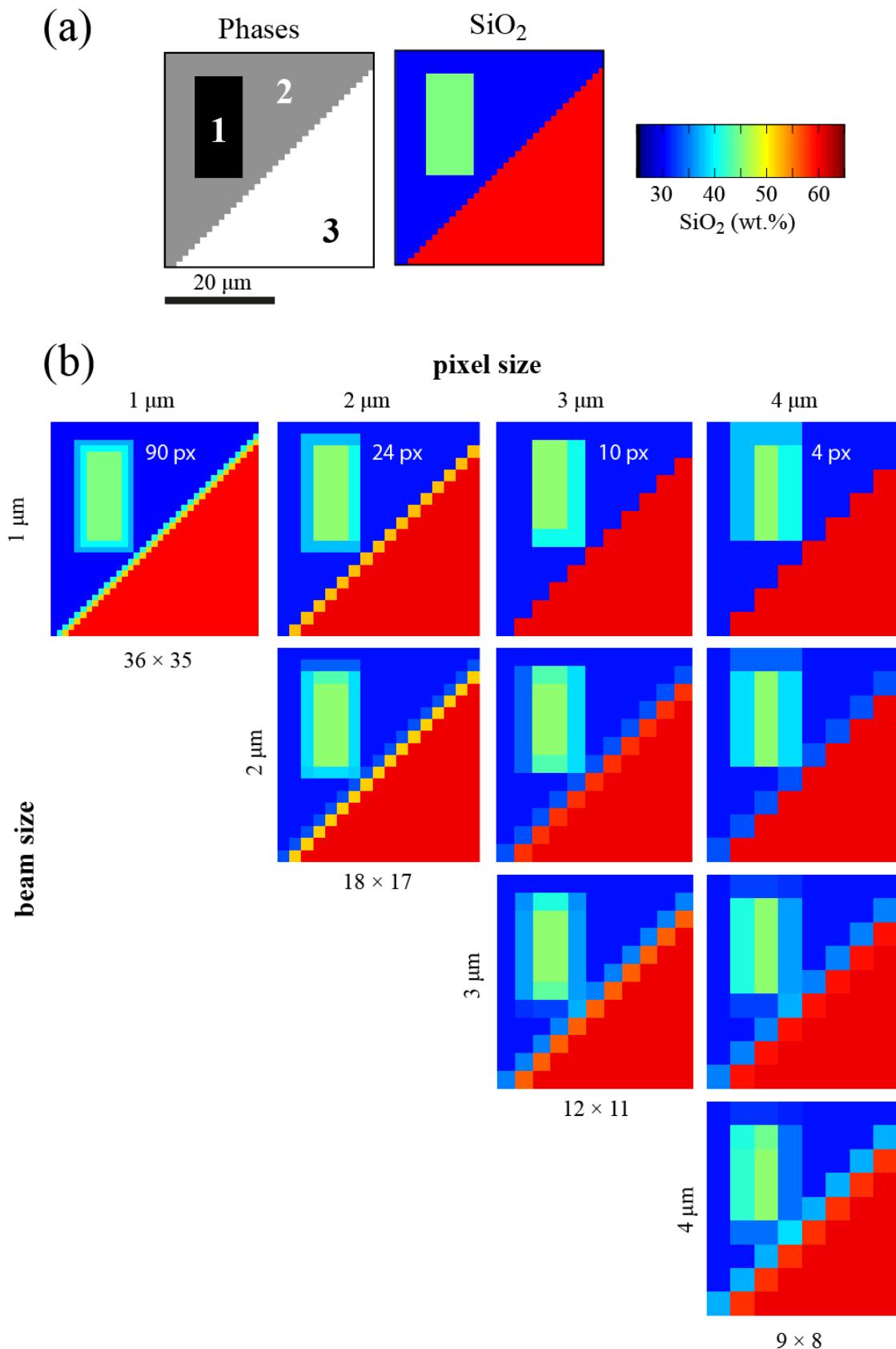


Figure 1.3 – Spatial resolution dependency to pixel size and beam size. (a) Images of the different phases (left) and compositions of SiO_2 (right). The phase compositions are assumed to be perfectly homogeneous with SiO_2 composition of 45 wt.%, 30 wt.% and 60 wt.% for phases 1, 2 and 3 respectively. The size of the small inclusion of phase 1 is $8 \times 16 \mu\text{m}^2$. (b) X-ray images generated for different resolutions and beam size of 1, 2, 3 and 4 μm (see text for details).

1.6.1.2 Chemical resolution

The chemical resolution for a given element depends on the dwell time $Td(s)$ used. The precision of microprobe measurement can be modeled using a Poisson law (Fig. 1.4):

$$P = \frac{2}{\sqrt{n}} \quad (1.2)$$

in which P is the precision (in % at 2σ), and n the number of recorded counts (intensity). This function has been plotted in figure 1.4. Consequently, 4,500 counts are required to reach a chemical precision of 3% (2σ), 10,000 counts for 2% (2σ), and 20,000 for 1% (2σ).

Example: A map of chlorite was acquire at the Institute of Geological Sciences (University of Bern) on a metasediment from the Western Alps, using an electron beam focussed at $1\mu m$, 15 KeV accelerating voltage, 100 nA specimen current, 200 ms dwell time and $3\mu m$ step size. The chlorite composition is $SiO_2 = 25.0\text{ wt-}\%$; $Al_2O_3 = 20.1\text{ wt-}\%$; $FeO = 32.1\text{ wt-}\%$; $MgO = 10.6\text{ wt-}\%$. The average number of counts recorded for each chlorite pixels is $Si = 3695$; $Al = 2612$; $Fe = 3302$; $Mg = 1551$. Analytical precision was derived using equation (1.2): $Si = 3.29\%$; $Al = 3.90\%$; $Fe = 3.48\%$; $Mg = 5.08\%$. Consequently, the limits to detect chemical zoning in chlorite is $SiO_2 = 0.82\text{ wt-}\%$; $Al_2O_3 = 0.78\text{ wt-}\%$; $FeO = 1.12\text{ wt-}\%$; $MgO = 0.534$ for the given analytical variations.

Example 2: An example of the propagation of this analytical uncertainty on structural formula compositions is described in [Lanari et al. \(2014b\)](#).

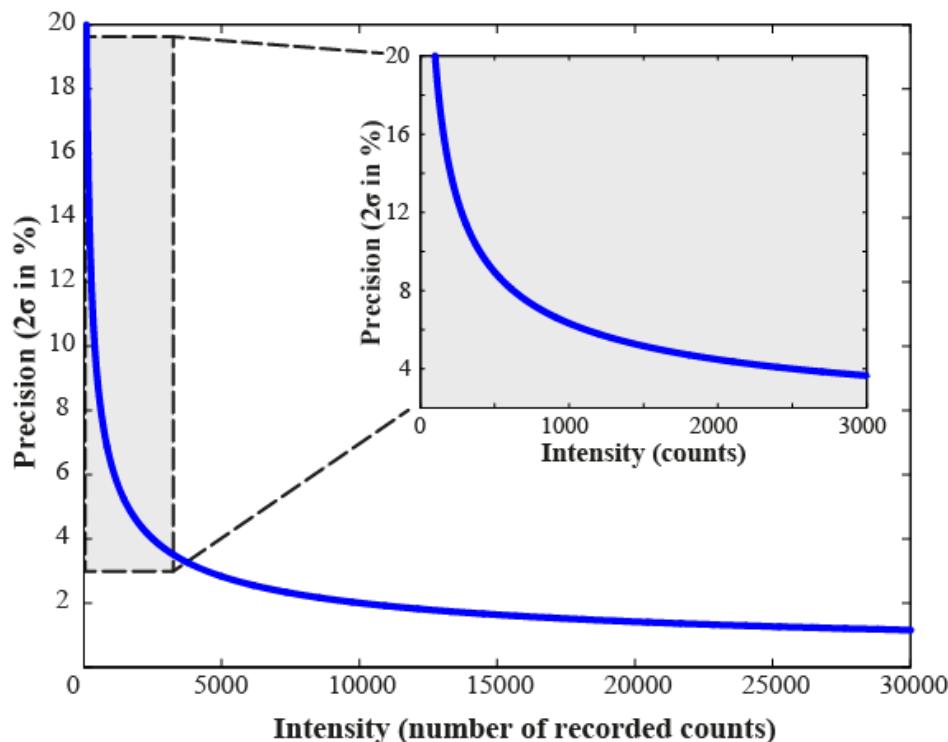


Figure 1.4 – Relation between the number of recorder counts and the analytical precision of an analysis

1.7 THEORETICAL CONSIDERATIONS

The following sections outline some fundamental aspects of quantitative mapping through theoretical descriptions. This section is expected to grow with time. If you have the feeling that something fundamental is missing and you want to participate, do not hesitate to contact me.

1.7.1 How to precisely determine local bulk composition from compositional maps?

1.7.1.1 Problem description

To estimate local bulk compositions, we need a standardized map for which we know the concentration of each pixels expressed in oxide weight percentage (wt-%). The aim of this section is to show you how to derive the bulk composition of a rock by extrapolating a 2D slice (map) into a 3D volume. In theory, this can easily be done if the following conditions are met:

- The thin section was made perpendicular to a schistosity or a foliation (extrapolation from 2D to 3D)
- The map was acquired on an unaltered rock surface devoid of compositional heterogeneities
- The size of the map is large enough to ensure a good sampling

Let first consider a domain of a rock composed by three phases Min_1 , Min_2 and Min_3 showing homogeneous compositions C_1^{wt} , C_2^{wt} and C_3^{wt} . The compositions are expressed in oxide weight percentage. The bulk composition of this domain (C_{bulk}) can be calculated as:

$$C_{bulk} = w_1 C_1^{wt} + w_2 C_2^{wt} + w_3 C_3^{wt} \quad (1.3)$$

with w_1 , w_2 and w_3 the mass fractions of Min_1 , Min_2 and Min_3 . This relation can be generalised for a map of this domain containing n pixels:

$$C_{bulk} = \sum_{i=1}^{i=n} w_i C_i^{wt} \quad (1.4)$$

with X_i^{wt} and w_i the mass fraction and composition in oxide weight percentage of pixel i . However the use of this relation is not straightforward because it requires the knowledge of the mass fraction of a given pixel. On the other hand side, a pixel fraction is a surface fraction (s_i) and can be converted into volume fraction (v_i).

For a rock made of 60 vol - % of quartz and 40 vol - % of andalusite equilibrated at 650K and 2000 bar, the bulk rock composition of this rock is exactly 60 wt - % of SiO_2 and 40 wt - % of Al_2O_3 . A compositional map of a representative portion of this sample would contain 60% of pixels with quartz measurement and 40% of pixels with andalusite measurement (volumes fractions of 0.6 and 0.4 respectively). In such case the surface fraction of a phase i (s_i) is extrapolated into a volume fraction (v_i) assuming

$$v_i = s_i \quad (1.5)$$

By contrast weight fractions of quartz and andalusite for the given example are of 0.36 and 0.64 respectively. The deviation between volume and weight fractions is caused by a density difference between the two solids. At 650K and 2000 bar the density of quartz is $2608 kg/m^3$ and andalusite $3126 kg/m^3$. The density of the mixture (bulk rock) made of 60 vol - % of quartz and 40 vol - % of andalusite is $2915 kg/m^3$.

For any mixture made of n homogeneous phases, the density of the mixture $\rho_{mixture}$ is

$$\rho_{mixture} = \sum_{i=1}^{i=n} v_i \rho_i \quad (1.6)$$

The density of phase i is the ratio of the mass (M_i) to the volume (V_i)

$$\rho_i = \frac{M_i}{V_i} \quad (1.7)$$

and consequently the mass of phase i is

$$M_i = \rho_i v_i \sum j = 1j = nV_j \quad (1.8)$$

As the mass fraction of a phase i in that mixture is the ratio of the mass of that phase (M_i) to the mass of the mixture ($M_{mixture}$)

$$w_i = \frac{M_i}{M_{mixture}} \quad (1.9)$$

By combining Eq. (1.8) and Eq. (1.9), it comes out that

$$w_i = \frac{\rho_i}{\rho_{mixture}} v_i \quad (1.10)$$

The mass fraction of each pixel may be convert into volume fraction of the pixel using Eq. (1.10) if the density of the corresponding phase and the density of the rock (mixture) are both known. The Eq. (1.4) become

$$C_{bulk} = \sum_{i=1}^{i=n} \frac{\rho_i}{\rho_{mixture}} v_i C_i^{wt} \quad (1.11)$$

If a significant density difference exists between the considered phase the local bulk composition is calculated from a *density-corrected map*. The oxide weight percentage of components of each pixel are multiplied by $\frac{\rho_i}{\rho_{mixture}}$. If $\frac{\rho_i}{\rho_{mixture}}$ is close to one for all the phases, the local bulk composition can be approximatively derived from the uncorrected oxide weight percentage maps. Accurate determination of local bulk composition require the knowledge of the phase density.

1.7.1.2 XMapTools procedure to export local composition

- (1) Use the standardization functions to generate standardized maps for all considered phases
- (2) Merge the standardized maps of interest using the function *merge standardized phases*  [B2401] to generate a standardized map that contain for all selected phases the pixels compositions in oxide weight percentage.
- (3) Duplicate the new standardized map using the function *duplicate Quanti file*  [B2106]
- (4) Use the functions *select and area and delete the pixels outside*  [B2409] or *select and area and delete the pixels inside*  [B2410] to remove pixels of any domain that is not in the area-of-interest from which you want to extract the local composition. It is really important to have in this standardized map only the pixels you need for the local composition estimate because the function that does the density correction needs to calculate the mean density of the considered pixels ($\rho_{mixture}$ in Eq. 3.24).

(5) Generate a density map from the selected mask file (in X-ray) using the function *generate a density map (from selected mask file)*  [B2406]. It is possible to define the phase densities in *Classification.txt* below the keyword *>2* (see example in Code 3.18). The order must be the same as the phases defined below *>1*. Each row must have only one number.

(6) You can display the density map by using the function *display the density map*  [B2407].

(7) Calculate a density-corrected map using the function *compute a density-corrected oxide map*  [B2408]. This map should only be used to export local compositions because each pixel is multiplied by $\frac{\rho_i}{\rho_{mixture}}$. The sum is not anymore 100 wt-%. The name of this Quanti file begins with *DCM- to remember you to not use it for other purpose. There is a warning if you try to use this density-corrected map for structural formula. I strongly suggest to delete this map after exporting the compositions

(8) The composition of this specific domain may be exported using the function *export local composition: map*  [B2402].

1.7.1.3 Method evaluation

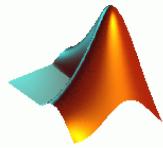
The description of this technique as well as some tests are provided in [Lanari and Engi \(2017\)](#).

HOW TO GET STARTED

2

2.1 REQUIREMENTS & COMPATIBILITY

XMAPTOOLS is a MATLAB-based software solution which requires MATLAB to run. There is no compiled version available and this will not change in the future. **Consequently, you need to have MATLAB installed on your machine if you want to use XMAPTOOLS.** Note: a cheap MATLAB student version can be purchased via the Mathwork website (www.mathworks.com).



XMAPTOOLS 3 is fully compatible with MATLAB version 8.4 release R2014b and more recent versions which are based on the new graphics engine HG2 (read [here](#)). It has been developed using a MacBook Pro with MATLAB version 8.6 release R2015a and it has been intensively tested on MATLAB R2017b and on Windows 10 with MATLAB R2015b.

XMAPTOOLS 3.3.1 seems to be fully compatible with MATLAB R2018b on MacOS. Older MATLAB versions (pre-R2014b) are no longer supported. If you wish to use XMAPTOOLS with an older MATLAB version, it is still possible to download the last compatible version XMAPTOOLS 2.6.4 (<https://www.xmaptools.com>).

XMAPTOOLS does not require any additional MATLAB toolbox such as *Statistic*, *Image Processing* toolboxes. However, add-ons may require the *Image Processing* MATLAB toolbox. It is strongly recommend to get the basic toolboxes while installing MATLAB as they could be very useful if you want to go further than what XMAPTOOLS does.

Note for compatibility and updates: Since the release of XMAPTOOLS 3.1), MATLAB R2014b or a more recent version is required. XMAPTOOLS no longer receive updates if used within old MATLAB environments (pre-R2014b). Please consider upgrading your MATLAB to ensure full compatibility with the most advanced version of XMapTools.

2.2 UPGRADE PROCEDURE: MIGRATING FROM XMAPTOOLS 2 TO XMAPTOOLS 3

If you have any version of XMAPTOOLS 2 installed on your computer, you can simply follow the automated update procedure for migrating to XMAPTOOLS 3 (this procedure is described below in section 2.5).

Restart MATLAB after completing the setup of XMAPTOOLS 3.

2.3 UPGRADE PROCEDURE: MIGRATING FROM XMAPTOOLS 1 TO XMAPTOOLS 3 (OLD PROCEDURE)

If you have been using XMAPTOOLS 1.6.5 or a previous version on your computer, it must be deactivated before to install XMAPTOOLS 3.

(1) Run MATLAB

(2) In the MATLAB menu, press *File* and *Set Path* (or in R2013b and more recent, in *Home*, *Environment*, press the button *Set Path*).

(3) In the Set Path window, select the installation path of XMAPTOOLS 1.6.5 and press *Remove*.

(4) Press the buttons *Save* and *Close*.

(5) You can manually remove the directory with the old XMAPTOOLS files

(6) Follow the installation procedure described below (section 2.4).

NB: The installation directory of XMAPTOOLS must be stored in the pathdef file of MATLAB. If the setup directory is not listed there (during step 3, see above), this means that XMAPTOOLS is not correctly working on your machine. You can directly install the new program (see below).

NB: In order to find the XMapTools setup directory, the MATLAB function which can be used: » *which XMapTools.p*. This function works only if the program is correctly installed on your computer. Otherwise, the function print out: '*XMapTools.p*' not found.

2.4 INSTALLATION PROCEDURE (DOWNLOAD, SETUP AND CONFIGURATION)

2.4.1 Download the latest XMapTools package

The full XMAPTOOLS package is required for a first installation. Further upgrades can be made via automatic updates (see section 2.5).

This XMAPTOOLS package contains the core files and programs as well as an installer *Install_XMapTools.p* to assist you with setup and configuration.

The latest package is available at: www.xmaptools.com in the section RESOURCES and *Download XMapTools*.

Registration on the website is required to access the download page. To register, users must provide an user name together with a valid email address. The server sends an automatically generated password that you will be able to edit in the next steps. *NB: The confirmation email could be considered as SPAM by your mail or webmail application, please check your SPAM box.*

We do not collect any Personal Data, usage or diagnostic information when you download, install or use XMAPTOOLS and during automatic updates. Check the [Privacy Policy](#) for additional information.

- (1) Login to XMAPTOOLS website using you username and password
- (2) Go to the download page [XMAPTOOLS 3.X]
- (3) Download the latest XMAPTOOLS package using the button **download**.

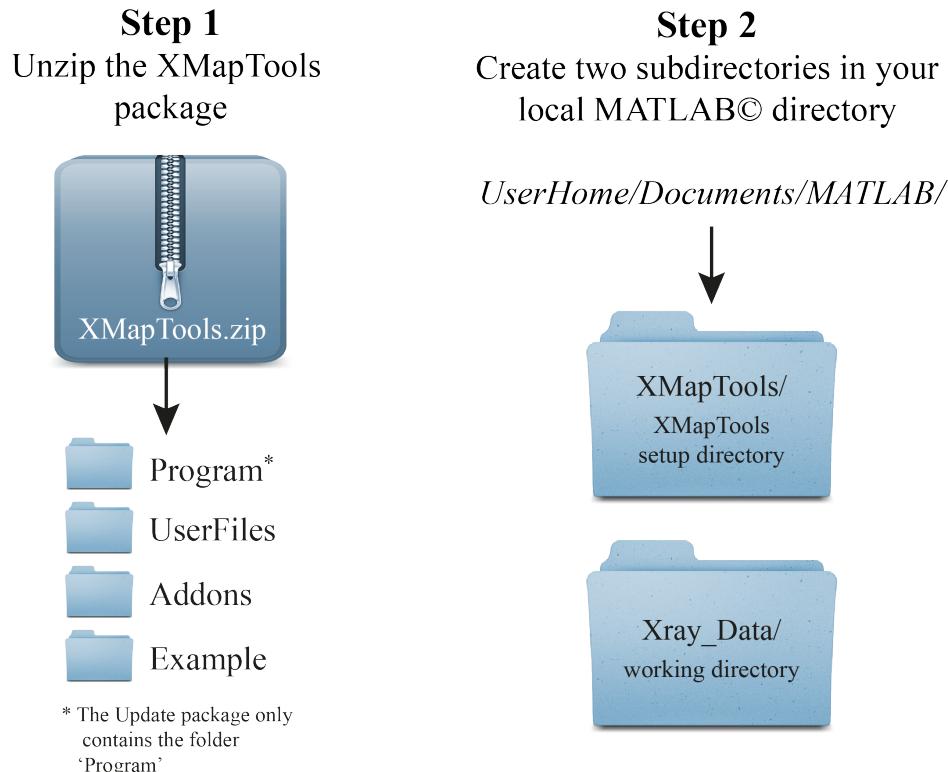
By downloading or using XMAPTOOLS, you accept the terms of the software license agreement (available in ??). XMAPTOOLS should be used only at the user's responsibility. Please note that XMAPTOOLS is free only for academic and public researchers. If you are working for a commercial institution, you should first get a licence. Please contact me before downloading the program

2.4.2 Install XMapTools

2.4.2.1 XMapTools package

- (1) Unzip the archive file *XMapTools-3.X.X-PackageXX.zip* in a suitable directory such as */User-Home/Documents/MATLAB/* (Fig. 2.1). It is strongly recommended to use this directory to install XMAPTOOLS. Here, MATLAB has the permissions to write in files. It is recommended not to have any blank (space) in the address of the location of MATLAB codes such as XMAPTOOLS.

The archive file contains four folders: *Program*, *UserFiles*, *Addon* and *Example*. *Program* contains the XMAPTOOLS core files and should be kept as it is. *UserFiles* contains user's additional functions and codes. The use of this functionality is explained in details in section 4.3 and is probably recommended to advanced users only. *Addon* contains the XMAPTOOLS' add-ons. Each subfolder in the *Addon* directory will be considered as a potential add-on. The description of the add-on system is provided in chapter 4.4. *Example* contains a set of microprobe X-ray maps that are used in the tutorial (see chapter 7).



Step 3
Move *Program/*, *UserFiles/* and *Addons/* to the setup directory:
UserHome/Documents/MATLAB/XMapTools/

Step 4
Move *Example/* to the working directory:
UserHome/Documents/MATLAB/Xray_Data/

Figure 2.1 – Description of XMAPTOOLS files and repertories. The setup package contains four folders: Program, UserFiles, Addons and Example. The user data must be stored in a different directory (e.g. Xray_Data).

- (2) Create two folders in your local MATLAB directory: .../UserHome/Documents/MATLAB/XMapTools/ for the program and .../UserHome/Documents/MATLAB/Xray_Data/ to store the X-ray data.
- (3) The folders *Program/*, */UserFiles* and */Addon* go in .../UserHome/Documents/MATLAB/XMapTools/.
- (4) The folder *Example/* goes in .../UserHome/Documents/MATLAB/Xray_Data/.

Warning: If any data file is stored in the folder *XMapTools/Program/*, it will be deleted during the next update. A warning message is displayed if one tries to start XMAPTOOLS from the setup directory.

2.4.2.2 Installation using Install_XMapTools.p

- (1) Open MATLAB

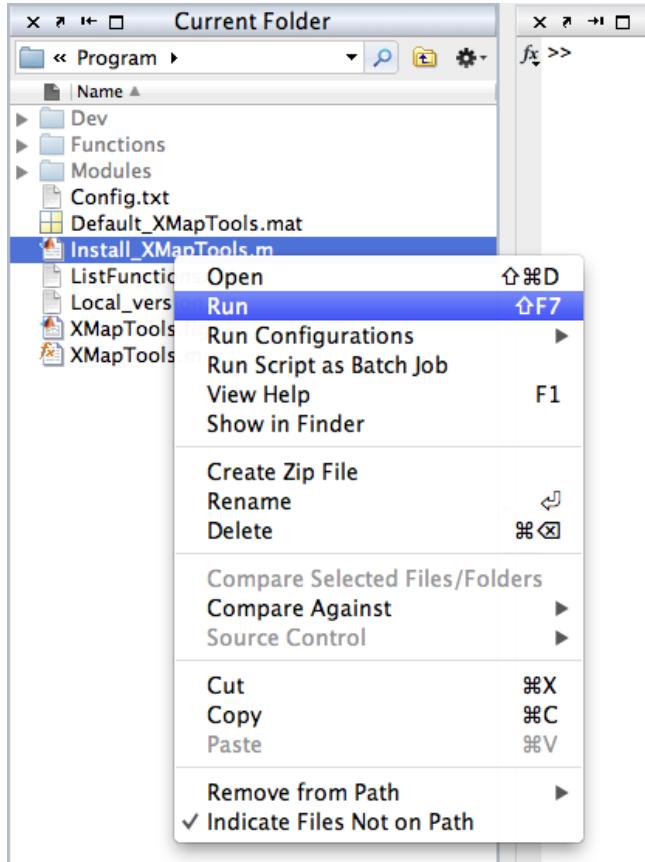


Figure 2.2 – XMAPTOOLS setup. Make a right-click on *Install_XMapTools.p* and press run to install XMapTools on your computer.

(2) Navigate to the XMAPTOOLS directory (*/Program*) using the *Current Folder* window in MATLAB

(3) Run the program *Install_XMapTools.p* (see Fig. 2.2, or using in the *MATLAB command window* the case-sensitive command: » *Install_XMapTools*)

(4) Press *Yes* to confirm that you would like to install XMAPTOOLS on your computer (Fig. 2.3a)

(5) After the setup, a confirmation message is displayed in a dialogue box. Two cases should be distinguished:

Case 1: Setup is completed (see message in Fig. 2.3b). This message is displayed if XMAPTOOLS was successfully installed in your computer. You can press *OK* and use XMAPTOOLS. If your setup is completed, you can run and use XMAPTOOLS from any folder, without the risk of modifying the main installation. Directly jump to the next section 2.4.3.

Case 2: Setup is not completed (see message in Fig. 2.3c). This message is displayed when XMAPTOOLS configuration failed. To solve this, try one of the two solutions below (5a and 5b):

(5a) In the MATLAB window, click on the icon *Set Path...* in the panel *ENVIRONMENT*. Press the button *Add folder* to add the directory *PROGRAM* to the MATLAB path. Then, press the button *Save* to update the MATLAB path. This file is loaded when MATLAB is opening. Usually, you will get a

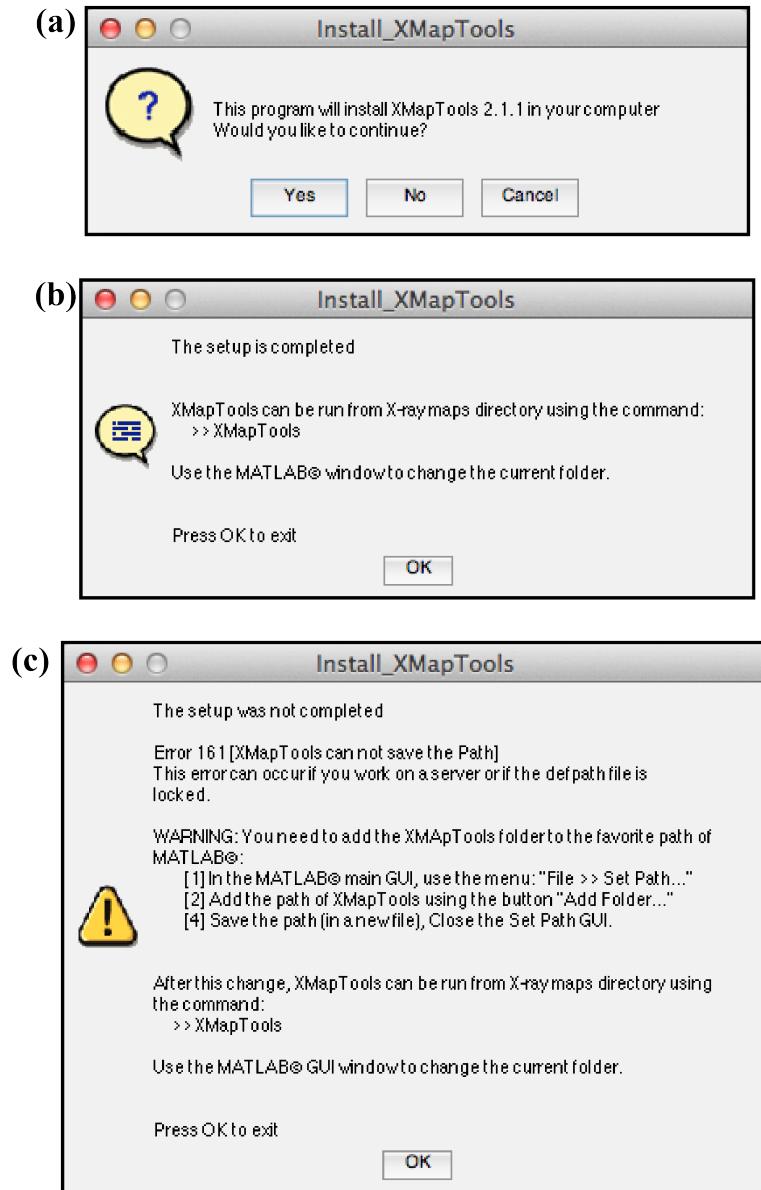


Figure 2.3 – XMAPTOOLS setup dialogue boxes

warning message saying that this file cannot be updated (you don't have the permission to update the file *pathdef.m*). In this case, you can simply save a copy of this file in */UserHome/Documents/MATLAB/*

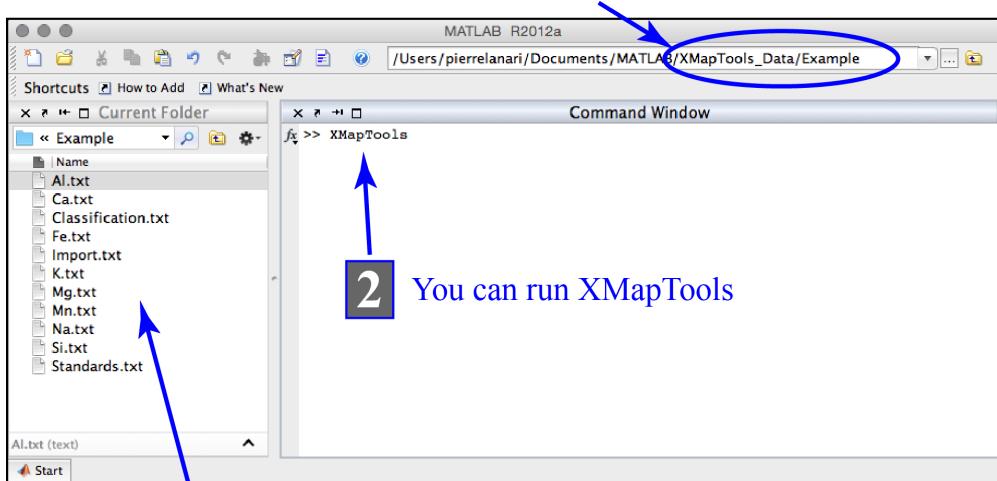
(5b) Open the file *pathdef.m* in your startup directory / or in *matlabroot/toolbox/local/* and change the file permissions. Then, try to run a new setup of XMAPTOOLS.

2.4.3 Run XMapTools

XMAPTOOLS can only be opened in MATLAB. The following steps detail how to run the program from the MATLAB command window.

Note: after a new installation or an update, close MATLAB and open it again. It seems that the

1 Check that you are in your project folder



This is good because in the working directory you have the Maps and the files Standards.txt and Classification.txt || XMapTools will generate new files here

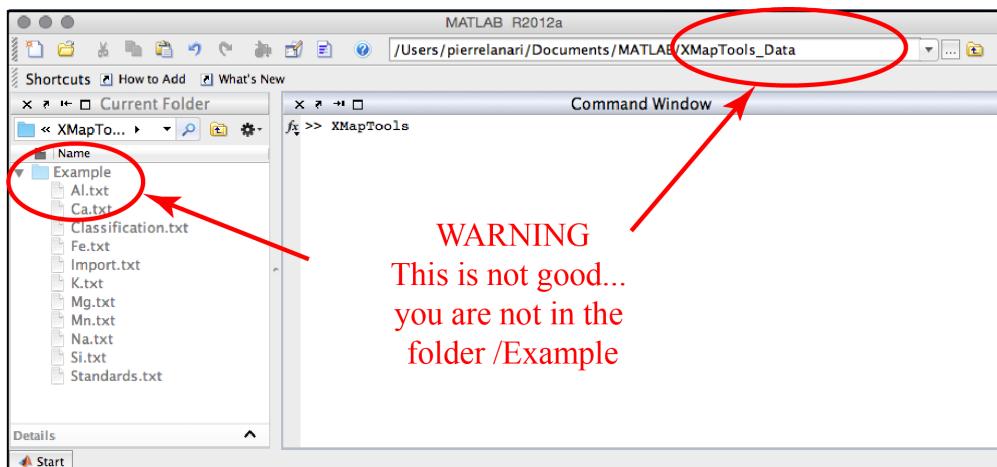


Figure 2.4 – Checking the working directory. (1) The full path to the working directory /Example is displayed; (2) the folded /Example is not opened! Double click on Example in the side window to get to state (1).

XMAPTOOLS graphic user interface experience issues after setup and update for some Windows' users. These can be easily solved by restarting MATLAB.

(1) Open MATLAB

(2) Set the MATLAB directory to your XMAPTOOLS working directory, where the X-ray maps are stored: .../UserHome/Documents/MATLAB/Xray_Data/ProjectX/. It is vitally important to set the MATLAB path to the working directory containing the maps and then to open XMAPTOOLS (see the warning below). While crunching data XMAPTOOLS generates files that are automatically saved in the working directory. Go to the data directory (see Fig. 2.1) using the *Current Folder* window in the MATLAB main window.

(3) Start XMAPTOOLS using the command: » **XMapTools** (case sensitive)

WARNING: Before to run XMAPTOOLS check that you are in the right working directory (See Fig. 2.4)

2.4.4 Open XMapTools and automatically load an existing project

A project can be loaded when you open XMAPTOOLS using the instruction *load* followed by the name of the project without the extension. If a project *aaa.mat* is available in the working directory you can use the case sensitive command:

```
>> XMapTools open aaa
```

Note: If the MATLAB path is not set to the working directory (see above 2.4.3), or if the project *aaa.mat* does not exist, XMAPTOOLS opens normally and do not load any project.

2.4.5 High definition mode (HD)

The graphical user interface of XMAPTOOLS is configured to run on a laptop with normal screen resolution. It happens that for some display setup, the icons are too small to be distinguished. In this case the high definition (HD) mode of XMAPTOOLS can be used. The command is:

```
>> XMapTools HD
```

Note that this command is fully compatible with other instructions, such as:

```
>> XMapTools HD open aaa
```

2.5 UPDATING XMAPTOOLS

A system that automatically check for updates is included in XMAPTOOLS 3. As soon as a new release becomes available XMAPTOOLS displays a dialog box when starting (Fig. 2.5). A connection to internet is required! It is possible to decide whether to use the automatic update system (press *Update now*) or to install it manually (press *Remind me later*). The main features of the new release can be displayed by selecting *Info*.

This automatic update system uses an Internet connection to automatically download the latest version of the software from the website (see details in section 2.5.1). Only the folder *Program* stored in the XMAPTOOLS setup directory is updated. This is NOT the case for: *Examples* and *UserFiles* that are kept as they are. The user files stored in *UserFiles* are not affected by the automatic update (provided that *UserFiles* is not stored in *Program*).

If you do not want to use automatic updates (in case you do not have access to the internet) an alternative procedure is also available (see section 2.5.2).

2.5.1 Automatic update procedure

The automatic update can be performed from any working folder in your computer as soon as a new release is available online.

(1) Open MATLAB

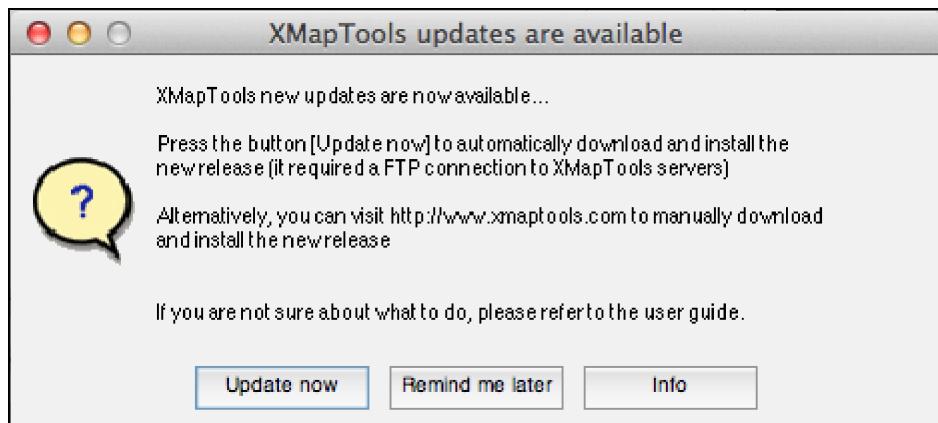


Figure 2.5 – XMAPTOOLS automatic update dialogue box

- (2) Start XMAPTOOLS (command: » XMapTools) and press the button *Update now*.
- (3) The update program asks for a confirmation; simply press *OK* to continue. The program will clean first all the files of the folder *program*. In a second time, the new version is downloaded and unzipped at the right location. At this stage, the update program will start the normal setup procedure (see details in section 2.4.2.2; (4) and following steps).

2.5.2 Manual update procedure

- (1) Login to the XMAPTOOLS website using you username and password and download the new package.
- (2) unzip the package. Navigate to the XMapTools setup directory and replace the old folder *Program* by the new one
- (3) Go to the XMAPTOOLS repertory (*Program*) using the *Current Folder* window in MATLAB and run the program *Install_XMapTools.p* (following the procedure described in section 2.4.2.2)

2.6 UNINSTALL XMAPTOOLS

- (1) Delete the setup repertory *Program* in which XMAPTOOLS setup files are installed. This operation deletes the core files. User data and functions if stored in a separate directory are kept unchanged.
- (2) Open the set path window in Matlab (*Menu > File > set path*). Select the XMAPTOOLS shortcut and remove it. Save and close this window.

2.7 REQUIRED DATA

2.7.1 EPMA

For a project involving EPMA data (X-ray images), it is recommended to use the following files that must be stored in the data repertory of this project.

Files	Type	Required
Si.txt - Al.txt - Fe.txt - Mn.txt - Mg.txt - Ca.txt - Na.txt - K.txt _P.txt - _S.txt - _Zr.txt - _Ni.txt	X-ray maps (WDS, type 1) with compatible names (see below)	Yes
TOPO.txt - SEI.txt Standards.txt	X-ray maps (EDS, type 2) with compatible names and the EDS code (_) Topo and SEI images used for corrections This file includes maps coordinates and spot analyses for the analytical standardization	Optional
Classification.txt	This file contains the name of the phases, the coordinates of the pixels used as composition inputs by the classification function and the average density of solid phases	Optional

Table 2.1 – *Required and optional files in a project folder for EPMA data. Note that the file names Standards.txt and Classification.txt (case sensitive) are automatically recognized by the program*

Examples of *Standards.txt* and *Classification.txt* files are provided in the XMAPTOOLS package (see the directory *Example*).

2.7.2 LA-ICP-MS

For a project involving LA-ICP-MS data (compositional maps in ppm), it is recommended to use the following files that must be stored in the data repertory of this project.

Files	Type	Required
7Li.txt, 9Be.txt, 11B.txt, 24Mg.txt, 27Al.txt, 29Si.txt, 31P.txt, 34S.txt, 35Cl.txt, 39K.txt, 45Sc.txt, 49Ti.txt, 51V.txt, 52Cr.txt, 55Mn.txt, 56Fe.txt, 59Co.txt, 60Ni.txt, 65Cu.txt, 66Zn.txt, 69Ga.txt, 71Ga.txt, 72Ge.txt, 73Ta.txt, 75As.txt, 81Br.txt, 82Se.txt, 85Rb.txt, 88Sr.txt, 89Y.txt, ...	LA-ICP-MS maps with compatible names (see below)	Yes

Table 2.2 – *Required and optional files in a project folder for LA-ICP-MS data.*

2.7.3 Map files

Map files must have *.txt, *.asc, *.dat or *.csv extension, no head line and a name compatible with the default elements names of XMAPTOOLS. The default list of element names is set in the file *XMapToolsSetupDirectory/Program/Dev/Xmap_Default.txt*. This file can be edited in order to add a new element.

The elements names available are Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Ag, Cd, Sn, Ce, As, Sb, Cs, La, Nd, Pb, Sr, Th, U, Yt (which is ytterbium not to be confused with "Y" coordinate), Sm, Gd, Dy, Pr.

The following isotopes names are available for LA-ICP-MS maps 7Li, 9Be, 11B, 12C, 13C, 23Na, 24Mg, 27Al, 28Si, 29Si, 31P, 34S, 35Cl, 39K, 43Ca, 44Ca, 45Sc, 47Ti, 49Ti, 51V, 52Cr, 53Cr, 55Mn, 56Fe, 57Fe, 59Co, 60Ni, 65Cu, 66Zn, 69Ga, 71Ga, 72Ge, 73Ta, 75As, 81Br, 82Se, 85Rb, 88Sr, 89Y, 90Zr, 93Nb, 95Mo, 105Pd, 107Ag, 111Cd, 115In, 118Sn, 121Sb, 125Te, 137Ba, 139La, 140Ce, 141Pr, 146Nd, 147Sm, 153Eu, 157Gd, 159Tb, 163Dy, 165Ho, 166Er, 169Tm, 172Yb, 175Lu, 178Hf, 184W, 192Os, 193Ir, 195Pt, 197Au, 202Hg, 205Tl, 204Pb, 206Pb, 207Pb, 208Pb, 209Bi, 232Th, 238U.

The oxides names available are SiO₂, TiO₂, Al₂O₃, FeO, MnO, MgO, CaO, Na₂O, K₂O.

The metalloids available are Fe_m, Cu_m.

The other maps types available are BSE (back-scattering electron image), SEI (secondary electrons) and TOPO (topography).

2.7.4 Map types

The following map types can be imported using the tool *Import map(s)*  available in the workspace (X-ray):

- Type 1: WDS maps (e.g. *Si*, *Al*, *Fe*, ...); they can be calibrated into maps of oxide mass fraction. The oxide corresponding to each element is defined in *Xmap_Default.txt* (see 2.7.3). A dead time correction is automatically applied to WDS maps when importing the maps.
- Type 2: EDS maps that can be calibrated in the same way as for type 1. Maps of type 2 are defined using the EDS code "_" in the file name. They are labeled "EDS_el" in the map menu. Note that there is no dead time correction applied to EDS maps.
- Type 3: Other maps such as TOPO, BSE and SE or calibrated EPMA (e.g. *SiO₂*, *Al₂O₃*, *FeO* ...) and LA-ICP-MS (e.g. 89Y, 90Zr, 93Nb, 95Mo) maps. These maps cannot be calibrated using any of the standardization functions. It is possible to transfer these maps to the workspace *Quanti* using the function *transfer to quanti* (see 3.8.6.4).
- Type 4: Background maps defined using the codes "*-" (lower background) and "*+" (upper background). A dead time correction is automatically applied to WDS background maps when importing the maps.
- Type 5: Maps generated using the *Generator Module* (see 3.11.5). These maps cannot be calibrated.

Note that the corrections (see 3.8.4) cannot be applied to all the map types. All the map types can be used in the chemical modules (see 3.11). The function *info*  in the workspace X-ray can be used to display the type of the selected map.

2.7.5 File Classification.txt

This file contains the name of the different phases to be classified as well as (optional) the coordinate of the input pixels that will be used by the classification function (see code 2.1). The phase names and the corresponding X and Y coordinates must be listed below the keyword >1. The phase names should not contain any blank (space).

The specific average density of the phases may be provided in the same file below the keyword >2. Those densities are used to calculate the local bulk composition of domains. *Note* that the phase name are not repeated in the second block.

```
>1 Put below the list of | Mask Name | X | Y | ...
Chloritoid    66    242
Chlorite     210    203
Phengite     186    119
Quartz       481     85

>2 Densities
3540
2650
2820
2620
```

Code 2.1 – *File Classification.txt*

2.7.6 File Standards.txt

This file contains (i) the map coordinates and (ii) the spot analyses used for the standardization (see code 2.2). The map coordinates must be listed within a single row below the keyword >1. The oxide order is set below the keyword >2. **X and Y must be the two last labels and must be listed in this specific order**. The internal standards analyses are listed below the keyword >3 corresponding to the oxide order defined above (keyword >2).

```
>1 Here paste the image coordinates (Xmin Xmax Ymin Ymax)
56.739    57.239    43.691    43.371

>2 Here define the oxides order
SiO2    MgO    FeO    Al2O3    X    Y

>3 Here paste the analyses
25.4800    11.2600    29.0500    21.1400    1.4800    68.310    39.999
52.9400    3.5300    3.0200    24.2300    0.0197    68.331    39.535
52.5800    3.6300    2.7900    24.7200    0.0195    68.338    39.511
```

Code 2.2 – *File Standards.txt*

Additional informations:

The map coordinates are defined as: $X_{min} \ X_{max} \ Y_{min} \ Y_{max}$

Example: for a map with 600 columns (X) and 800 rows (Y), the system of XMAPTOOLS' coordinates is defined as: 0 600 800 0 (note that Y_{min} and Y_{max} are switched because the Y axis is reversed).

2.8 EPMA CONVERTER

This section introduces the *EPMA Converter*, a tool that automatically transform raw data generated by JEOL microprobes to a XMAPTOOLS' friendly format.

This module can be opened via the main menu of XMAPTOOLS in *File » EPMA Converter*.

2.8.1 Main steps

Each conversion involves the following steps:

1. Open XMAPTOOLS and the *EPMA Converter* via the menu
2. Select the *Type of Raw Data* in the top right drop-down menu. Once the recipe is selected, a description of the data required is displayed in the interface. More detailed explanations are provided in Tables 2.3 and 2.4
3. Press the button *Set a destination folder* and select/create the directory were the converted data will be stored
4. Press the button *Import Maps* and select the folder containing all the map files. Only files with compatible names will be selected (see Tables 2.3 and 2.4). Once this action is accomplished, the names of the original and converted files are listed in a table. The map coordinates required for XMAPTOOLS are calculated and displayed in the same window.
5. Press the button *Generate Classification.txt*. This file is generated in the destination folder
6. Press the button *Add Standard Data*. Several windows successively open to select the number of files required for each dataset. Select the files in the right order (e.g. summary data first for SUN and then stage data). The spot analyses, their compositions and coordinates are displayed in a table. You can repeat this operation to add data from different files.
7. Press the button *Generate Standards.txt* to generate the file in the destination folder. This action closes the *EPMA Converter* window and changes the working directory to the destination folder.
8. Import the maps in XMAPTOOLS

2.8.2 Compatible format

The mapping data acquired with the following instruments are compatible with the *EPMA Converter*:

- *EPMA - JEOL (SUN)* for old JEOL microprobes running with SUN (see Tab. 2.3)
- *EPMA - JEOL (WINDOWS)* for new JEOL microprobes (see Tab. 2.4)

Type	Files	Required
Map information	0.cnd	yes
X-ray map for element El1	1_map.txt (matrix of intensity), 1.cnd (information) 1_El1.pm, 1.map-Z (JEOL files)	yes no
X-ray map for element El2	2_map.txt (matrix of intensity), 2.cnd (information) 2_El2.pm, 2.map-Z (JEOL files)	yes no
...		
Oxide data	OxideDataset1_summary.txt OxideDataset2_summary.txt	yes optional
...		
Spot coordinates	OxideDataset1_stage.txt OxideDataset2_stage.txt	yes optional
...		

Table 2.3 – Raw files used by the EPMA Converter; option: EPMA JEOL (SUN)

Type	Files	Required
X-ray map for element El1	data001.csv (matrix of intensity), data001.cnd (information)	yes
X-ray map for element El2	data002.csv (matrix of intensity), data002.cnd (information)	yes
...		
Oxide data	OxideDataset1.txt OxideDataset2.txt	yes optional
...		

Table 2.4 – Raw files used by the EPMA Converter; option: EPMA JEOL (WINDOWS); The file containing the oxide data should be exported with the option ALL

PROGRAM DESCRIPTION

3

3.1 INTRODUCTION

This chapter provides a detailed description of all the functions available in XMAPTOOLS. By contrast, the tutorial "Electron microprobe X-ray maps processing" (chapter 7) explains how to use these functions to perform the successive steps of processing (e.g. classification, analytical standardization, thermobarometry).

This program description is divided into three sections: the general functions (section 3.5), the display functions (section 3.6) and the processing functions (sections 3.8, 3.9 and 3.10). All buttons and menus available in the GUI are shown in Figs. 3.1, 3.2 and 3.3, 3.4.

3.1.1 Quick access to function descriptions

Main menu:

File - [New] - [Close] - [Open Project] - [Save] - [Save as...] - [EPMA Converter] - *Import*: [Add Map(s)] [Mosaic] [Mosaic & Standards] - [Export Image] - [Export Mask Image] - [Preferences] - *Add-ons*: [Manage Extensions] - [About XMapTools]

Edit - [Copy] - [Clean Figure]

Image - [Image Info] - [Mask File Info] - [Resampling]

Sampling - [Line] - [Path] - [Area] - [Integrated Line (stripe)] - [Sliding Window] - [Sampling options]

Modules - [Histogram] - [Binary] - [TriPlot] - [RGB] - [Generator] - [Spider]

Workspace - [Xray] - [Quanti] - [Results]

Help - [Download Documentation] - [Download Tutorial Data]

General:

Drop-down lists: [M5601]

Buttons - *add-ons* [B5601] - *Other options* [B4403]

Display and corrections:

Buttons: *figure/display tools* [B5101] [B5102] [B5103] [B5104] [B5105] [B5106] [B5107] [B5108] [B5109] - *Color palette* [M1302] [B1301] - *Mask File* [M1301] - *Other tools* [B4402] - *X-pad navigator* [B5401] [B5402] [B5403] [B5404] [B5405]

Input fields: *figure/display tools* [C5101] [C5102] - *sampling tools* [C5201]

Xray:

Drop-down lists: *X-ray images display* [M1101] [M1102] - *classification* [M1201] [M1202] - *maskfiles* [M1301] - *corrections* [M1401] - *standardization* [M1601]

Buttons: *X-ray images display* ([B1101] [B1102] [B1103] [B1104] [B1105] [B1106] [B1107] [B1108]) - *classification* [B1201] - *maskfiles* [B1301] [B1302] [B1303] - *corrections* [B1401] - *standards* [B1501] [B1502] [B1503] [B1504] [B1505] [B1506] - *standardization* [B1601]

Correction methods:

Buttons: [BRC] [TRC] [MPC] [SPC] [IDC] [BA1] [RM1]

Quanti:

Drop-down lists: *standardized maps* [M2101] [M2102] - *external functions module* [M2301] [M2302] [M2303]

Buttons: *standardized maps* [B2101] [B2102] [B2103] [B2104] [B2105] [B2106] - *info* [B2201] [B2202] [B2203] - *external functions module* [B2301] [B2302] - *Pixel size* [B2413] - *local com-*

positions module [B2401] [B2402] [B2403] [B2404] [B2405] [B2406] [B2407] [B2408] [B2409] [B2410] [B2411] [B2412]

Results:

Drop-down lists: *results from external functions* [M3101] [M3102]

Buttons: *results from external functions* [B3101] [B3102] [B3103] [B3104] [B3105] - *Other* [B3302] [B3303]

3.1.2 XMapTools strategy

The strategy behind XMAPTOOLS is intensively described in [Lanari et al. \(2014b\)](#) and [Lanari et al. \(2019\)](#). However to get started, it is important for the new user to know some decisions that have been made during the development of the software.

Following the original idea of microprobe X-ray image processing using an Castaing's approach ([De Andrade et al. 2006](#)), XMAPTOOLS software is divided into three workspaces *Xray*, *Quanti* and *Results*. They are activated using the corresponding tabulation buttons *Xray*, *Quanti* and *Results* or the items in the menu *Workspace* (see section [3.2.6](#)) and display specific objects such as groups of buttons.

X-ray workspace is automatically selected when XMAPTOOLS opens. This workspace is important for (1) adding data, displaying and manipulating raw data such as X-ray maps, (2) classifying the pixels, i.e. computing masks and identifying mineral phase(s) via a supervised multi-channel classification, (3) correcting raw X-ray data, (4) loading standard files containing the spot analyses to be used as internal standard, (5) correcting the positions of the maps and the spot analyses as well as for selecting/unselecting spots and finally for (6) standardizing the raw data to maps of oxide wt(%) concentrations.

Quanti workspace is devoted to treatment of the maps of oxide mass concentrations. It is possible to (1) export analyses of the entire map or of a selected area, (2) merge standardized map and export local bulk compositions ([Lanari and Engi 2017](#)), (3) calculate maps of structural formulas, (4) apply empirical to semi-empirical geothermobarometers to evaluate P-T conditions of formation ([Lanari et al. 2013](#)).

Results workspace displays the calculated results (mineral structural formulas, P-T maps).

General functions are provided in all the workspaces such as: (1) plot options, (2) filters, (3) sampling functions and (4) external modules: BINARY,TRIPLOT, RGB and GENERATOR. These functions are accessible via the XMAPTOOLS menu (see section [3.2](#)) or the button panel located on the left part of the interface.

LA-ICP-MS data can also be proceeded via XMAPTOOLS. The standardized maps are imported in the workspace *X-ray* and directly sent to the workspace *Results* using the functions *Transfer to Quanti* and *Transfer to results*. The module SPIDER allows spider diagrams to be generated (including the creation of videos from spider diagrams).

XMAPTOOLS projects can be saved as *.mat files which contain all the variables. These are easily accessible from the MATLAB command window. Type in the command window ">> open MyProjectName.mat" and ">> whos" to display XMAPTOOLS variables (and data).

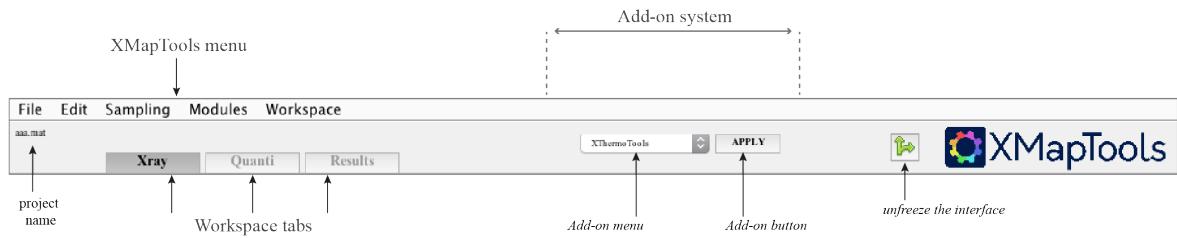
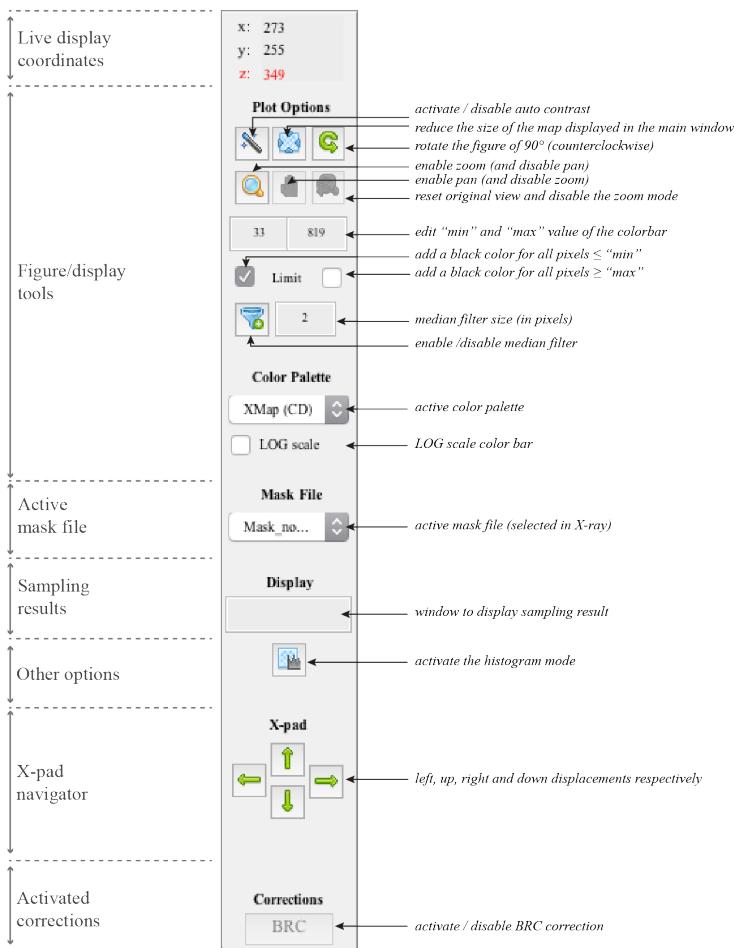
(a) General**(b) Display and corrections**

Figure 3.1 – *XMapTools objects and corresponding functions for (a) "general" and (b) "display" windows.*

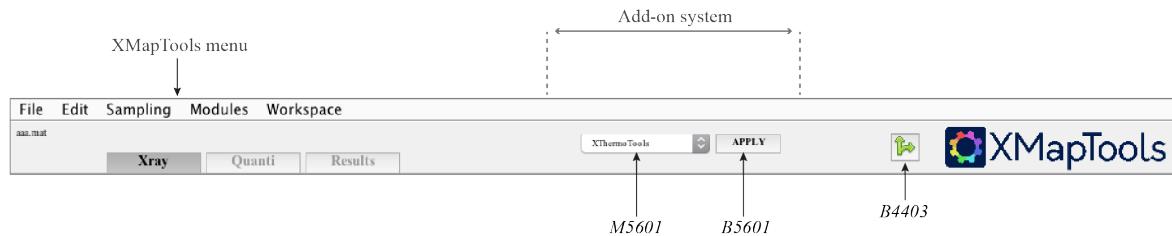
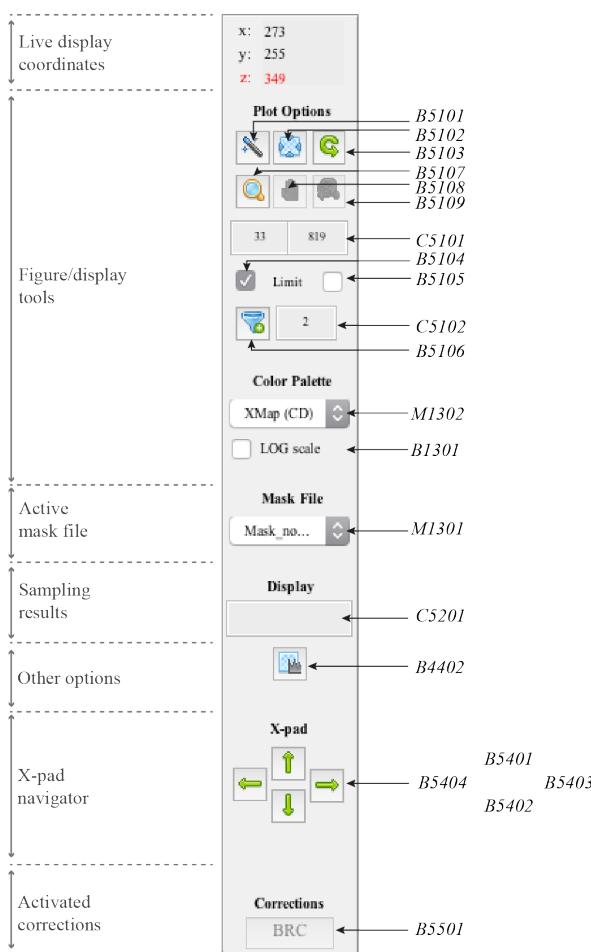
(a) General**(b) Display and corrections**

Figure 3.2 – XMapTools objects and corresponding functions for (a) "general" and (b) "display" windows.

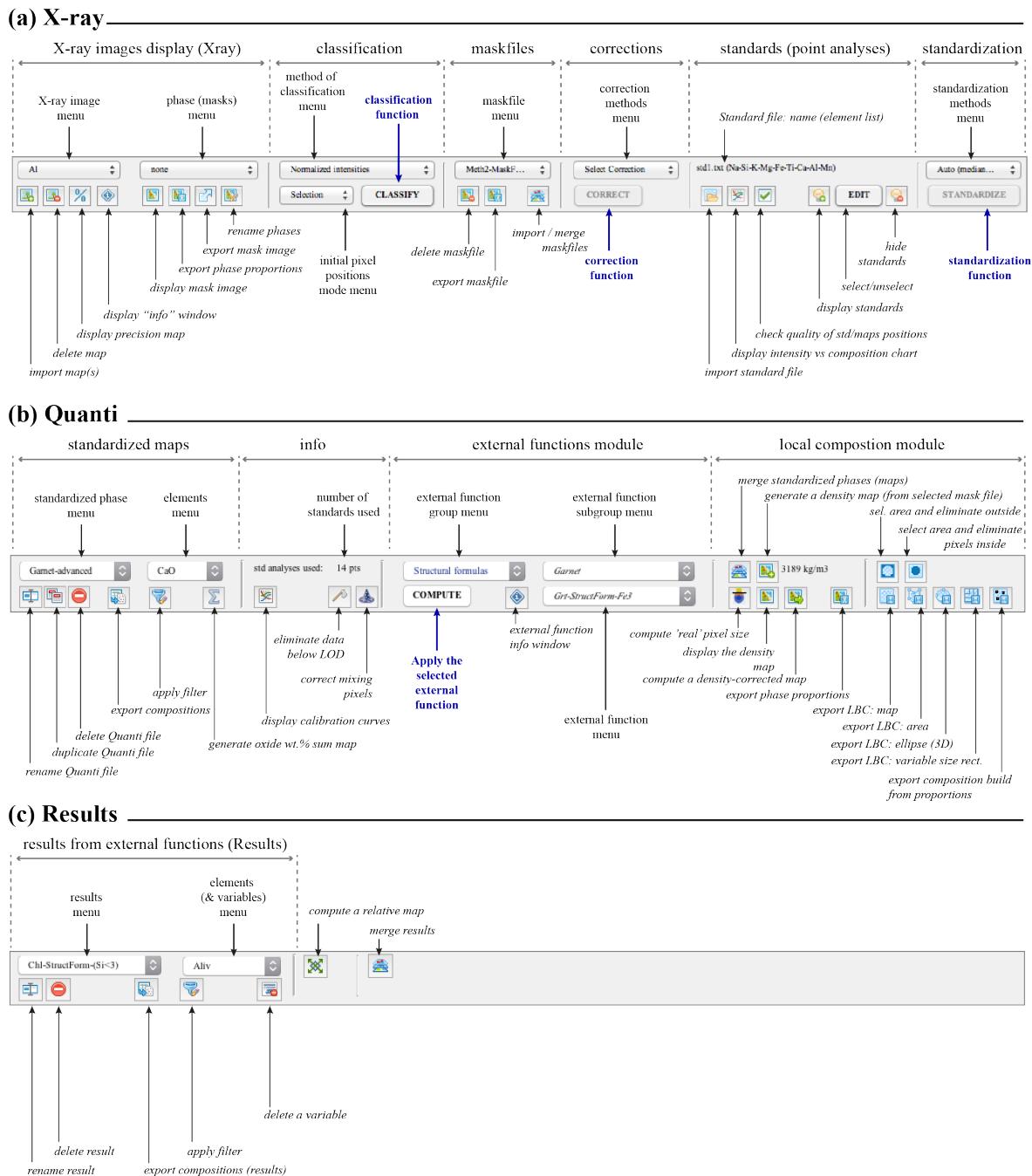


Figure 3.3 – *XMapTools* objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.

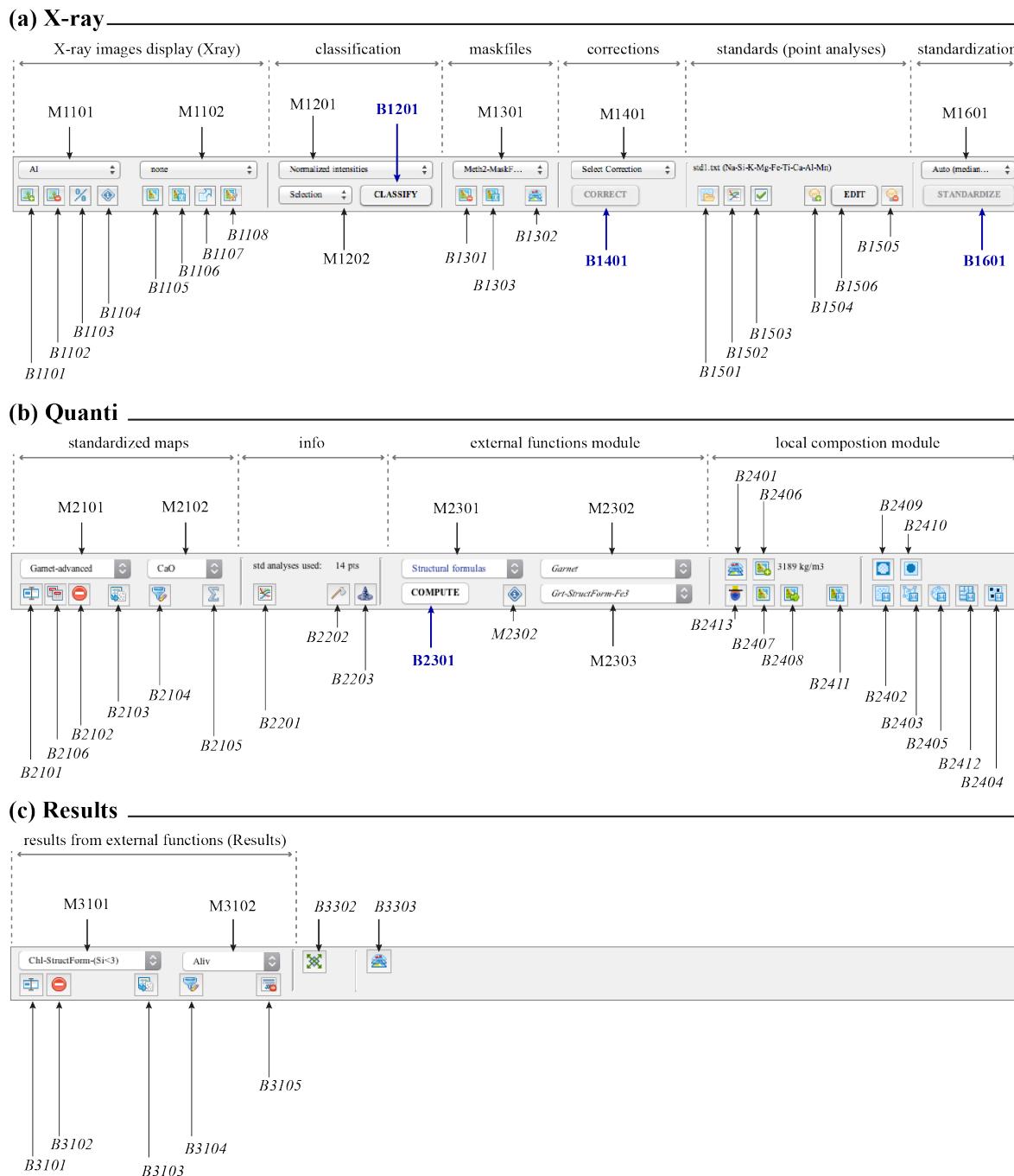


Figure 3.4 – *XMapTools* objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.

3.2 MAIN XMAPTOOLS MENU

3.2.1 File

The following functionalities are available in the menu *File* (Fig. 3.5-a):

[New] Close the active XMAPTOOLS window and open a new window. *Shortcuts:* *ctrl-N (WIN); cmd-N (MAC)*

[Close] Close the active XMAPTOOLS window. *Shortcuts:* *ctrl-W (WIN); cmd-W (MAC)*

[Open Project] Select and open an existing project consisting of a MATLAB file (.mat) generated by XMAPTOOLS (see section 3.5). *Shortcuts:* *ctrl-O (WIN); cmd-O (MAC)*

[Save] Save the active project. *Shortcuts:* *ctrl-S (WIN); cmd-S (MAC)*

[Save As...] Save as a new project.

[EPMA Converter] Open the EPMA converter that automatically transform raw data generated by JEOL microprobes to a XMAPTOOLS' friendly format. A detailed description of the *EPMA Converter* is given in chapter 2.8.

[Import] Import data to XMAPTOOLS:

- **[Add Map(s)]** Import new maps (normal procedure, see 3.3.2) *Shortcuts:* *ctrl-A (WIN); cmd-A (MAC)*
- **[Mosaic]** Combine maps and create a mosaic (see 3.3.3)
- **[Mosaic & Standards]** Merge maps in a referenced system based on their original coordinates (see 3.3.4)

[Export Image] Export a copy of the image displayed in the main XMAPTOOLS window. This figure can be saved using the standard MATLAB tools. In the menu of the new window, select *File, Save As...* (see details in section 3.4)

[Export Mask Image] Export a copy of the mask image of the selected mask file (see section 3.8.2). This figure can also be saved using the standard MATLAB tools (see above).

[Preferences] Display the settings window (see the description below in section 3.5.2).

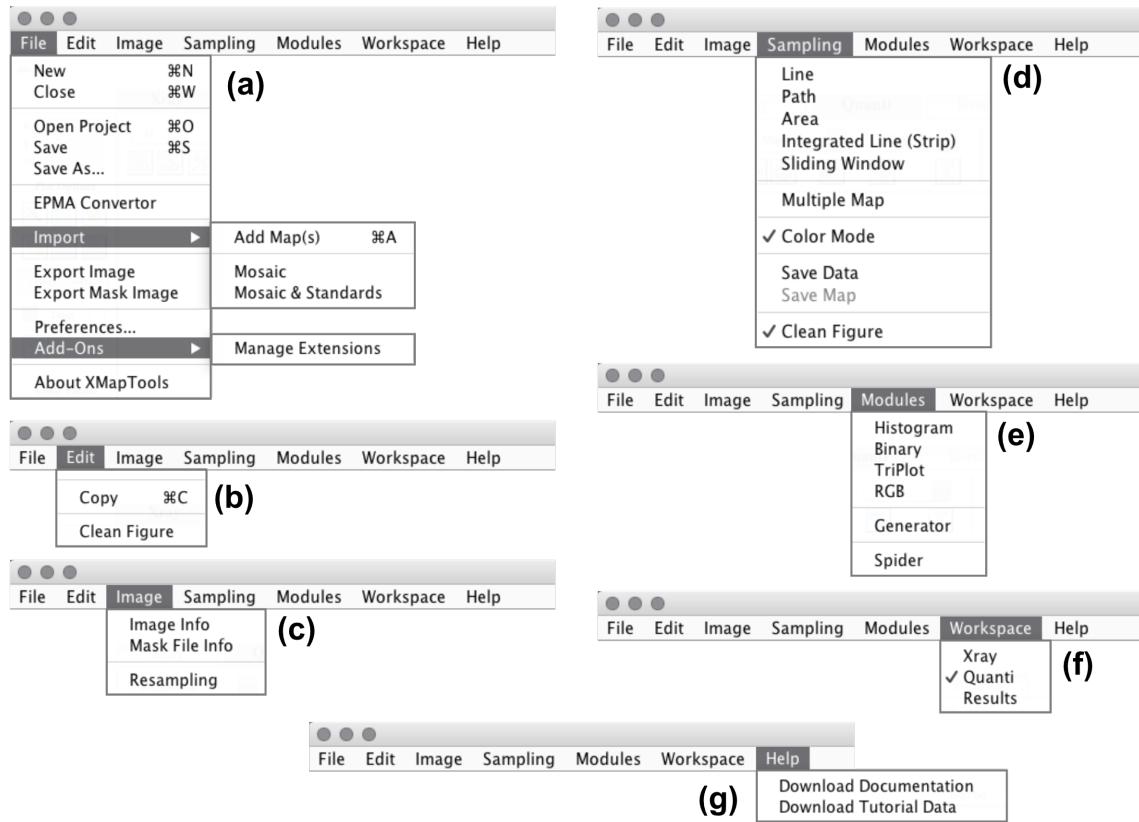


Figure 3.5 – Main menu

[Add-ons: Manage Extension] Manage XMAPTOOLS add-ons (see in section 6).

[About XMapTools] Display the last release notes and a short description of the program.

3.2.2 Edit

The following functionalities are available in the menu *Edit* (Fig. 3.5-b):

[Copy] Copy the displayed image to the clipboard. A confirmation message is displayed once this operation is done. Note that it is also possible to obtain a vectorized image by using first the function *Export Image* (see above) and then the default copy function of MATLAB *Copy Image* available in the figure menu *Edit*.

[Clean Figure] Restore the image by deleting any extra object that was plotted (e.g. lines, points, curves, text, etc.).

3.2.3 Image

The following functionalities are available in the menu *Image* (Fig. 3.5):

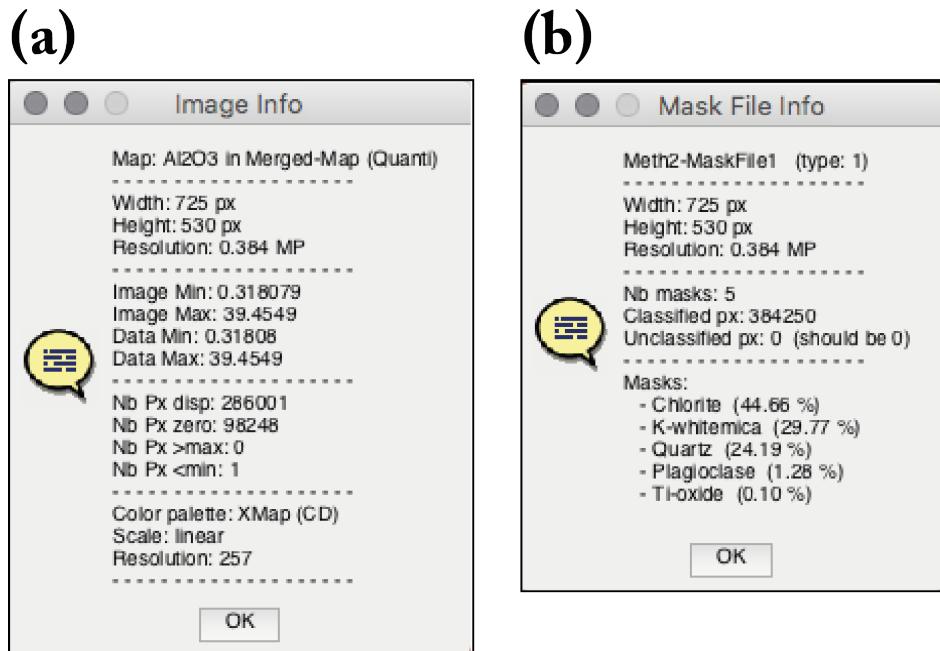


Figure 3.6 – Image information: (a) for the active map, (b) for the selected mask file.

Information	Description
Name	Shows the name of the map including information on the data
Map size	Reports the width and height in pixels (px) and resolution in mega-pixel (MP)
Data (1)	Displays the min and max values of the displayed image (color bar limits) and of the data
Data (2)	Shows the number of pixels displayed in the range (<i>min; max</i>) and outside this range as well as the number of pixels with the value of zero
Color palette	Shows the name of the selected color palette, the scale (linear/log) and the resolution

Table 3.1 – List of information displayed by Image Info (see Fig. 3.5-c)

[Image Info] Display detailed information of the map plotted in the main figure (Fig. 3.6-a and Table 3.3).

[Mask File Info] Display detailed information of the active mask file (Fig. 3.6a).

[Resampling] Duplicate the selected *Quanti file* and adjust manually the resolution. The new map is generated using a gridded interpolant. The interpolated values are based on linear interpolation of the values at neighboring grid points in each respective dimension.

This option can be used to increase the resolution of a quantitative map, for example to generate smoother images (Fig. 3.7-d). It can also be used to decrease the resolution when, for example, intensive computations are applied to the map via one of the external functions (Fig. 3.7-b).

Procedure:

Information	Description
Name	Displays the name of the selected mask file
Mask file size	Shows the width and height in pixels (px) and resolution in mega-pixel (MP)
Masks (1)	Displays the number of masks and the number of pixels that are classified ($value > 0$) and unclassified ($value = 0$). The later should always be 0.
Masks (2)	Lists the maskfile with their relative fraction (in %)

Table 3.2 – List of information displayed by Mask File Info (see Fig. 3.5-b)

1. Navigate to the workspace *Quanti* and select a map to adjust its resolution
2. In the main menu, select *Image* and *Resampling*
3. Set the new width. The actual width is displayed as default. Increasing the value increases the resolution whereas decreasing the value decreases the resolution. The new height is recalculated automatically to maintain the aspect ratio of the image.

Note: this option is only available in the workspace *Quanti*.

3.2.4 Sampling

XMAPTOOLS contains several sampling tools which can be used to extract data from the maps. These tools and their options are available in the menu *Sampling* (Fig. 3.5-d). The description of the sampling tools is provided in section 3.7.

3.2.4.1 Sampling tools

[Line] Extract a composition profile between two points *A* and *B* (see description in section 3.7.2.1).

[Path] Extract a composition profile along a path composed by $n - 1$ linear segments defined n points (see description in section 3.7.2.2).

[Area] Extract the average composition from an area-of-interest polygon (see description in section 3.7.2.3).

[Integrated line (stripe)] Extract the average composition profile from a rectangular area by averaging the composition of each transect (see description in section 3.7.2.4).

[Sliding window] Extract an average composition profile using a rectangular area sliding along a path composed by $n - 1$ linear segments defined n points (see description in section 3.7.2.5).

3.2.4.2 Sampling options

These options should be set before using a sampling tool. A detailed description of the option is provided in section 3.7.2

[Multiple Map] Activate the mode multiple-map allowing to sample across several dimensions.

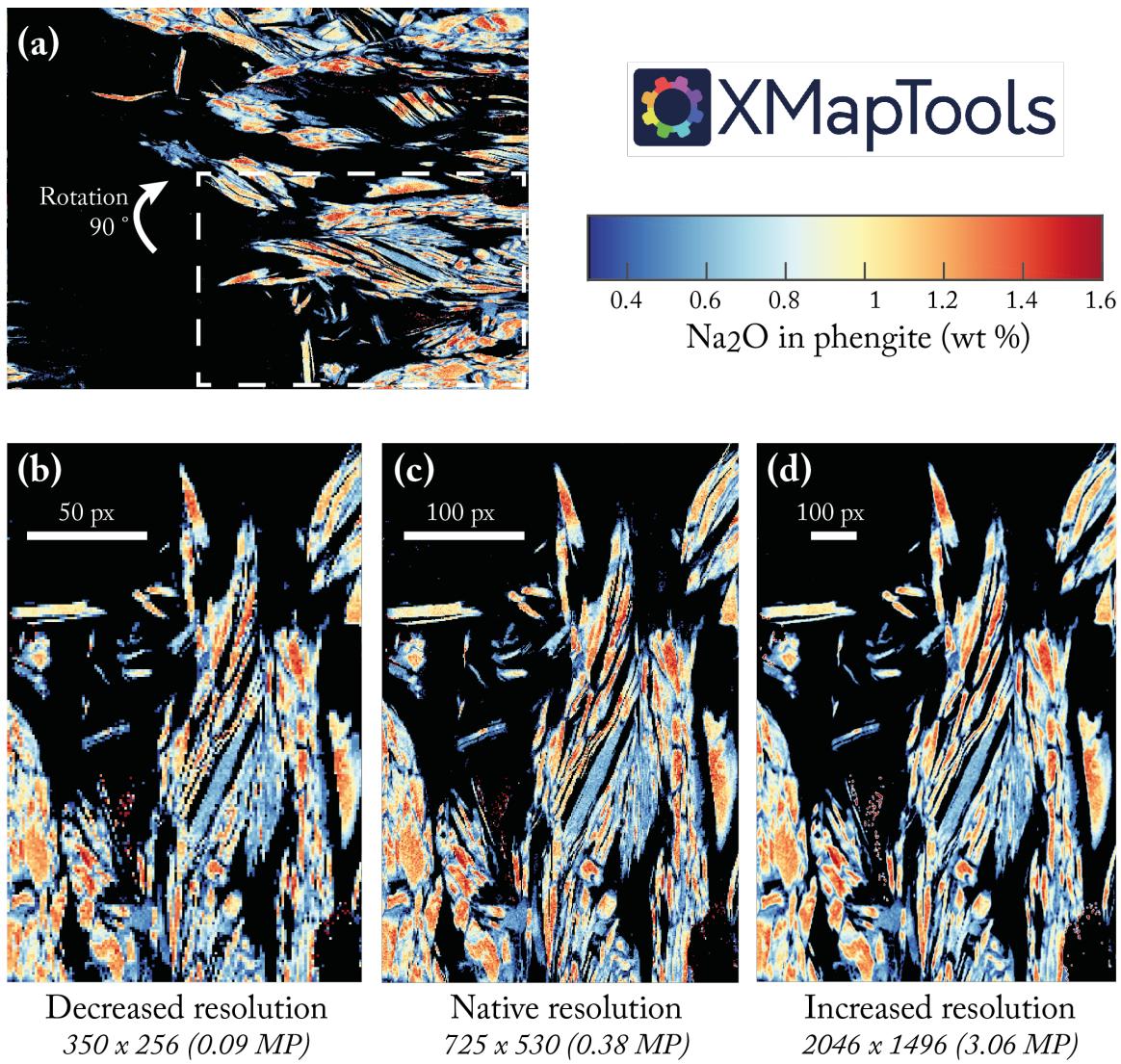


Figure 3.7 – Resampling quantitative maps. (a) original map of Na₂O. A small area delimited by the white dashed line was selected and turned by 90° to display (b), (c) and (d) using the same color scale. The resolution in (b), (c), and (d) refer to the original image.

[Color Mode] Plot the compositional profile using colored points based on the colormap and limits of the defined color bar.

[Save Data] Save the results such as figures (compositional profile(s), comparison(s)) and data tables.

[Save Map] Save the map displayed in the main window. This option is only available if the data are saved (option *Save Data* above).

[Clean Figure] Clean the figure before processing to the next sampling stage.

Module	Type	Requirements
Histogram	Histogram diagrams	available in all workspaces requires at least one map
Binary	Binary diagrams	available in all workspaces requires at least two maps
TriPlot	Ternary plot via triangular diagrams	available in all workspaces requires at least two maps
RGB	RGB image (multi-channel image)	available in all workspaces requires at least two maps
Generator	Generate new maps	available in all workspaces requires at least two maps
Spider	Spider diagrams	only in the workspace <i>RESULTS</i> requires trace element maps in ppm

Table 3.3 – *List of modules, data and possible restrictions*

3.2.5 Modules

XMAPTOOLS contains several modules which can be used for data exploration and visualization. These modules are available in the menu *Modules* (Fig. 3.5-e). The type of data and possible requirements are listed in Table 3.3.

[Histogram] Open the module *Histogram*. The description of this module is available in section 3.11.1.

[Binary] Open the module *Binary*. The description of this module is available in section 3.11.2.

[TriPlot] Open the module *TriPlot*. The description of this module is available in section 3.11.3.

[RGB] Open the module *RGB*. The description of this module is available in section 3.11.4.

[Generator] Open the module *Generator*. The description of this module is available in section 3.11.5.

[Spider] Open the module *Spider*. The description of this module is available in section 3.11.6.

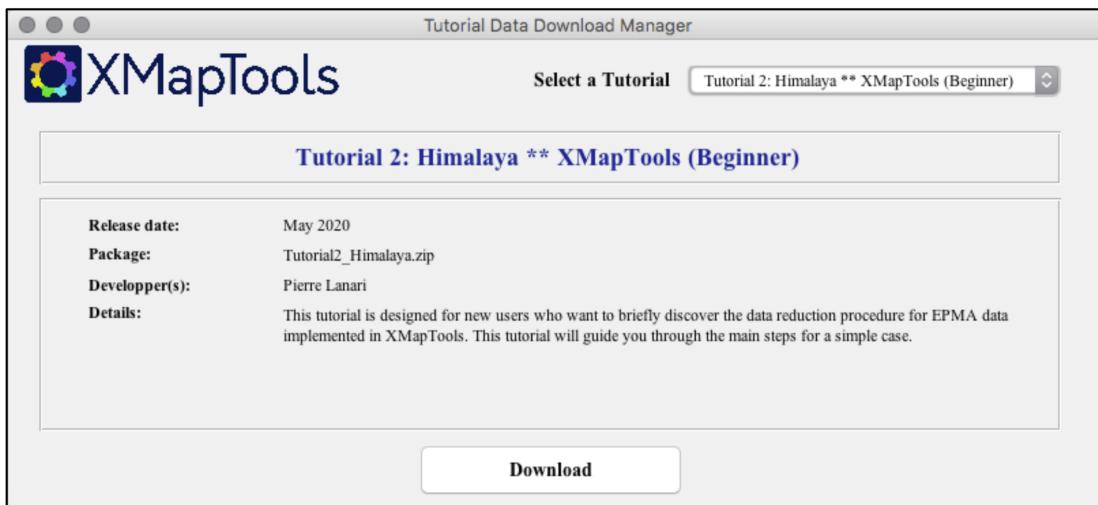


Figure 3.8 – *Tutorial Data Download Manager* window

3.2.6 Workspace

Menu *Workspace*. Switch between the three workspaces *X-ray*, *Quanti* and *Results*. Additional information is provided in section 3.1.2.

3.2.7 Help

The menu *Help* provide tools for downloading help material such as the user guide and tutorial data.

[Download Documentation] Download the last version of the user guide in the specified directory. Note that the user guide is updated for each major release (e.g. 3.4; 3.5, etc.)

[Download Tutorial Data] Download the data used in the tutorials. Select a tutorial in the menu (top right) and press the button *Download* to get the data in the specified directory. Note that this action can take up to several minutes depending on the file size and the speed of your connection. The progress of the download is not monitored so be patient...

3.3 IMPORTING DATA

This section described the procedure to import maps in XMAPTOOLS.

3.3.1 Converting raw data to XMapTools' format

The programs listed below are included in the XMAPTOOLS package and allow raw data exported from instruments to be automatically converted to the correct XMAPTOOLS' format.

This is work in progress, feel free to contact me if your instrument is not yet covered.

3.3.1.1 JEOL converter (SUN version)

The program *XConvert_JEOL_SUN* allows raw data generated with a JEOL microprobe (SUN operating system only) to be converted to a XMAPTOOLS' friendly format.

This program requires the following files (names are case-sensitive):

- The map files with their original name (e.g. *1_map.txt*; *2_map.txt*, etc.)
- The file *O.cnd* containing the mapping conditions
- A file *summary.txt* containing the table of the oxide mass fractions (format: row + spreadsheet)
- A file *stage.txt* containing the table of the X, Y and Z coordinates (format: row + spreadsheet)

To use the converter, navigate with MATLAB to the map directory and use the command (case-sensitive): `>> XConvert_JEOL_SUN`

If you only want to convert the maps (not generate *Classification.txt* and *Standards.txt*), use the command: `>> XConvert_JEOL_SUN -s`

The generated data are stored in a subfolder *Project_XMapTools* which can be copied to the MAP DIRECTORY.

3.3.2 Import map(s)

The maps can be loaded together or separately. Files must be text files and have *.txt; *.asc; *.dat or *.csv extensions containing a rectangular matrix with no header line (see file format in 2.7.3). Note that the *import map* function can also read data organized as single column. In this case, it is necessary to provide the size of the map to reshape each vector into a matrix.

The function *import map* available in the menu *Edit* (see section 3.2.1) checks the file names one by one in an attempt to recognize the corresponding element name. A dialog box is displayed if the file name does not match any element in the database that can be detected via the *automated indexation* technique. It is mandatory to select an element name to import a map in XMAPTOOLS; the name of the map is set to the corresponding element.

The *Import Tool* GUI opens once the data are loaded (Fig. 3.9). It contains several corrections that can be applied to the maps. Select the corrections required depending on the type of data (see below) and press *Apply Corrections* to validate and import the corrected maps in XMAPTOOLS.

Three types of corrections are available, the first two being applied respectively to EPMA and LA-ICP-MS maps:

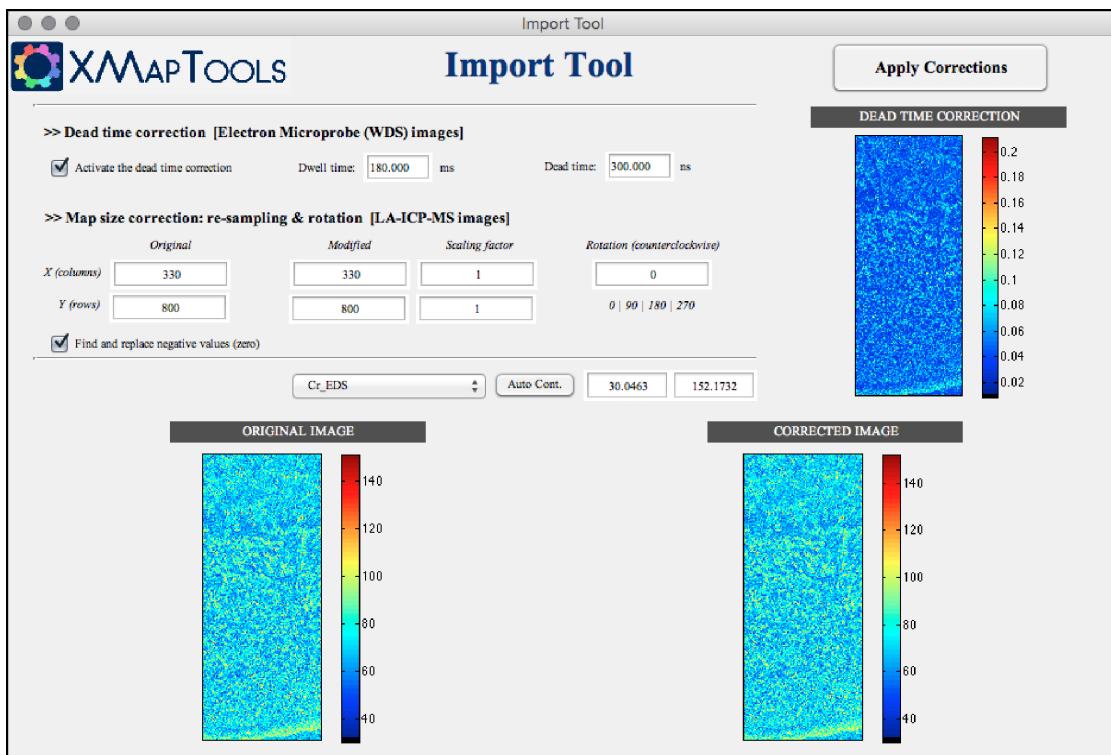


Figure 3.9 – Import module of XMapTools

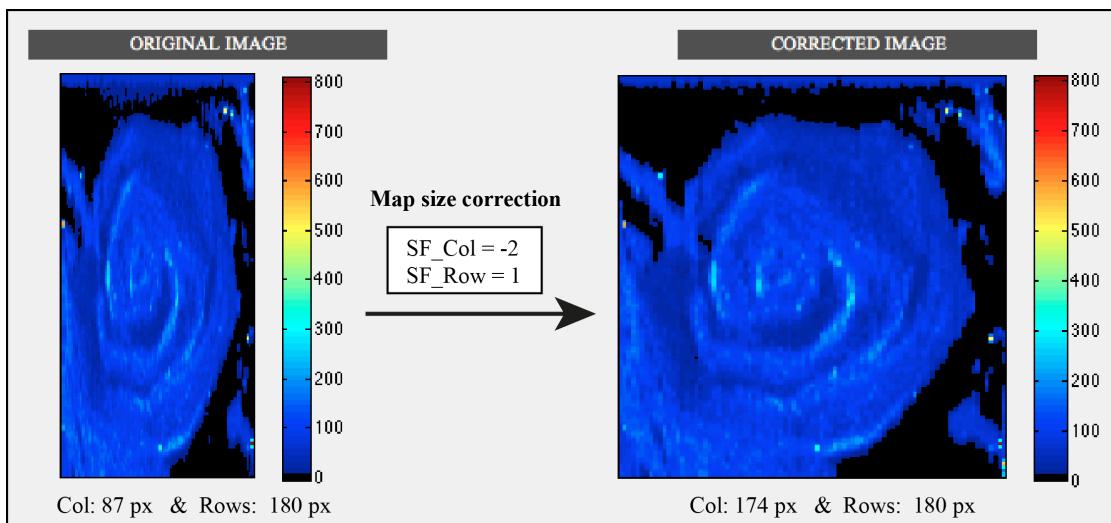


Figure 3.10 – Example of map size correction for LA-ICP-MS images

- *EPMA*: Select the option that activates the dead-time correction. Note that the dead-time correction is apply to WDS maps only (type 1, see insert 3.2). The following dead-time equation is used:

$$I_{corr} = \frac{I_{measured}}{1 - DT \times 10^{-9} \times I_{measured}} \quad (3.1)$$

with I_{corr} and $I_{measured}$ the corrected and measured X-ray intensities in counts per second and DT the dead time of the detector in ns (default 300 ns).

- *LA-ICP-MS*: Map-size correction: re-sampling and rotation. Scaling factors (integers) can be use to modify the size of the map. Positive scaling factors shrink the image using re-sampling, whereas negative scaling factors expand the image by duplicating the pixels. An example of re-sampling is provided in figure 3.10.
- *All*: Find and replace negative values (zero). If this option is activated all the negative values of the images are replaced by zero.

Any useful information regarding the corrections is printed out in the MATLAB command window (see examples for EPMA insert 3.1 and LA-ICP-MS insert 3.2 below)

Warning: Do not apply any rotation correction to EPMA maps, otherwise the map coordinates provided in Standard.txt will not work anymore. The rotation correction may only be used with standardized maps such as LA-ICPMS images.

```
Import Tool ... (apply corrections) ...
  - Map: Cr_EDS [type: 2]
  - Map: Si      [type: 1]
    * Dead time correction applied: DwellT(180); DeadT(300)
  - Map: TOPO   [type: 3]
    * Negative values are replaced by zero
Import Tool ... (Saving Import.txt) ... OK
```

Code 3.1 – Example: Import EPMA images (EDS + WDS)

```
Import Tool ... (apply corrections) ...
  - Map: 88Sr   [type: 3]
    * Map corrections applied: SF_col(-2); SF_lin(1); Rotation(0)
    * Negative values are replaced by zero
  - Map: 89Y    [type: 3]
    * Map corrections applied: SF_col(-2); SF_lin(1); Rotation(0)
  - Map: 139La  [type: 3]
    * Map corrections applied: SF_col(-2); SF_lin(1); Rotation(0)
    * Negative values are replaced by zero
  - Map: 140Ce  [type: 3]
    * Map corrections applied: SF_col(-2); SF_lin(1); Rotation(0)
Import Tool ... (Saving Import.txt) ... OK
```

Code 3.2 – Example: Import LA-ICP-MS images and map correction

3.3.3 Import maps (Mosaic)

The *mosaic tool* combines several maps together by creating a mosaic. This function is helpful to show maps of individual grains on a single image and visualize possible changes in composition. The original coordinates of each map are not preserved. The spot analyses to be used as internal standard needs to have X and Y defined in the XMAPTOOLS' coordinate system after merging. For an alternative option, see the function *Import maps (Mosaic & Standards)* in section 3.3.4.

Procedure & Requirements:

- Set the *working directory* to a directory containing a folder *Mosaic* (case sensitive) and open XMAPTOOLS
- The folder *Mosaic* should contain a set of maps with the same elements. Each dataset has to be stored in a separate subfolder. Note that the folder name is used to define the order of the map in the mosaic. Use folder names such as 01_Map34; 02_Map4; 03_Map1 to adjust the order before importation.
- If the name of a folder starts with a minus symbol (-), the folder will be skipped and not imported to create the mosaic.
- Important: the maps must have the same spatial resolution. If a map has a different spatial resolution, the resolution has to be adjusted first. Note that XMAPTOOLS assumes that the maps have the same resolution and does not check this during the creation of the mosaic.
- In the menu *File*, select *Import* and *Mosaic*
- Define the number of columns in the dialog box
- XMAPTOOLS generates the mosaic, save the maps in the working directory and run the normal import procedure (see section [3.3.2](#)).

This tools will be progressively improved in the future.

3.3.4 Import maps (Mosaic & Standards)

This import function merges several maps in a referenced system based on their original coordinates. It also calculates the coordinates of the new map for the file *Standards.txt*. This means that spot analyses obtained during the same probe session can be directly provided and used to calibrate the mosaic.

Procedure & Requirements:

- Set the *working directory* to a directory containing a folder *Mosaic* (case sensitive) and open XMAPTOOLS
- The folder *Mosaic* should contain a set of maps with the same elements. Each dataset has to be stored in a separate subfolder and already at the XMAPTOOLS' format. Note that the folder name is used to define which map is read first and this impacts the mosaic creation. In case of overlap, the latest map that is read will be shown on top. Use folder names such as 01_Map34; 02_Map4; 03_Map1 to adjust the order before importing the maps. Each folder should contain the file *Standards.txt* containing the coordinates of the map. If a file *Classification.txt* exists, it will be skipped.
- The spatial resolution of each map will be adjusted automatically to the settings of the map with the higher spatial resolution. Resampling is performed using a linear interpolant for gridded data.
- In the menu *File*, select *Import* and *Mosaic & Standards*
- XMAPTOOLS generates the mosaic, save the maps in the working directory, generate a file *Standards.txt* containing ONLY THE FIRST BLOCK with the map coordinates and run the normal import procedure (see section [3.3.2](#)). The order of oxide (second block) and the analyses (third block) need to be added manually.

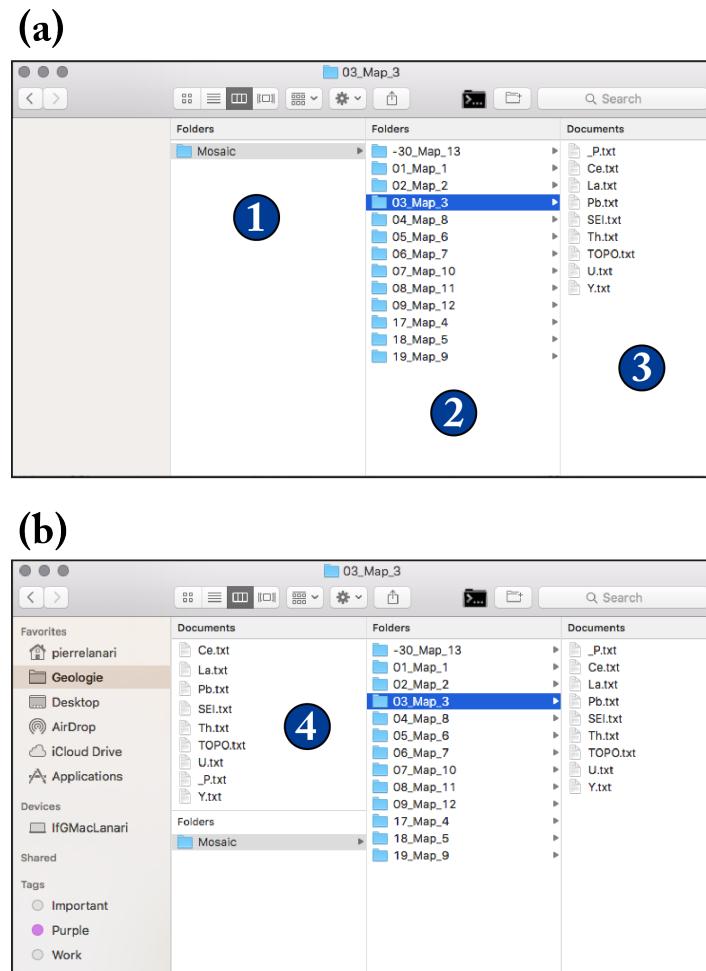


Figure 3.11 – (a) Requirements for using the mosaic tool. 1. The directory Mosaic; 2. The subdirectories containing each maps. Note that the first one will be ignored because the folder name starts with the symbol minus. 3. Maps in each subfolders. (b) The mosaic maps have been created in the working directory (see 4.)

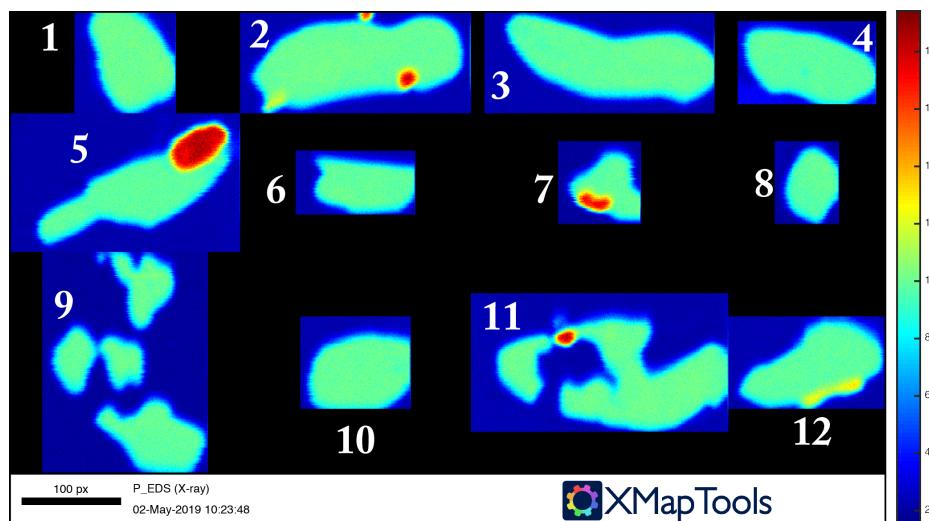


Figure 3.12 – Example of mosaic generated from the folder configuration presented in Figure 3.11. In this case, 12 maps have been used to generate the mosaic with up to 4 maps per column. The map order is shown on the figure.

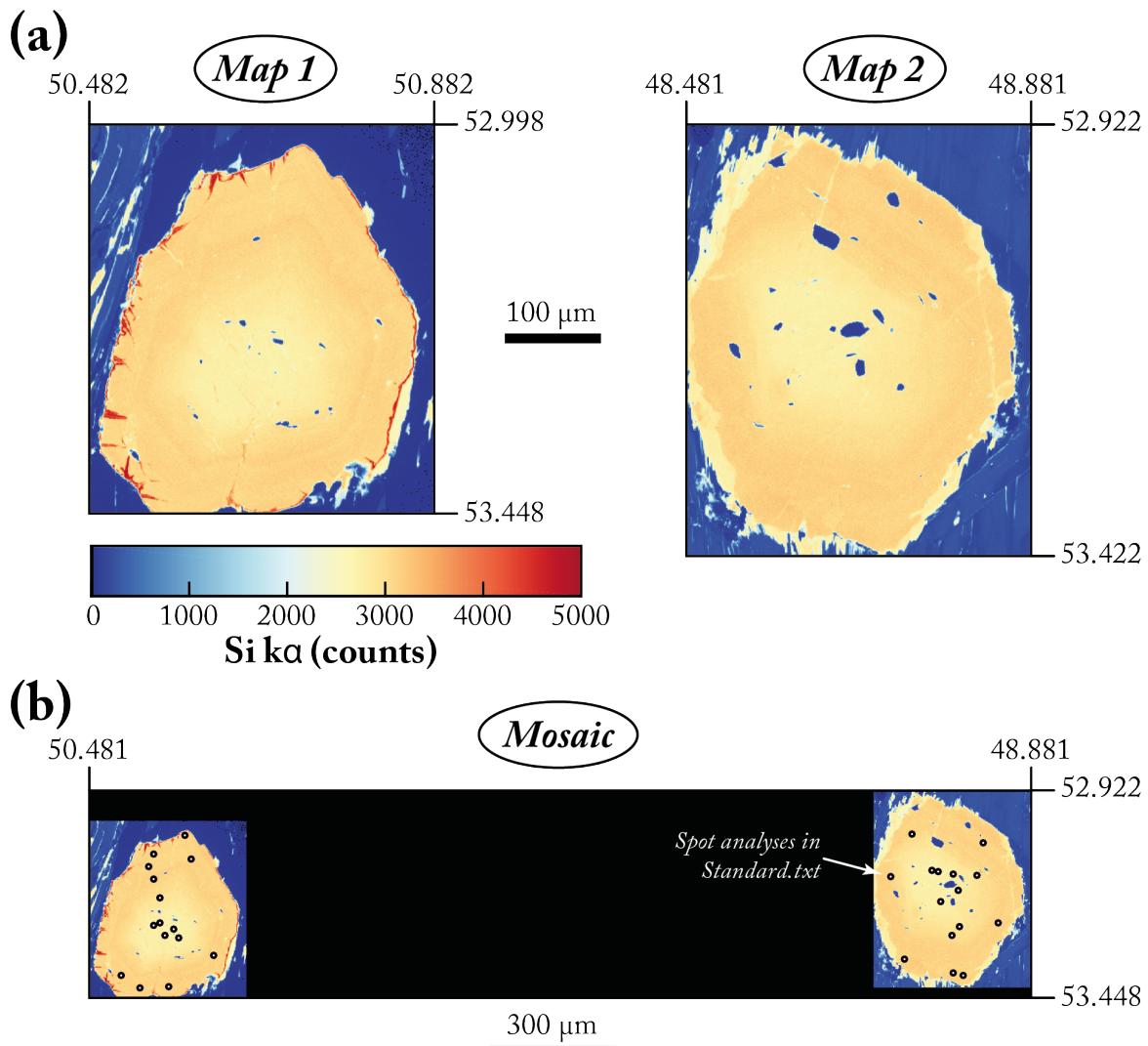


Figure 3.13 – Example of mosaic. In this case, 2 maps have been used to generate the mosaic. The spot analyses are displayed in the final mosaic.

Note that the file *Standards.txt* must be edited to add the two missing blocks.

An example is shown in Figure 3.13. Two garnet maps and spot analyses were acquired during the same analytical session, i.e. in the same coordinate system (Fig. 3.13a). The mosaic shows the maps in their original coordinate system (Fig. 3.13b).

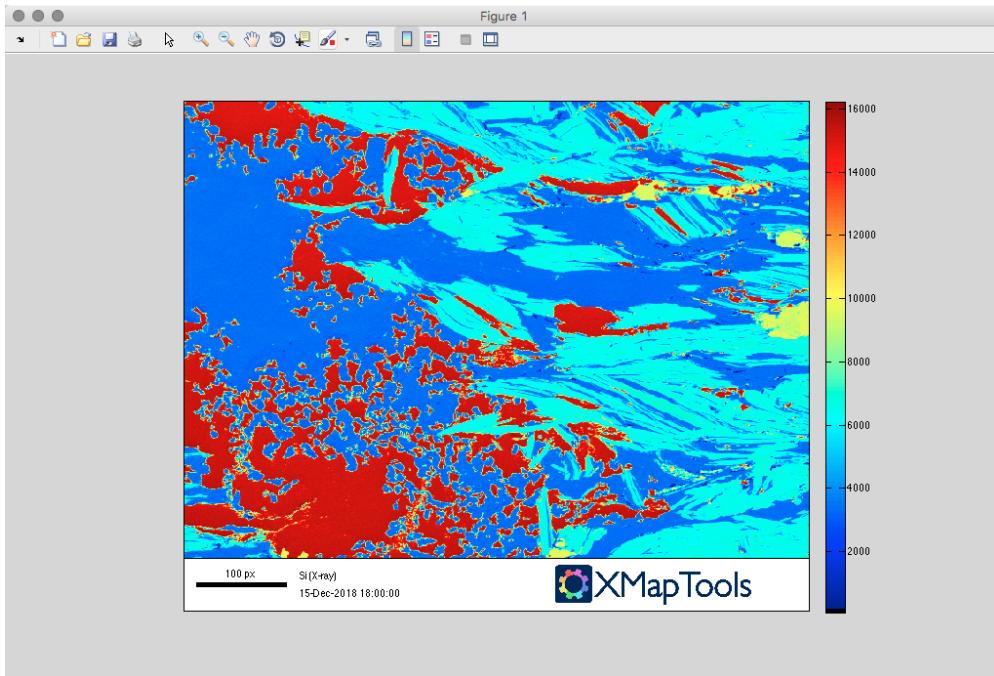


Figure 3.14 – MATLAB Window with the exported figure (see button [B5102])

3.4 EXPORTING AND SAVING IMAGES

Two functions are available in the menu *File*:

- **Export image.** Export the image plotted in the main figure window
- **Export mask image.** Export the mask map of the selected mask file

3.4.1 Export image

This function available via the menu *File* exports the active figure. It generates a copy of the figure displayed in the main XMAPTOOLS window (including images and user's selections, points, lines...) in a new MATLAB figure window. This function can also be used to export the histogram and probability density diagram.

An example of exported figure is given in figure 3.14. The date and a scale-bar of 100 pixels are printed in the exported figure. This figure can be saved in different picture formats. In the menu, select *File > Save as* and choice the image format: *.fig, *.eps, *.jpg, *.pcx, *.pbm, *.pdf, *.pgm, *.png, *.ppm, *.pkm and *.tif. Pdf files are convenient as they can be easily edited using a program such as Adobe Illustrator.

3.4.2 Export mask image

This function available via the menu *File* opens the mask image of the selected mask file (in menu [M1301]) in a new window. This figure can be saved using the menu *file > save as*. Several image formats are available: jpeg, .pdf, .eps or .png. This function is also available via the men *File, Export Mask Image* (see 3.2.1)

3.5 GENERAL FUNCTIONS

3.5.1 Project

XMAPTOOLS project files are MATLAB formatted binary files (MAT-file, extension: `*.mat`). The following structure variables are saved: *Corrections*, *Data*, *Directory*, *ListMap*, *MaskFile*, *Profils*, *Quanti* and *Results*.

NB: The backup files are relatively heavy (more than 100 Mb for a project including 10 maps, 12 standardized maps and 20 results). Be patient when XMAPTOOLS is reading or writing the project files, it can take up to several minutes.

The projects are managed via the menu *File* (see the menu description in section [3.2.1](#)).

Open Project Select and load an existing project. The name of the active project is displayed below the menu.

Save Save the active project. If the project is saved for the first time, the program calls the function *Save as...*

Save as... Save the project as a new project.

It is strongly recommended to close the XMapTools window between each session, especially if you want to open an other project. Closing the window clears all data that are not yet saved.

3.5.2 Preferences

XMAPTOOLS settings and preferences are accessible via the the main menu *File*, *Preferences* (see the menu description in section [3.5.2](#)).

The settings window is displayed in the center of the screen. The buttons *APPLY AND SAVE* or *APPLY* can be used to validate the preferences and hide the settings window. All the other functionalities of XMAPTOOLS are disabled when the preference window is displayed.

3.5.2.1 General options

- **Display help in XMAPTOOLS window [default: enabled]** Display help instructions at the bottom of the main graphical user interface (blue/red text).
- **Activate the diary [default: disabled]** Save all the info displayed in the MATLAB command window in a diary file. The diary must be deactivated using the command `» diary off` if XMAPTOOLS is not closed using the menu *File* and *Close*, or the close button in the top-left corner.
- **Display live coordinates [default: enabled]** Display the live coordinate in the main window (top left, see description in section [3.6](#)). This option may in some rare instances cause notable slowing down during the use of the software; it can be disabled here.

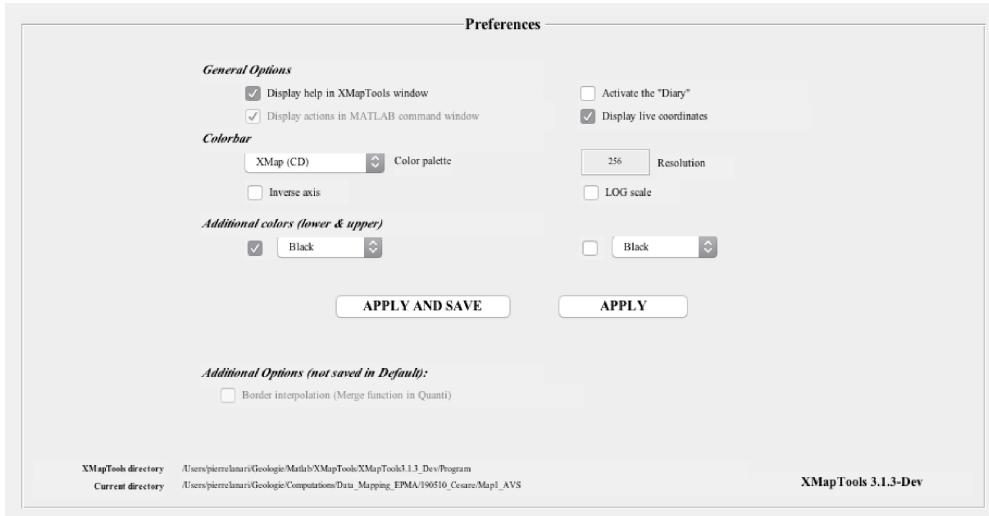


Figure 3.15 – Settings window. This window can be displayed via the menu File and Preferences.

3.5.2.2 Color options

- **Color palette [default: XMap (CD)]** Set the color palette to be used in the colorbar throughout XMAPTOOLS. The recommended color palettes are: XMap (default), Spectral, SingleRed, Frenchy, Fruity, Ocean, Forest, Blues, Reds, B&W, Horizon, Watermelon and Purples. JET is still supported but not recommended. A description of the color palettes is given in section 3.6.3.
- **Colormap resolution [default: 256]** Set the number of colors used in the colormap (i.e. the resolution of the color bar). The color palettes defined with more colors are resampled.
- **Inverse axis [default: disabled]** Inverse the order of the color palette. This option is only applicable for the color palettes defined in */XMapTools/Program/Dev/XMap_ColorMaps.txt*
- **LOG scale [default: disabled]** Set the color bar to a logarithmic axis. If this option is not selected a linear scale is applied instead.

3.5.2.3 Additional colors (lower & upper)

- **Lower [default: selected, black]** Add a layer at the bottom of the color palette. If selected, the layer can be set either to *Black* or *White*
- **Lower [default: disabled, black]** Add a layer at the top of the color palette. If selected, the layer can be set either to *Black* or *White*

Note that these options change the resolution of the color bar set above by +1 each.

3.5.2.4 Additional options (not saved in Default)

- **Border interpolation (merge function in Quanti) [default: unselected]** activates the border interpolation option in the function merge [B2401].

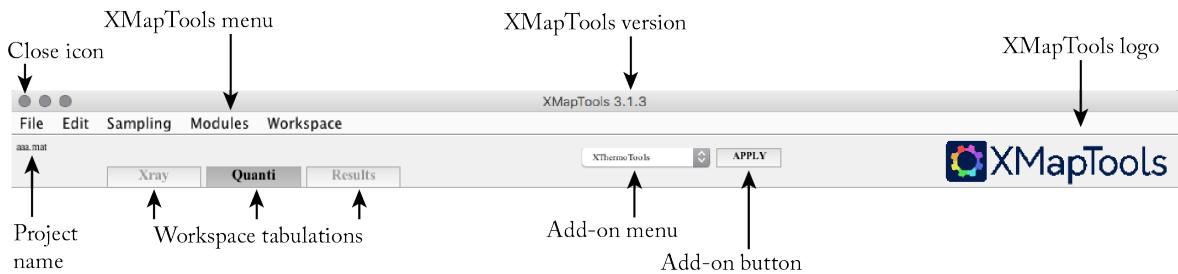


Figure 3.16 – XMAPTOOLS menu, workspace and add-on functionalities.

3.5.2.5 Saving the settings

User's personal settings are updated when the button *APPLY AND SAVE* is pressed. The saved settings are used by default. The settings are stored in the file *Default_XMapTools.mat* located in the directory */Program*.

NB: XMAPTOOLS update will reset the personal settings; new personal settings must be redefined after each software update.

The XMAPTOOLS release number, the setup directory and current working directories are also displayed in the *Settings window*.

3.5.3 About XMapTools

The release notes and a short description of XMapTools can be displayed via the menu *File* and the option *About*.

3.5.4 Workspaces

The tabulations *Xray*, *Quanti* and *Results* allows the user to switch between the three workspaces (see Fig. 3.16).

3.5.5 Add-ons

[M5601] *Add-on Menu* (see Fig. 3.16) List all the compatible add-ons available in .../*UserHome/Documents/MATLAB/XMapTools/Addons/*. The selected add-on can be called using the button [B5601] *OPEN*.

[B5601] The button *OPEN* run the add-on selected in the add-on menu [M5601].

3.5.6 Figure options

[B4403] *Unfreeze the interface* . A description of this functionality is given in section 5.3.1.
Note: to be only used if the program is crashed!

3.6 DISPLAY FUNCTIONS

3.6.1 Live coordinates display window

The *Live coordinates display window* provides the X and Y coordinates of the cursor in the image displayed into the main figure window. This option can be enabled/disabled in the *Settings window* (see complete description in section 3.5.2). Note that the Y axis is inverted.

NB: The coordinates reported in the *Live coordinates display window* are the matrix coordinates of the initially loaded X-ray image. The displayed coordinates for one selected pixel are the same for all the rotate positions (i.e. this value is *corrected* for the rotation, see function [B5103])

The value displayed as Z is the value for the pixel that is located exactly under the cursor. The unit of the number displayed depends on which image is displayed. It can be number of counts, oxide wt%, atoms per formula unit, end-member fraction, equilibrium conditions, density or reference number of a phase.

3.6.2 Figure/display tools

3.6.2.1 Map display

[B5101] *Apply auto-contrast.* Apply an optimized color-scale to the displayed image. If the auto-contrast mode is active then the same button can be used to disable the auto-contrast (*disable auto-contrast*) restoring to the default values. The default *lower* and *upper* values of the color bar are the *min* and *max* values of the displayed map.

[C5101] *Edit 'min' and 'max' values of the colorbar* Manually adjust the lower and upper values of the color-scale.

NB: Use this button to turn the auto-contrast mode on/off.

[B5102] *Change the size of the display window* Adjust the size of the map display window. Three different sizes are available (full screen, intermediate, small) and the button permits to switch between these sizes.

[B5103] *Rotate the figure of 90° (counterclockwise).* Change the orientation of the image displayed in the main figure by 90°. It is possible to rotate the map to the following orientations:

- Orientation 1 - 0° [Default], see figure 3.17a
- Orientation 2 - 90°, see figure 3.17b
- Orientation 3 - 180°, see figure 3.17c
- Orientation 4 - 270°, see figure 3.17d

NB: The default orientation (1, Fig. 3.17a) is automatically set when you run XMAPTOOLS without loading a project. Press the function *rotate the figure of 90° (counterclockwise)* to change the orientation. The selected orientation will be applied during the active session and saved in the project file for the next sessions. Note that a few functionalities remain not compatible with the rotate function. In this case a warning message will be displayed inviting to restore the original orientation.

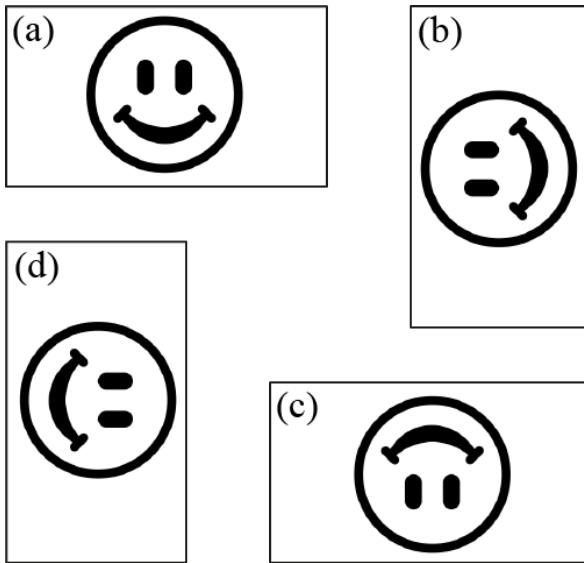


Figure 3.17 – Orientation positions available for the main figure display (see rotate function [B5103])

The coordinates reported in the *Live coordinates display window* (see section 3.6.1) are the matrix coordinates of the initially loaded X-ray image. The displayed coordinates for a given pixel are the same for all the rotate positions.

[B5104] The check box *Lower black layer* allows a black color layer to be added to the color bar for all the values lower or equal to the 'min' value defined in [C5101].

[B5105] The check box *Upper black layer* allows a black color layer to be added to the color bar for all the values greater or equal to the 'max' value defined in [C5101].

[B5106] *Activate/disable median filter.* Activate or disable the median filter. If selected, this function applies a median filter to the displayed image along two dimensions using a square window. Each output pixel contains the median value in the M-by-M neighborhood around the corresponding pixel in the input image. M value is defined in [C5106]. The median filter is only applied to the displayed images. The data stored in the software are kept unchanged.

[C5102] The cells *median filter size* allows to set the size in pixel of the median filter [C5106]. Every time a number is enter, the median filter applied to the displayed figure is updated.

3.6.2.2 Zooming and panning

[B5107] *Activate zoom mode.* Turns the zoom mode on. Turning on the zoom mode disables the pan mode (and vice versa).

When zoom mode is enabled, pressing a mouse button while your cursor is within the displayed map zooms into the point or out from the point beneath the mouse (note that each mouse click or scroll wheel click zooms in or out by a factor of 2.). When using zoom, you can:

- Zoom in by positioning the mouse cursor where you want the center of the plot to be and either (1) press the mouse button or (2) rotate the mouse scroll wheel away from you (upward).

- Zoom out by positioning the mouse cursor where you want the center of the plot to be and either (1) simultaneously press *Shift* and the mouse button, or (2) rotate the mouse scroll wheel toward you (downward).
- Clicking and dragging over an axes when zooming in is enabled draws a rubberband box. When you release the mouse button, the figure is adjusted to zoom in to the region enclosed by the rubberband box.

Note: If only a region of an image is displayed (after zoom or pan was used), this specific view is maintained when using most of the functions within one workspace (*Xrax*, *Quanti* or *Results*). However, a few functionalities still require resetting the display to the original image.

[B5108]  *Activate pan mode.* Turns the pan mode on. Turning on the pan mode disables the zoom mode (and vice versa). Note that panning is only available if a zoom is applied.

When the pan mode is active, holding the mouse button while your cursor is within the displayed map permits panning the view of display interactively.

[B5109]  *Reset zoom & pan* disables both zoom and pan modes and restore the original view of the displayed image.

Note: the original view is restored when the program switches between the three workspaces.

3.6.3 Color palette

[M1302)] Select the active color palette used throughout XMAPTOOLS. Navigate to the menu *File*, *Preferences* and press *APPLY AND SAVE* to save as default.

XMAPTOOLS includes a large choice of color palettes in line with the general recommendations for good scientific practices¹. These palettes are shown in Figure 3.18 and listed in Table 3.4 (above the *other*).

The color palettes are defined in the file */XMapTools/Program/Dev/XMap_ColorMaps.txt*.

The old palettes are still proposed at the bottom of the list (below *other* in Tab. 3.4). It is not recommended to use the color palettes *Jet*, *ColdWarm* and *FreezeWarm* as they introduce significant artifacts caused by non-linear and changing gradient slopes.

These recommendations are not applicable to logarithmic color bars (see below).

3.6.3.1 Logarithmic color bar

[B1301)] Apply a logarithmic color bar to the main figure. Navigate to the menu *File*, *Preferences* and press *APPLY AND SAVE* to save the choice as default.

¹The color palettes are largely inspired from www.ColorBrewer.org by Cynthia A. Brewer, Geography, Pennsylvania State University.

Color Palette	Recommended	Linear (L)	Colorblind friendly (C)	Divergente (D)	Printing friendly (P)
XMap	yes	no	yes	yes	no**
Spectral	yes	no	yes	yes	no**
SingleRed	yes	no	yes	yes	no**
Frenchy	yes	no	yes	yes	no**
Fruity	yes	no	yes	yes	no**
Ocean	yes	no	yes	no	yes
Forest	yes	no	yes	no	yes
Blues	yes	no	yes	no	yes
Reds	yes	no	yes	no	yes
B&W	yes	yes	yes	no	yes
Horizon	yes	yes	yes	no	yes-
Watermelon	yes	yes	yes	no	yes-
Purples	yes	yes	yes	no	yes
Other					
WYRK	yes	no	n.t.	no	n.t.
ColdWarm	no	no	n.t.	no	n.t.
FreezeWarm	no	no	yes	no	n.t.
Jet	no	no	no	no	no
Parula	yes	no	n.t.	no	n.t.
Bone	yes	yes	yes	no	yes
Copper	yes	yes	yes	no	yes
Pink	yes	yes	yes	no	yes

** see Fig 3.19

- low contrast

n.t. not tested

Table 3.4 – Characteristics of the color palettes available in XMAPTOOLS. Note that the color palettes below other are either proposed by users or generic MATLAB color palettes.

3.6.4 X-pad navigator

[B540X] The buttons of the X-pad navigator - [B5401] up, [B5402] down, [B5403] right, [B5404] left - can be used to move objects during the corrections. Standard position can be adjusted during the SPC correction (see section 3.8.4.4) and X-ray maps during the MPC correction (see section 3.8.4.3).

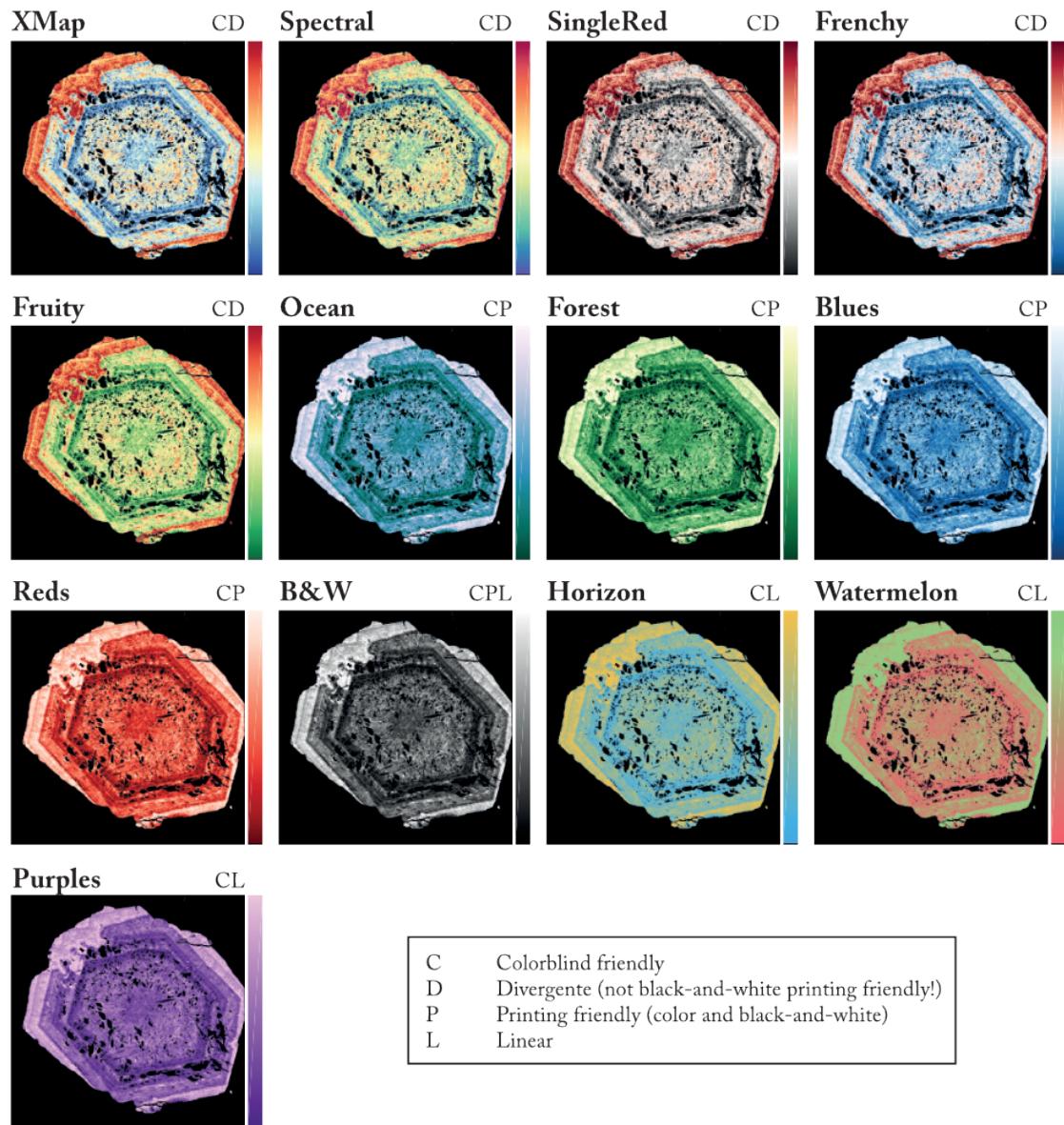
[B5405] *Apply*. Exit the correction mode and apply the modifications made.

3.6.5 Other options

[B4402]  *Activate/disable histogram mode* Switch to the histogram mode (or vice versa, switch back to the mapping mode). In histogram mode all the values of the pixels displayed in the main figure window are used and plotted as histogram (bottom) and probability density function (top).

3.6.6 Activated corrections

[B5501] The button *BRC* allows the BRC correction to be displayed (selected) or hidden (unselected). This button becomes available once the BRC correction has been calculated using the correction function (see section 3.8.4.1).

Figure 3.18 – *Color palettes available in XMAPTOOLS*

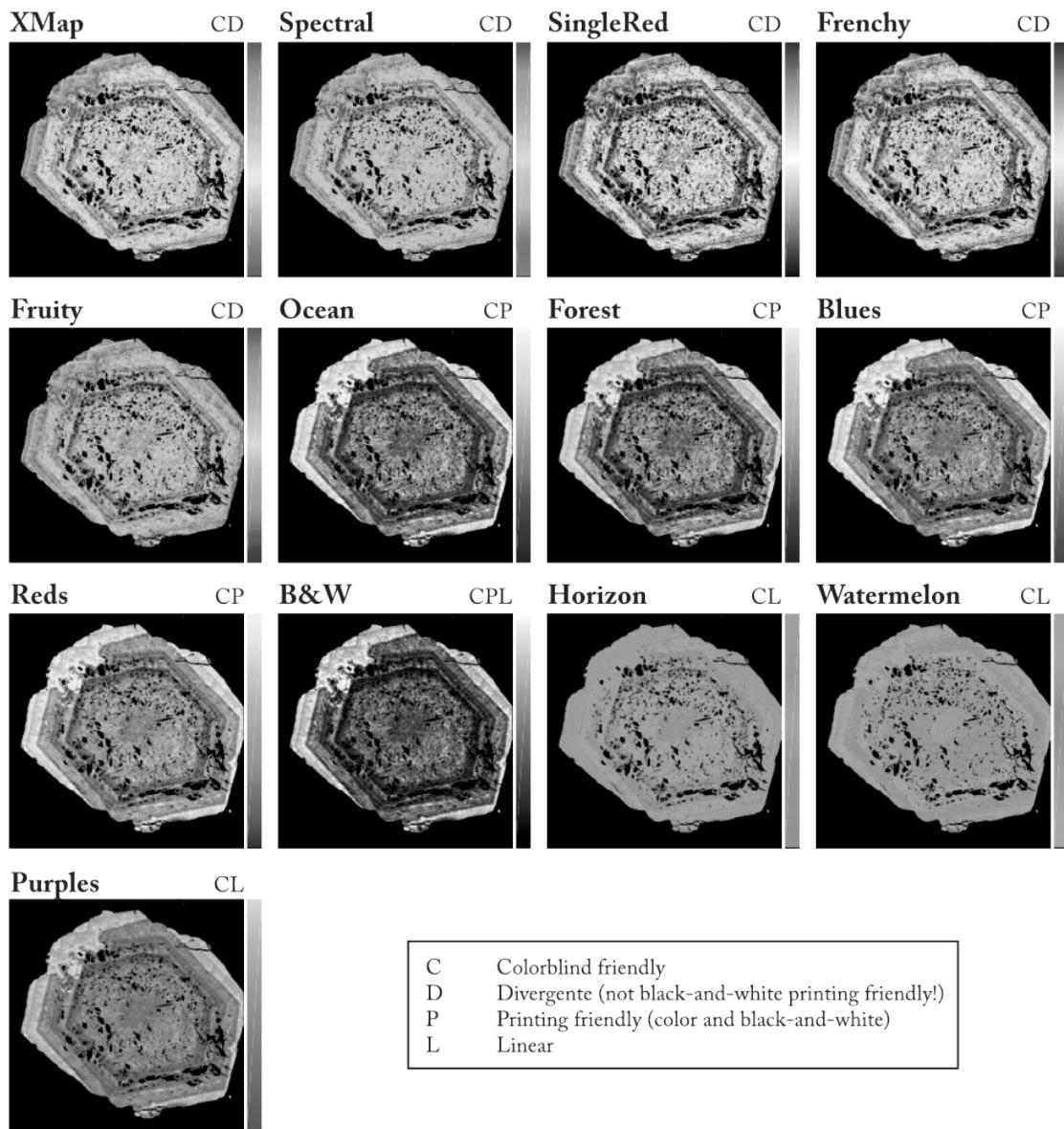


Figure 3.19 – Color palettes available in XMAPTOOLS transformed to black-and-white for simulating BW printing. Note that the divergence palettes (D) are not printing friendly. The two gradients cannot be distinguished from each other in the black-and-white version of those palettes

3.7 SAMPLING TOOLS

XMAPTOOLS contains several sampling tools which can be used to extract data from the maps (see Fig. 3.20). These tools and their options are available via the menu *Sampling* (Fig. 3.5-d). A description of the menu items is provided in section 3.2.4 and the technical description is reported below.

[C5201] *sampling results* (cell). Display some results from the sampling functions.

XMAPTOOLS includes several options that can be set before using the sampling tools. These options are described first in the next section.

3.7.1 Description of the sampling options

The sampling options are:

- **Multi-map**, a mode allowing the data to be exported for more than one elements at the same time (i.e. more than one map). If this mode is active, a dialog box is displayed to select the map(s) from which the data will be extracted
- **Color mode**, a mode in which the data points of the compositional profiles are shown in color, following the active color scheme of the displayed map. Note that the scale is automatically adjusted if the mode *Multiple-map* is also active.
- **Save data**, a mode allowing all the data and corresponding figures to be automatically saved in the folded */Export-sampling*
- **Save map**, a mode to export and saved a copy of the active map along with the data
- **Clean the figure**, a mode in which the main figure window is cleaned up between each sampling action

Note: These options must be set via the menu first before using the sampling functions.

The compatibility of these options for each sampling mode is described in Table 3.5:

Method	Multi-map	Color mode	Save data	Save map	Clean figure
Line	yes	yes	yes	yes**	yes
Path	yes	yes	yes	yes**	yes
Area	yes	no	yes	yes**	yes
Integrated lines (stripe)	yes	no	yes	yes**	yes
Sliding window	yes	no	yes	yes**	yes

** Save map is only available if the data are also saved

Table 3.5 – *Sampling functions and their options*

3.7.2 Description of the sampling tools

3.7.2.1 Line

Extract compositional profile(s) along a linear transect. Each sampling line is defined by two spots 1 and 2; the direction in the plot is always from spot 1 (left) to spot 2 (right; see Fig. 3.20). Select

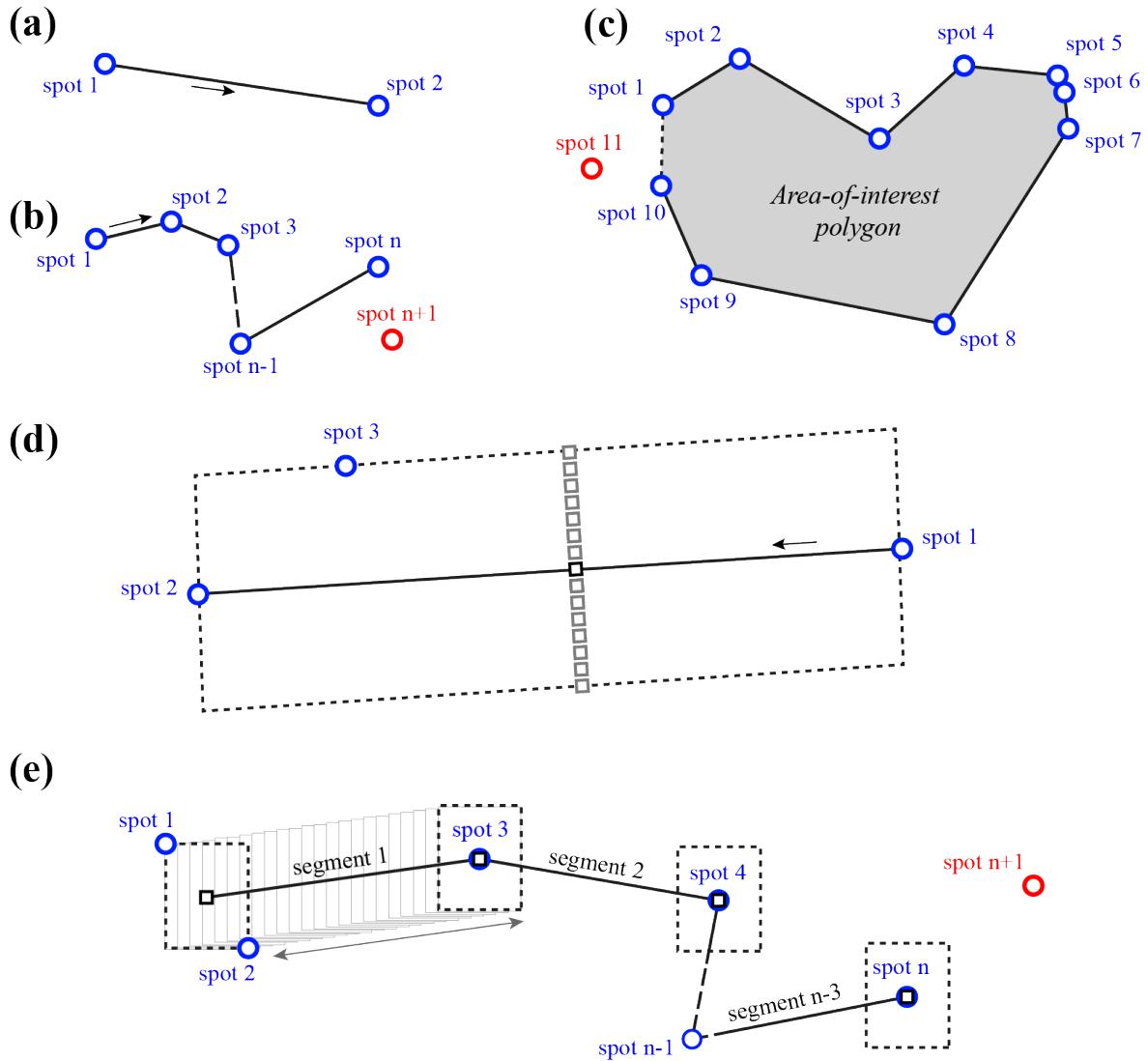


Figure 3.20 – Sampling functions: (a) Line (see description in section 3.7.2.1); (b) Path (see 3.7.2.2), (c) Area (see 3.7.2.3); (d) Integrated lines (see 3.7.2.4); (e) scanning window (see 3.7.2.5)

the sampling item *Line* in the sampling menu and click twice on the active map to define A and B. Note that once the function is selected, the program is expecting two points to be defined (other functionalities and buttons are frozen).

This function can be used in black-and-white mode (e.g. Fig. 3.21c) or color mode (e.g. Fig. 3.21b) and is fully compatible with the multi-map mode (see Tab. 3.5)

The figure of the active map is displayed in a new figure window and save via the menu *File Save as...*

If the mode *Save data* is active, the plotted data are saved as an ASCII file (in *.txt, see Ex. 3.3). This file is automatically stored in the repertory */Export-sampling*. If this repertory does not exist, the program creates a new one in the working directory.

If the mode *multi-maps* is active, the figures generated by the software are saved both as FIG and PDF files in a new folder that is located in the */Export-sampling* directory. Note they are saved but not displayed! Two additional figures that contain all the elements (linear and logarithmic axes) are

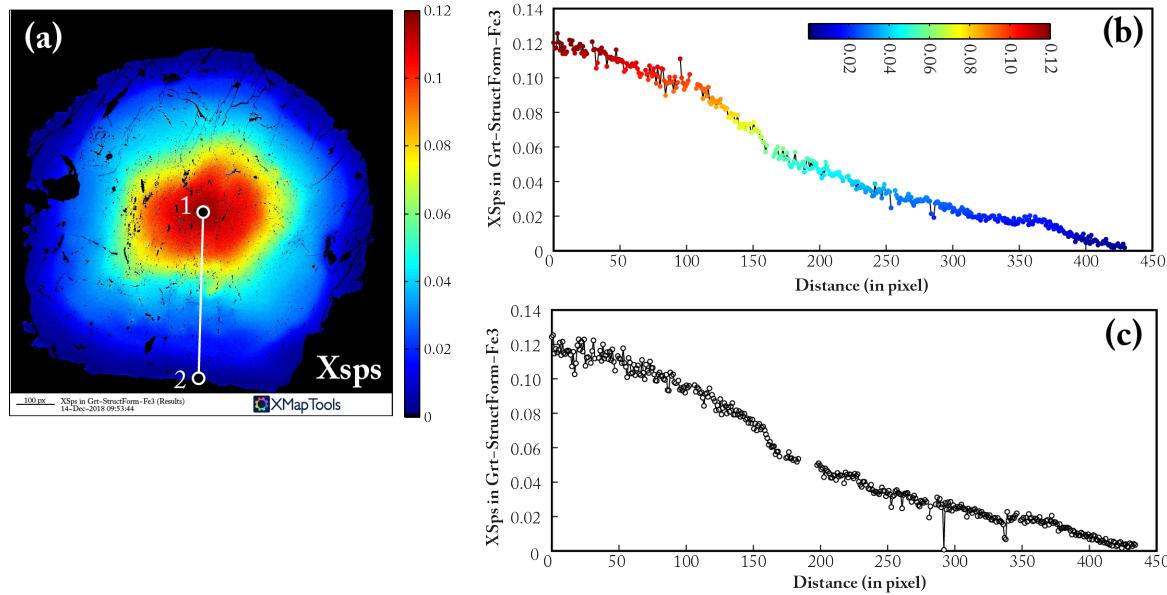


Figure 3.21 – Example of line sampling across a garnet porphyroblast using (a) the map fraction of spessartine (X_{Spss}). (b) mode Single Map (color). note that the color of is the same as the corresponding pixel on the map. (c) mode Single Map (bw).

also saved and kept for display. For a profile AB extracted from four maps (elements), twenty-two files are generated. In this case the data are saved as a matrix in which each column corresponds to a given element.

Sampling data exported from XMapTools		
02-May-2019 14:07:01		
Sampling mode: Line		
Ref	Distance (px)	Value
1	0	5184.0498
2	1.0113	4334.6294
3	2.0226	5190.0685
4	3.034	5050.6411
5	4.0453	3814.3598
6	5.0566	4290.5155
7	6.0679	5260.2881
8	7.0792	5206.1184
9	8.0906	5320.4787
10	9.1019	5180.0373
11	10.113	5367.6295

Code 3.3 – Example of exported file (sampling mode line; single map). This example is not related to Fig. 3.21

NaN	7.0626458e-01	4.2383406e-02	8.0733279e-02
1.0147566e+00	6.5981714e-01	5.6531633e-02	8.3051179e-02
2.0295131e+00	6.7420776e-01	3.5311783e-02	8.2939191e-02
3.0442697e+00	6.4783629e-01	6.1009299e-02	8.2588029e-02
4.0590263e+00	6.4783629e-01	6.1009299e-02	8.2588029e-02
5.0737829e+00	6.6443397e-01	6.2993626e-02	8.3669548e-02
6.0885394e+00	6.8620576e-01	4.4191272e-02	8.2615855e-02
7.1032960e+00	6.7362292e-01	5.8242926e-02	8.3168996e-02
8.1180526e+00	6.8470315e-01	5.3741117e-02	7.4112187e-02
9.1328092e+00	6.9712853e-01	4.6606671e-02	7.8347844e-02
1.0147566e+01	6.8852298e-01	4.5695592e-02	8.1875825e-02
1.1162322e+01	6.7977865e-01	4.6299546e-02	8.3027452e-02
1.2177079e+01	6.7977865e-01	4.6299546e-02	8.3027452e-02

Code 3.4 – Example of exported file (sampling mode line; multiple map). In this case the first column corresponds to the distance in pixels (NaN = 0) and the next columns contain the profile corresponding to each element. Not related to Fig. 3.21

3.7.2.2 Path

Extract compositional profile(s) along a path composed by multiple linear segments (Fig. 3.20-b). A path is defined by n spots corresponding to $n - 1$ segments. Select the sampling item *Path* in the sampling menu and click on the figure to generate your path and right-click to validate and plot the compositional profile. This sampling function cannot be interrupted by any other way than right-clicking.

This function can be used in the same way as the function *Line* described above. An example is given in Fig. 3.22.

3.7.2.3 Area

Extract the average composition of a region-of-interest. The region-of-interest is set by selecting spots that define segments of a polygon which is converted by the program into a mask (see spots 1 to 10 Fig. 3.20b). The polygon is closed without considering the right clicking position, see dashed line in figure 3.20b.

The result is displayed in the cell [C5201] in the vertical tool box. The displayed result includes, the average and standard deviation (1σ).

If the mode *Save data* is selected (see Tab 3.5), the results also include the number of pixels used to derive the average and the associated standard error (1σ).

For a pixel i with composition X_i from an area containing n pixels, the values shown in 3.5 are obtained using:

$$Value = \bar{x} = \frac{\sum X_i}{n} \quad (3.2)$$

$$StdDev = \sigma = \sqrt{\frac{\sum(X_i - \bar{x})^2}{n}} \quad (3.3)$$

$$StdErr = \frac{\sigma}{\sqrt{n}} \quad (3.4)$$

If the mode *Multi-map* is selected, it is possible to select both multiple maps and multiple areas. In this case a figure shows the compositional changes between the successive areas.

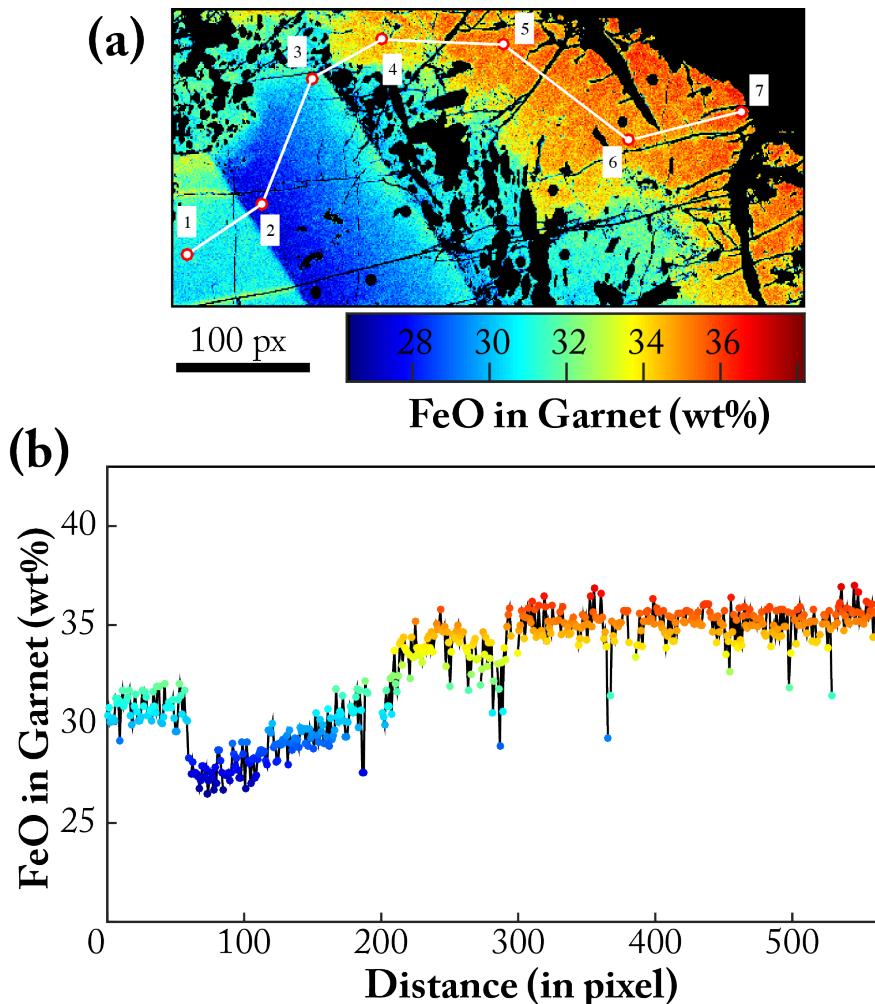


Figure 3.22 – Example of Path sampling across a garnet porphyroblast: (a) Map of FeO in Garnet; (b) Compositional profile.

An example is given in Fig. 3.23 and Ex. 3.5. This file is automatically stored in the repertory /Export-sampling.

```

Sampling data exported from XMapTools
14-Dec-2018
Sampling mode: Area (multiple maps/areas)

#1 | Nb pixels = 1325
Ref      Name      Value      StdDev   N       StdErr
1.0000  XSps     0.1163    0.0035   1325    0.0001

#2 | Nb pixels = 865
Ref      Name      Value      StdDev   N       StdErr
1.0000  XSps     0.0508    0.0042   865     0.0001

#3 | Nb pixels = 3453
Ref      Name      Value      StdDev   N       StdErr
1.0000  XSps     0.0039    0.0014   3453    0.0000

```

Code 3.5 – Example of exported file (sampling mode area, see Fig. 3.23)

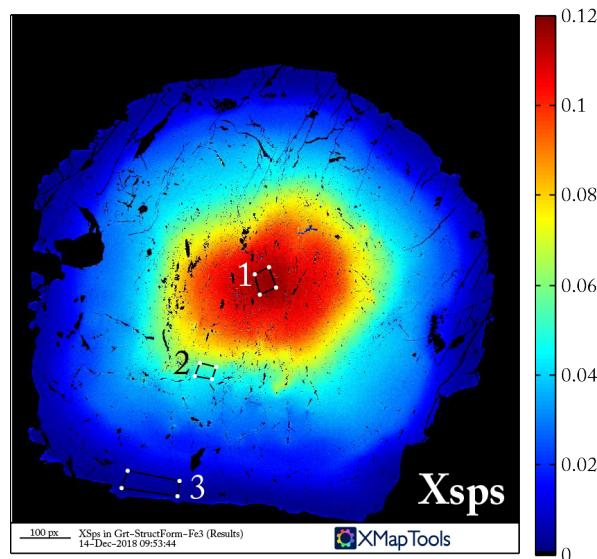


Figure 3.23 – Three areas used to export the average X_{Sps} (see 3.5)

3.7.2.4 Integrated lines (stripe)

Extract the average composition profile from a stripe with a rectangular shape by averaging the composition of each transect. For a given pixel on the central transect, the value is calculated as the mean of the pixel compositions perpendicular to the reference transect (see Fig. 3.20d). The central transect is defined first by two spots, whereas the third spot defines the height of the rectangular area.

Two figures are generated by this sampling function:

- A figure showing the evolution of the mean including the standard deviation envelope (see Fig. 3.24b)
- A figure with two separate plots (see Fig. 3.24c): the upper diagram showing all the transects in gray as well as the mean and median transects in red and blue respectively; the lower diagram shows the evolution of the fraction of pixels used to generate the average transect. Note that unused pixels have a value of 0 and are therefore ignored while calculating the average value.

Data can also be saved if the mode *Save data* is active. An example is shown in Fig. 3.24 and Ex. 3.6.

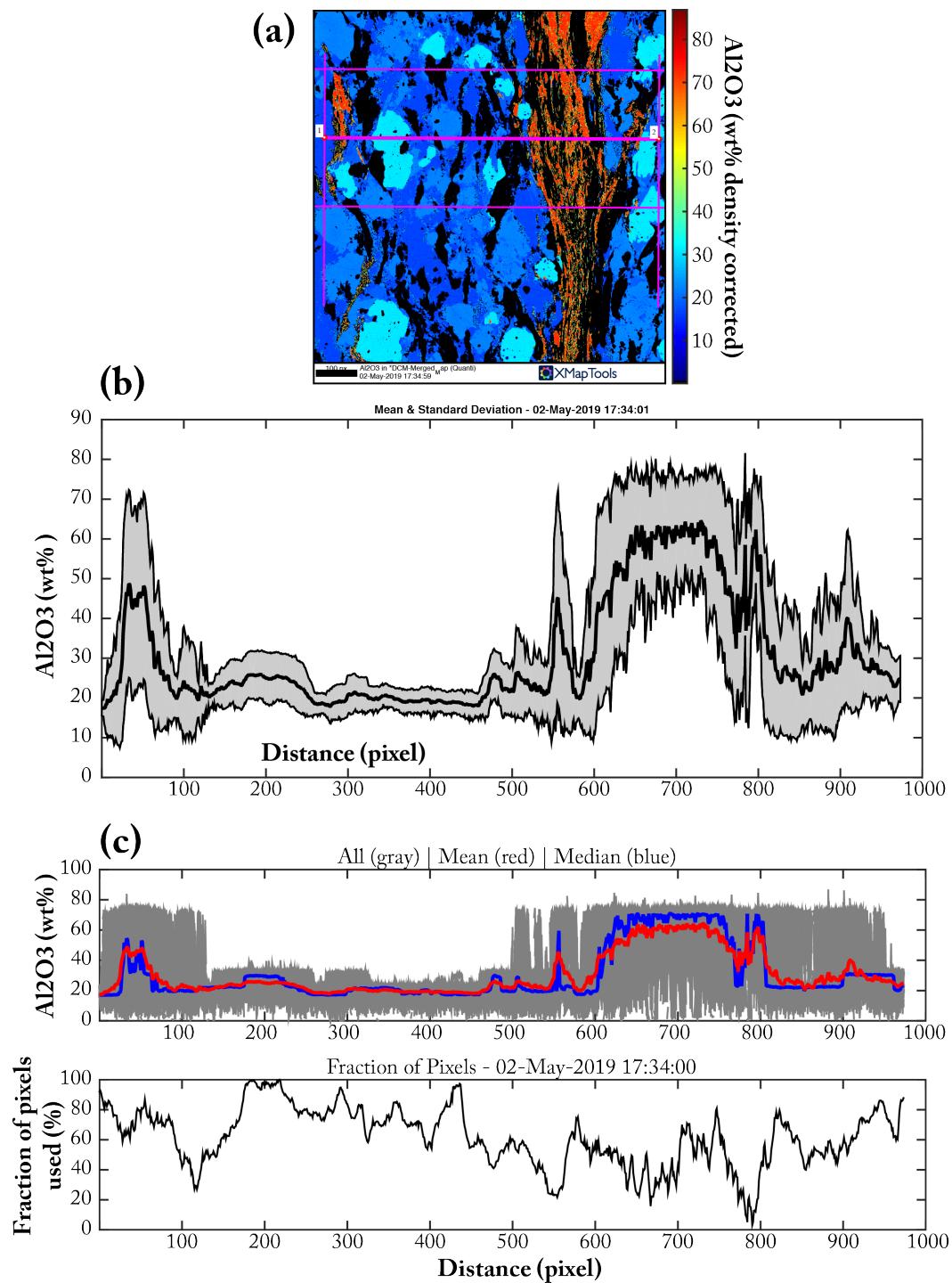


Figure 3.24 – Sampling: Integrated lines (stripe) on quantitative map of Alumina (corrected for density differences between the phases). (a) Compositional map showing the rectangular area; note that the reference profile goes from left to right. (b) Compositional changes of Al₂O₃ from left to right (mean + standard deviation envelope). (c) Upper plot: all transects (gray), mean (red), median (blue); lower plot: fraction of pixel used. Note that this value changes along the profile because of the presence of quartz in this sample.

Sampling data exported from XMapTools				
02-May-2019 17:34:15				
Method: Integrated Area				
Columns: Distance (px) Mean Median Std Frac. Pixel (%)				
0.00000000	17.53304668	17.00537705	1.97578032	92.00000000
1.00000000	17.40780069	17.06151210	2.01730203	92.75000000
2.00000000	17.45544626	17.07748472	2.11132433	91.25000000
3.00000000	17.46201992	17.01333969	4.00269996	88.50000000
4.00000000	17.53795322	16.98533287	4.98548763	86.25000000
5.00000000	18.29509240	17.04573629	7.32770999	83.25000000
6.00000000	18.45975458	17.05951679	7.45648841	80.75000000
7.00000000	19.69604802	17.10250719	9.90641147	85.00000000
8.00000000	18.92646198	16.96473802	8.44213952	84.25000000
9.00000000	19.26462865	17.03576723	9.03272135	82.25000000
10.00000000	19.23550957	17.07197563	8.673363453	83.75000000
11.00000000	19.41361754	17.10139080	8.82599782	86.00000000
12.00000000	20.28463405	17.11553340	10.27648576	85.50000000
13.00000000	20.43134306	17.10895356	10.06648718	83.75000000
14.00000000	20.68205128	17.10314485	11.11304613	82.75000000
15.00000000	21.81339800	17.10159137	13.62204274	82.75000000
16.00000000	21.78075563	17.18632971	13.05048223	78.75000000
17.00000000	20.69364885	17.16891474	10.99522319	75.75000000
18.00000000	22.12034036	17.19984969	13.18999470	76.50000000

Code 3.6 – Example of exported file (sampling mode integrated area). Same data as Fig. 3.24

3.7.2.5 Scanning window (rectangular)

Calculates a composition profile using a moving average window. This sampling mode requires first to define a rectangular area with two spots (see Fig. 3.20e) followed by the definition of a path, similar to the sampling function *Path*, along which center of the scanning window will move. This function is available in the menu *Sampling*. Once the menu item has been selected, click on the figure to set the rectangle (first two spots) and the path. Similarly to the function *Path*, right-clicking validate the selection and generate the plot. This sampling function cannot be interrupted by any other way than right-clicking.

An example of sampling window is provided in Figure 3.26. the rectangle is displaced along 3 segments from the starting spot (left on Fig. 3.26-a) to the end of the path (right on Fig. 3.26-a). The average composition of the pixels for every step is calculated together with the standard deviation and are plotted in a new figure window (Fig. 3.26-b).

Note that in XMAPTOOLS the distance unit used is pixel. In figure 3.26, distances have been converted from pixels to μm .

An example of output is provided in Ex. 3.7

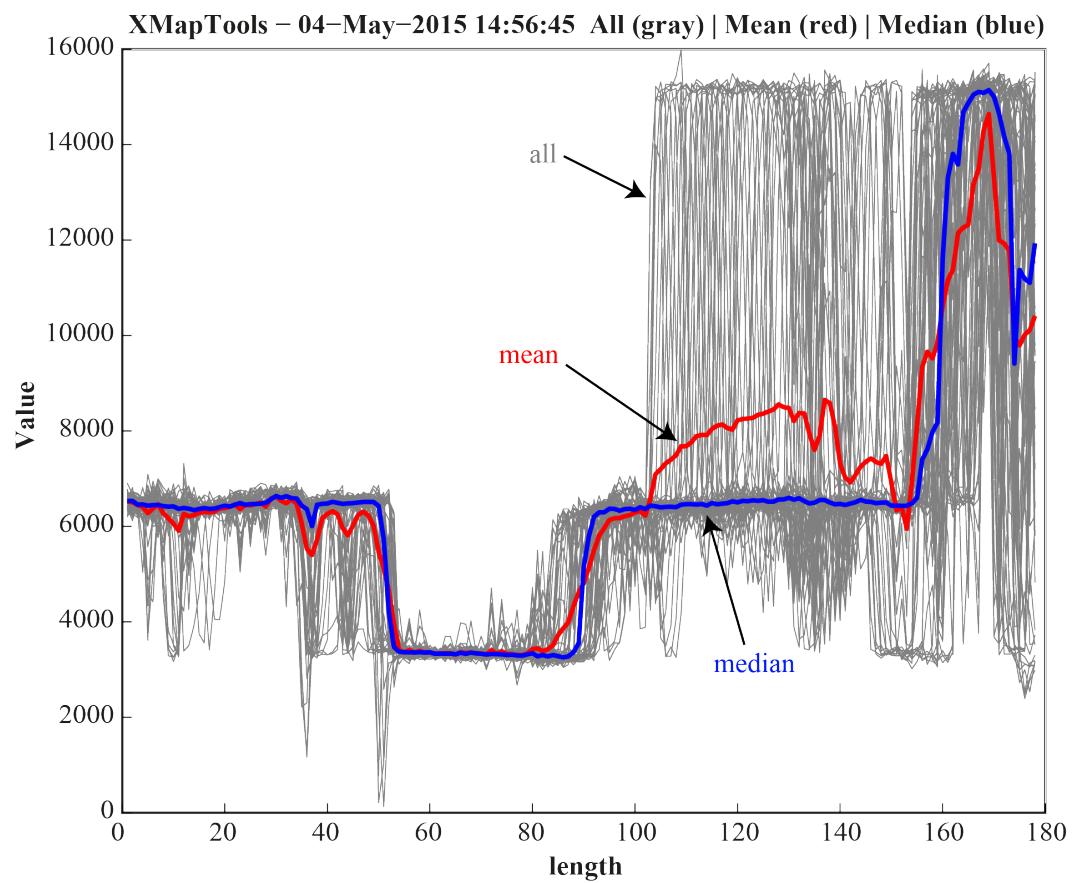


Figure 3.25 – Example of sampling integrated lines mode.

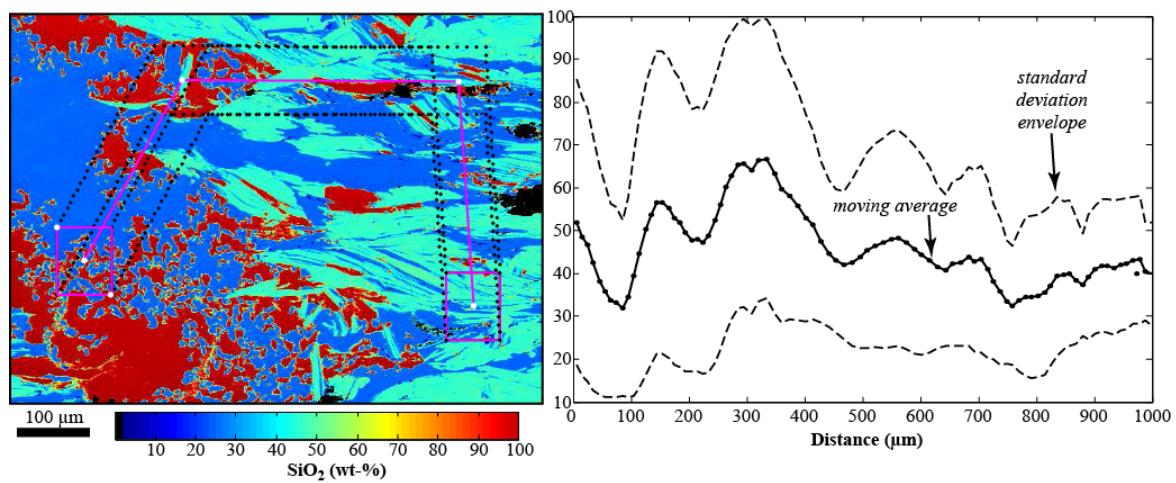


Figure 3.26 – Example of sampling using (a) a scanning window and the exported (b) the moving average and standard deviation.

Sampling data exported from XMapTools		
04-May-2019 07:48:23		
Method: Sliding Window		
Columns: Distance (px) Mean Std		
1.01115467	0.07042017	0.00434901
2.02230934	0.07026298	0.00446547
3.03346401	0.07004675	0.00442742
4.04461868	0.06991756	0.00444096
5.05577335	0.06986120	0.00429657
6.06692802	0.06979739	0.00427235
7.07808269	0.06971791	0.00414286
8.08923736	0.06932858	0.00509202
9.10039203	0.06922548	0.00540427
10.11154670	0.06914304	0.00553828
11.12270137	0.06938213	0.00590496
12.13385604	0.06941252	0.00589785
13.14501071	0.06939695	0.00608730
14.15616538	0.06903524	0.00785494
15.16732006	0.06899280	0.00823086
16.17847473	0.06885037	0.00834379
17.18962940	0.06865828	0.00902304
18.20078407	0.06860217	0.00942488
19.21193874	0.06833886	0.00958221
20.22309341	0.06806243	0.01033523
21.23424808	0.06772410	0.01045512
22.24540275	0.06766251	0.01063467
23.25655742	0.06761547	0.01058769
24.26771209	0.06778431	0.01061411
25.27886676	0.06788618	0.01054925
26.29002143	0.06796660	0.01031684
27.30117610	0.06789530	0.01004517
28.31233077	0.06777310	0.01015705
29.32348544	0.06762824	0.01001430
30.33464011	0.06796718	0.00855412
31.34579478	0.06794971	0.00839101
32.35694945	0.06816555	0.00784839
33.36810412	0.06823258	0.00671204
34.37925879	0.06811918	0.00669923
35.39041346	0.06813346	0.00645991
36.40156813	0.06814059	0.00623433
37.41272280	0.06834628	0.00551073
38.42387747	0.06828218	0.00518582
39.43503214	0.06822461	0.00511663
40.44618681	0.06807220	0.00509531
41.45734148	0.06795047	0.00510995
42.46849615	0.06805163	0.00448413
43.47965082	0.06818091	0.00396966
44.49080550	0.06815204	0.00393970
45.50196017	0.06828982	0.00391321

Code 3.7 – Example of exported file (sampling mode scanning window)

3.8 X-RAY

3.8.1 Image display

[M1101] *X-ray image* Menu to select the map to be displayed in the main figure window. All the maps that have been previously imported with the function *add map(s)* (see section 3.3.2) are listed in this menu.

[M1102] *Phase (mask)* Menu to only show the pixel compositions belonging to a given mask. Note that the masks available are those of the active mask file (see menu *maskfile* [M1301]). The element map selected in [M1101] is displayed in the main figure window for the phase selected in menu [M1102].

Masks are generated during the classification. They can also be imported from a mask file using the button import ([B1302], see below). If *none* is selected (first choice in the menu), all the pixels of the map selected in [M1101] are displayed in the main figure window.

[B1101]  *Import map(s)* in XMAPTOOLS (see section 3.3.2).

Note: The procedure on how to import map(s) is given in the section 3.3.2.

[B1102]  *Delete map*. Delete the selected map. This functionality is only available if two or more maps have been loaded.

[B1103]  *Display precision map*. Generate a map showing the precision in % at 2σ (see general concept and equation in §1.6.1.2). This image is opened in a new window. The color contrast values are the lower and upper values of the precision map. The precision is computed for a given element (menu [M1101]) and the selected phase provided that a mask is selected in the menu [M1102].

[B1104]  *Info*. Display a the information of the selected map. This info window contains: (1) the name of the selected element (with a number corresponding to the internal reference in the element database); (2) the selected mask, if a mask selected in menu [M1102]; (3) the map size in pixels: format rows / columns, corresponding to Y / X; (4) the mean intensity of the displayed pixels (if a phase is selected in [M1102] the mean is calculated from the intensities of this phase only) and the corresponding uncertainty at 2σ ; (5) median intensity of displayed pixels and the corresponding uncertainty at 2σ ; (6) standard deviation; (7) lower and (8) upper intensity values; (9) BRC, (10) TRC and (11) MPC correction info (see section 3.8.4).

[B1105]  *Display mask image*. Display the mask image of the selected mask file (menu [M1301]) in the main GUI. This image can be exported from the menu *File* (see 3.2.1).

[B1106]  *Export phase proportion*. Export the phase proportions expressed in surface fraction of the selected mask file (menu [M1301]). A folder *Exported-PhaseProportions* is automatically generated and the file is saved. Phase proportions are printed in pixel-% that correspond to surface-%.

[B1107]  *Export mask image*. Open the mask image of the selected mask file (in menu [M1301]) in a new window. This figure can be saved using the menu *file > save as*. Several image formats are available: .jpeg, .pdf, .eps or .png. This function is also available via the men *File, Export Mask Image* (see 3.2.1)

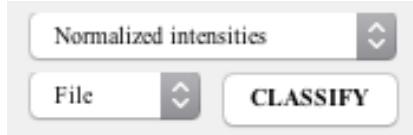


Figure 3.27 – Classification module including the menus 'Method of classification' [M1202] and 'Initial pixel composition mode' [M1202] and the button 'Classify'

[B1108] *Rename phases.* Change the assigned phase names. A dialog box opens and names can be edited. When the button *OK* is pressed, a new mask image is plotted with the new labels.

NB: It is strongly mandatory to use single-word phase names (i.e. without blank or space in the name).

3.8.2 Classification

[M1201] *Method of classification* Menu to select the method that will be used by the classification function (button [B1201]). Two automated methods are available: *classic computation* or *normalized intensities*. The differences between both methods are described in details in [Lanari et al. \(2014b\)](#). Masks files can be derived using each method and compared. The differences stand in the magnitude of the differences between the composition of phases. For optimal results it is generally recommended to give a try to both methods.

[M1202] *Initial pixel composition mode* Menu to select the method for defining the coordinates of the initial pixels to be selected. The compositions of these pixels will be used by the classification function (button [B1201]) to define the first groups. Two options are available: *selection* and *file*. The mode *selection* enables to define initial pixels by clicking directly into the map during the classification. This mode requires a map on which all the mineral phases are visible. If the mode *file* is selected, the classification function reads a file containing the coordinates of the initial pixels. The format of this file is described in [2.7.5](#). If the file is named *Classification.txt* (case sensitive), then the program automatically proposes to read this file.

[B1201] *Classify.* Perform a semi-automated classification, which aims to attribute each pixel of the image to a distinct chemical phase (also termed mask here). This function uses a clustering approach (k-means function) and the method selected in menu [M1201] from compositions of initial pixels selected by user (see menu [M1202] and Fig. 3.27). A complete description of the classification function is provided in [Lanari et al. \(2014b\)](#).

The classification function requires selecting the set of maps that will be used to define the chemical system. If the mode *selection* is selected and if a file *Classification.txt* exists in the working directory, the program proposes to use this file to specify the initial pixel set during the classification. Press *yes* to continue and *no* to read an other file.

3.8.3 Mask files

[M1301] *Mask file.* Menu to select the mask file that will be applied (1) to display phases using the menu [M1102], (2) to display masks and calculate phases proportions using the buttons [B1105] and [B1106] (3) for the standardization using the button [B1601].

[B1301]  *Delete mask file.* Delete the mask file selected in menu [M1301]. This functionality is only available if two or more mask files have been generated. Note that there is no undo functionality in XMAPTOOLS.

[B1302]  *Import / merge mask files.* Import or merge mask file(s) generated with the chemical modules *Binary* and *TriPlot*. The function import the mask file if a single file is selected and merge mask files if more mask files are selected. The mask files are generally stored in the folder */Maskfiles*. If several files are selected, XMAPTOOLS generates a new mask file by merging them. The name of the new mask file can be edited via the dialog box.

NB: during merging of mask files, the n masks (could be from several mask files) are scanned and the pixels are allocated to new n mask. If a pixel is selected twice or more, it will be allocated to the last scanned mask containing this pixel. The pixels that are unselected (0) in the mask file are detected by the function and not used during the merging step. In the end, all the pixels that are not allocated are transferred into a *unselected pixels* group (the last mask). Details and information regarding the import / merge function are printed into the command window of MATLAB (see example below).

Example: Four mask files (Chlorite.txt; Phengite.txt; Plagioclase.txt; and Quartz.txt) generated from *Binary* module have been imported. Some pixels are not allocated to any group and there are transferred toward a new mask number 5: *unselected pixels*. The number added after the mask file names (-1 in this examples) corresponds to the reference of the mask in the corresponding file.

```
Mask importing ... (Merged-Maskfile) ...
Mask importing ... (Nb Masks: 5)
Mask importing ... (Phase: 1 name: Chlorite -1 < 36.3654\% >)
Mask importing ... (Phase: 2 name: Phengite -1 < 23.3991\% >)
Mask importing ... (Phase: 3 name: Plagioclase -1 < 0.81197\% >)
Mask importing ... (Phase: 4 name: Quartz -1 < 18.991\% >)
Mask importing ... (Phase: 5 name: Unselected pixels < 20.4325\% >)
Mask importing ... (Merged-Maskfile) ... Done
```

Code 3.8 – Example: Import / merge mask function (printed output)

[B1303]  *Export mask file* Export the mask file selected in menu [M1301] and save it as a text file in the folder */Maskfiles*. A dialog box is displayed to select which mask will be saved. Note that any unselected pixel is set to zero and will be classified as *unselected_pixels* by the *iImport and merge function* [B1302].

3.8.4 Corrections

[M1401] The menu *correction method* allows a correction method to be selected. This correction will be applied using the button [B1401]. List of requirements and button strings are shown in tab. 3.6. The corrections are described in the following sections.

[B1401] The button *activate / set / apply correction* enables applying the correction selected in menu [M1401]. Corrections involving a correction mode (see details in Tab. 3.6) need to be validated in order to apply the correction and exit the correction mode.

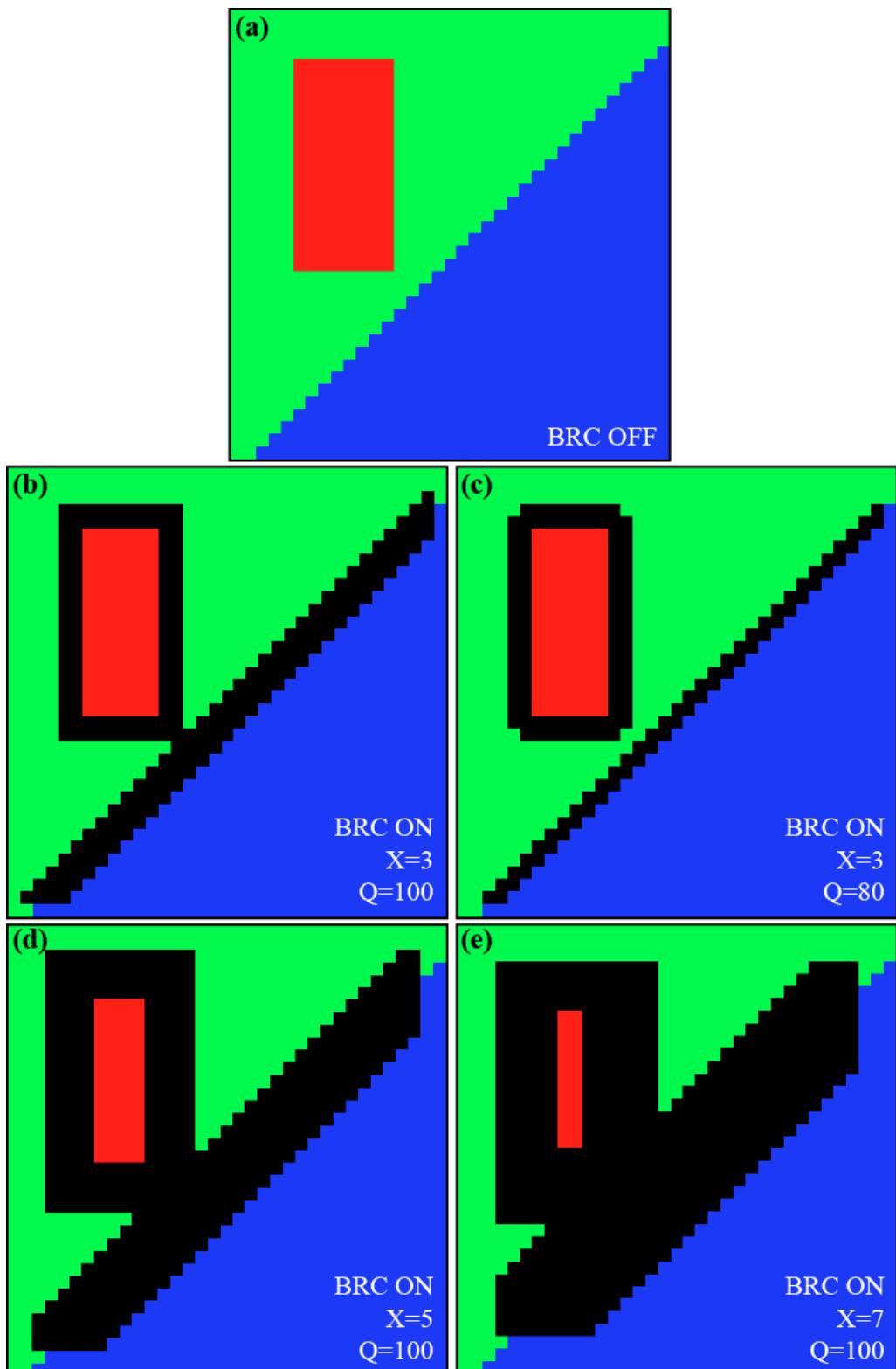


Figure 3.28 – Examples of BRC correction with various X and Q parameters. This small map ($35 \times 35 \text{ pixels}^2$) exhibits three phases (Phase 1 in red; Phase 2 in green; Phase 3 in blue). Pixels removed by BRC are plotted in black. A complete description of this map can be found in Fig. 1.3.

Abbreviation	Name	Button string	Correction mode	Requirements
BRC	Border-removing correction	APPLY	No	existing mask file
TRC	Topo-related correction	SET	Yes	TOPO map
MPC	Map position correction	ACTIVATE	Yes	Standards analyses
SPC	Standard position correction	ACTIVATE	Yes	Standards analyses
IDC	Intensity drift correction	APPLY	No	Phase selected
BA1	Background correction (using maps)	APPLY	No	Background maps
RM1	Clean pixels (area; all maps)	SELECT	Yes	...

Table 3.6 – Type of corrections available in XMAPTOOLS, abbreviation, name, button string, activation of the correction mode and prerequisites

3.8.4.1 BRC - Border-removing correction

Border-removing correction (*BRC*) is a correction function that aims to remove the pixels located at the contact between two phases. *BRC* can be applied after the classification and before the analytical standardization. It is strongly recommended to apply *BRC* before to standardize phases if you are interested in maps of structural formulas because *BRC* will help to avoid the mixing pixels. However, *BRC* should not be used to standardize phases that will be merged to calculate local bulk compositions. Indeed, *BRC* strongly affects the phase proportions as shown in Figure 3.28. When the computation is achieved, it is possible to deactivate or activate the *BRC* using the *BRC* button in the correction window [B5501].

BRC is a very simple mathematical correction based on the mask file only. *BRC* does not take into account the chemistry of the pixels. This is the reason why it belongs to the user to check the size of the mixing zone and to select the correct set of parameters to remove the right amount of pixels.

Considering a mask i.e., a matrix with ones where the pixels are allocated to the selected phase, and a given pixel:

$$px(i, j) \quad (3.5)$$

with

$$((X - 1)/2) < i < i_{max} - ((X - 1)/2) \quad (3.6)$$

and

$$((X - 1)/2) < j < j_{max} - ((X - 1)/2) \quad (3.7)$$

This pixel is removed by the *BRC* function ($BRC(i, j) = 0$) if

$$\sum_1^{X^2} (px(i - (X - 1)/2 : i + (X - 1)/2, j - (X - 1)/2 : j + (X - 1)/2)) < X^2 \frac{Q}{100} \quad (3.8)$$

with X the size of the scanning window in pixel (odd number ≥ 3) and Q the reject criterion in %. This filtering procedure is applied to all the pixels of all the masks.

The equation (3.8) implies that the *BRC* may not filter the pixels located at the rim of the map. The width of this rim is exactly $(X - 1)/2$ pixels.

Examples of *BRC* correction are given in fig. 3.28. Corrections are applied to a small map exhibiting three phases plotted with three colors (red, green and blue in Fig. 3.28a). Several combinations of X and Q parameters have been tested and results are reported in figs. 3.28b, c, d and e. For a fixed Q of 100%, it comes out that $(X + 1)/2$ pixels are removed for both horizontal and vertical boundaries.

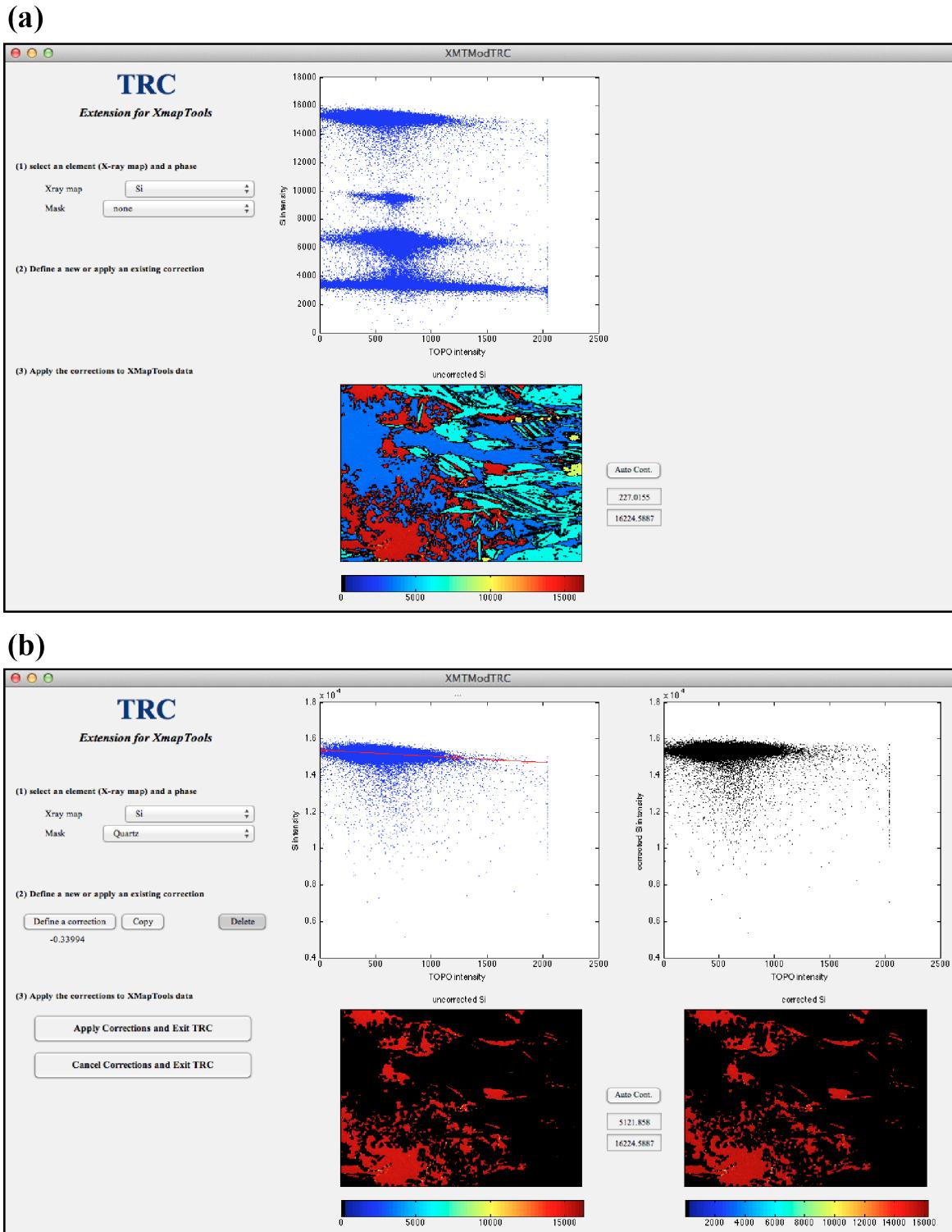


Figure 3.29 – Example of TRC correction for Si using the TRC module. In this example, BRC correction has been applied and the black contours are visible in the map in (a). In the diagram X-ray intensity against TOPO intensity, each cloud is a mineral. (a) display mode; (b) correction mode with a phase selected.

3.8.4.2 TRC - Topo-related correction

Topo-related correction (*TRC*) is a correction function that aims to correct X-ray intensity variations generated by topographical variations on the surface of the sample. *TRC* may be applied after the classification and before the analytical standardization. Masks are required to apply *TRC* because the correction of one element is phase-dependent because of different matrix effects.

TRC correction are done using the *TRC* module (Fig. 3.29) that is activated by selecting *TRC* in menu [M1401] and pressing the button [B1401].

NB: The *BRC* correction may be applied before to use the *TRC* correction. If the pixels showing mixing compositions are removed, the variations of chemistry correlated with topographical variations can easily be characterized.

An example of *TRC* correction is given in figure 3.29. One element (e.g. Si) can be selected using the menu *X-ray maps* (Fig. 3.29a). Two plots are generated: a diagram *Si intensity* against *TOPO intensity* and a map of *Si intensities*.

The correction may only be applied for one element and one phase because the variations of X-ray intensities with TOPO intensities are matrix-dependent. In figure 3.29b the phase quartz is selected to correct for Si. A linear relationship (red line in Fig. 3.29b) is defined by user after pressing the button *Define a correction*. The corrected intensities are reported in a new diagram *Si intensity* against *TOPO intensity* and in a map of *Si intensities* (right diagrams in Fig. 3.29b).

The correction straight line defined above may be written as:

$$\Delta I = a \times I_{topo} \quad (3.9)$$

with ΔI the intensity correction and a the slope of this line. ΔI is used to transform the measured intensities (I_{meas}) into corrected intensities (I_{corr}):

$$I_{corr} = I_{meas} - \Delta I \quad (3.10)$$

Together with Eq. 3.9 this gives:

$$I_{corr} = I_{meas} - a \times I_{topo} \quad (3.11)$$

As the corrections have been defined, the parameter a can be copied (button *Copy*) to be directly applied to an other phase by using the button *paste*. A correction can be removed by using the button *Delete*.

Once all the phases have been corrected, the corrections can be applied using the button *Apply corrections and exit TRC*. This function closes the correction module and send back the corrected data to XMPTOOLS.

A confirmation window is operating before to exit the correction module because the *TRC* correction is an irreversible process. The new intensities corrected for *TRC* replace the raw intensities. However, original data are still preserved in the X-ray files. Obviously, *TRC* may be applied many times on the same data.

3.8.4.3 MPC - Map position correction

Map position correction (*MPC*) is a correction function that aims to correct X-ray maps position such as X and Y shifts that may have occurred during the acquisition. *MPC* may be applied before the

classification. The function *Check quality of std/map positions* [B1503] allows to use the standard analyses in order to detect shift in X and Y coordinates. More details regarding this function are provided in the function description [B1503]. When *MPC* is activated, the program suggests to calculate a correlation map for different spot analyses positions using the function *Check quality of std/map positions* [B1503].

MPC correction mode may be activated by selecting *MPC* in menu [M1401] and pressing the button [B1401].

The selected map position can be edited by using the arrow buttons. Use the button [B5501] arrow up to move up, the button [B5502] arrow down to move down, the button [B5503] arrow right to move right and the button [B5504] arrow left to move left.

The *MPC* correction mode is disabled when the user presses the button apply [B1505] located below the arrows. The corrections are applied to the selected X-ray map.

3.8.4.4 SPC - Standard position correction

Standard position correction (*SPC*) is a correction function that aims to correct the standard X and Y positions that can have occurred during the acquisition. *SPC* may be applied before the standardization in order to guaranty that the positions of the spot analyses used as internal standard are not shifted. The functions *Display intensity vs composition chart* [B1502] and *Check quality of std/map positions* [B1503] allow to detect such shifts. When *SPC* is activated, the program suggests to calculate a correlation map for different spot analyses positions using the function *Check quality of std/map positions* [B1503].

SPC correction mode may be activated by selecting *SPC* in menu [M1401] and pressing the button [B1401].

The spot analyses used as internal standards can be moved by using the arrow buttons. Use the button [B5501] arrow up to move the analyses up, the button [B5502] arrow down to move the analyses down, the button [B5503] arrow right to move the analyses right and the button [B5504] arrow left to move the analyses left.

The *SPC* correction mode is disabled when the user presses the button apply [B1505] located below the arrows. The corrections are applied to position of the standards.

3.8.4.5 IDC - Intensity drift correction

Intensity drift correction (*IDC*) is a correction function that aims to correct any time-dependent intensity drift that can have occurred during the acquisition. Relatively slight drifts (few %) are systematically reported on some EPMA instruments mainly caused by variations of the beam current at the specimen surface. To be corrected the time-dependent intensity drift has to be characterized in a mineral showing homogeneous compositions such as Si in quartz or garnet and widely distributed across the mapped area. The correction *IDC* may be applied right after *TRC* to avoid unwanted correction of any intensity variation related to the topographical variations.

TRC correction are done using the *IDC* module (Fig. 3.30) that is activated by selecting *IDC* in menu [M1401] and pressing the button [B1401]. It is strongly recommended to apply this correction to a homogeneous phase (e.g. quartz for Si).

An example of intensity drift is reported in figure 3.30. The measured map of Si in titanite (Fig. 3.30a) exhibit vertical variations of the number of counts for Si. this variation is caused by a time-dependent drift caused by variation of the vacuum conditions in the gun. The relative range of variation is about 14% in this example. All the elements recorded during the same pass are affected in a similar way.

In the correction parameters (Fig. 3.30) it is possible to specify the direction of acquisition, i.e. *horizontal* or *vertical* (vertical in the example shown in Fig. 3.30). A *BRC* correction can be used in the correction module. Note that this correction is only used to generate the composition profile and is not sent back to the main program after correction. The interpolation method can be chosen among:

- *Linear* (linear interpolation)
- *Pchip* (shape-preserving piecewise cubic interpolation)
- *Spline* (piecewise cubic spline interpolation)
- *Nearest* (nearest neighbor interpolation)

The lines (vertical mode) or columns (horizontal mode) of intensities of the selected element are summed up and displayed as a 1D profile (Fig. 3.30). The red dot show the average intensity of each line or column with the relative error and standard deviation uncertainty envelope (at 2σ).

A correction scheme can be defined by pressing the button *Add a new correction*. The interpolation points used to define the correction function are selected by clicking onto the figure (see black points in Fig. 3.31). This selection is always done from left to right; a new point is registered only if the *X* coordinate is higher than the previous point. At least 2 points are required to define a correction function. The selection mode is deactivated by doing a right-clic.

The correction function used the method defined in the correction parameter (see above) to interpolate the points (green curve in Fig. 3.31). The interpolation method can be changed after the selection of the points.

The correction map (see map in Fig. 3.31 in percentage) is obtained by duplicating the correction function for the number of columns (vertical mode) or rows (horizontal mode). The corrected profile is also displayed.

Note that the message in the *display* window change once the correction has been applied to a given element (compare Fig. 3.30 and Fig. 3.31).

The selected correction scheme can be applied to other element, for example if they have similar intensities and have been measured during the same pass. Press *Apply* to apply the correction scheme to a selected element. Press *Edit* to change the selected correction scheme. Press *Reset* to reset the correction of the selected element.

Once all the element have been corrected for time-dependent drift, the corrections can be applied using the button *Apply corrections and exit IDC*. This function closes the correction module and send back the corrected data to XMAPTOOLS.

A confirmation window is operating before to exit the function because the *IDC* correction is also an irreversible process (except if you manually proceed to the exact inverse correction in a new run). The new intensities corrected for *IDC* replace the raw intensities stored in the X-ray workspace. However,

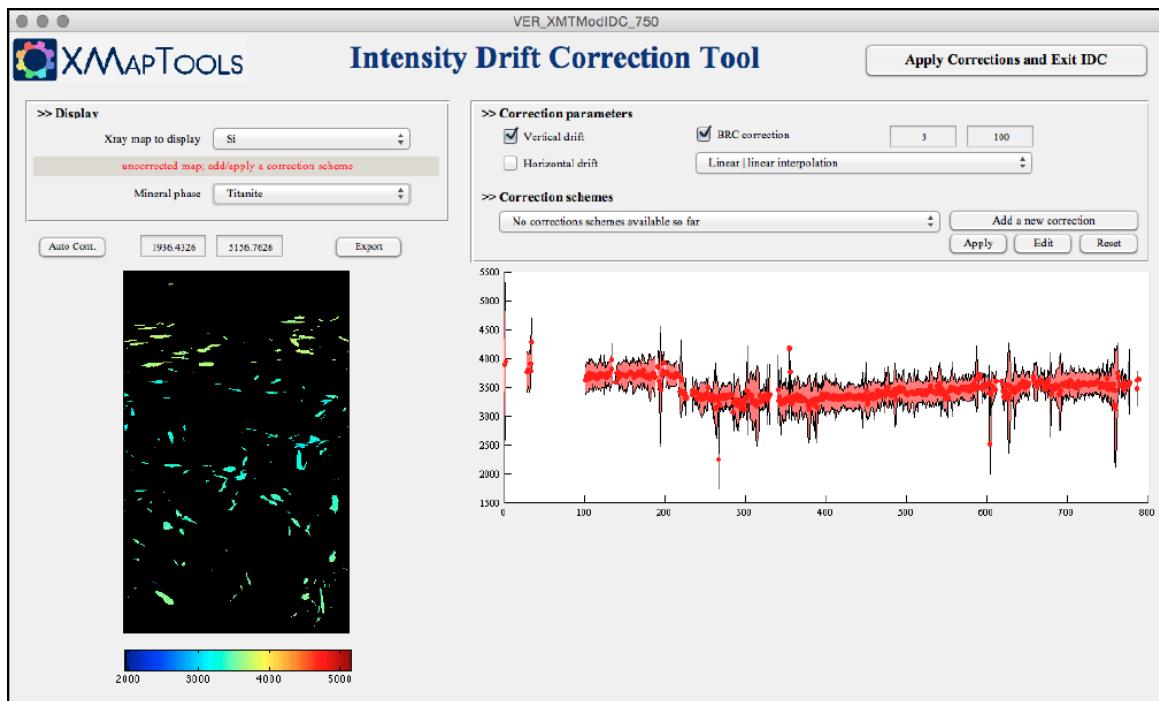


Figure 3.30 – Module to perform the IDC correction. In this example, Si in titanite is used to detect the time-dependent intensity drift (in counts) during the first scan. Note that the abrupt decrease of intensity was caused by a vacuum failure in the gun.

original data are still preserved in the X-ray files. Obviously, IDC may be applied many times on the same data.

It is also possible to export the corrected maps as text files. The files are automatically stored in the working directory in a subfolder *CorrectedMaps*. These maps can be imported in XMAPTOOLS using the *import* function [B1101]. Be careful to not apply twice the deadtime correction.

3.8.4.6 BA1 - Background correction (map)

This function is not yet available for public use yet. Please contact Pierre Lanari if you want to use this function.

An example of background correction is given in [Lanari et al. \(2019\)](#) to be compared with the *advanced standardization method*.

3.8.4.7 RM1 - Eliminate pixels (area; all maps)

This function allows the user to define a region-of-interest and to eliminate all the pixel compositions within this area for all the maps of the workspace *X-ray*. Two modes are available in the *RM1* function; the mode can be selected in the menu appearing once the button *SELECT* is pressed.

- Inside the selected region-of-interest
- Outside the selected region-of-interest

The region-of-interest is a polygon for which each - consecutive - corner is set by clicking onto the image (see spots 1 to 10 Fig. 3.20b). the selection mode is disabled using right-clicking (spot 11, in

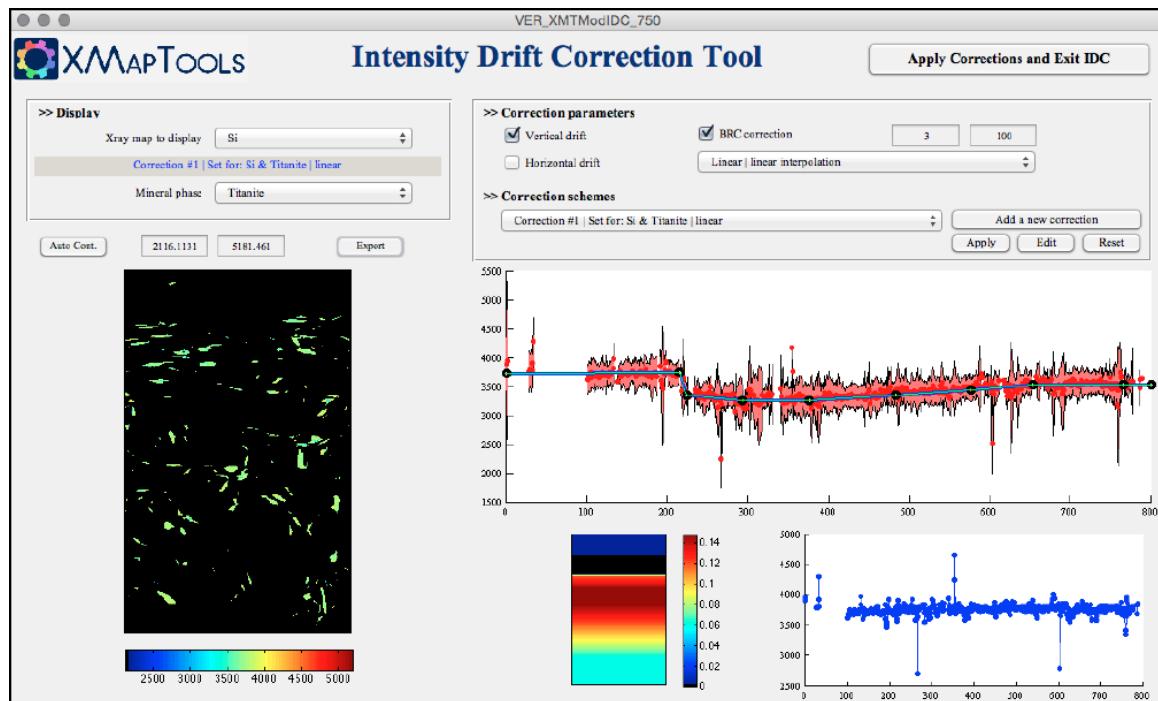


Figure 3.31 – Module to perform the IDC correction. The correction for Si in titanite has been defined in the chemical diagram.

Fig. 3.20b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.20b. For all the maps available in the workspace X-ray and the phase in selected [M1102] all pixels inside or outside the region-of-interest are eliminated.

The eliminated pixels cannot be recovered. Note that it is still possible to reload the original maps.

3.8.5 Internal standards (spot analyses)

[B1501] *Import standard file* Load a file containing standard data for calibration. The standard file must have *.txt extension and the an adequate format (see the detailed description of the file format in section 2.7.6). The *import standard file* function (i) reads the file, (ii) extract the map coordinates, the oxide order and the chemical data and (iii) perform the projection of the spot analyses onto the map using the map and spot coordinates given in the file.

Example: The file *Standards.txt* has been read. Ten oxides are provided and the corresponding elements are printed out in the command window (Si, Mn, K, Na, Fe, Al, Cr, Ca, Mg, Ti). The X-ray maps having these names can be standardized by using the composition of the spot analyses. In this example, 139 spot analyses have been read and correctly imported.

```
Import standard file ... (File name: Standards.txt) ...
Import standard file ... (Elements: (Si-Mn-K-Na-Fe-Al-Cr-Ca-Mg-Ti)
Import standard file ... (Number of analyses: 139)
Import standard file ... (Validity: 1 1 1 1 1 1 1 1 1 1)
Import standard file ... (Standards.txt) ... Ok
```

Code 3.9 – Example: Import standard file

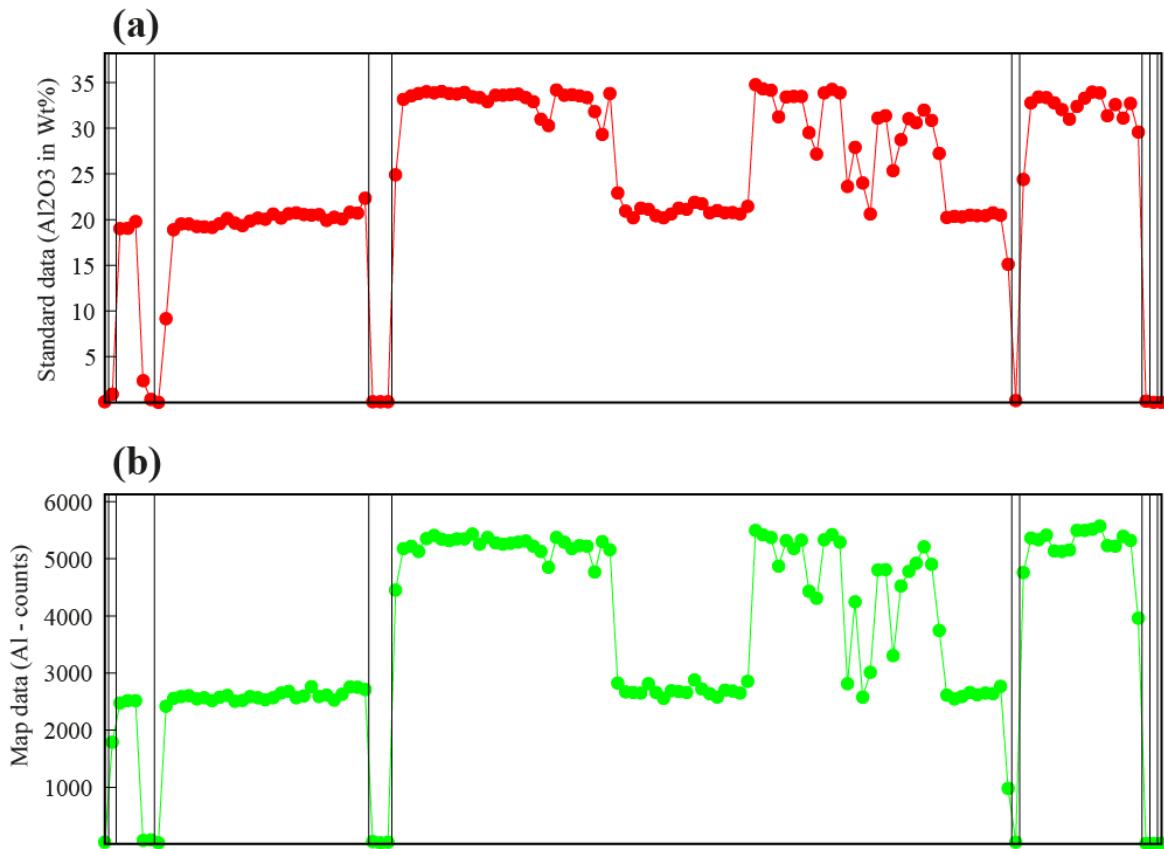


Figure 3.32 – Function display intensity vs composition chart

[B1502] *Display intensity vs composition chart.* Plot the compositions of the internal standard (spot analyses) against the intensities of the corresponding pixels of the map selected in the menu [M1101].

Example: The function *Display intensity vs composition chart* has been used to compare the compositional data for Al in spot analyses (in wt.% Al₂O₃ in Fig 3.32a) and in the X-ray map Al (Fig 3.32b). The correlation coefficient is 0.97 (see Ex. 3.10).

```
Standards testing ... (Element: Al) ...
Standards testing ... (Correlation: 0.96754)
Standards testing ... (Element: Al) .... Ok
```

Code 3.10 – Example: function display intensity vs composition chart

[B1503] *Check quality of std/maps positions* Test the positions of the internal standard via a comparison against the intensities of the X-ray maps. This function checks all the map names and search for the corresponding oxides or elements provided with the spot analyses. All the imported maps must have a corresponding element in the standard files. If maps such as *TOPO* or *BSE* or *SEI* are loaded, they must be deleted (button [B1102]) before to use this function.

```
Check ... [ Quality Check – Standard/Maps positions ]
The following maps have no corresponding elements in the standard data: TOPO
Check ... CANCELLED
```

Code 3.11 – Example: error "check quality of std/maps positions"

This function automatically searches the optimal positions of the spot analyses (internal standard) on the maps. For each element the correlation between the compositions of the spot analyses (in oxide wt-%) and the compositions of the corresponding pixels (in counts) is calculated. The user should define ΔX and ΔY two variables expressed in pixels. For a given spot analysis with the initial coordinate X_j and Y_j , the map of the correlation coefficient (τ) for the element El_i is calculated from the position:

$$(X_j - \Delta X, Y_j - \Delta Y) \quad (3.12)$$

to the position

$$(X_j + \Delta X, Y_j + \Delta Y) \quad (3.13)$$

The resulting variable $\tau(El_i)$ is a matrix with $(2 * \Delta Y - 1)$ rows and $(2 * \Delta X - 1)$ columns.

Two figures are generated by the function *check quality of std/maps positions*. The first figure contains the maps of the correlation coefficients $\tau(El_i)$ (Fig. 3.33). The original position (X_j, Y_j) is located in the middle at coordinates $(0, 0)$ and marked by a black star (white squares in Figs 3.33 and 3.34). The axis values are given in pixels from $-\Delta X$ to ΔX and from $-\Delta Y$ to ΔY . In this example the default values $\Delta X = 10px$ and $\Delta Y = 10px$ are used.

The second figure 3.34 can be used to obtain the optimal position (higher number) for all the elements and is calculated as the sum of square of correlation coefficients (M):

$$M = \sum El = 1n(\tau_i)^2 \quad (3.14)$$

This method works provided that the individual maps from figure 3.33 show contrasted τ values ranging from $0.2 - 0.4$ to $0.9 - 1$. If no good correlation exists, the higher value of the second figure could not be the optimal position. In this case a problem should have occurred with the transformation of the map coordinates or the best position can be out of range. Greater values of ΔX and ΔY might be used.

[B1504]  *Display standards*. Display spots on the main figure marking the location of the spot analyses (purple circles). The function *select/unselect standards* [B1506] is available only when the spot analyses positions are displayed.

[B1505]  *Hide standards*. Clean the map shown in the main window.

[B1506] *Select/unselect standard (Edit)*. Activate the selection mode allowing the internal standards to be selected/unselected. This button is only displayed (i.e. the function is available) when the location of the spot is displayed in the map (i.e. after pressing the button *display standards*  [B1504]). When the button *Edit* is pressed, the editing mode is activated. Spot analyses may be selected or unselected by a single click close to their respective locations. Right-clicking disables the editing mode. Zoom is not allowed during in editing mode, but it can be used before to activate to the editing mode.

Why do I have to select or unselect spot analyses? The analytical standardization is performed separately for each phase using a linear relationship between the oxide wt-% compositions of the point analyses (internal standards) and the corresponding pixel intensities from the X-ray maps. The calibration line is defined using the median values of the wt-% compositions and the intensities (Lanari et al. 2014b). For an optimal standardization only the good compositions and intensities must be used. This means that all the spot analyses showing mixing compositions (i.e. located between two phases) or in fractures, should not be used and consequently unselected.

NB: Unselected analyses are displayed in black and are ignored during the analytical standardization.

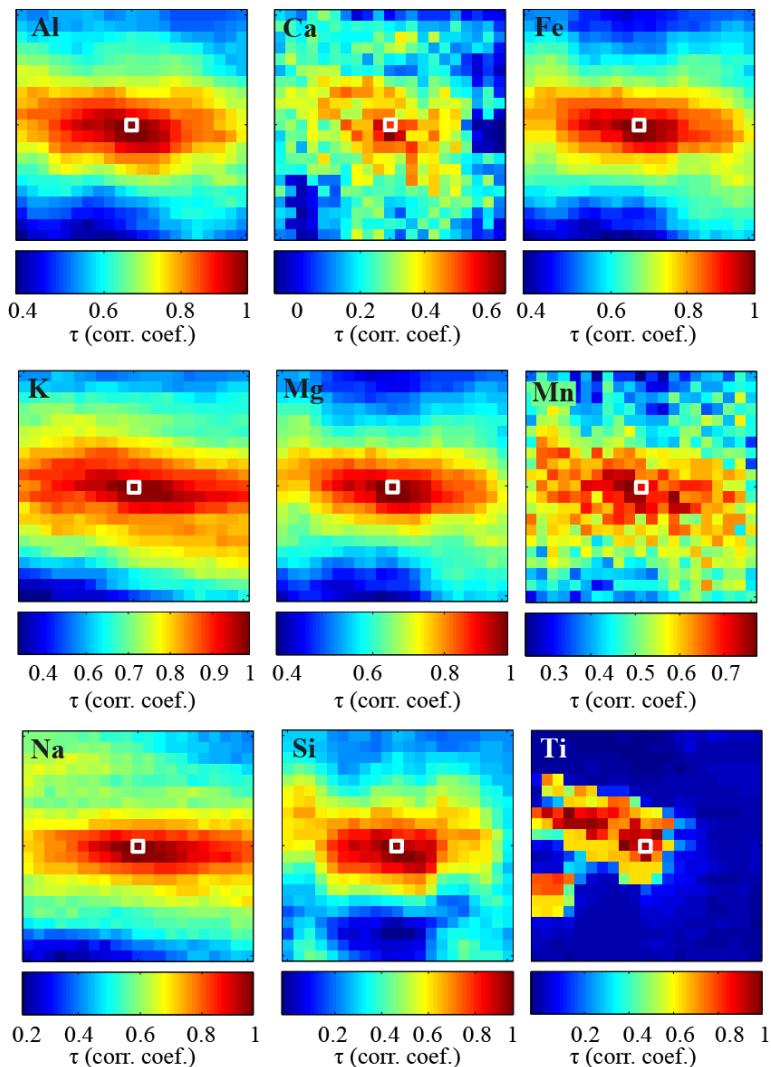


Figure 3.33 – Function: *check quality of std/maps positions*. Correlation coefficients (τ) maps for each element (El_i) (see text for details)

3.8.6 Standardization

When all required steps are accomplished it is possible to process to the analytical standardization, i.e., to transform each phase X-ray maps into maps of weight percentage oxide concentration. More details about this calibration are given in XMAPTOOLS' publications [Lanari et al. \(2014b\)](#) and [Lanari et al. \(2019\)](#).

[M1601] The menu *standardization methods* is used to select the standardization method that will be applied by the standardization function.

Four standardization methods are available:

- *Advanced standardization* is a semi-automatic method of standardization that includes a pseudo-background correction ([Lanari et al. 2019](#)). The advanced standardization is applied using the module *XMTStandardizationTool* (see §3.8.6.4). This method is the default method and is recommended for most applications.
- *Auto (median approach)* is an automatic method of standardization in which the calibration

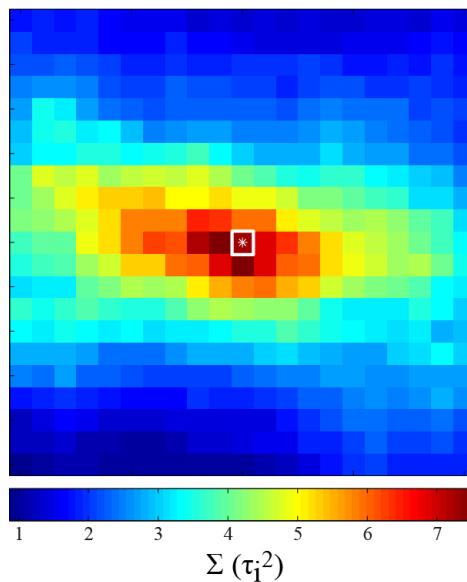


Figure 3.34 – Function: check quality of std/maps positions. $\Sigma (\tau_i^2)$ (see text for details)

curves are defined using a median approach. Note that this method is not optimal for low concentrations as the background may strongly affect the slope of the calibration curve ([Lanari et al. 2019](#)).

- *Manual (User's selection)* allows you to graphically define the calibration curves for each element. This method should be used when the automatic function fails to correctly standardize the element(s) of a given phase. However, in most cases it has been shown that the problems may be solved by unselected some bad spot analyses (see procedure in subsection 3.8.5).
- *Manual (Homogeneous phase)* allows homogeneous phases to be standardized using a known composition such as for quartz (100% of SiO_2). Each calibration curve is defined using the median values of the intensities of the internal standards and the reference composition provided during calibration.

The following function is available to transfer the map(s) to the next workspace (*Quanti*):

- *Transfer to Quanti* to send the raw data from the *X-ray* workspace to the *Quanti* workspace without standardization. If the raw data are directly standardized map this function is used to transfer them to the *Quanti* workspace. Several conversions are possible (conversion factors are defined in *XMap_ConversionFactors.txt* and *XMap_OxideData.txt* in *Program/Dev/*).
 - From wt% of element to ppm of element
 - From wt% of oxide to ppm of element
 - From ppm% to wt%
 - From ppm of element to wt% of oxide
 - From wt% of element to wt% of oxide

[B1601] STANDARDIZE Proceed through the analytical standardization using the method selected in [M1601]. Only the compositions of the pixels belonging to the phase selected in [B1102] are considered during the calibration.

NB: When the standardization is achieved the program generates a *standardized phase* containing the standardized data and switches automatically to the next workspace *Quanti* updating accordingly the associated objects. The displayed map is also updated and the standardized data (first oxide in the list) is plotted (see the next section 3.9).

3.8.6.1 Classical standardization and the problem of background

The classical standardization as defined in [Lanari et al. \(2014b\)](#) uses the median position C (X_C, Y_C) of the i calibration points P_i (X_{P_i}, Y_{P_i}). The calibration curve is simply defined as:

$$Y = \frac{Y_C}{X_C} X \quad (3.15)$$

Note that the position of C can be automatically or manually defined (see the list of the methods above).

The X-ray intensities of a given phase p (Y_i^p) are standardized into oxide weight percentage (X_i^p) using the following relationship:

$$X_i^p = \frac{X_C}{YX_C} Y_i^p \quad (3.16)$$

Any calibration curve defined with the equation 3.15 intersects the X- and Y-axis origin (0, 0). This assumption generates systematic deviations for the low-concentrated elements and result in a biased standardization.

Example: An example of the advanced standardization of garnet is shown in Figure 3.35. The advanced standardization is compared with the automated approach for element showing low concentrations such as MnO and MgO. A complete discussion is provided in [Lanari et al. \(2019\)](#).

3.8.6.2 Pseudo-background correction in XMAPTOOLS

A function that approximate the background value for every element is available in the *advanced standardization*. In this case, each calibration curve is defined by the center of the cluster C (X_C, Y_C) determined either automatically or manually, and the background point B (0, Y_B). A calibration curve taking into account the background is defined as:

$$Y = \frac{Y_C - Y_B}{X_C} X + Y_B \quad (3.17)$$

and the standardization of the X-ray intensities for a given phase p (Y_i^p) into oxide weight percentage (X_i^p) is obtained using the relationship:

$$X_i^p = (Y_i^p - Y_B) \frac{X_C}{Y_C - Y_B} \quad (3.18)$$

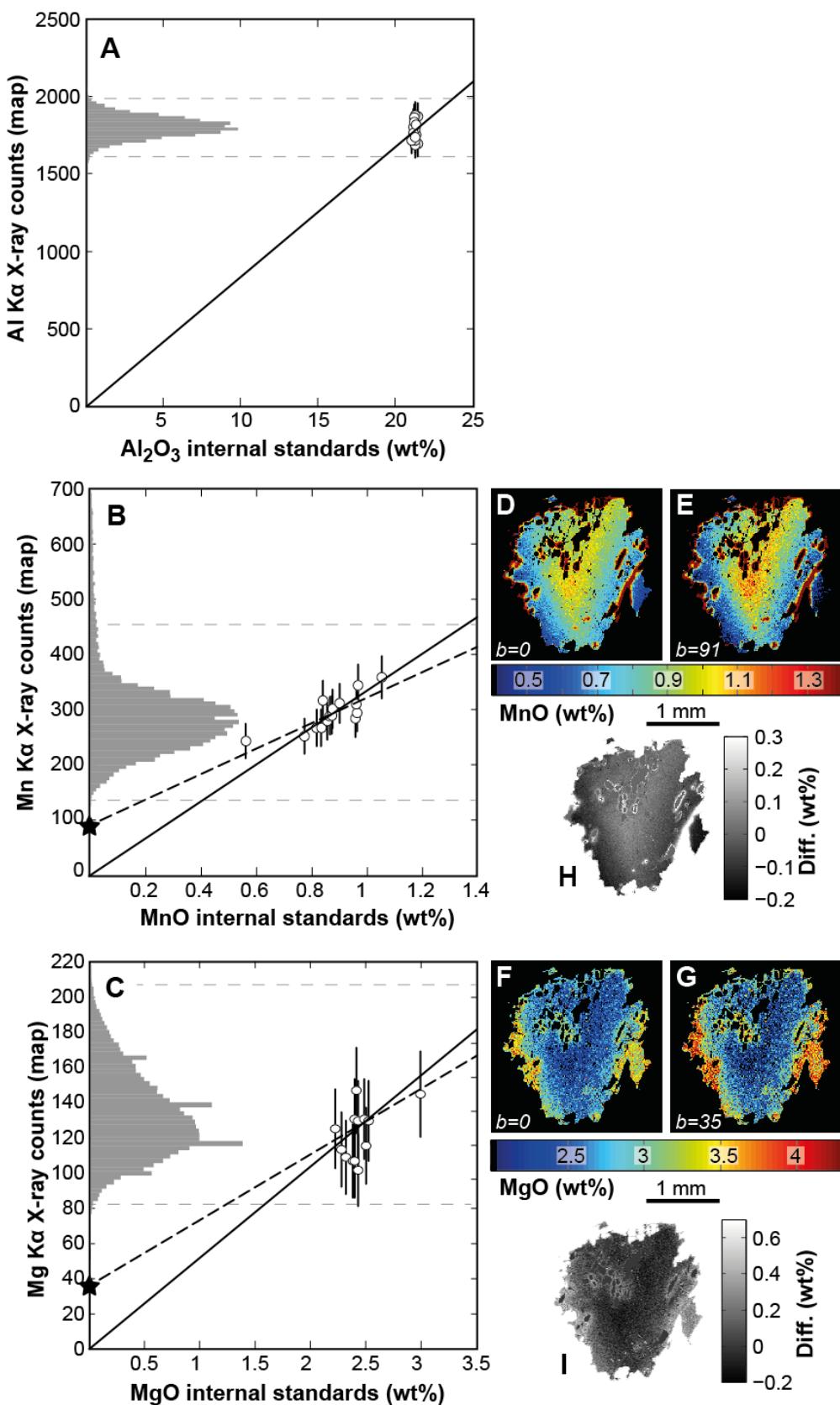


Figure 3.35 – Example of standardization for a garnet of the Central Alps after Lanari et al. (2019).

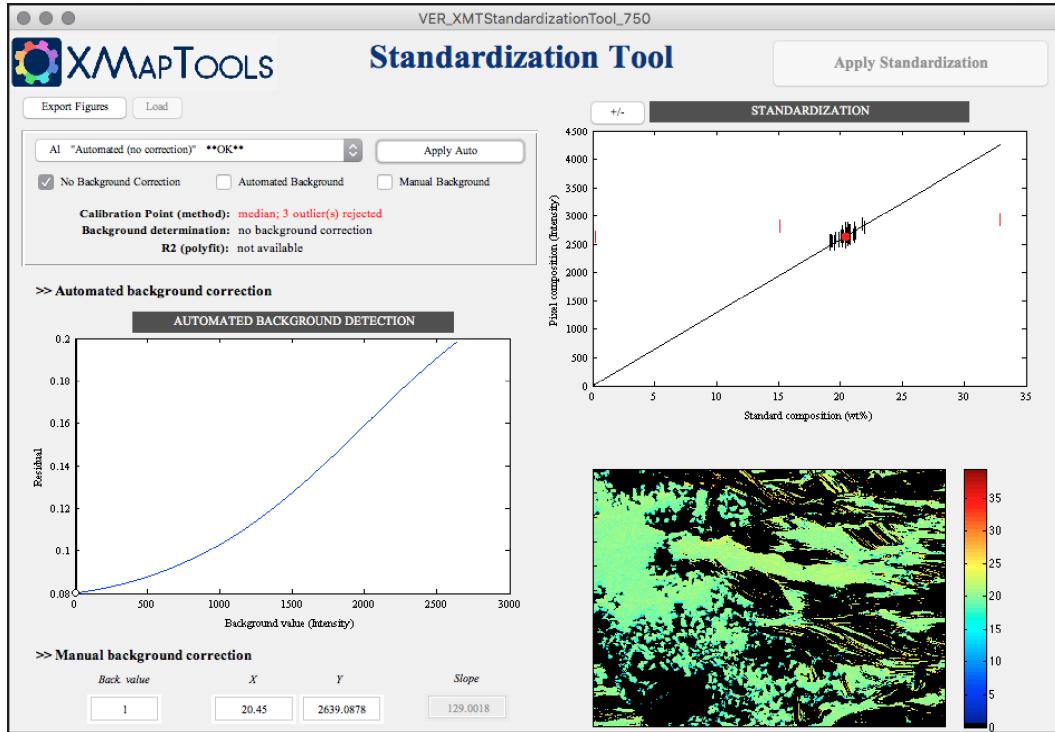


Figure 3.36 – Advanced standardization; case: automated - no background correction (here Al in chlorite)

3.8.6.3 Limit of detection

A theoretical limit of detection is calculated for each element during the advanced standardization. A file is saved in the folder *LOD* and can be used for filtering in the workspace *Quanti*. Note that this limit of detection is not the real limit of detection of the instrument but a limit of detection for a given phase and the mapping conditions.

For a given element, the calibration curve is defined by its slope a :

$$a = \frac{Y_C - Y_B}{X_C} \quad (3.19)$$

and its intercept b corresponding to the background:

$$b = Y_C - aX_C \quad (3.20)$$

The relative uncertainty s of the background expressed in counts and calculated at the 1σ level is:

$$s = \frac{b}{\sqrt{b}} \quad (3.21)$$

with a corresponding limit of detection (in concentration of oxide) calculated as:

$$LOD = \frac{s}{a} \quad (3.22)$$

3.8.6.4 Module XMT_StandardizationTool

The module *Standardization Tool* is used to define the calibration curves if the method *advanced standardization* is selected in menu *standardization methods* [M1601].

The elements are listed in the main menu (Fig. 3.36). It is required to go through the element list and to set the calibration curves. Each item in the element menu is a string containing the element name, the status and (optional) the method used to define the calibration curve. For a given element, here aluminium (Al), the string can be:

- Al "Not checked" **??** - No calibration curve is defined yet for this element (the button *Apply auto* has not been pressed)
- Al "Automated (no correction)" **OK** - A calibration curve is defined and the automated method is applied (no background correction). This is diagnostic is made for high X-ray intensity as the background effect on the calibration curve can be neglected (Lanari et al. 2019).
- Al "Automated (with background correction)" **OK** - A calibration curve is defined and the automated method is applied including a pseudo-background correction. Several techniques can be employed to approximate the background value of an element (see below).
- Al "Manual" **OK** - A calibration curve is defined and the manual mode was used. In this case, a background correction may or may not be applied, depending on the inputs *X*, *Y* and *Back. value*.

The button *Apply Auto* calls an automated calibration function which return either the option *No Background Correction* or the option *Background Correction* determined using the *least-square* method or the *polyfit* method. This button must be pressed once for each element. Pressing this button again resets the automated calibration mode (for example if manual mode was active). Note: for elements showing a small intensity-to-background ratio, the background value is approximated from the intercept of the calibration curve. For elements showing a high intensity-to-background ratio, the background correction is neglected (Lanari et al. 2019).

The check buttons *No background correction*, *Automated background* and *Manual background* display the mode being used for the selected element. Select *Manual background* to activate the manual mode. Press *Apply Auto* to reset the display to the automated mode.

Additional informations are also displayed:

- *Calibration point*: shows the method used to define the calibration point. It can be (1) *median*, defined using the median values of the oxide compositions of the internal standards and intensities of the corresponding pixels; (2) *polyfit*, using a point slightly outside the upper limit of the compositional range on the polyfit function; (3) *manual*, if the user switched to manual mode.
- *Background determination*: shows the method used to define the background value. It can be (1) *no background correction*, for high intensity-to-background values; (2) *auto (least-square) with or without outlier rejection*, if the minimum of the least-square residual function is used; (3) *auto (polyfit) with or without outlier rejection*, if the spread is large enough to ensure a good approximation of the background value; (4) *manual background*, if the user switched to manual mode.
- *R² (polyfit)*: is displayed if the polyfit function has been used.

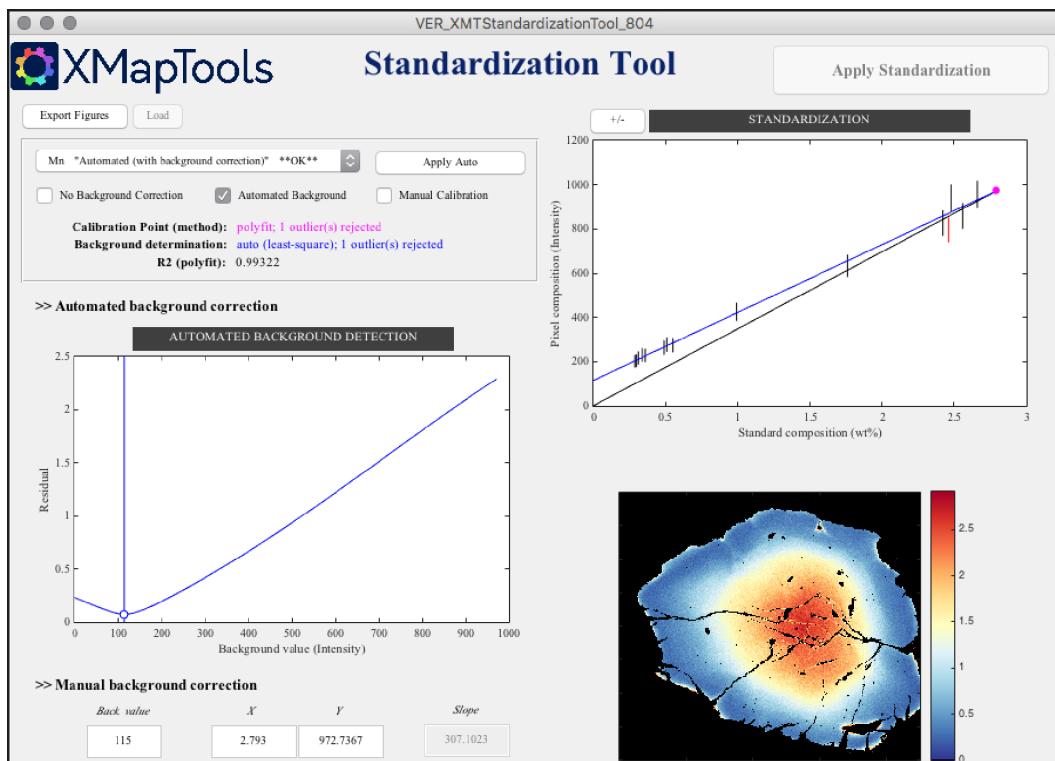


Figure 3.37 – Advanced standardization; case: automated - background correction (here Mn in garnet)

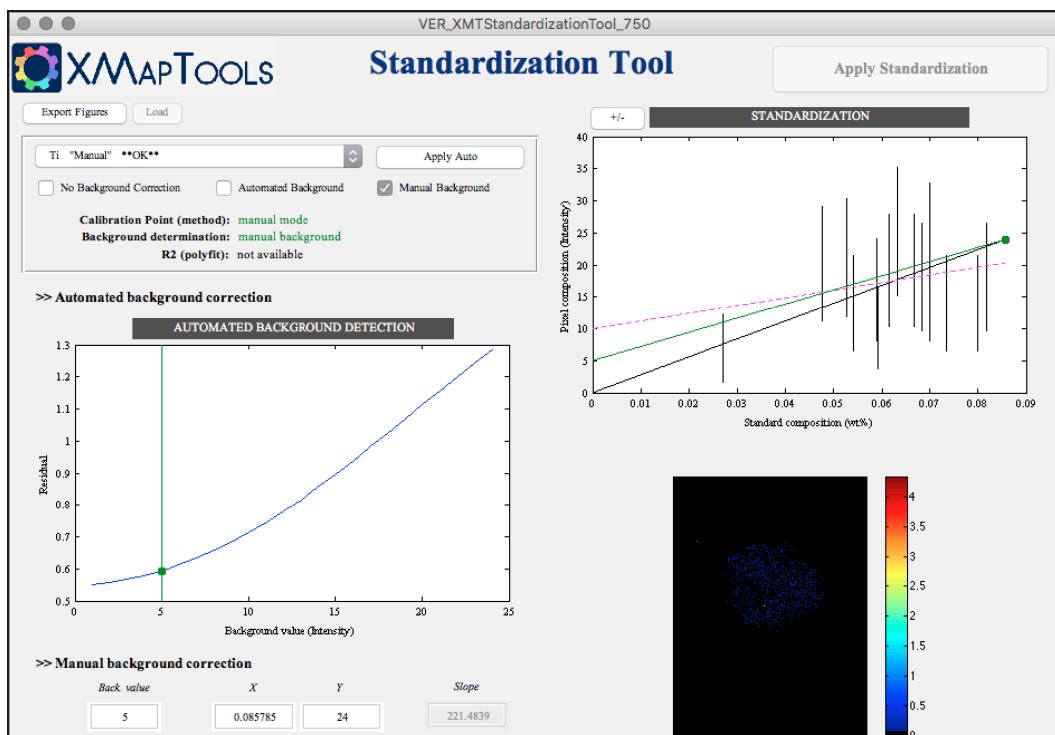


Figure 3.38 – Advanced standardization; case: manual - background correction (here Ti in garnet)

The figure *Automated background correction* shows the evolution of the residuals with the background value (e.g. Fig. 3.37). The residuals are computed as the square of the sum of the distances between the calibration curve and the internal standards for different background values.

The background value as well as the X and Y coordinates of the calibration point are shown in the window *Manual background correction* (Fig. 3.37). These values can be edited if the manual mode is active.

The window *Standardization* contains a figure displaying the calibration curve(s) together with the internal standards. The calibration curve without background correction is displayed in black. The calibration point determined using the median values in red and the one determined using the polyfit approach in magenta. The calibration curves based on the polyfit approach are shown in magenta (dashed line, not used, continuous line, used). The calibration curve based on the least-square residual approach is shown in blue.

The button +/- permits to include (shown in black) or to exclude (shown in red) any point from the calibration set. A single point has to be either added or excluded every time the button is pressed. The excluded analyses are treated as outliers by the program. The automated optimization is performed every time a standard analysis is added or removed to the calibration set.

The *map figure* displays the calibrated map based on the calibration curve defined in the *standardization* figure. The color range is fixed to *Min* and *Max* values for non-zero concentrations. A warning message is displayed in the *standardization* figure if some pixels have a composition greater than 110 % (for the selected element only). Note that this map allows you to visualise the composition of the mixing pixels.

Three examples are shown in Figures 3.36, 3.37 and 3.38:

- (1) Automated calibration curve, method median (red dot) without any background correction (Al in chlorite, see Fig. 3.36). The calibration curve is plotted in black. Three outliers were found and automatically rejected by the program.
- (2) Automated calibration curve with background correction (Mn in garnet, see Fig. 3.37). In this case, the calibration curve is plotted in magenta as the *polyfit* method is used. Note that the best solution of the least-square method is show as a blue dot.
- (3) Manual calibration curve with background correction (Ti in garnet, see Fig. 3.38). The calibration curve is plotted in green (manual). The dashed curve show the result of the polyfit function (not used here), the black curve the automated correction without background correction (not used here).

Warnings concerning the advanced standardization method

- It seems that the automated method works fine for > 98% of the cases. For the more complicated ones, it may be needed to switch to the *manual mode*. Keep in mind that the goal is to obtain a reasonable calibration curve for the mineral of interest.
- It is critical to avoid spot analyses (standards) showing mixing compositions to obtain an accurate standardization. The quality of the standardization should always be tested by displaying the sum of the oxide maps (button *generate oxide wt-% sum map* [B2105], see below). Examples of bad standardizations are given in the tutorial 7 (see §7.2.7.6).

- For the old project files (older than XMAPTOOLS 2.4.1), it might be necessary to re-standardize each phase to be able to use all the new features.

3.9 QUANTI

3.9.1 Standardized maps

[M2101] *Standardized phase* Select the quantitative map (corresponding to a *standardized phase*) to be displayed in the main figure window. All the *standardized phase* are listed in this menu.

NB: For coding reasons, the first *standardized phase* name is always *none*. If none is selected, nothing happens in the plotting areas and the buttons of the workspace are inactive.

[M2102] *Elements*. Menu to select the oxide of the *standardized phase* that is displayed in the main figure window. This menu is updated for each *standardized phase* selected in [M2101].

[B2101]  *Rename Quanti file* Edit the name of the *standardized phase* selected in [M2101]. This name is usually automatically set during the standardization (format: *[mineral name]-[method used]*).

[B2106]  *Duplicate Quanti file*. Duplicate the selected *standardized phase*.

[B2102]  *Delete Quanti file*. Delete the *standardized phase* selected in [M2101]. This functionality is only available if two or more *standardized phase* have been computed.

[B2103]  *Export compositions*. Export oxide analyses from the *standardized phase* selected in [M2101]. The generated file is saved in the directory */Exported-Oxides*. If this directory does not exist the program create it as a new folder in the working directory. Different methods are available for exporting data (see Fig. 3.39)

The data are exported to a text file containing a header block and a table with a row for each analysis. The exported data can easily be imported in Microsoft Excel. Two formatting options are available: (i) the definition of the oxide order and (ii) the format of the delimiter.

The **oxide order** must start with the keyword *Ref* which allows to print out the reference number of each pixel. All the oxide names corresponding to those listed in are separated by a dash (-). If the software does not recognize the oxide name, a value of zero is automatically allocated for the corresponding column. Example: in the default order, zero values are allocated to Fe₂O₃ and XFe₃+ if there are no corresponding map available. The **format of the delimiter** can be either *blank* or *tabulation*.

```
Ref-SiO2-TiO2-Al2O3-FeO-Fe2O3-MnO-MgO-CaO-Na2O-K2O-Fe3-
```

Code 3.12 – Default oxide order

```
Oxide mineral compositions (Wt%) from XMapTools
16-Mar-2015
Analyses: 170611
Standardized phase: Chlorite-auto
Order: Ref-SiO2-TiO2-Al2O3-FeO-Fe2O3-MnO-MgO-CaO-Na2O-K2O-Fe3-
65.00 18.58 0.02 20.39 26.76 0.00 0.74 7.85 0.03 0.02 0.18 0.00
66.00 17.36 0.02 17.85 29.55 0.00 0.47 9.74 0.03 0.02 0.10 0.00
107.00 40.71 0.04 12.53 12.25 0.00 0.32 3.91 0.08 0.20 0.07 0.00
```

Code 3.13 – Example of exported file

The methods available to export data are called : [method reference] method name (what is required). The required actions / files can be: *selection* of an area by the user or *maskfile*, a file with a selection of pixels generated by XMAPTOOLS. The description of the methods is provided below.

- [1] *All pixels* - Export all the compositions of the *standardized phase* selected in [M2101] as oxide weight percentage analyses. If the map size is very large, the generated file could have a lot of rows. Some text editing programs can have troubles to read this file (insufficient memory warning message).
- [2] *Selection of pixels (area)* - Export all the compositions included in an area defined by the user of the *standardized phase* selected in [M2101]. This mode requires to select an area and press right click to finish. This last action will automatically close the area.
- [3] *Random pixels* - Export a specified number of compositions randomly selected into the *standardized phase* selected in [M2101]. This number may be specified (default, 100).
- [4] *Average of groups (maskfile)* - This method allows exporting average oxide compositions of *standardized phase* selected in [M2101] for all the groups of pixels specified into a given maskfile. The maskfile may be generated using the modules BINARY and TRIPLOT.
- [5] *All of a group (maskfile)* This method allows exporting the oxide compositions of a Quanti file selected in [M2101] for the pixels belonging to one group of a given maskfile. User can select which mask is used.
- [6] *Average of a group (maskfile)* - This method works the same way as the method [4]. However in this case only the average oxide composition of one group is exported including average, standard deviation and the median values (column format).
- [7] *Average of all pixels* - This method allows exporting the average oxide composition of all the compositions of the Quanti file selected in [M2101]. Exported values are average, standard deviation and median (column format).
- [8] *Average + std of selected pixels (area)* - Export the average composition and associated standard deviation of pixels included in an area defined by the user of the *standardized phase* selected in [M2101]. This mode requires to select an area and press right click to finish. This last action will automatically close the area. This function can also apply the external function selected in [M2303] to the estimated average composition. If the user press yes, the function runs a Monte Carlo simulation in order to estimate average and standard deviation values of all the output of the selected external function. The exported file could be easily imported into Excel. This function is useful to estimate the average composition of an homogeneous domain of a given phase with a good approximation of the analytical uncertainties on the structural formula.

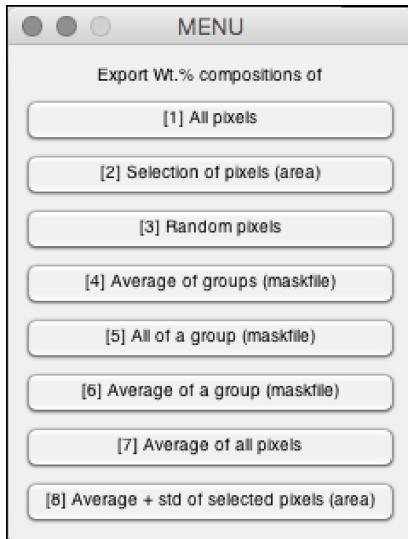


Figure 3.39 – *Menu listing the methods available to export oxide analyses from the selected Quanti file*

[B2104] *Apply filter.* Generate a new *standardized phase* from the selected *standardized phase*, but only with the composition values ranging between the minimum and maximum values of the color bar set in [C5101]. This method has been used by [Lanari et al. \(2013\)](#) to divide each phase into subgroups of compositions prior to the thermobarometric study.

[B2105] *Generate oxide wt-% sum map.* Display a new map showing the sum of the oxide wt-% compositions. This map can only be displayed via this function for checking purposes (no for computations, as it is not saved in the project). Color bar minimum and maximum values can be adjusted and the image exported using the function export ([B5102]). A similar map can also be generated via the *Generator* module.

3.9.2 Standardization Info & corrections

All the detailed explanations regarding the techniques used to test the quality of the analytical standardization are intensively described in [Lanari et al. \(2014b\)](#).

[B2201] *Display calibration curves.* Plot the composition of the standards (spot analyses, in oxide wt-%) against the composition of the corresponding pixels (X-ray maps, in number or counts) and the calibration curves in a new figure.

Warning: This functionality is not available in the version 2.4.1 (and the following updates) for standardizations that have been computed with 2.3.1 and previous versions. In this case, it is recommended to re-standardize your phases. Note that the following function is not affected and can still be used to check the quality of the standardization.

[B2202] *Eliminate data below LOD.* Apply a filter eliminating the data below detection limit. This functionality requires a dataset of detection limit in the same unit of the maps. The selected *Quanti map* is duplicated before applying the correction.

LOD data can either be stored in a file *LOD.txt* in the working directory or in a file */LOD/LOD_QuantiName.txt*, with *QuantiName* the name of the selected Quanti map. The element and the limit of detection (one per line) need to be provided below the keyword > (see examples

in inserts 3.14 and 3.15). Note that the LOD files are automatically generated for EPMA data during the *Advanced Standardization* (see section 3.8.6.3 for a description of how the LOD is calculated).

Example of LOD files is given for EPMA (insert 3.14, unit oxide weight percentage) and for LA-ICP-MS data (insert 3.15, unit ppm of element)

```
>
SiO2      0.115403
Al2O3     0.079747
CaO       0.321135
FeO       0.035126
MgO       0.767588
MnO       0.109571
```

Code 3.14 – Example of LOD file for garnet EPMA data

```
>
89Y      22.2
139La    10.6
140Ce    10.4
141Pr    7.2
153Eu    10.2
158Gd    23.9
159Tb    5.0
163Dy    20.1
165Ho    4.8
169Tm    4.2
172Yb    18.9
175Lu    3.8
178Hf    12.8
```

Code 3.15 – Example of LOD file for garnet LA-ICP-MS data

[B2203]  *Correct mixing pixels.* Apply a correction to filter the pixels having a sum above a given threshold. This function contains an algorithm that will automatically propose a correction based on the distribution of the data (Fig. 3.40a). These values can be defined manually if the button *NO* is clicked (Fig. 3.40b).

3.9.3 External functions module

The external function module can be used to call an external function added to XMAPTOOLS. The program includes a large set of external function and the amount of them is continuously increasing.

NB: Before the first use of a function, user should perform tests in order to check the results of the function (see the section 4.3.3 *How can I check the results of an external function?*)

[M2301] The menu *external function group* lists the groups of external functions available and can be used to set which group is active. The external functions are grouped in five groups:

- **Structural formulas:** Structural formula functions groups the function to calculate structural formulas of the selected standardized phase.
- **P,T and P-T /Map mode:** These functions aims to calculate temperature (T) and/or pressure (P) of crystallization for a given phase, for each selected pixel of the map, which is turned into P, T, or P and T maps. For each pixel of the input map, the equilibrium conditions are derived

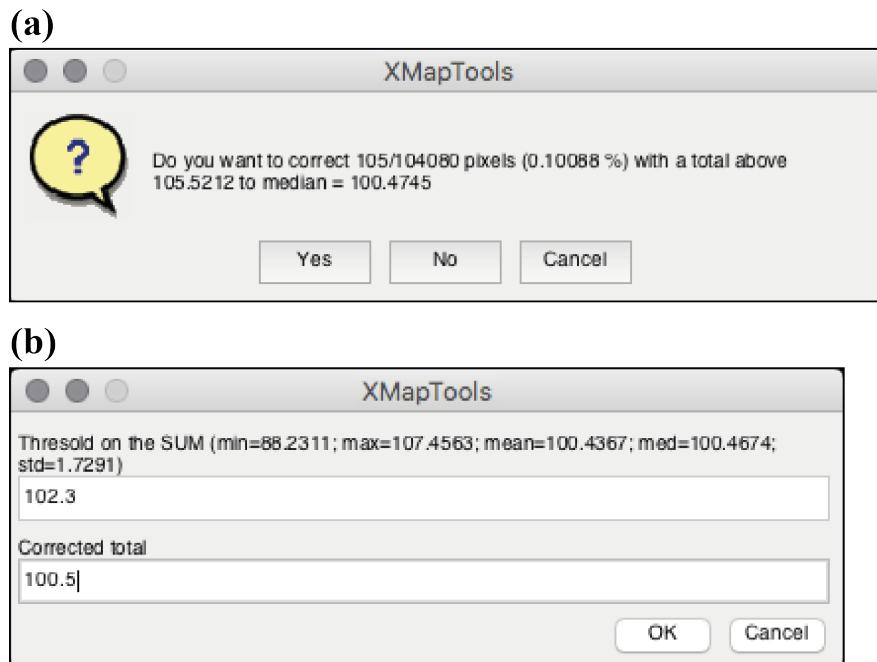


Figure 3.40 – Options of the function Correct mixing pixels

using the pixel composition and fixed variables such as coexisting phase composition, or P or T.

- **P,T and P-T /Spot mode:** These functions aims to calculate T and/or P of crystallization for a given set of pixel. XMAPTOOLS generates a composite chemical map displaying the compositions of the phases of interest. Set of pixels may be selected directly on the image and the corresponding compositions are used to estimate the equilibrium conditions.
- **General functions:** Additional external functions used in XMAPTOOLS.
- **Density functions** External functions calculating density maps from the compositions of solid solutions
- **Transfer to Results** Send the selected Quanti

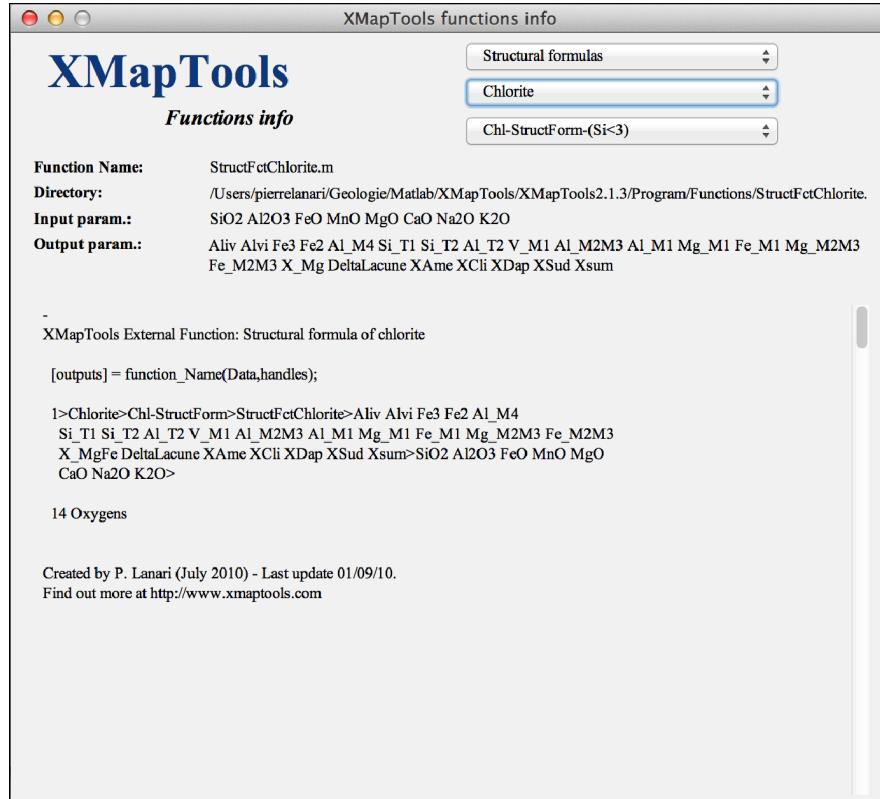
[M2302] *External function subgroup.* Menu listing the subgroups of external functions available in a given group set in [\[M2301\]](#).

[M2303] *External functions.* Menu listing the external functions available in a given subgroup set in [\[M2302\]](#).

[B2301] *COMPUTE.* Apply the external function selected in [\[M2303\]](#). The data of the *standardized map* selected in [\[M2101\]](#) are used as input data.

[B2302] *External function info window.* Display the external function info window (see Fig. 3.41). This module aims to provide an easy access to each external function description including:

- **External function name** the name of the MATLAB function file with .m extension

Figure 3.41 – *XMapTools function info GUI*

- **Directory** the location of the selected external function
- **Input parameters** as defined in *ListFunctions.txt* (or if used the user's file *ListFunctions_USER.txt*). NB: The name of the variables should be compatible with the XMAPTOOLS element names defined in *Xmap_Default.txt*
- **Output parameters** Names of the output variables generated by the external function
- **Comment block** displaying the first command block of the selected *standardized map* to the workspace *Result*

3.9.4 Real pixel size

[B2413]  *Compute the 'real' pixel size.* The real pixel size is evaluated by approximating the interaction volume of the electron beam. This functionality requires a density map (see below).

The real pixel diameter d is approximated using the following a biexponential model valid for an accelerating voltage of 15 KeV and a beam size of 1 μm as proposed by (Lanari and Piccoli 2019):

$$d = 4.034e^{-0.02139Z\rho^2} + 1.548e^{-0.006457Z\rho^2} \quad (3.23)$$

with Z the mean atomic number and ρ the density of the material.

The procedure to approximate real pixel sizes in XMAPTOOLS is the following:

- **Part 1** Generate a density map (see [B2406])

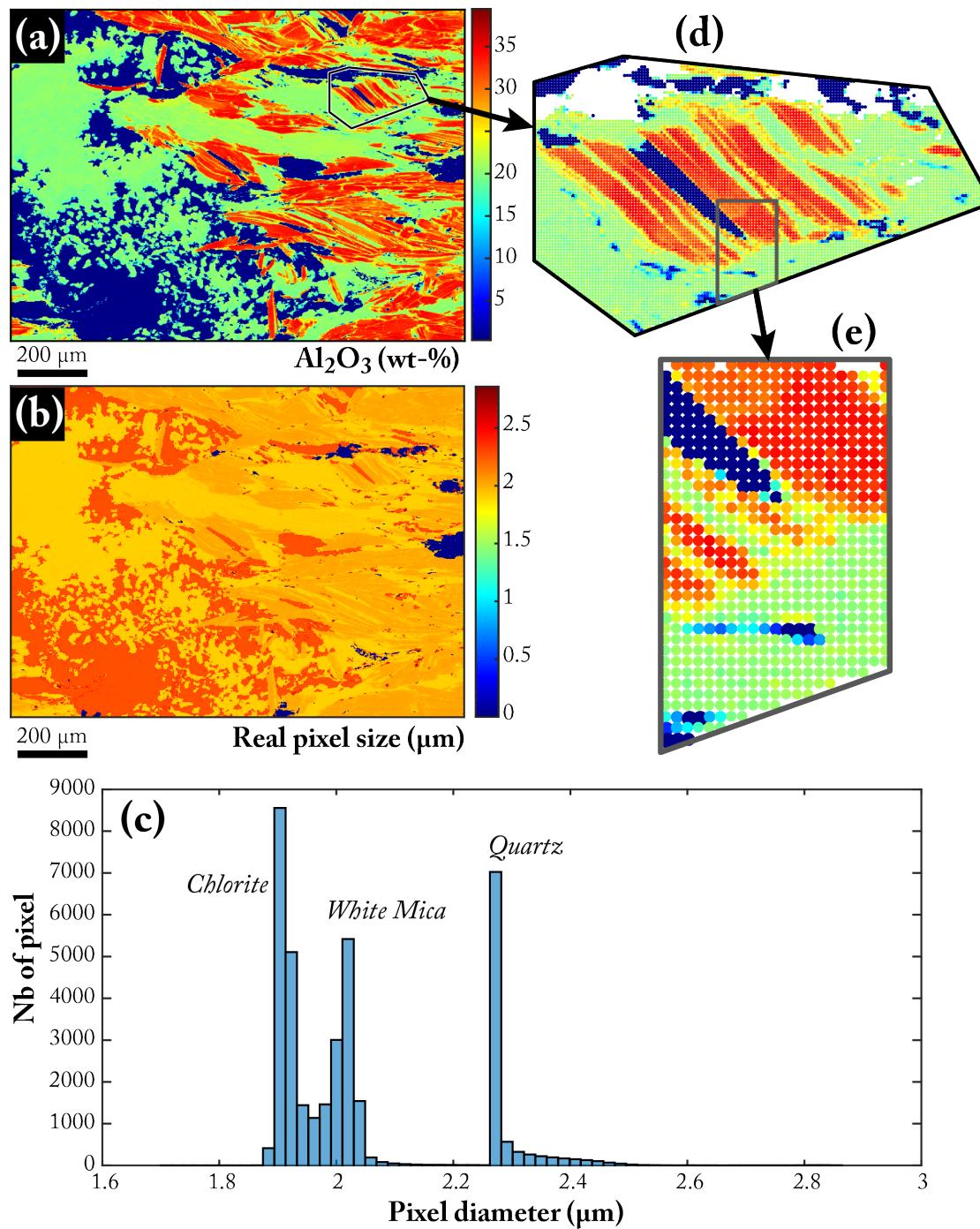


Figure 3.42 – Plotting the real pixel size. (a) map of alumina (Al_2O_3) of a metapelite from the Western Alps (sample from Aude Verly). (b) map colored by pixel size (in μm). (c) distribution of pixel sizes; the three populations correspond to the pixels of chlorite, white mica (phengite) and quartz. (d) Map plotted with the real pixel size. (e) zoom. The pixel size is 2 μm .

- Select the map of interest in *Quanti* (merged maps are good) and adjust the contrast of the color bar before clicking the button 
- **Part 2** Once the function has been called, a dialog box appears to decide whether the program should assume that $H_2O = 100 - \sum oxide$ or not. This decision will affect the estimation of the mean atomic number (MAN)
- The MAN value for each pixel is calculated from the oxide composition
- The program applies Eq. 3.23 and displays a map in which each pixel is colored by the corresponding pixel size (Fig. 3.42b). These data are also plotted in a histogram diagram (Fig. 3.42c).
- **Part 3** A dialog box is shown to set the pixel size of the map (in μm)
- The same compositional map is plotted in a new window in which you can select an area-of-interest polygon (click on the image and right-clicking for validating the selection). It is strongly recommended to select a relatively small area (max 300×300 pixels) because the computer becomes very slow when two many round-shape pixels are being plotted.
- The program generates a new maps of this area using round-shape pixels showing reflecting the real pixel size (see examples in Fig. 3.42d-e)

3.9.5 Local composition module

[B2401]  *Merge standardized phases.* Merge the selected standardized phases and generate a new quantitative map. The phases are selected via a dialog box and the function generates the merged map.

The function *merge standardized phases* sums up the selected standardized phases. This function does not check if the same standardized phases is selected twice, e.g. same phase but with two different standardizations. If the composition of one pixel is provided in two or more standardized phases, the result will be the sum of the compositions. As explained before the function *generate oxide wt-% sum map* [B2105] should be used to check that the oxide wt-% sum values are coherent with the expected values for the occurring mineral phases.

If the check box *Border interpolation* is selected, a reference element is needed to perform the border interpolation. This reference element is used to estimate the composition of the missing pixels between the two surrounding phases. This interpolation is done only there is missing pixel between phases. Two additional parameters (*X-n->X+n* and *OnGarde*) are required. *X-n->X+n* is the size of the window in pixel used for the interpolation. *OnGarde* is a parameter defining the sensibility of the correction (ranging between 0.1 and 1). The default values, 2 and 0.5 respectively, are the optimal value for most cases.

[B2406]  *Generate a density map (from selected mask file).* Create a density map assuming a constant density value for each phases of the selected mask file. Such density map may be used to generate a density-corrected oxide map or approximate the real pixel size. The procedure to export local compositions is discussed in the section 1.7.1. Density of phases may be defined in the file *Classification.txt* below the keyword >2 (see example in code 3.18). Nb: The order of the density values is the same as the mask above. If phase densities are not provided in *Classification.txt*, a new window opens allowing user to define them.

```
>1
Biotite      367      556
Paragonite   433      741
Nepheline    307      801
Albite       177      224
Rutile       500      415

>2
2918
2921
2590
2599
4203
```

Code 3.16 – File Classification.txt including specific density (after the keyword >2)

[B2407] *Display the density map.* Plot the density map in the main window. This function is available only if a density map was calculated. Local density along profiles or within domains can be estimated using the sampling functions [B5201], [B5202], [B5203] and [B5204]);

[B2408] *Compute a density-corrected oxide map.* Generate a density-corrected oxide map from the selected oxide map. The name of this new map can be edited in the dialog box that appears once the button has been pressed. The default name begin with *DCM abbreviation of density-corrected map. As detailed in the section 1.7.1, DCM value of a pixel i (DCM_i) is computed from the composition in oxide weight percentage of this pixel (C_i^{wt}) using the following relationship

$$DCM_i = \frac{\rho_i}{\rho_{mixture}} C_i^{wt} \quad (3.24)$$

with ρ_i the pixel density that is the density of the corresponding phase and $\rho_{mixture}$ the local average density of the selected pixels, i.e. those having a non-zero composition.

Information regarding the density-correction are reported in the MATLAB Command Window (see code 3.17). Note that in this exemple the map average density and the local average density are different. This is because not all the pixels have a defined composition. Thus it is important to correct only the phases that will be used to estimate local compositions in order to have a good approximate of the local average density (see discussion in section 1.7.1).

```
DCM ... (Density corrected map) ... processing
DCM ... - Maskfile: Meth2-MaskFile2
DCM ... - Map average density: 2703.7063
DCM ... - Selected pixels: 813246/870400
DCM ... - Local average density: 2688.646
DCM ... - New Quanti file: *DCM-Merged_Map_BioAlpine
DCM ... (Density corrected map) ... done
```

Code 3.17 – Information regarding the density-correction displayed in the MATLAB Command Window

[B2411] *Export phase proportions.* Extract the phase proportions from the selected map using the selected mask file. The pixels having a sum of composition of zero are not considered.

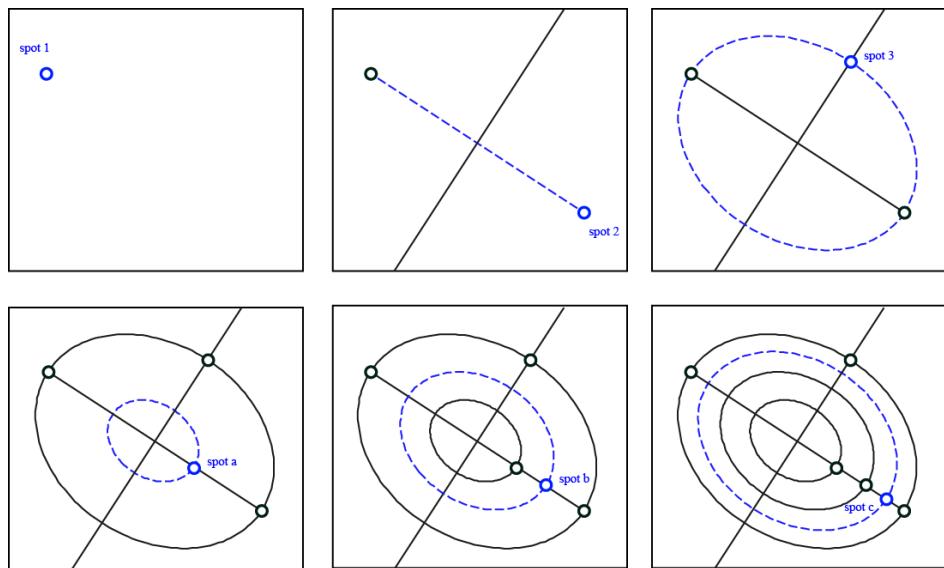


Figure 3.43 – Procedure to define an ellipse and export composition extrapolated in 3D

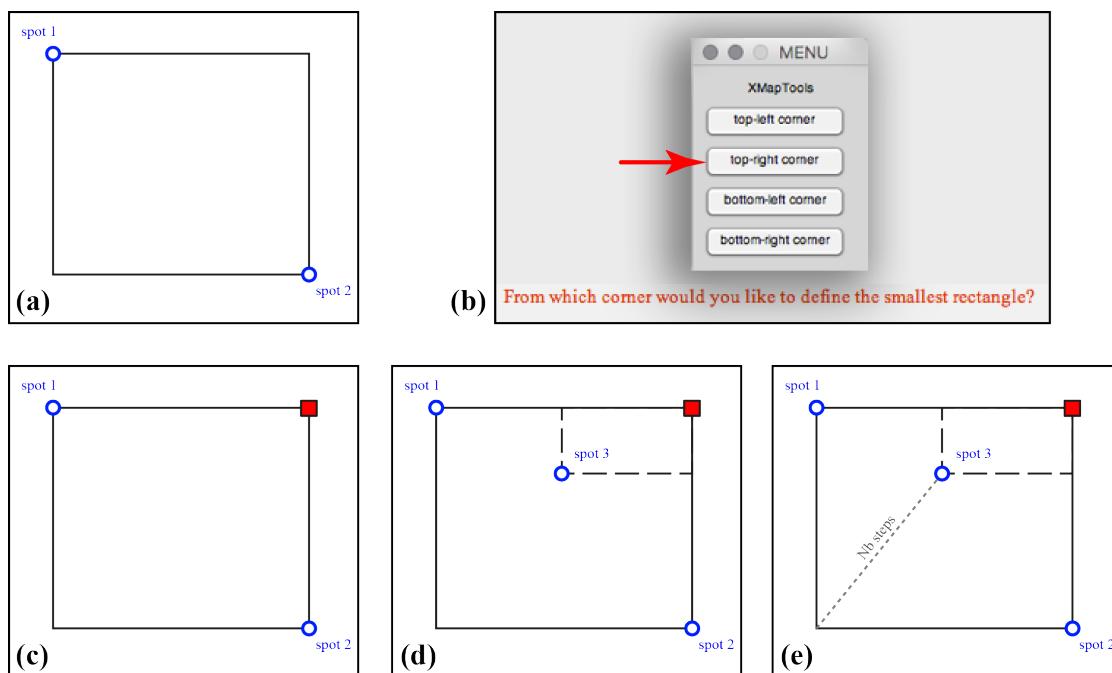


Figure 3.44 – Procedure to export compositions with a variable-size rectangle

[B2409]  *Select an area and eliminate pixels outside.* Eliminate pixels outside a region-of-interest. This region-of-interest is defined by selecting spots that define a polygon which is converted by the program into a mask (see spots 1 to 10 Fig. 3.20b). Selection mode is disabled using right-clicking (spot 11, in Fig. 3.20b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.20b. For the standardized phase selected in [M2101] all pixels outside the region-of-interest are eliminated.

[B2410]  *Select an area and eliminate pixels inside.* Eliminate pixels inside a region-of-interest (description of the selection mode is given above). For the standardized phase selected in [M2101] all pixels inside the region-of-interest are eliminated.

[B2402]  *Export local composition: map.* Calculate and save the average oxide composition of the *oxide map* or *density-corrected map* selected in [M2101]. This function has been designed to work with merged maps with or without density correction (see function [B2401]). The generated file (see code 3.18) is exported in the directory *Exported-LocalCompos*. If this directory does not exist the program makes it in the working directory.

Local composition (Map) from XMapTools	
Al ₂ O ₃	24.3961
CaO	0.021694
Cr ₂ O ₃	0.057805
FeO	19.6617
K ₂ O	3.6851
MgO	6.8446
MnO	0.35621
Na ₂ O	0.33612
SiO ₂	34.833
TiO ₂	0.18467
SUM	90.3769

Code 3.18 – Example of exported file in /Exported-LocalCompos

[B2403]  *Export local composition: area.* Calculate and save the average oxide composition of pixels included in an area defined by the user of the map selected in [M2101]. This mode requires to select an area and press right click to finish. This last action will automatically close the area. The generated file is exported in the directory *Exported-LocalCompos*. If this directory does not exist the program makes it in the working directory.

[B2405]  *Export local composition: ellipse (3D).* Calculate and save the average oxide composition of pixels included in ellipse defined by the user of the map selected in [M2101]. The composition of each small ellipse is extrapolated from 2D surface to 3D volume of an ellipsoid (e.g. code 3.19).

This mode requires to define a primary ellipse with a long axis between point 1 and 2 and a short axis with point 3 (Fig. 3.43). Then integrations are defined from the center to the rim of the primary ellipse (see points a, b and c on Fig. 3.43).

Local composition (Ellipsoid) from XMapTools 12-Nov-2015					
Reference ellipse information:					
Center position (X,Y)					
Slope Major axis					
Radius Major axis					
Radius Minor axis					
Surface (Nb of pixels)					
Surface (in px ²)					
Integrations:					
Number of integrations					
Integration values					
Volumes integrations (px ³)					
Volumes fractions					
Nb pixels integrations					
Surface integrations (px ²)					
Surface fraction (from px)					
Surface fraction (in px ²)					
Compositions integrations:					
Al ₂ O ₃	24.920	25.508	23.386	22.140	
CaO	0.088	0.170	0.275	0.497	
FeO	1.873	1.010	0.571	0.607	
K ₂ O	2.560	1.701	1.520	1.100	
MgO	4.150	2.046	1.091	0.882	
MnO	0.057	0.055	0.059	0.060	
Na ₂ O	7.985	9.470	11.300	11.425	
TiO ₂	1.529	2.183	1.775	0.360	
SiO ₂	54.799	56.254	59.698	62.701	
Extrapolated (ellipsoid) local Compositions:					
Al ₂ O ₃	23.421				
CaO	0.336				
FeO	0.758				
K ₂ O	1.439				
MgO	1.388				
MnO	0.058				
Na ₂ O	10.754				
TiO ₂	1.249				
SiO ₂	59.928				
SUM	99.3309				

Code 3.19 – Example of exported file in /Exported-LocalCompos

[B2412]  Export local composition: variable-size rectangle. Calculate and plot the changes in local bulk composition between two rectangular areas along n steps (Fig. 3.44 and 3.45).

The procedure consists of the following steps:

- Defining the reference domain with a rectangle shape by clicking two pixels (see Fig. 3.44-a).
- Choosing from which corner of this rectangle you want to define the smallest rectangle (see Fig. 3.44-b). The available options are: *top-left corner*, *top-right corner*, *bottom-left corner*, *bottom-top corner*. In the example shown in figure 3.44-c, the *top-right corner* is selected (red arrow in b).
- Defining the smallest rectangle from the selected corner (see Fig. 3.44-d).

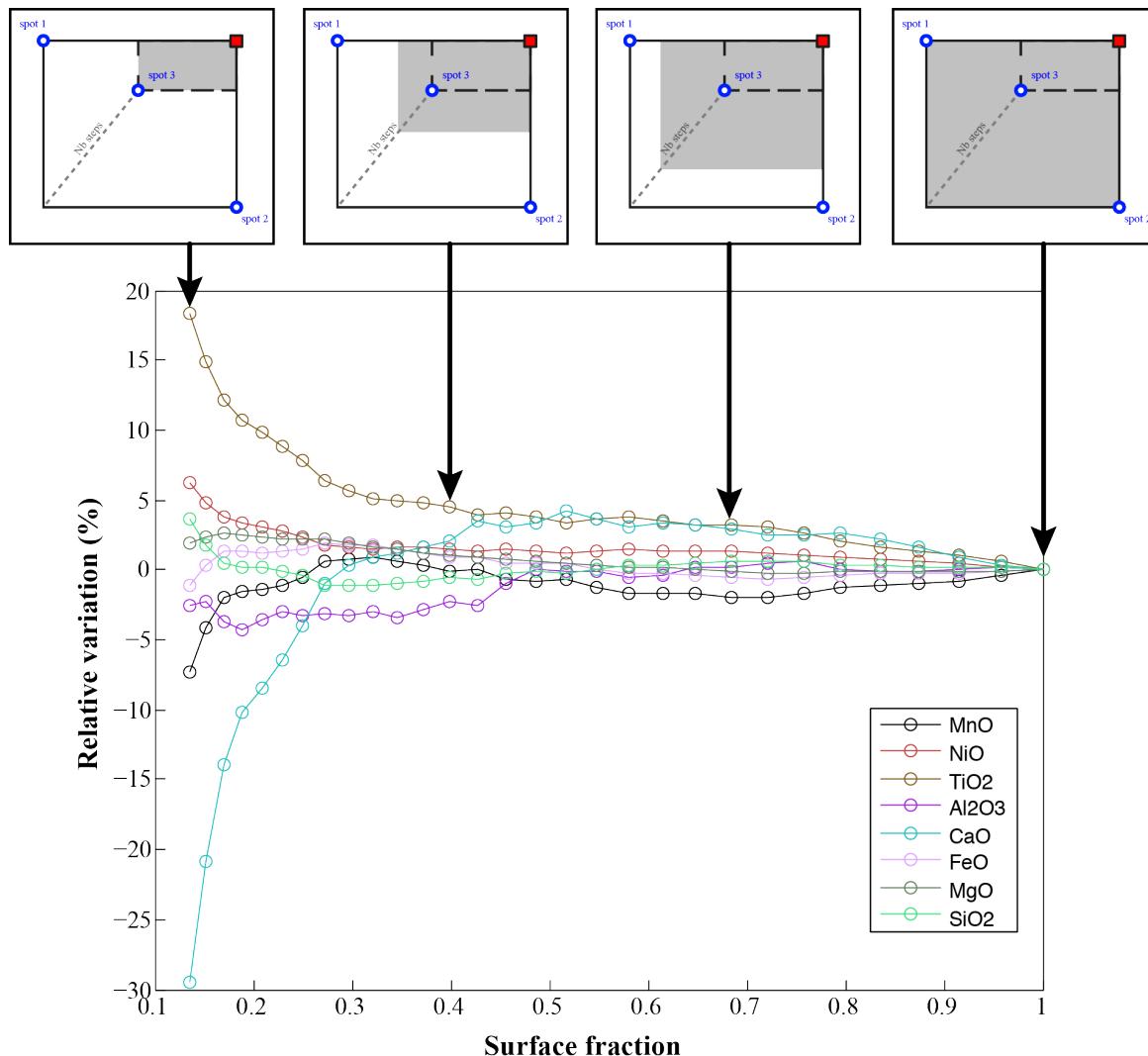


Figure 3.45 – Result exporting compositions with a variable-size rectangle

- Defining the number of steps, i.e. the number of samples along the dashed line in figure 3.44-c

Three figures are generated plotting some variables against the surface fraction of the reference rectangle:

- The first figure shows the relative difference (in %) for the local bulk composition of the available oxide (see for example the diagram in Fig. 3.45). As the relative difference of the local bulk composition is expressed relative to the reference rectangle, it comes out that for $x = 1$, $y_i = 0$.
- The second figure shows the variation of the concentration expressed in the unit of the standardized maps, usually oxide weight percentage.
- The third figure shows the absolute difference in the unit of the standardized maps, usually oxide weight percentage.

Note: This function does not save any file with the composition of the successive domains.

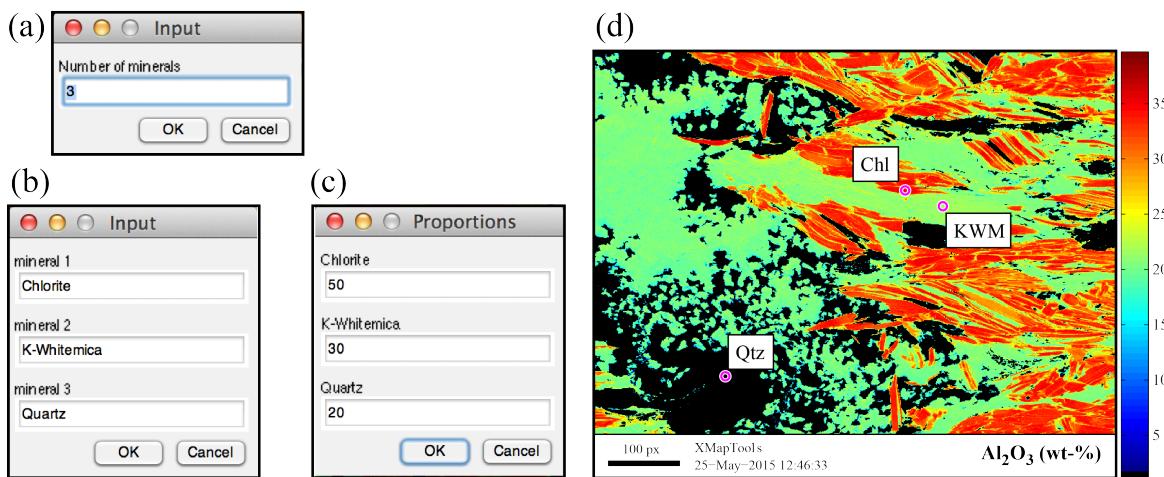


Figure 3.46 – Procedure to export composition build from proportions. (a) number of phases and their (b) names, (c) modal proportion, and (d) compositions.

Warning: The function *Export local composition: variable-size rectangle* does not work with rotated maps. If the rotate function is being used, the program will ask you to restore the original orientation.

[B2404] *Export composition build from proportions* Calculate and save a bulk composition based on mineral compositions and mineral proportions. For example, it is possible to estimate the bulk composition of an assemblage made of 50% chlorite 30% K-white mica and 20% quartz using this function (see Fig. 3.46). In this case, the unit is weight fraction of phases (density is not considered).

The following steps are required:

- Defining the number of phases to be considered
- Setting the phase names
- providing the phase modal proportions as percentage
- Setting the input compositions for each phase by selecting one pixel on the displayed map

The generated file (see code 3.18) is exported in the directory *Exported-LocalCompos*. If this directory does not exist the program makes it in the working directory.

Local composition (Proportions) from XMapTools**(1) Mineral proportions:**

Chlorite	50
K-Whitemica	30
Quartz	20

(2) Mineral compositions:

	Chlorite	K-Whitemica	Quartz
Al ₂ O ₃	21.6714	34.5545	0.0000
FeO	31.0584	1.454	0.0000
K ₂ O	0.0094	9.0293	0.0000
MgO	12.2202	1.2115	0.0000
Na ₂ O	0.018231	1.4428	0.0000
SiO ₂	25.3511	46.49	99.612
TiO ₂	0.029867	0.36857	0.0000

(3) Local Composition:

Al ₂ O ₃	21.202
FeO	15.9654
K ₂ O	2.7135
MgO	6.4736
Na ₂ O	0.44197
SiO ₂	46.5449
TiO ₂	0.1255

Code 3.20 – Example of exported file in /Exported-LocalCompos

3.10 RESULTS

3.10.1 Results from external functions (Results)

[M3101] *Results phase.* Menu to select the *result* (corresponding to the output of an *external function*) to be displayed in the main figure window. All the available *results* are listed in this menu.

NB: For coding reasons, the first *result* name is always *none*. If none is selected, nothing happens in the plotting areas and the buttons of the workspace are inactive.

[M3102] *Elements & variables.* Menu to select the variable of the *result* to be plotted. This list is updated for each *result* selected in [M3101].

[B3101] *Rename result.* Edit the name of the *result* selected in [M3101]. This name is automatically defined during the computation of the external function (format: *[FunctionName]*).

[B3102] *Delete result.* Delete the *result* data selected in [M3101]. This button is available only if two or more *results* have been computed.

[B3103] *Export compositions (results).* Extract and save variables from the *result* selected in [M3101]. One file is generated for each selected variable. The generated files are matrices with the same size as the original map. The files are saved in the directory */Exported-Results*. If this directory does not exist the program creates it as a subfolder in the working directory.

```
Export ... (RESULTS in ascii format) ...
Export ... (mineral: K-WhiteMica) ...
Esport ... (method: Phg-StructForm) ...
Export ... (reshape: 530/725) ...
Export ... (Si4 has not been saved ** User Request **) ...
Export ... (Al_T2 has not been saved ** User Request **) ...
Export ... (Si_T2 has not been saved ** User Request **) ...
Export ... (V_M1 was saved [...] /Exported-Results/TEST-V_M1.txt]) ...
Export ... (Fe_M1 was saved [...] /Exported-Results/TEST-Fe_M1.txt]) ...
Export ... (Mg_M1 was saved [...] /Exported-Results/TEST-Mg_M1.txt]) ...
Export ... (Al_M2M3 was saved [...] /Exported-Results/TEST-Al_M2M3.txt]) ...
Export ... (Mg_M2M3 was saved [...] /Exported-Results/TEST-Mg_M2M3.txt]) ...
Export ... (Fe_M2M3 has not been saved ** User Request **) ...
Export ... (XMg has not been saved ** User Request **) ...
Export ... (K_A has not been saved ** User Request **) ...
Export ... (V_A has not been saved ** User Request **) ...
Export ... (Na_A has not been saved ** User Request **) ...
Export ... (RESULTS in ascii format) ... Ok
```

Code 3.21 – Export results (info reported in the Command Window)

[B3104] The button *APPLY FILTER* allows a new *result* to be created from the one selected in [M3101], containing only the pixels within the compositional range defined in [C5101]. If the range is *min – max*, then this function duplicates the selected result.

[B3105] *Delete a variable.* Eliminate the variable selected in [M3102] of the *result* selected in [M3101]. This action cannot be reversed (no undo).

3.10.2 Other functions for trace element maps

[B3302] Compute a relative map  Compute a compositional map relative to the composition of a reference pixel. A reference pixel shall be defined by clicking on the image (Fig. 3.47a). New maps are generated and saved in a new *result*; these maps show the relative variation of each pixel composition to the composition of the reference pixel. A new *result* is generated with the name *REL_NameOriginalResult*. Two maps are included:

- **Diff_rel** shows the relative difference in composition for each pixel to the composition of the reference pixel (e.g. Fig. 3.47b). This map has no unit. For a map A (matrix) and a reference pixel with a composition R , $Diff_{rel}$ is simply obtained by:

$$Diff_{rel} = \frac{A}{R} \quad (3.25)$$

- **Diff_per** shows the relative difference in composition for each pixel to the reference pixel expressed in percentage (e.g. Fig. 3.47c).

$$Diff_{per} = \frac{(A - R)}{R} \times 100 \quad (3.26)$$

Note 1: The undefined pixels are plotted with a relative difference of -100 %.

Note 2: The function *enable auto-contrast*  does not work properly with relative maps that can contain negative value (as the one shown in Fig. 3.47c). Only the pixel with positive values are considered by the *auto-contrast* function.

[B3303] Merge results  Merge two or more results into a new result dataset.

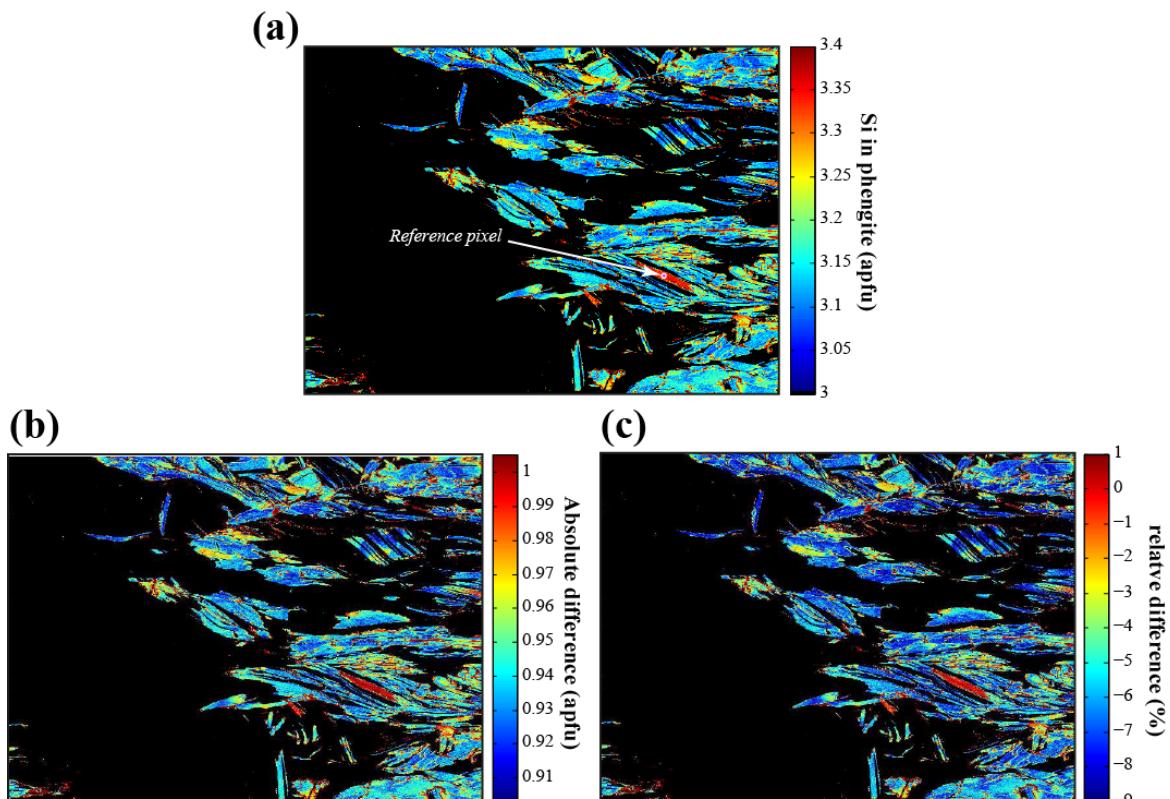


Figure 3.47 – Relative maps. (a) Silicon map of phengite in atom per formula unit (apfu). The reference pixel used to compute (b) and (c) was selected in the Si-rich phengite (3.37 apfu) and is plotted in magenta. (b) Map of Si in phengite showing the relative composition of each pixel to the reference pixel (see Eq. 3.25). (c) Map of relative differences expressed as percentage (see Eq. 3.26).

3.11 MODULES FOR DATA VISUALIZATION AND EXPLORATION

For advanced data exploration, any map displayed in the main window (e.g. *X-ray maps*, *compositional map*, *merged map*, *result*) can be visualized in a histogram, or combined with other maps to be plotted in binary diagrams (Fig. 3.52a), in ternary diagrams (Fig. 3.52b) or also displayed as composite RGB image (Fig. 3.57). Data from trace element maps can be represented in spider diagrams using the module SPIDER .

It is also possible to generate new maps (variables) from existing maps (variables) using mathematical expressions using the GENERATOR module.

The modules HISTOGRAM, BINARY, TRIPLOT, RGB, GENERATOR and SPIDER can be opened via the menu (see section 3.2.5) provided that enough maps (i.e. variables) are available. A description of each module is provided in the following sections.

Trace element concentration maps such as REE can be plotted in spider diagrams using the chemical module *Spider* [B3301]. Note that this module is only available in the workspace *Results* and will work only with LA-ICP-MS maps in ppm having compatible names (see §2.7.2).

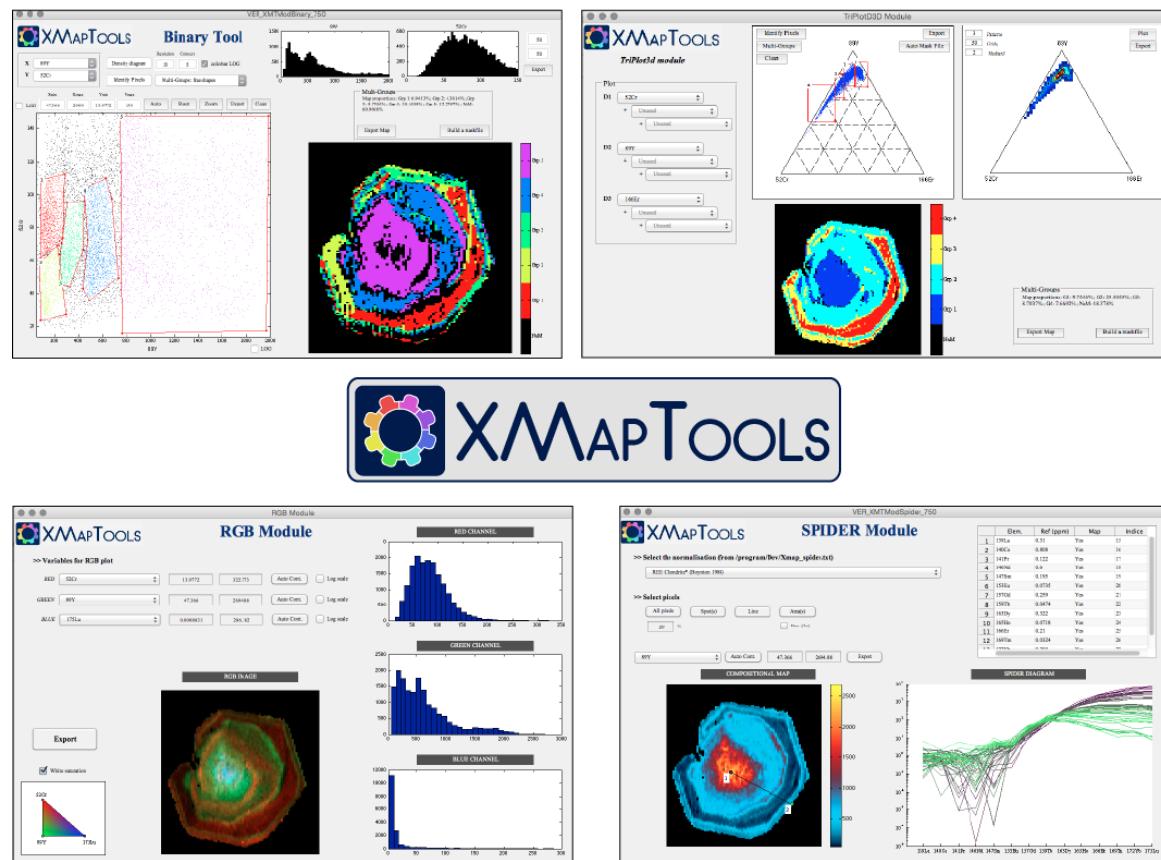


Figure 3.48 – Selection of additional modules available in XMAPTOOLS

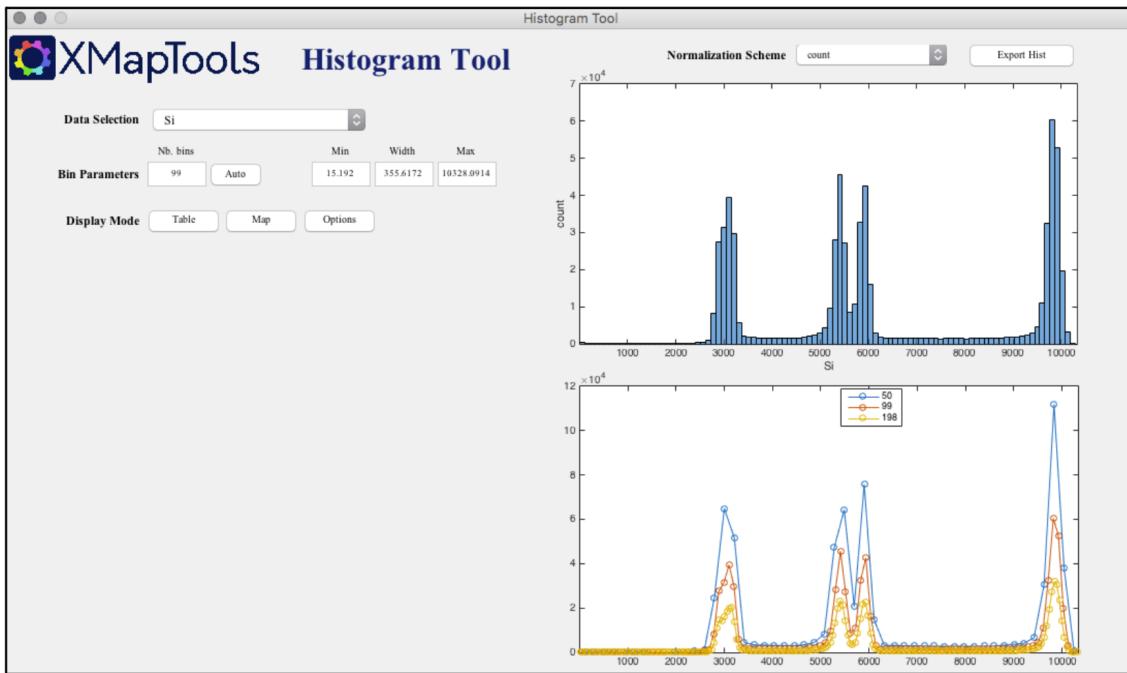


Figure 3.49 – Chemical module HISTOGRAM

3.11.1 Histogram

HISTOGRAM is an additional user interface (module) provided in the XMAPTOOLS’ package. HISTOGRAM is accessible in any of the three workspaces via the main menu *Modules* and *Histogram* (see section 3.2.5) provided that a map is available in the active workspace. This module is independent from the the main XMAPTOOLS window; both can be used at the same time.

In the following, this module is described using the example of a X-ray map of Si-K α of high-grade metapelite with garnet, biotite, plagioclase, sanidine, quartz and sillimanite (see tutorial 2 in chapter 8).

Two figures are displayed (see Fig. 3.49):

- *Histogram* (top plot) displays an histogram bar plot of the data
- *Curves* (bottom plot) displays curves, which shows the height of each bin of the histogram without the bars. This figure generates three curves: (1) for the same number of bins (orange); (2) for half the number of bins (blue); (3) for double the number of bins. This figure can be used to evaluate the effect of the bin number on the distribution.

The main buttons and options are available in the *Binary* module (see Fig. 3.49) are:

Normalization Scheme (option, top right) for setting the normalization scheme of the histogram values. The normalization scheme affects the scaling of the histogram along the vertical axis. The following options are available:

- *Count (default)*: the height of each bar is the number of observations in each bin, and the sum of the bar heights is the number of considered pixel values
- *Probability*: the height of each bar is the relative number of observations (number of observations in bin / total number of observations), and the sum of the bar heights is 1

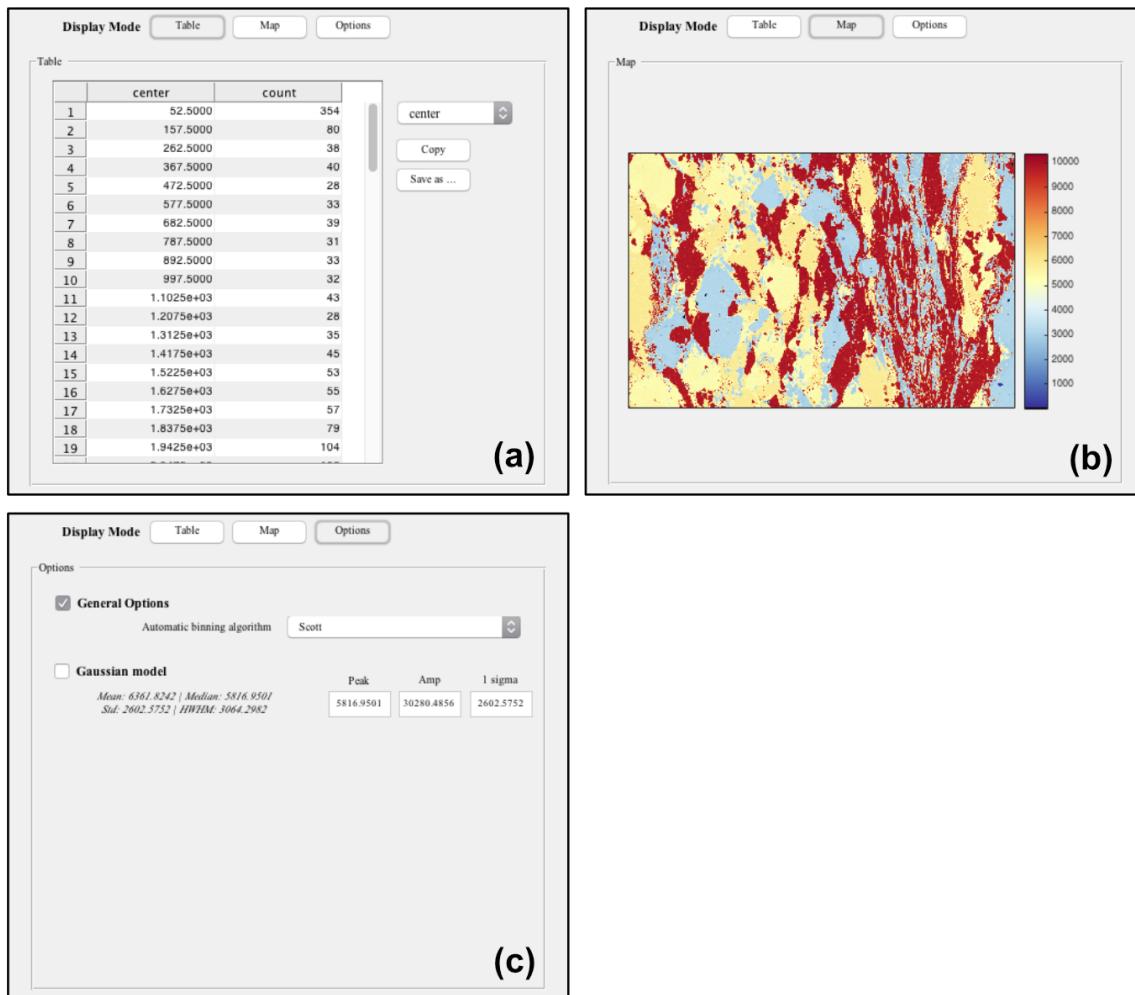


Figure 3.50 – Display modes of the module HISTOGRAM: (a) Table; (b) Map; (c) Options

- *Pdf*: probability density function estimate; The height of each bar is, (number of observations in bin) / (total number of observations * width of bin). The area of each bar is the relative number of observations, and the sum of the bar areas is 1
- *Cumcount*: the height of each bar is the cumulative number of observations in each bin and all previous bins. The height of the last bar is the number of considered pixel values
- *Cdf*: cumulative density function estimate; the height of each bar is the cumulative relative number of observations in each bin and all previous bins. The height of the last bar is 1.

Data Selection (menu, left) for selecting the map data to be plotted in the histogram. Selecting a new element resets all the settings (number of bins, etc.) to default values

Bin Parameters (options, left) for adjusting the plotting options of the histogram figure. Selecting a new element resets all the settings (number of bins, etc.) to default values.

- *Number of bins* display the number of bins used to plot the histogram. This number can be adjusted manually.
- *Auto* adjust automatically the number of bins using the automatic binning method selected in *Options / General Options* (see below)

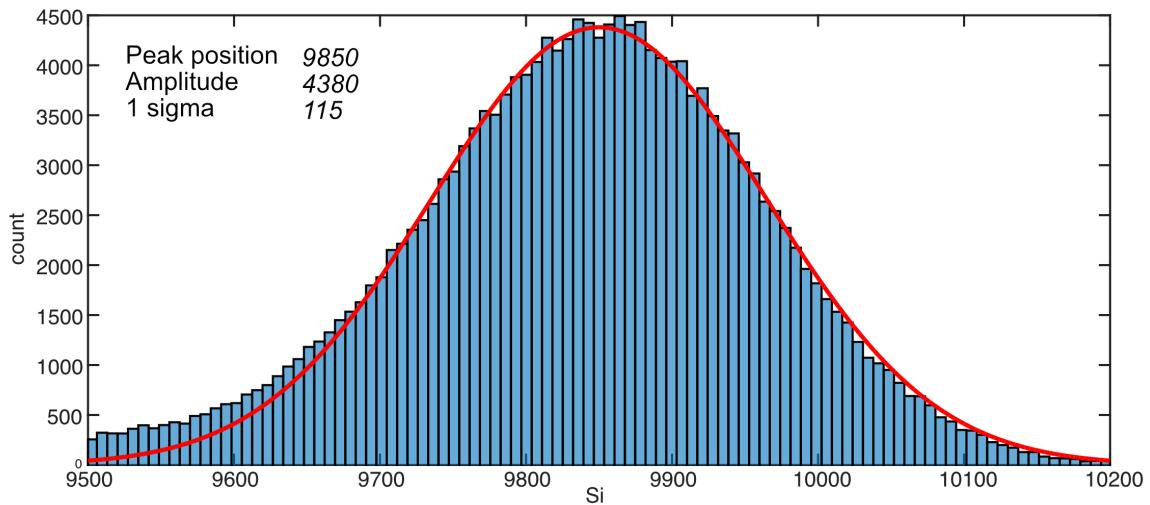


Figure 3.51 – Gaussian model for Si-in-quartz (unit: counts of $\text{Si}\alpha$)

- *Min*, *Width*, *Max* display the values used to generate the plots. These numbers can be adjusted manually. Adjusting *Width* causes a change of the number of bins. But if the number of bin is changed by any method, *Width* is automatically updated.

Display Mode allows additional results and options to be displayed (Fig. 3.50). Press each button to activate the corresponding display mode.

3.11.1.1 Table mode

Once this mode is activated by pressing the button *Table*, a table containing the data used to generate the histogram is displayed. The position of the bars are reported in the first table, using either the value for each (1) bin center, (2) lower bin, or (3) upper bin. The second columns show each value corresponding to the normalization scheme selected.

The data can be saved to a text file using the button *Save as ...* or copied to the clipboard in an Excel-compatible format by pressing the button *Copy*.

3.11.1.2 Map mode

Displays a map of the selected variable. Note that the range of the color bar is automatically adjusted to match the range of data plotted in the histogram.

3.11.1.3 Options

Two options are available in this module:

Automatic binning algorithm used by the button *Auto*. The following methods are available:

- *Scott*: Scott's rule is optimal if the data is close to being normally distributed, but is also appropriate for most other distributions. It uses a bin width of: $3.49 * \text{std}(X) * \text{numel}(X)^{-\frac{1}{3}}$

- *Freedman-Diaconis*: the Freedman-Diaconis rule is less sensitive to outliers in the data, and may be more suitable for data with heavy-tailed distributions. It uses a bin width of $2 * iqr(X) * numel(X)^{-\frac{1}{3}}$; iqr is the interquartile range
- *Sturges*: Sturges' rule is a simple rule which chooses the number of bins to be $\lceil 1 + \log_2(numel(X)) \rceil$
- *Sqrt*: The Square Root rule is another simple rule; it chooses the number of bins to be $\lceil \sqrt{\text{numel}(X)} \rceil$

A Gaussian function can be plotted on top of the distribution as shown in an example in Figure 3.51. The values of peak position, amplitude and standard deviation of the Gaussian distribution can be adjusted manually.

3.11.2 Binary Module

BINARY is an additional user interface included in the XMAPTOOLS' package. BINARY is accessible in the three workspaces *X-ray*, *Quanti* and *Results* via the main menu *Modules* and *Binary* (see section 3.2.5) provided that at least two maps are available. This module is independent from the the main XMAPTOOLS window; both can be used at the same time.

In the following, this module is described using the example of a merged map of oxide wt-% compositions of chlorite, phengite and quartz for which SiO_2 is plotted against MgO (Fig. ??a). The sample used in the figure is a greenschist facies metapelite from the western Alps investigated by Aude Verly during her Master at the University of Grenoble.

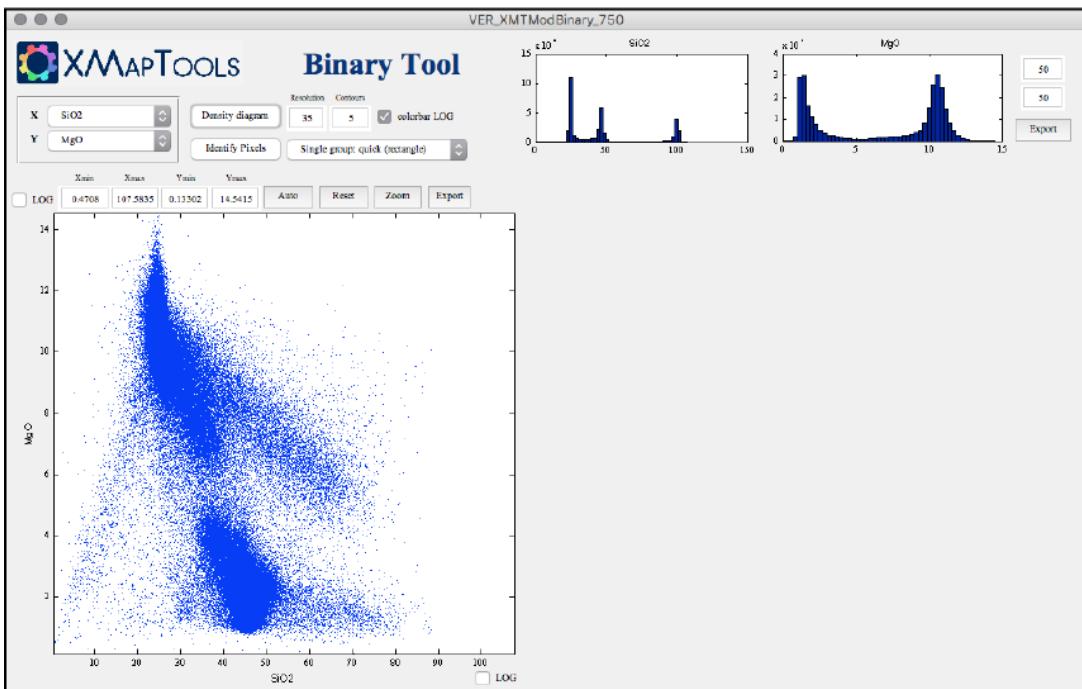
The main buttons and options are available in the *Binary* module (see Fig. 3.53) are:

Main menus (X & Y) to select the maps used as input for the variables X and Y (e.g. SiO_2 vs MgO in Fig. 3.53). The maps listed in these menus depend on the workspace from which *Binary* is called. Changing the workspace in the main XMAPTOOLS window does not affect the BINARY module.

Plot options contain some tools controlling the display of the binary diagram.

- *Xmin*, *Xmax*, *Ymin*, *Ymax* display the range of composition displayed for X and Y axes.
- *Auto (button)* automatically adjust the range of each axis to have exactly 99.9 % of the pixels compositions plotted.
- *Reset (button)* resets the original display and plot all the pixel compositions.
- *Zoom (button)* sets the range of each axis using a rectangle defined by clicking on the figure to select 2 points.
- *Export (button)* opens the figure in a new window (check the description of [B5102] to see how to save figures).
- *LOG (x-axis)* the mode of the horizontal axis is set to *log* if this option is selected.
- *LOG (y-axis)* the mode of the vertical axis is set to *log* if this option is selected.
- *Histogram options* to set the number of bins (default 50) and to export the figures.

(a)



(b)

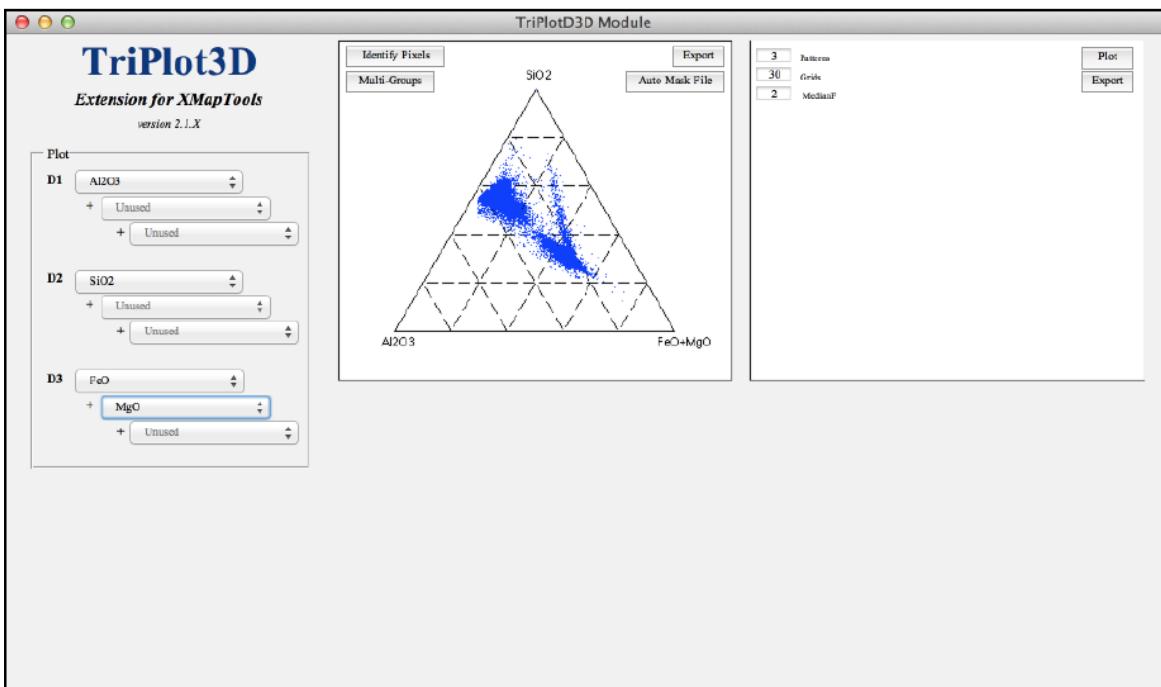


Figure 3.52 – Chemical modules (a) Binary and (b) TriPlot

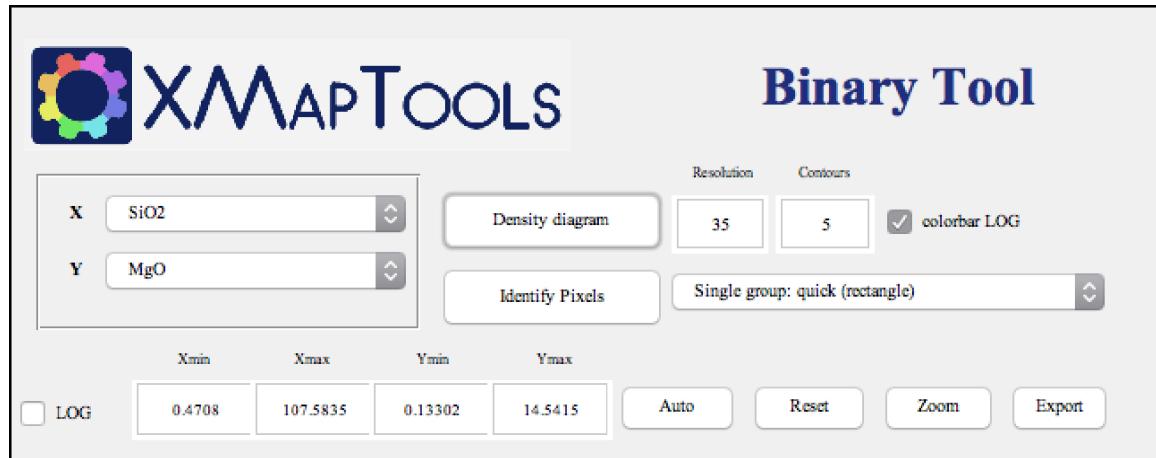


Figure 3.53 – Buttons and options of the Binary module

Note 1: If *log* axis are shown when a selection is made to Identify Pixels, the shape of the polygon is not correct, whereas the color of the selected pixels are.

Note 2: The *log* axis are not compatible with the density plot and the export function.

3.11.2.1 Density diagrams in the Binary module

Density diagram (button) generate a density diagram from the points plotted in the binary diagram. The resolution (default 300 pixels) can be changed before generating the density map. The resolution is defined as the number pixels in the density image for both vertical and horizontal dimensions. Note that the density map is plotted using a color bar with a logarithmic scale if the option *colorbar LOG* is selected.

Two types of density diagrams are available:

- *Density map (quick)* is an image in which each pixel shows the number of points (density) within the corresponding surface.
- *Spots colored by density (slow)* is a binary plot in which each spot is displayed with the color of the corresponding pixel on a density map.

The density map is quick to generate, whereas the second diagram can take up to several minutes to be displayed, depending on the number of points to be displayed. This plot can also slow down significantly the BINARY module.

The displayed density diagram can be eliminated by clicking on the close button displayed in the top-left corner of the plot. It is also possible to export a density plot by clicking the button *Export* located near the *Density* button.

3.11.2.2 Identify pixels (and show their distribution)

Identify Pixels (button) allows the position of pixels within a specific range of composition to be displayed on the map. This function includes the following modes that can be selected in the menu (e.g. *Single group: quick (rectangle)* is selected in Fig. 3.53):

- *Single group: quick (rectangle)* uses a rectangle defined by two points; one group

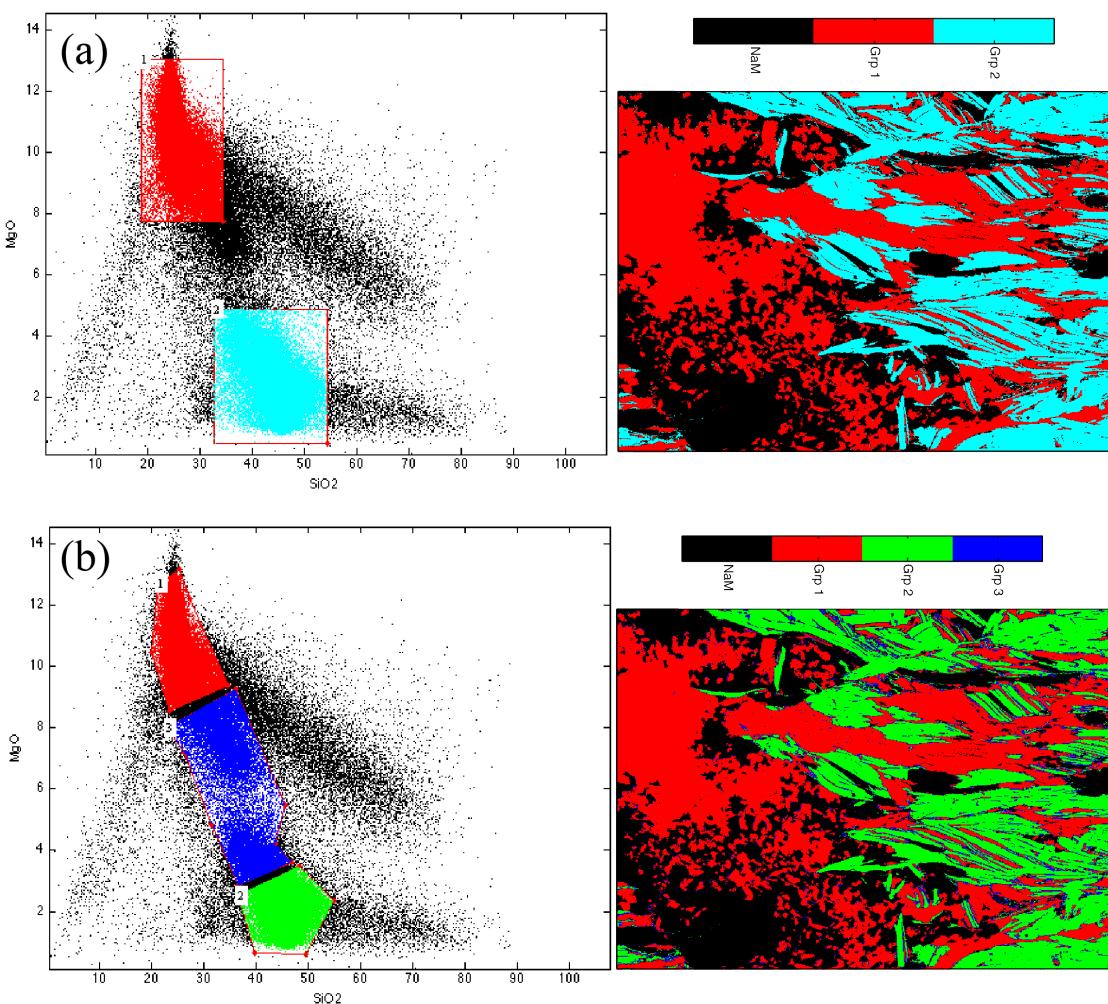


Figure 3.54 – Multi-Groups functions in the Binary module. (a) Quick (rectangle) using 2 groups: chlorite (red) and phengite (blue). (b) Free shape using 3 groups: chlorite (red), phengite (green) and the mixing pixels between them (blue)

- *Single group: free shape* uses a polygone defined by n points (right-clicking to validate); one group
- *Multi-group: quick (rectangle)* uses several rectangles, each of them defined by two points (right-clicking to validate); several groups
- *Multi-group: free shape* uses several polygones, each of them defined by n_i points (right-clicking to validate each group); several groups. A menu is displayed once each group is selected asking if an additional group should be added or not.

An example of the Multi-group function is shown in Figure 3.54.

Note: Details such as the relative proportion of each group are displayed in a small window above the map.

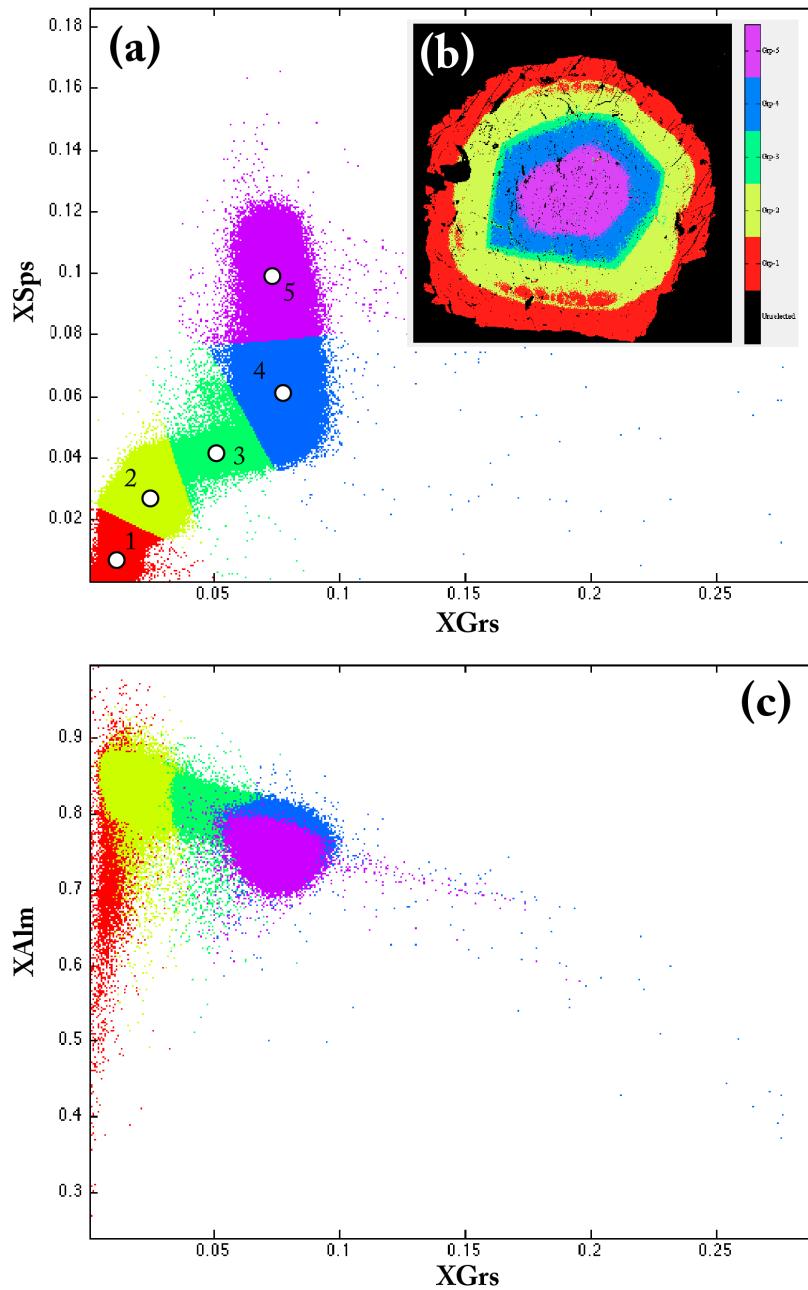


Figure 3.55 – k -means clustering in the Binary module. (a) clustering in the system $[X_{Grs}, X_{Sps}]$ using 5 clusters (see the spots for the initial centroids) and the method sqEuclidian. (b) map showing the spatial distribution of each final cluster. (c) The clusters are plotted in a binary diagram X_{Alm} vs X_{Grs} . Note that the cluster distribution was computed in a different binary system, it allows possible relationships (or absence of relationships) to be identified. In this example, the groups 4 and 5 have similar compositions in Fe (X_{Alm}) and Ca (X_{Grs})

3.11.2.3 K-means clustering in the Binary module

K-means (button) performs k-means clustering to partition the compositions of the selected binary system into k clusters. The other elements are not considered during this classification. The k initial centroids are defined by clicking on the figure. Any click outside the axes (or alternatively right-clicking) validates the selection and generate a mask file.

The k-means algorithm computes centroid clusters based on one of the following method (can be selected in the menu *method*):

- *sqEuclidean* - Squared Euclidean distance (recommended). Each centroid is the mean of the points in that cluster.
- *cityblock* - Sum of absolute differences. Each centroid is the component-wise median of the points in that cluster.
- *cosine* - One minus the cosine of the included angle between points (treated as vectors). Each centroid is the mean of the points in that cluster, after normalizing those points to unit Euclidean length.

Clustering large datasets might take time. A window is displayed when the k-means function is working; please wait until the waiting window disappears before using the *Binary module*.

K-means (Maskfile menu) lists the mask files generated by the *k-mean function* in the Binary module. It is possible to select a mask file to display the corresponding clusters.

Plot (button) this button allows the original binary diagram in which the clusters of the selected mask file were generated to be plotted. This button is only available when a mask file is selected.

Map (button) displays a map showing the spatial distribution of each cluster of the selected mask file.

3.11.3 TriPlot Module

TRIPLOT is an additional user interface included in the XMAPTOOLS' package. TRIPLOT is accessible in any workspace via the main menu *Modules* and *Ternary* (see section 3.2.5) provided that at least three maps are available. Similarly to BINARY, this module is independent from the the main XMAPTOOLS window; both can be used at the same time.

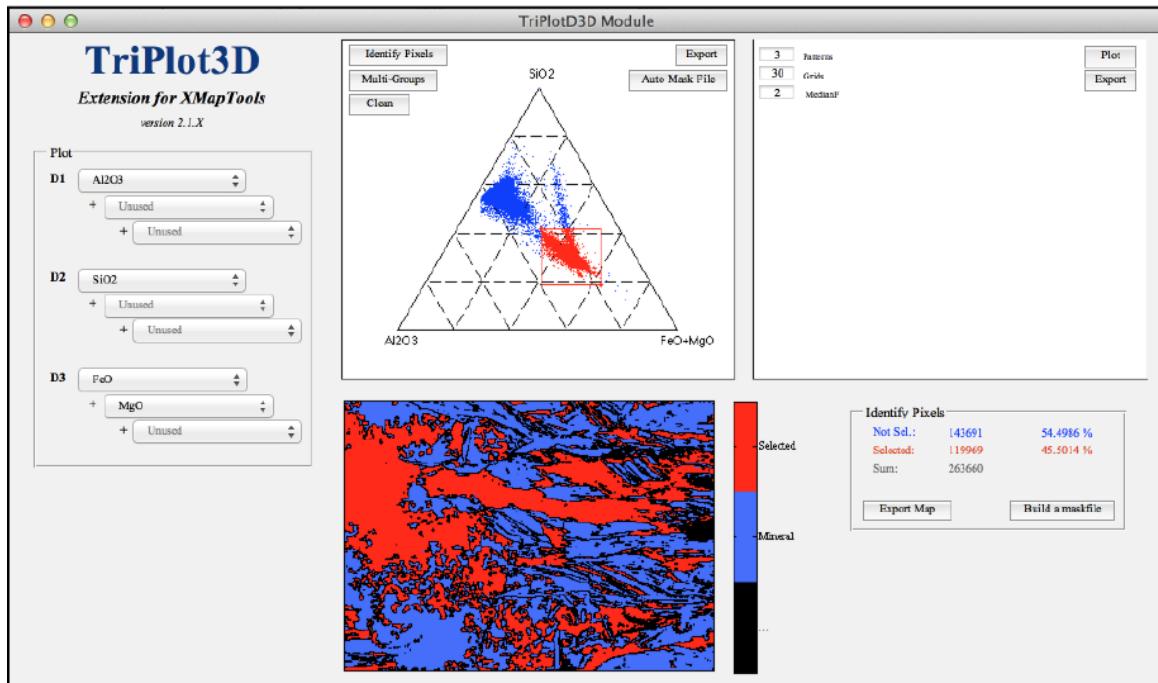
The functions available in TRIPLOT (Fig. 3.56) are similar to those described above for the BINARY module. This section of the user-guide as well as the module will be improved in a future update.

3.11.4 RGB Module

RGB is an additional user interface included in the XMAPTOOLS' package generating three channels composite images (RGB for red, green and blue) from maps. RGB is accessible in any workspace via the main menu *Modules* and *RGB* (see section 3.2.5) provided that at least three maps are available. In figure 3.57, a garnet from Peaked Hill shear zone, Reynolds Range, central Australia mapped by LA-ICP-MS is used to illustrate the use of the *RGB module* (information and sample description are available in [Raimondo et al. 2017](#)).

The *variables for RGB spot* window (Fig. 3.57) contains the menus for selecting the three maps to be combined as a single RGB map. The *auto-contrat* buttons works in the same way as those available

(a)



(b)

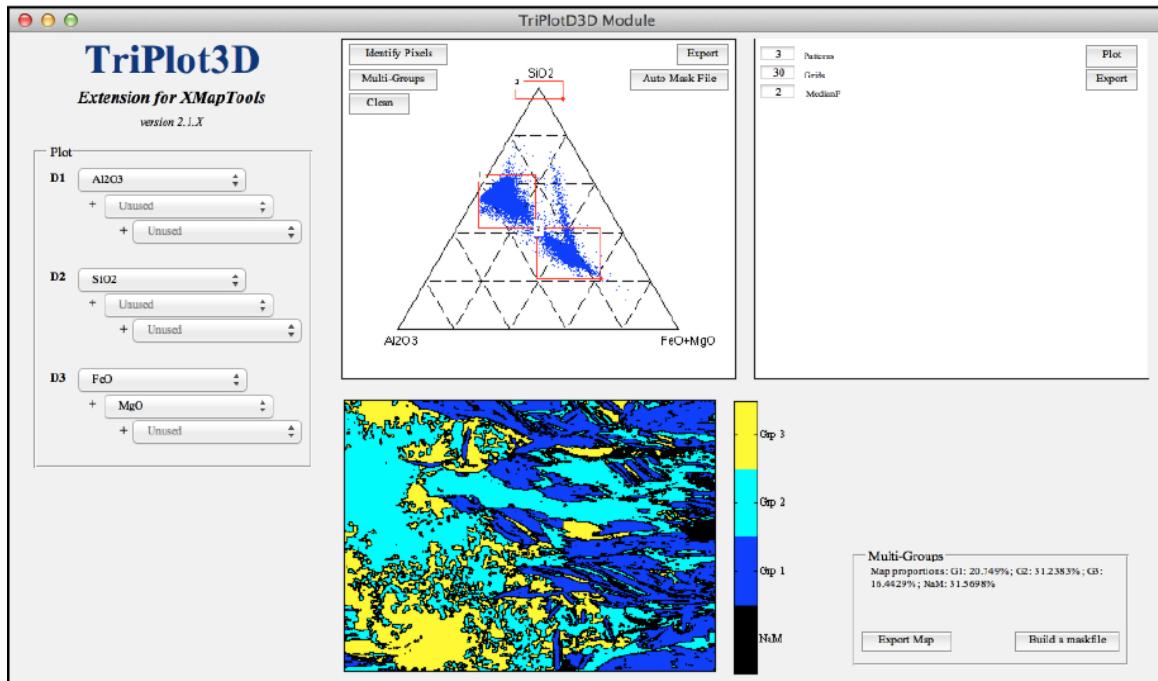


Figure 3.56 – Chemical modules TriPlot (a) identify pixels, (b) multi-group

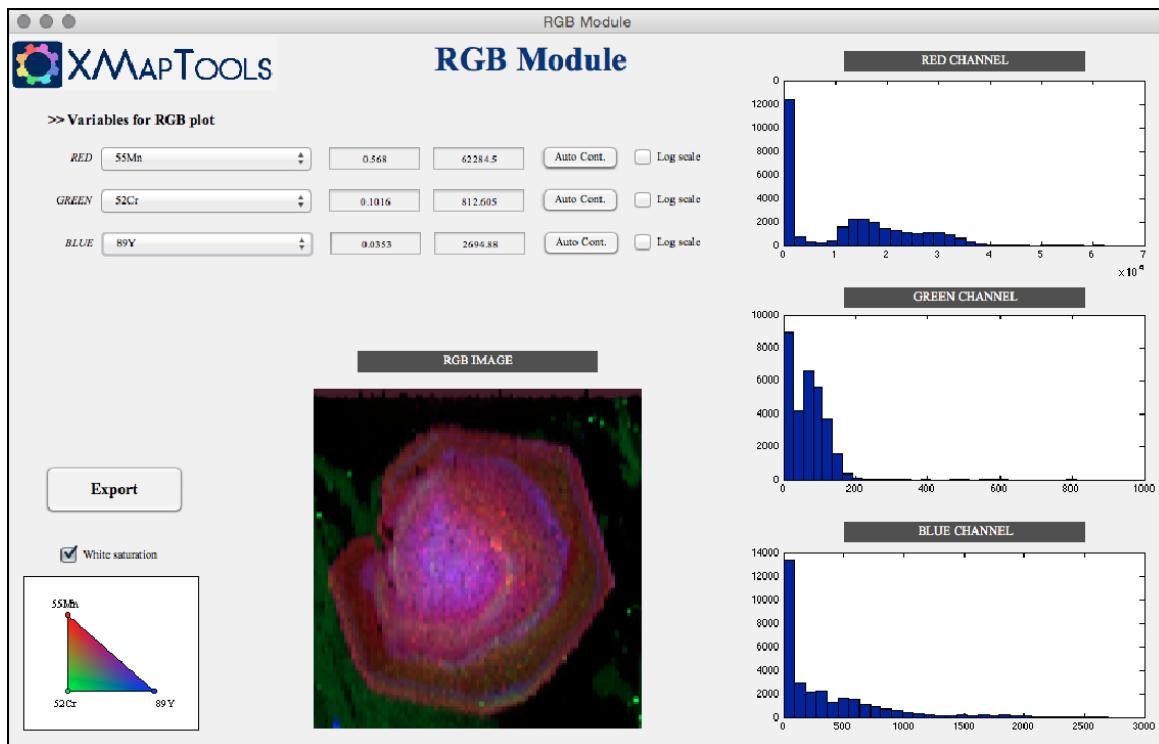


Figure 3.57 – Chemical modules RGB (see text for details)

in XMAPTOOLS. If an element is selected again using the corresponding menu, the program restores the original limits, i.e. the *min* and *max* non-zero values of the selected map. The button *Log scale* allows to use a log scale in the corresponding histogram figure.

The *RGB image* is updated and plotted with a special colorbar. The button *export* allows the figure to be opened in a new MATLAB figure window (check the description of [B5102] to see how to save the figures).

If the contrasts of some of the channels are restricted to narrow ranges of composition, some pixels of the image can turn white. In order to avoid this, there is an option available below the *export* button.

3.11.5 Generator Module

GENERATOR is an additional user interface included in the XMAPTOOLS' package that can be used to generate new maps (i.e. variables) from existing maps in any workspace (*X-ray*, *Quanti* or *Results*). The GENERATOR is accessible via the main menu *Modules* and *Generator* (see section 3.2.5). Once the new maps are generated they can be added to XMAPTOOLS. Note that the main XMAPTOOLS window is frozen when the GENERATOR module is in use. Close the GENERATOR window to unfreeze XMAPTOOLS.

3.11.5.1 Code format

Standard MATLAB code format is used by the GENERATOR to combine existing maps and create new variables. The format is:

$$[Output] = [Operation] \quad (3.27)$$

with:

- [*Output*] the name of the new map. This name is not required to be a valid variable name, in this case XMAPTOOLS will generate a valid variable name (see the example below). Note that for several reasons the name cannot have any space in it.
- [*Operation*], an arithmetic operation defined by the rules of linear algebra or array arithmetics. The operation can contain empty spaces between variables digits and operators. Array operators (with the period character ".") must be used if maps are divided or multiplied by each other. Use of semicolon at the end of the instruction is optional.

A+B	% addition
A-B	% subtraction
A.*B	% Element-wise multiplication
A./B	% Element-wise division
A.^B	% Element-wise power

Code 3.22 – Array arithmetic commands in MATLAB using the period character “.”

Additional information regarding the MATLAB operators can be found at https://www.mathworks.com/help/matlab/matlab_prog/matlab-operators-and-special-characters.html

Example 1 - Let’s consider two compositional maps with identical size, Fe and Mg expressed in atom per formula unit. The ratio map Mg divided by Fe can be obtained using the following code:

$$Fe/Mg = Fe./Mg; \quad (3.28)$$

Note that element-wise division is used “.” in order to divide the two arrays element by element. The module generates a new map with the display name *Fe/Mg*, the corresponding variable name is *Fe0x2FMg*. Indeed / cannot be used in variables name and the GENERATOR needs to create a valid name to be used in further operations.

Example 2 - Let’s consider the same maps Fe and Mg. The Mg# map can be obtained using the following code:

$$Mg\# = (Mg./ (Mg + Fe)) * 100 \quad (3.29)$$

Note that element-wise division is again used “.” whereas the multiplication is arithmetic (*) as an array is multiplied by a number. In this example, all the elements are multiplied by 100. The GENERATOR module generates a new map with the display name *Mg#*, the corresponding variable name is *Mg0x23*. Indeed # cannot be used in variable names.

Example 3 - Let’s consider two compositional maps with identical sizes showing the concentration of ^{175}Lu and ^{147}Sm in garnet, expressed in ppm. The average slope of the HREE normalized to chondrite can be obtained using the following code:

$$HREE_slope = (x175Lu/0.0381)./(x147Sm/0.231) \quad (3.30)$$

Note that the valid variable name of the map $175Lu$ is *x175Lu* as a variable name always starts with a letter. This conversion is automatically done by XMAPTOOLS: any map name starting with a number will have a variable name starting with *x*. Element-wise division is used “.” to divide the two normalized maps, while each normalization is performed with arithmetic division. The GENERATOR module generates a new map with the display name *LREE_slope*. In this case the variable name is identical.

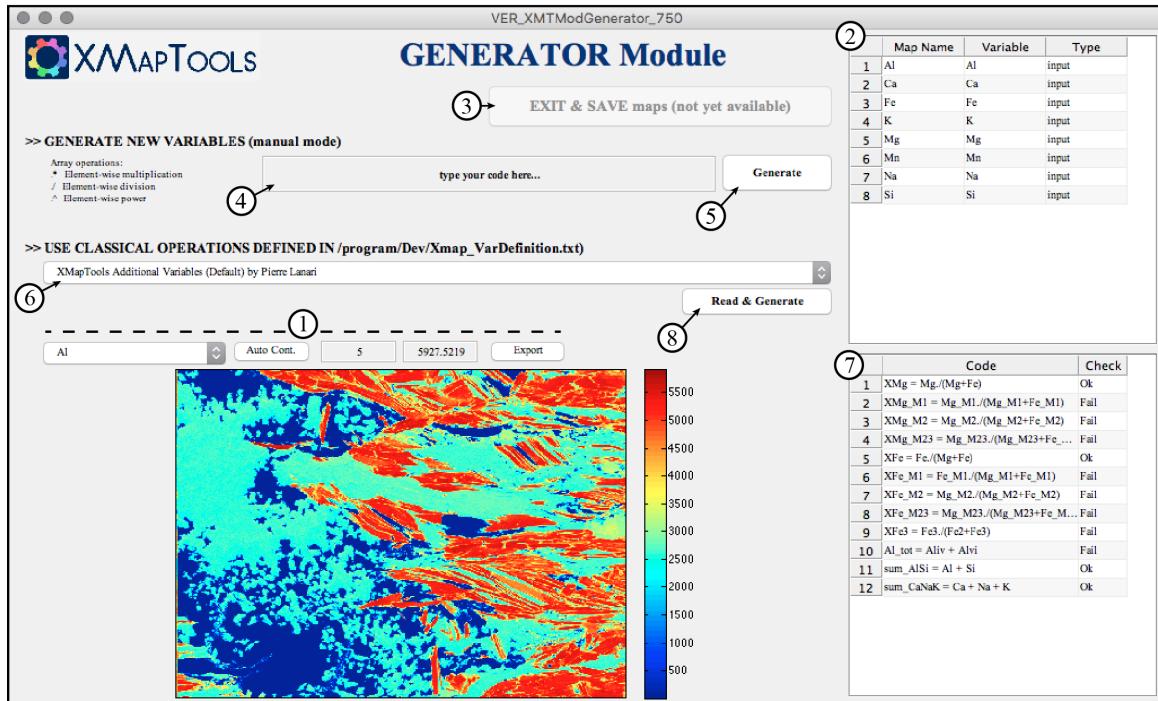
Additional information regarding the variable names can be found at https://www.mathworks.com/help/matlab/matlab_prog/variable-names.html

3.11.5.2 Graphical User Interface of the Generator module

The interface of the GENERATOR module is shown in Figure 3.58. The description is divided into two parts:

Before to generate new maps:

(a)



(b)

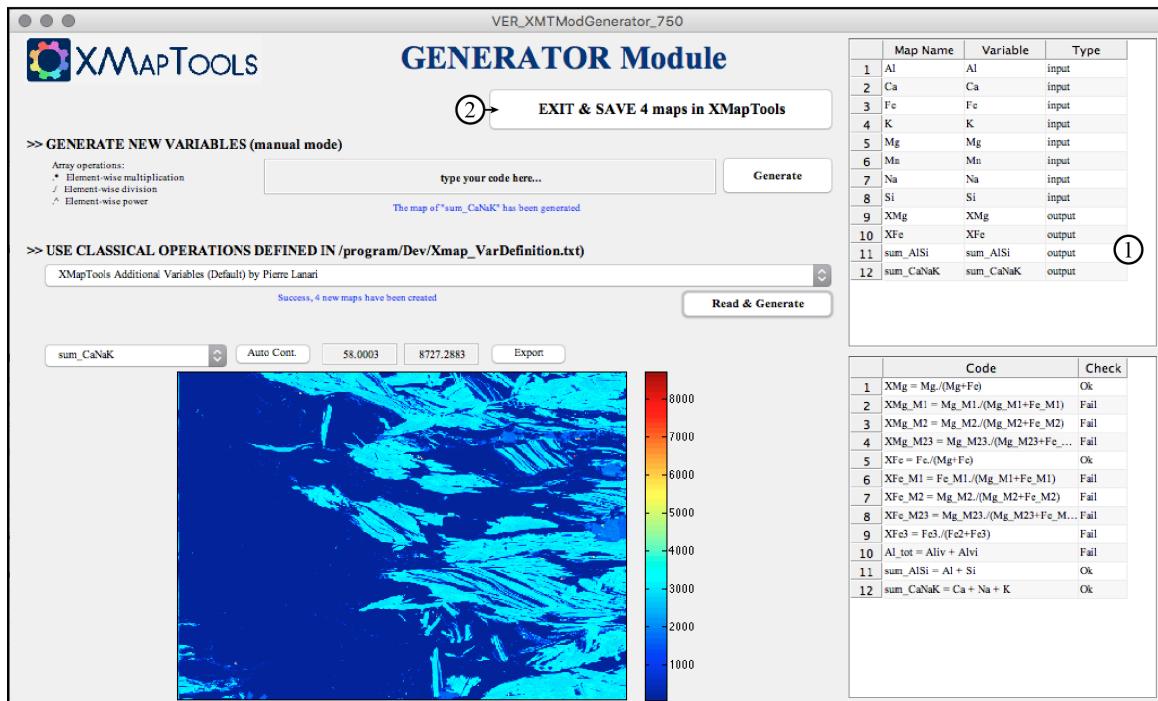


Figure 3.58 – GENERATOR module graphical user interface (a) before to generate a new map; (b) after generating new maps

[1] Plot options (Fig. 3.58a) The menu can be used to select the map to display. The function *Auto Cont.* automatically adjusts the colorbar limits (see [B5101] for details). Select a map in the menu to reset the display to min and max values. The *Min* and *Max* fields allows the colorbar limits to be manually adjusted (note that *Max* must be greater than *Min*). The function *export* opens the displayed map in new MATLAB windows (see [B5102] for details).

[2] List of maps (Fig. 3.58a) This table shows the maps and the corresponding variable names available in the GENERATOR module. If the map name is a valid variable name, this name is used as variable name (default). Map type are:

- *Input*: map sent by the main XMAPTOOLS program to the GENERATOR module; cannot be modified. These maps are not exported when the GENERATOR module is closed.
- *Output*: map created by the GENERATOR module that is transferred to the main XMAPTOOLS program when the GENERATOR module is closed using the button *Exit and Save maps*.

[3] Exit and Save maps (Fig. 3.58a) This button is available only when new maps have been created. To close the interface and unfreeze XMAPTOOLS, use the *close* button in the top left corner.

[4] Code input (Fig. 3.58a) Input for the code that will be evaluated to generate new variables (maps).

[5] Generate (Fig. 3.58a) Button to generate the map using the code given in (4).

[6] Classical operations (Fig. 3.58a) Menu listing the type of classical operations available in XMAPTOOLS. Each menu item correspond to a block of operations. The input file containing the bloc definitions is available in *Program/Dev/Xmap_VarDefinition.txt*.

[7] List of operation (Fig. 3.58a) Table showing the operations available in the block selected in the menu (see step 6). The results of the test function are listed in the the column *check*:

- *Ok*: All the maps are available to create this new variable and the variable does not already exist.
- *Fail*: At least one of the map used in the code is missing; this variable cannot be created.

[8] Read and Generate (Fig. 3.58a) This function create all the variables of the block selected in (6) that passed the test (see column check in (7)).

Once maps have been generated:

[1] List of maps (Fig. 3.58b) The new maps are added to the table. The corresponding variables can be used; the maps can be sent back to XMAPTOOLS (see below).

[2] Exit and Save maps (Fig. 3.58a) This button is available only when new maps have been generated. To close the GENERATORinterface and unfreeze XMAPTOOLS without saving the new maps, use the *close* button in the top left corner.

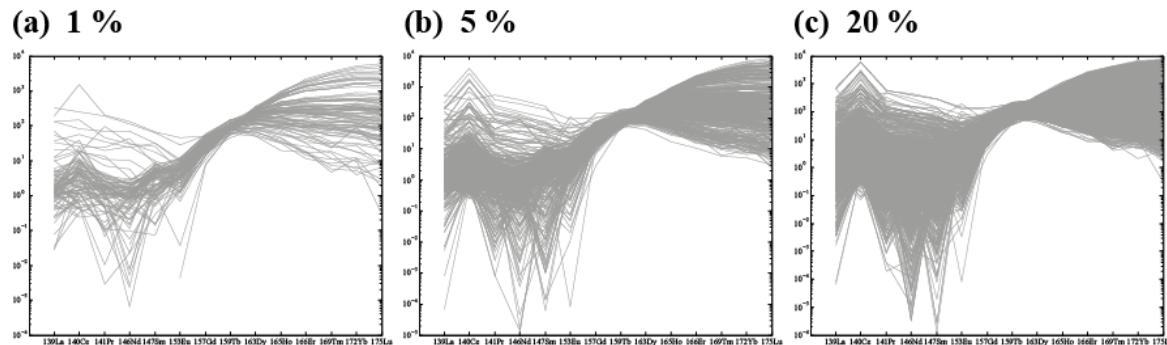


Figure 3.59 – *Spider diagram of REE in garnet using (a) 1%, (b) 5% and (c) 20% of the pixels of the map. See Fig. 3.60 for x labels.*

3.11.6 Spider Module

The SPIDER module (Fig. 3.48) generates spider diagrams of trace element maps. The SPIDER module is available in the workspace *Results* via the menu *Modules* and *Spider* (see section 3.2.5), provided that trace element maps of isotopes are available (see §2.7.2). The list of the isotopes and the reference compositions used in the selected normalization are shown in the table (see 1 in Fig. 3.61)

To compute and display a spider diagram, it is necessary to:

- Select a normalization in the normalization menu (2 in Fig. 3.61)
- Select a color scheme in the color menu (3 in Fig. 3.61)
- Select pixels of the map using the sampling functions: (1) All; (2) Spot(s); (3) Line; (4) Areas (see below)

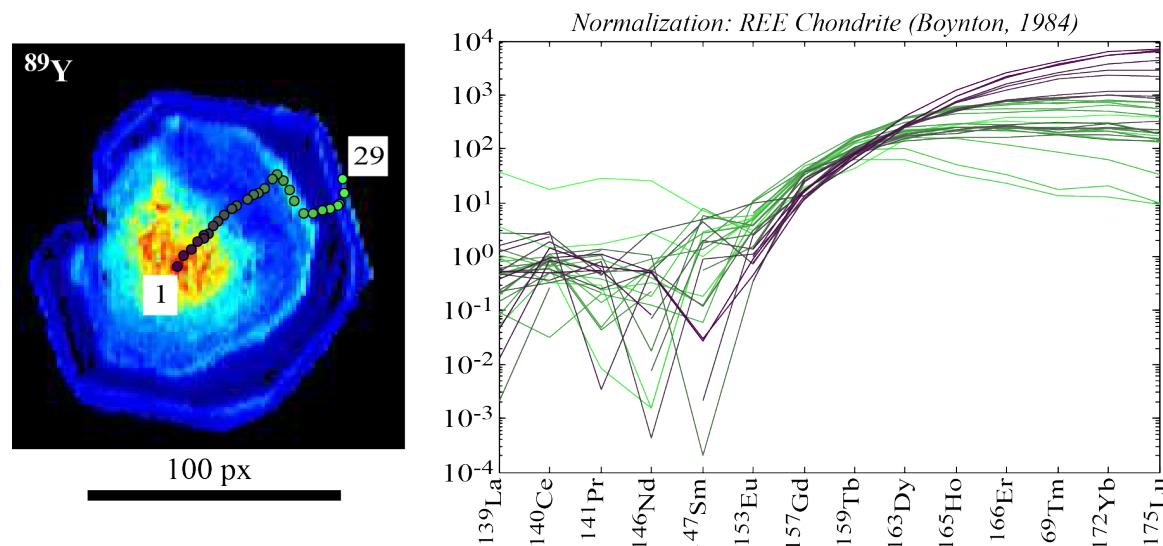


Figure 3.60 – *Spider diagram of REE in garnet using the sampling method: spot analyses. Map: ^{89}Y (red high concentration, blue low concentration, in ppm, see Fig. 3.61 for color scheme)*

3.11.6.1 Sampling functions

[1] All pixels: The button *All pixels* enables activating the display of a given fraction of the total number of pixels displayed in the field below (in %). The pixels are randomly selected. Any new call of the function (made by pressing the button or changing the number of the fraction of pixels) plots a new selection of pixels. An example of pixel fractions of 1%, 5% and 20% are reported in figure 3.59. Note that in this example, there is no significant difference between 20% and 100% because of the large number of pixels used.

[2] Spot(s): The button *Spot(s)* enables selecting pixels to plot in the spider diagram. As usual in XMAPTOOLS, use right-clicking to leave the selection mode. An example of selection of 20 spots from garnet core to the rim is provided in figure 3.60. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram.

[3] Line: The button *Line* enables selecting two pixels and plotting the composition of the pixels along the line. An example of selection of line from garnet core to the rim is provided in figure 3.61. Note that the colors of the first and last spots correspond to the colors of the lines in the spider diagram.

[4] Area(s): The button *Areas* enables selecting one or more area(s) and plotting the corresponding average compositions of the pixels. An example of selection of three areas from garnet core to the rim is provided in figure 3.62. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram. In this case the standard deviation (1σ) envelopes are displayed together with the average. This mode can be activated using the option below the button *Area(s)*. The envelope is not displayed if $(mean - std) < 0$ or $(mean - std) = 0$.

The curves are plotted using the color scheme defined in the corresponding menu (see below).

The map and the spider diagram are cleaned every time a new sampling tool is used. The option *hold on* (see Fig. 3.61) can be selected in order to add a new set of curves onto an existing spider diagram.

3.11.6.2 Figure and colors

The map can be managed using the following functions (see 5 in Fig. 3.48):

- *Plot* menu to select the map to be displayed in the figure window
- *Auto Cont.* button to automatically adjust the colorbar limits (see [B5101] for details)
- *Min and Max* values to manually adjust the colorbar limits (note that *Max* must be greater than *Min*)
- *Export* this function allows the map and spider diagrams to be exported in new MATLAB windows (see [B5102] for details).

The following color schemes are available to draw curves using the spot and line modes:

- *Original* violet to green (Fig. 3.63a)
- *Bred* blue to red (Fig. 3.63b)
- *Greyl* green to yellow (Fig. 3.63c)

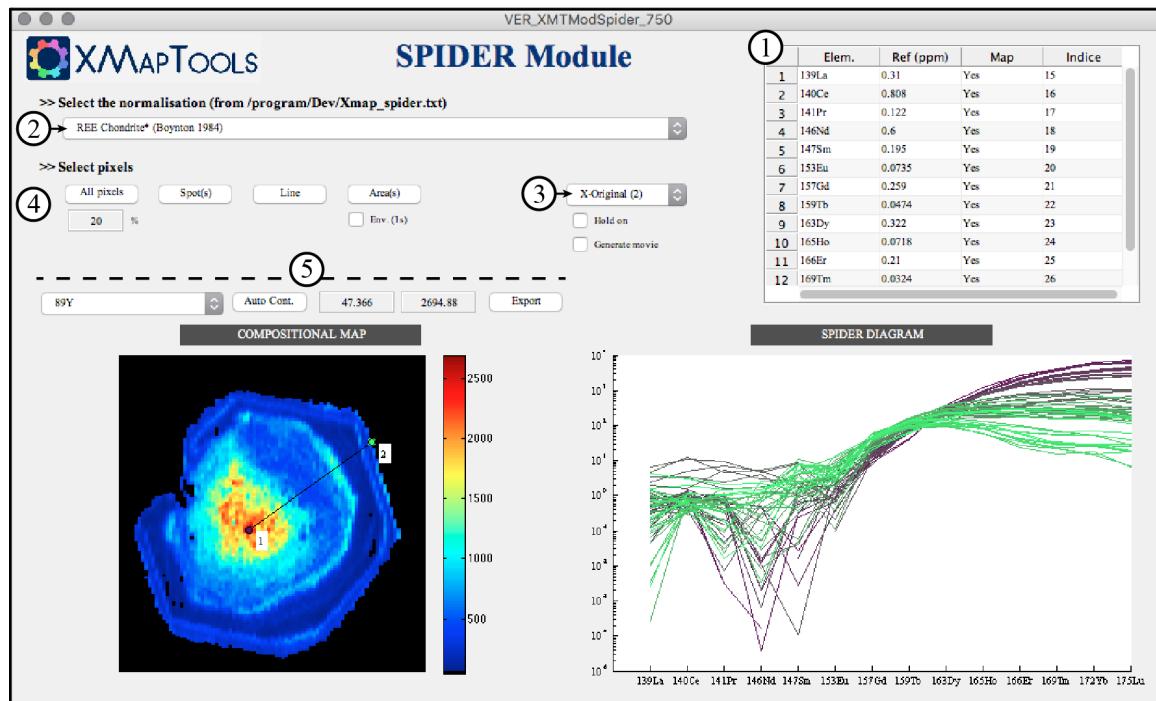


Figure 3.61 – Spider diagram module; sampling mode: line.

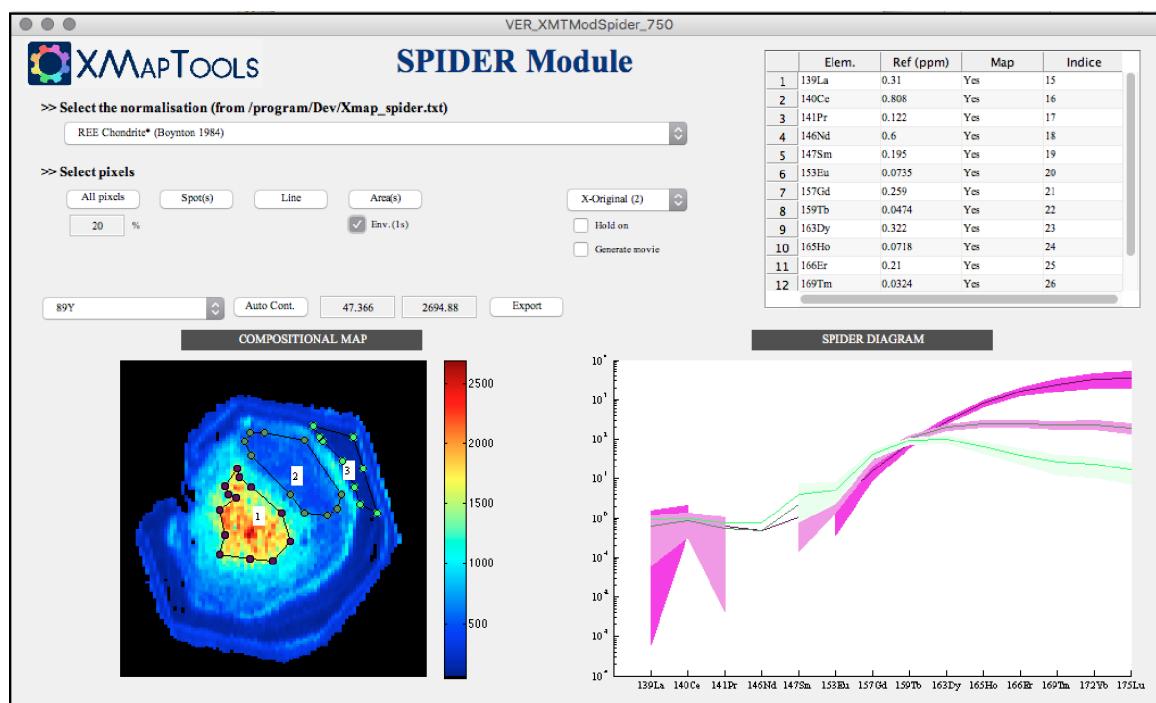


Figure 3.62 – Spider diagram module; sampling mode: area(s)

- *Pinor* pink to orange (Fig. 3.63d)
- *Shicy* braun to green to blue (Fig. 3.63e)
- *Jet (4)* blue to green to orange to red (Fig. 3.63f)

Note: it is possible to change the active color scheme between each plot.

3.11.6.3 Create a movie with the Spider diagram

If the sampling modes *spot* or *line* are used, it is possible to generate and save a video of the spider diagram. The steps to follow are:

- Select your favourite color scheme using the color menu (e.g. X-Bred (2) in Fig. 3.64a).
- Unactivate the option *hold on*
- Activate the option *Generate movie*: two new fields appear (see Fig. 3.64a)
- Set the duration (in second)
- Set the quality (in %, generally between 50 % and 100 %)
- Select your sampling mode (*spot* or *line*) and click on the corresponding button
- Define a trail of spots or a line (see above).
- A new window opens; resize the window and press the button *RESIZE THE FIGURE AND CLICK HERE* to continue and to generate the movie (Fig. 3.64b)
- The frames are generated (note that the duration depends on your computer and on the number of points; it is independent of the movie duration) and this figure disappears.
- The video *myfile.avi* is saved in your working directory. Rename this file. Note that if a file with the same name already exists it will be automatically replaced.

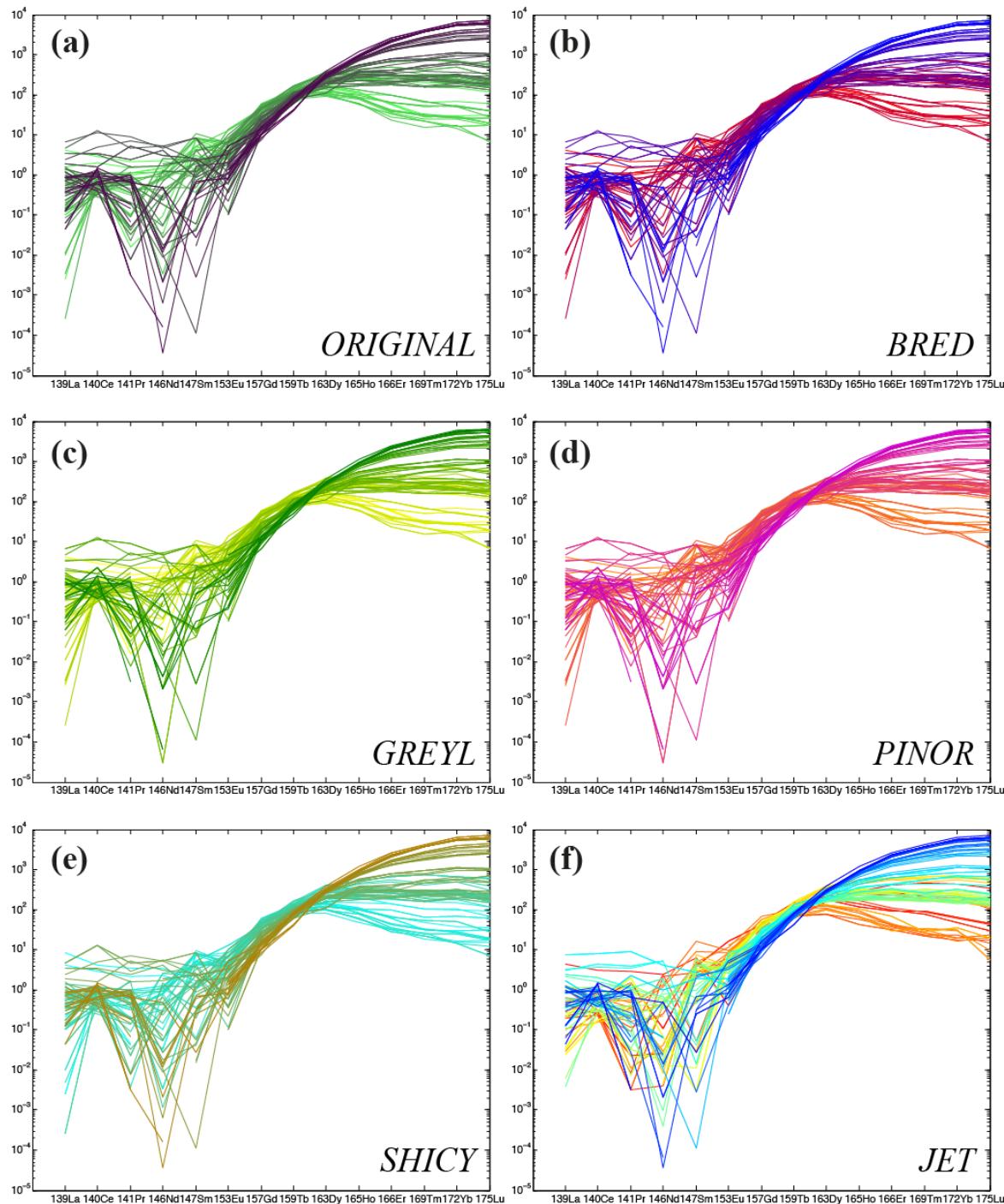


Figure 3.63 – Color schemes available in the SPIDER module

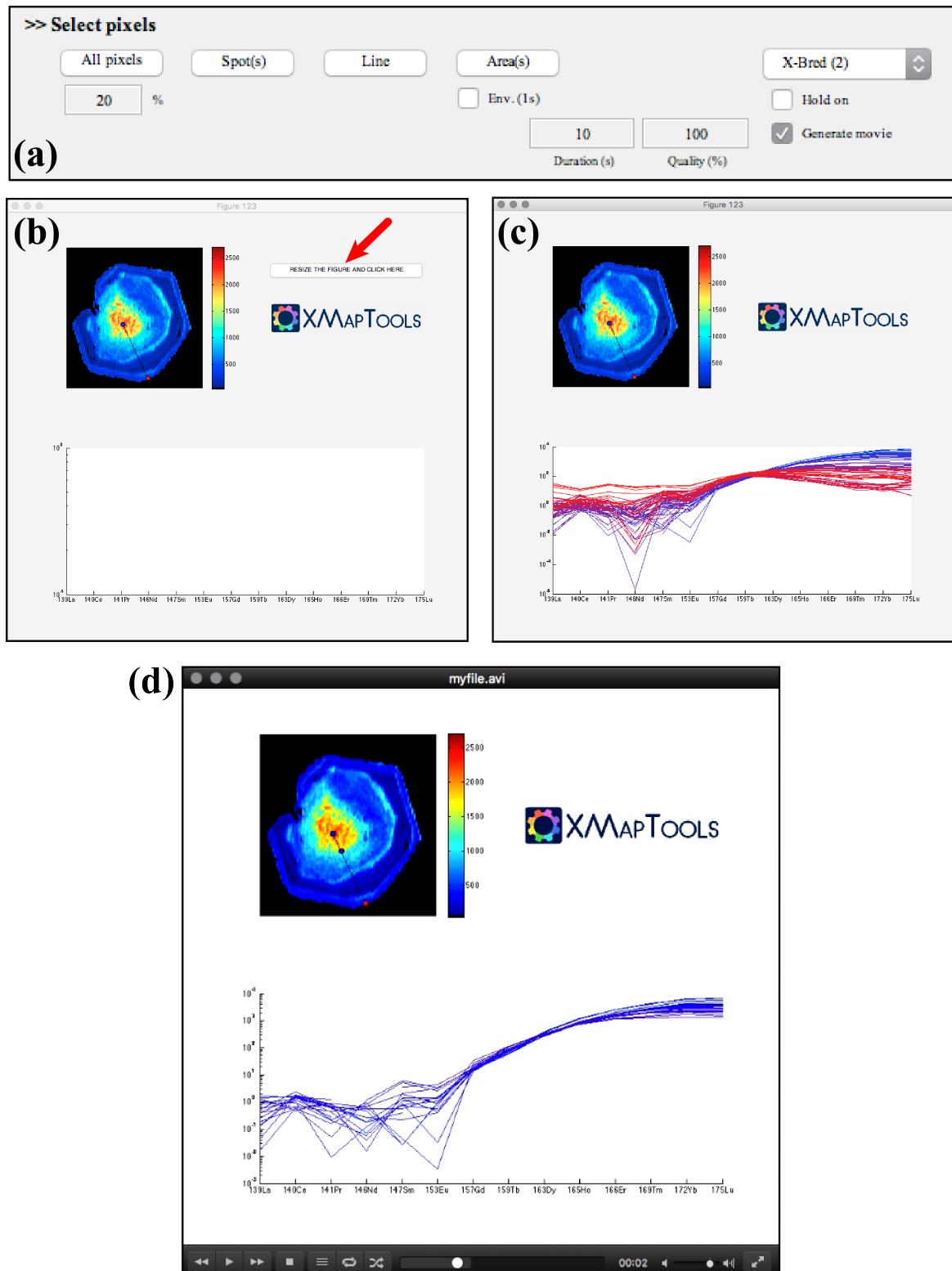


Figure 3.64 – Video mode of the SPIDER module. (a) The option Generate movie is active and it is possible to edit the duration of the video in second and the quality (between 10 and 100 %). (b) Figure used to generate the movie; this figure can be resized before to start recording the movie. (c) live mode. (e) video (myfile.avi)

4

ADDITIONAL TIPS AND ADVANCED FUNCTIONALITIES

4.1 XMAPTOOLS AND NEGATIVE NUMBERS

In theory, a compositional map should not have any pixel with a negative value. Consequently, the pixels having negative values are generally ignored and/or replaced by zeros in *XMapTools* (e.g. during the standardization). Pixel with negative values are not shown when a map is displayed in the main window because the functions setting the colorbar range such as the auto contrast [B5101] are designed in a way that pixels with negative values are ignored.

However, it is possible to force the program to show negative values by setting the displayed range manually in [C5101].

Example: The amount of vacancies on the A-site of phengite has been calculated using the *Generatore Module* and the formula: $Vac = 1 - (Na_A + K_A)$. This calculation will generate pixels with negative values if the sum of $Na + K$ is greater than one; this can be the case for misclassified pixels. The results are shown in Figure 4.1:

- If the vacancy map is selected for display, the limits of the colorbar are automatically set considering only the pixels with positive values (see Fig. 4.1a). All the pixels having a negative value are shown with the first (bottom) color of the colorbar.
- If the lower limit is changed manually to force the display of pixels with negative values (e.g. -0.5 in Fig. 4.1b), these pixels appear on the map (see the black arrows). However the pixels that do not belong to phengite are have a color that correspond to a value of zero and are no longer plotted in black.

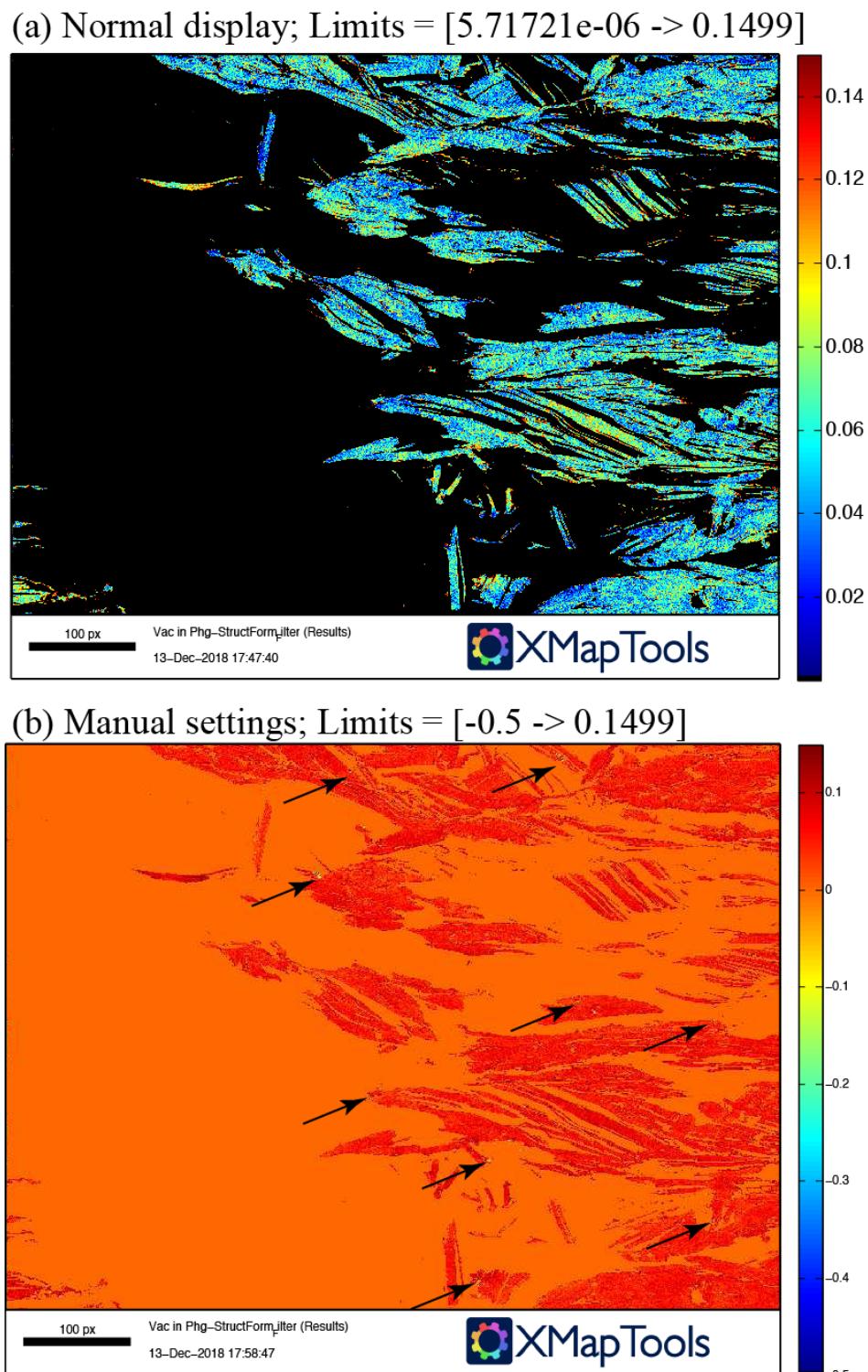


Figure 4.1 – Example of image with negative values that are (1) ignored by the automatic display; (2) visible if the lower limit of the displayed values is set manually

4.2 EXPORT MASK IMAGES WITH PERSONALIZED COLORS

It is possible to use the figure tools of MATLAB to edit the colors of the mask image.

[1] Export a mask image (Fig. 7.1-1) using the button  The button *export mask image* in the workspace *Xray*. An example of mask image is reported in figure 4.2.

[2] Functions are available and can be activated using the icons available below the menu. Press the last one *Show plot tools and Dock figure*. MATLAB turns the figure window into editing mode (Fig. 4.3).

[3] With pop-up menu color map, select *Custom*. A new window *Colormap editor* opens (Fig. 4.4) and you can select the colors for each mineral by pressing on the color arrows (see examples in Fig. 4.4).

[4] When new colors are defined, it the figure can be saved using the figure menu and the function *Save as...*

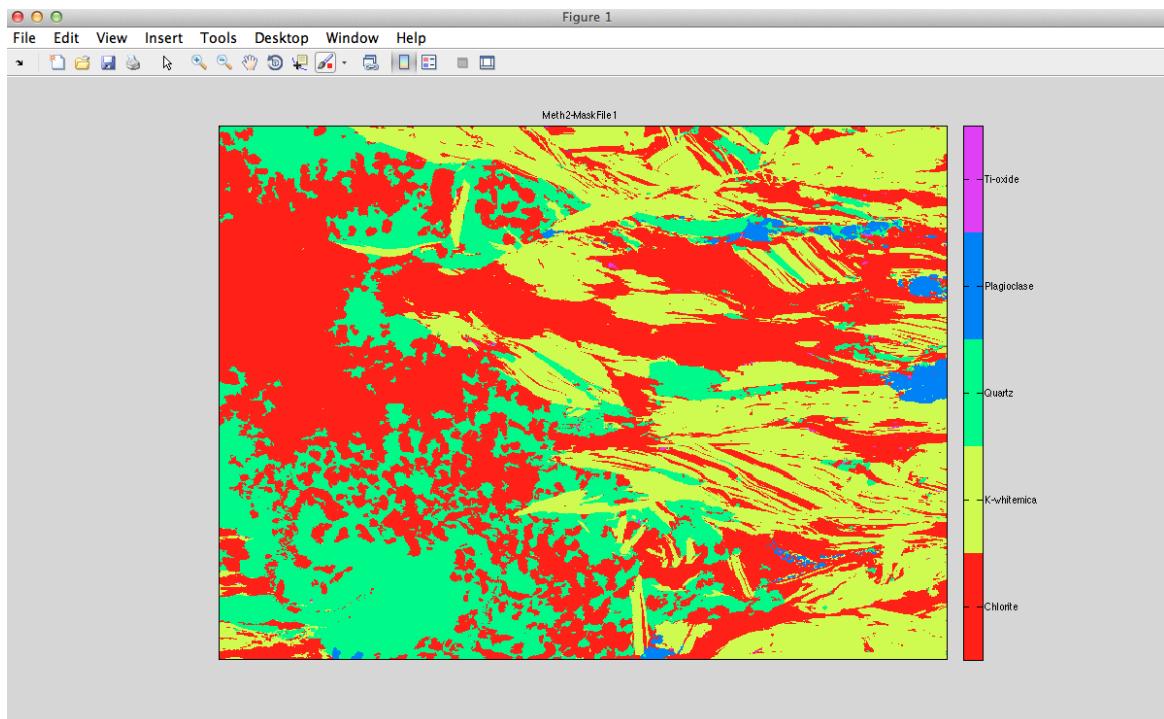


Figure 4.2 – Mask image exported using the function *export mask image* (see text)

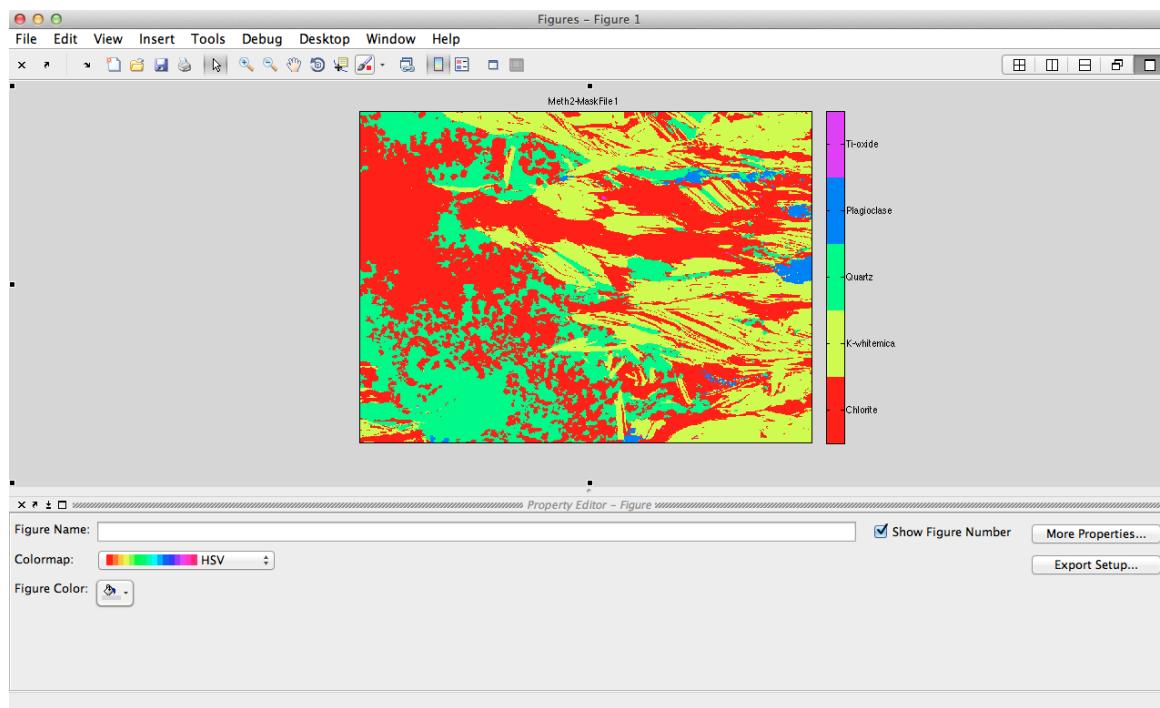


Figure 4.3 – Mask-image with the Figure editor

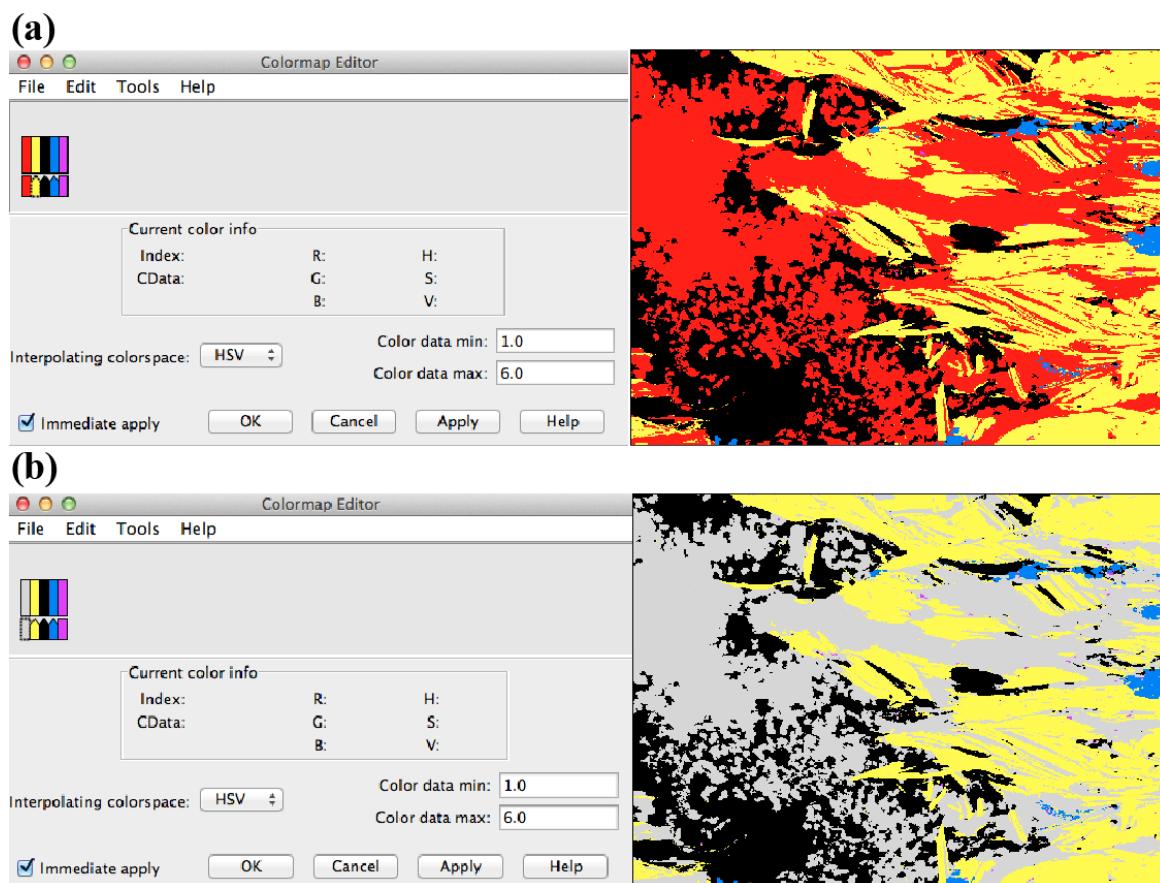


Figure 4.4 – Colormap Editor with the new colors

4.3 USER'S EXTERNAL FUNCTIONS

The repertory *UserFiles* located in the main setup directory can be used to add external functions to XMAPTOOLS. It is crucial to store the user's files in this directory which is not affected by automatic updates of XMapTools. All the files stored in the */program* directory are automatically deleted during updates.

In this section, I explain the procedure to add a personalized *ListFunction.txt* file (called *ListFunctions_USER.txt*). In a second part, the procedure to generate your own external functions and to add them to XMAPTOOLS is also described.

4.3.1 List of user's external functions (file *ListFunctions_USER.txt*)

All the external functions provided with XMAPTOOLS are listed in the file *ListFunctions.txt* which is located in the setup directory (*/program*). This file is used by XMapTools to define all the options required to run an external function. Each line corresponds to one function and provides the following information:

- **Function type** that correspond to the function category. Possible indexes are: [1] Structural formulae; [2] P, T and P-T map mode; [3] P, T and P-T spot mode; [4] General Functions; [5] Density functions.
- **Mineral(s)** that correspond to the name(s) of mineral phase(s) for which the function may be applied. For example, to add a function that calculate the structural formulae of chlorite, the code line must includes the keyword *Chlorite* in order to indicate to XMapTools that this function belong to the category *Chlorite* within the type: *Structural formulae*. If a different name is used such as *ChloriteDT*, a new category will be automatically generated.
- **Name** is the name of the function that is displayed in XMAPTOOLS.
- **Function name** is the name of the function without the extension. External functions are MATLAB functions files (*.m). For example, the function name *StructFctChlorite* is reported for the file *StructFctChlorite.m*.
- **Output variables** is the list of output variable names.
- **Input variables** is the list of input variable names that are the names of the standardized maps generated by XMAPTOOLS. The oxide names available are: Na₂O, MgO, Al₂O₃, SiO₂, P₂O₅, SO₂, Cl₂O, K₂O, CaO, TiO₂, V₂O₅, Cr₂O₃, MnO, FeO, CoO, NiO, CuO, ZnO, ZrO₂, AgO, CdO, SnO₂, Ce₂O₃, As₂O₅, Sb₂O₃, Cs₂O, La₂O₃, Nd₂O₃, PbO, SrO, ThO₂, UO₂, Y₂O₃, Sm₂O₃, Gd₂O₃, Dy₂O₃, Pr₂O₃. The metalloids names available are: Fe_ms, Cu_ms.
- **External variables** (optional for function of type [3]) are variables that can be edited by the user at each iteration. Such variables must be provided together with a default value, for example: *PressureKbar(10)*.

All these options are separated by the delimiter >.

This file *ListFunctions.txt* should never be edited by any user. If additional functions are needed, the following procedure can be applied:

- [1] Close XMAPTOOLS and go to the setup directory (*/program*).
- [2] Copy the file *ListFunctions.txt* into the repertory */UserFiles*.

(a) XMapTools default function

```
Loading ... (XMapTools paths) ... Ok
Loading ... (User files path) ... Ok
Loading ... (Setting GUI parameters) ... Ok
Loading ... (Help texts) ... Ok
Loading ... (External functions: ListFunctions.txt [default]) ... Ok
```

(b) User's function (located in /UserFiles)

```
Loading ... (XMapTools paths) ... Ok
Loading ... (User files path) ... Ok
Loading ... (Setting GUI parameters) ... Ok
Loading ... (Help texts) ... Ok
Loading ... (External functions: ListFunctions_USER.txt [user file]) ... Ok

WARNING - You are not using the XMapTools default file ListFunction.txt (see above) !!!
```

Figure 4.5 – *XMapTools info displayed in the command window at the launching of the program. (a) The file ListFunctions_USER.txt has not been detected in the repertory UserFuntons and the default file is loaded and a warning message displayed. (b) The file ListFunctions_USER.txt exists and has been loaded.*

[3] Rename *ListFunctions.txt* as *ListFunctions_USER.txt* (case sensitive).

[4] Come back to the working directory and restart XMAPTOOLS. If the user's function is read by the program a warning message is displayed in the Command Window when XMapTools is launching (Fig. 4.5b). If this warning is not displayed (Fig. 4.5a) the default file has been loaded by the program. Check the external function name in */UserFiles* that must be *ListFunctions_USER.txt*.

4.3.2 Procedure to add an external function to XMAPTOOLS

The official external functions are provided in the directory *XMapTools/Program/Function/*. It is not recommended to edit a function located in this directory as changes will be lost during the automated updates.

4.3.2.1 Source-code of the external functions

The external functions in XMAPTOOLS are distributed as m-files. These script files contain the source-code and can be opened in MATLAB or in any other text editor.

4.3.2.2 Function definition file: *ListFunctions.txt*

Each external function is defined in the file *XMapTools/Program/ListFunctions.txt*. This file contains the basic definition needed for the function to communicate with XMAPTOOLS. Note that this file is read while XMAPTOOLS is opening. Changes are only applied after restart.

This file should not contain any empty row. Each row not starting with the comment symbol ! is interpreted as a function definition. Each definition contains the following blocks delimited by the symbol >. The general format is:

Code 4.1 – *Test functions*

Type > Mineral > Name > Function > Output > Input >

A complete description is provided in section 4.3. In the following we will create a user-function for calculating the sum of oxide.

- 1** Duplicate the file *XMapTools/Program>ListFunctions.txt* to *XMapTools/UserFiles/* and edit the file name to *ListFunctions_USER.txt*. If you start XMAPTOOLS the program will indicate that the USER file was read and display the following warning:

Code 4.2 – *Test functions*

```
Starting ... (External functions: ListFunctions_USER.txt [user file]) ... Done
WARNING - You are not using the XMapTools default file ListFunction.txt (see
above) !!!
```

Let's create a function that calculate a simple sum of oxide. The input parameters are the maps of oxide concentratiton (SiO_2 , TiO_2 , Al_2O_3 , FeO , MnO , MgO , CaO , Na_2O , K_2O) and the output parameters: $SumOxi$, $XSiO2$. The corresponding definition is:

Code 4.3 – *Test functions*

```
4>General>Gnrle-SumOxi>FctOxiSum>SumOxi XSiO2>SiO2 TiO2 Al2O3 FeO MnO MgO CaO
Na2O K2O>
```

4.3.2.3 Building the external function

The external function should have the following format (see example in insert ??):

- A function definition line (first row): `function [ListOutputVariables] = FunctionName(Data,handles)`. The list of output variables should match the order of the definition file. The input variable *Data* contains the maps as a single array (one column for one element) and *handles* contain the XMAPTOOLS variables to interact with the GUI
- A function description (second row and following ones until the row $n + 1$ does not start with %)
- Variable pre-allocation (mandatory if a loop is used as in example ??). Output variables are single row vectors! Note that each output variables must be sent back via single row vectors having the same number of columns as the number of rows in *Data*.
- Communication with the XMAPTOOLS' waiting bar using the function `XmapWaitBar(VALUE,handles)`; with VALUE ranging between 0 (display empty waiting bar) to 1 (full and hidden). DO NOT UPDATE the wait bar at every iteration or the function will be very slow. Use a counter as shown in the example ???. If you use the wait bar, the function should finish with the instruction `XmapWaitBar (1 , handles)`;
- Computation
- End the function code with the instruction `return`

Note that in the present case the external function can be written without using any loop (see example 4.5). This version does not require a waiting bar as the computation takes less than a second on a personal computer.

Code 4.4 – Function *FctOxiSum* calculating $\text{SumOxi} = \text{sum}(\text{oxide})$ and $X\text{SiO}_2 = \text{SiO}_2/\text{sum}(\text{Oxide})$

```

function [SumOxi,XSiO2] = FctOxiSum(Data,handles)
% -
% DESCRIPTION
% ...
%
% Variable pre-allocation
SumOxi = zeros(1,length(Data(:,1)));
XSiO2 = zeros(1,length(Data(:,1)));

% Activate the waiting bar in XMapTools
XmapWaitBar(0,handles);

hCompt = 1;
for i = 1:size(Data,1)

    % Update of the colorbar
    hCompt = hCompt+1;
    if hCompt == 1000; % if < 150, the function will be slow
        XmapWaitBar(i/length(Data(:,1)),handles);
        hCompt = 1;
    end

    SiO2 = Data(i,1);
    TiO2 = Data(i,2);
    Al2O3 = Data(i,3);
    FeO = Data(i,4);
    MnO = Data(i,5);
    MgO = Data(i,6);
    CaO = Data(i,7);
    Na2O = Data(i,8);
    K2O = Data(i,9);

    SumOxi(i) = SiO2+TiO2+Al2O3+FeO+MnO+MgO+CaO+Na2O+K2O;
    XSiO2(i) = SiO2/SumOxi(i);

end

% Deactivate the waiting bar in XMapTools
XmapWaitBar(1,handles);
return

```

Code 4.5 – Alternative function *FctOxiSum*

```

function [SumOxi,XSiO2] = FctOxiSum(Data,handles)
% -
% DESCRIPTION

SumOxi = sum(Data,2)';
XSiO2 = zeros(size(SumOxi));
Indx = find(SumOxi);
XSiO2(Indx) = Data(Indx,1)'./SumOxi(Indx);

return

```

4.3.3 How can I check the results of an external function?

Before the first use of an external function, the user is strongly recommended to perform tests in order to check the quality of the results generated by the function. The following procedure may be used to test an external function:

- [1] Close XMAPTOOLS and go to the setup directory (*/program*) and open the file *ListFunctions.txt*. As described in section 4.3.1, this file reports all the characteristics of the external functions. This file provides the list of input and output parameters for each functions.

4.3.3.1 Two names functions (P, T and P-T functions)

In this example, we can test the thermometer chlorite-chloritoïd of Vidal et al. (1999). The setup line in *ListFunctions.txt* corresponding to this external function is:

3>Chlorite+Chloritoid>T- Vidal etal 1999>NThermoCCVidal1999>T lnKd>SiO₂ TiO₂ Al₂O₃ FeO MnO MgO CaO Na₂O K₂O>

- **Function type** [3] corresponds to P, T and P-T spot mode
- **Mineral(s)** The thermometer is indexed in the group *Chlorite+Chloritoid*
- **Name** displayed is *T- Vidal etal 1999*
- **Function name** is *NThermoCCVidal1999.m*
- **Output variables** are: T and lnKd
- **Input variables** are SiO₂, TiO₂, Al₂O₃, FeO, MnO, MgO, CaO, Na₂O, K₂O
- **External variables** are not used in this case (no pressure dependency).

the input data are organized as a matrix in which the first line is the composition of the chlorite and the second line the composition of the chloritoid (same order of the name: Chlorite+Chloritoid). The compositions order is given by the input variables: [SiO₂, TiO₂, Al₂O₃, FeO, MnO, MgO, CaO, Na₂O, K₂O].

The following analyses of chlorite and chloritoid PSB9210b are used from Table 2 in Vidal et al. (1999).

- **Chlorite:** 25.63 0.03 23.37 22.82 0.22 15.13 0.06 0.02 0.02
- **Chloritoid:** 24.15 0 40.80 22.81 0.16 3.02 0.04 0.01 0.02

- [2] Open the directory */program/Functions* with the MATLAB *Current Folder* tool. Use the following code into the *Command Window* to test the function:

Code 4.6 – Test functions

```
Compos(1,:) = [25.63 0.03 23.37 22.82 0.22 15.13 0.06 0.02 0.02]; % Chl first row
Compos(2,:) = [24.15 0 40.80 22.81 0.16 3.02 0.04 0.01 0.02]; % Ctd second row
[T ln_Kd] = NThermoCCVidal1999(Compos)
```

The predicted temperature is 492°C and the ln_Kd is 1.61 in line with the results of Vidal et al., (1999).

4.3.3.2 Single name functions (P, T and P-T and structural formulae functions)

The same test can be conducted with the *One name* functions. In this second case, only one composition is required. However, for the test the two following lines in the function code must be commented (using %):

Code 4.7 – Test functions

```
XmapWaitBar(0, handles);
XmapWaitBar(1, handles);

% must be replaced by:
%XmapWaitBar(0, handles);
%XmapWaitBar(1, handles);
```

The function *Chl-StructForm-(Si<3)* can be tested. The corresponding setup line in *ListFunctions.txt* is:

1>Chlorite>Chl-StructForm-(Si<3)>StructFctChlorite>Aliv Alvi Fe3 Fe2 Al_M4 Si_T1 Si_T2
Al_T2 V_M1 Al_M2M3 Al_M1 Mg_M1 Fe_M1 Mg_M2M3 Fe_M2M3 X_Mg DeltaLacune XAme
Xcli XDap XSud Xsum>SiO2 Al2O3 FeO MnO MgO CaO Na2O K2O>

Open the function *StructFctChlorite.m* in MATLAB and comment the two lines of the function *XmapWaitBar* (see above). Save the file and use the following code into the Command Window to test the function:

Code 4.8 – Test functions

```
% WARNING: In the tested function comment first (using %) the lines % XmapWaitBar
(0, handles);
% XmapWaitBar(1, handles);
handles = 0;
% SiO2 Al2O3 FeO MnO MgO CaO Na2O K2O
Data(1,:) = [25.63 23.37 22.82 0.22 15.13 0.06 0.02 0.02]; %Chl
[Aliv, Alvi, Fe3, Fe2, Al_M4, Si_T1, Si_T2, Al_T2, V_M1, Al_M2M3, Al_M1, Mg_M1, Fe_M1, Mg_M2M3
, Fe_M2M3, X_MgFe, DeltaLacune, XAme, Xcli, XDap, XSud, Xsum] = StructFctChlorite(
Data, handles)
```

After testing, take care to remove the comments (%) on the two lines of the function *XmapWaitBar* and save again the file.

4.4 XMAPTOOLS ADD-ONS

4.4.1 List of compatible add-on

There is no official add-on published so far.

4.4.2 How to install and use the XMapTools' add-on

- [1] Download and unzip the add-on package.
- [2] Copy the add-on folder.
- [3] Close XMAPTOOLS, go to the setup directory (*/Addon*) and paste the add-on folder.

The add-on is ready to be used in XMAPTOOLS and is available in the add-on menu. If the add-on is not listed in the add-on menu, there is either something wrong with the package or some files are missing.

Note: Some add-on may require an additional setup that will be done during the first call of the add-on.

4.4.3 Procedure to create a new add-on

Not yet available...

Please contact me if you are interesting in developing a XMAPTOOLS' add-on.

GENERAL ERRORS AND SOLUTIONS

5

5.1 INTRODUCTION

In this sections the main errors codes that may be displayed by XMapTools are described and solutions are given.

Fast and easy access to the error descriptions:

Setup errors: [ES0145]

In case of display issues caused by the screen resolution, check the section *XMapToolsHD*.

5.2 SETUP ERRORS (ES01XX)

[ES0145] /UserFiles not found

Code 5.1 – Error ES0145

Loading ... (User files path) ... Error ES0145 – /UserFiles not found

This error occurs during the launching when XMapTools is not able to find */UserFiles* that should be in the setup repertory (containing *XMapTools/Setup* and *XMapTools/UserFiles*). If this directory doesn't exist and if additional functions have to be used, create a new */UserFiles* folder and put it in the setup repertory. More details about the strategy are given in section 2.4.2.1.

5.3 INTERFACE ERRORS

The up to date list of identified bug is available at https://www.xmaptools.com/?page_id=84

5.3.1 How to unfreeze the interface in case of error in an external function

The buttons of the main XMAPTOOLS interface are frozen as soon as the program is in a busy state (Fig. 5.1b), i.e. the program is waiting for results from an external function or module. The busy state is activated for example if an external function has been called or if you are using the *import tool*, the *advanced standardization* module, the corrections *TRC* or *IDC* or the *GENERATOR* module. If an error occurs in the external function or in a module, the main interface gets stuck waiting for an answer that will never come.

To overcome this problem, a function that can force the program to exit the busy state has been added in XMAPTOOLS 2.5.1. The button *unfreeze the interface*  allows the interface to be unfrozen if the program is stuck.

Cases in which this button must not be used (see the warning message display by XMAPTOOLS in Fig. 5.2):

- The program is waiting you to click on the figure to select one or more specific pixels. Examples: the classification function, the function to select/unselect the standards and for all the functions asking you to define a region-of-interest. In this case, do not press the button *unfreeze* and use right click instead to end the selection mode. Note: several rick clicks may be required if the function has been called several times.
- The *correction mode* is active (e.g. *SPC*, *MPC*). Solution: press the button *APPLY* located below the *X-pad* navigator. Note that the unfreeze function does not work if the correction mode is active.

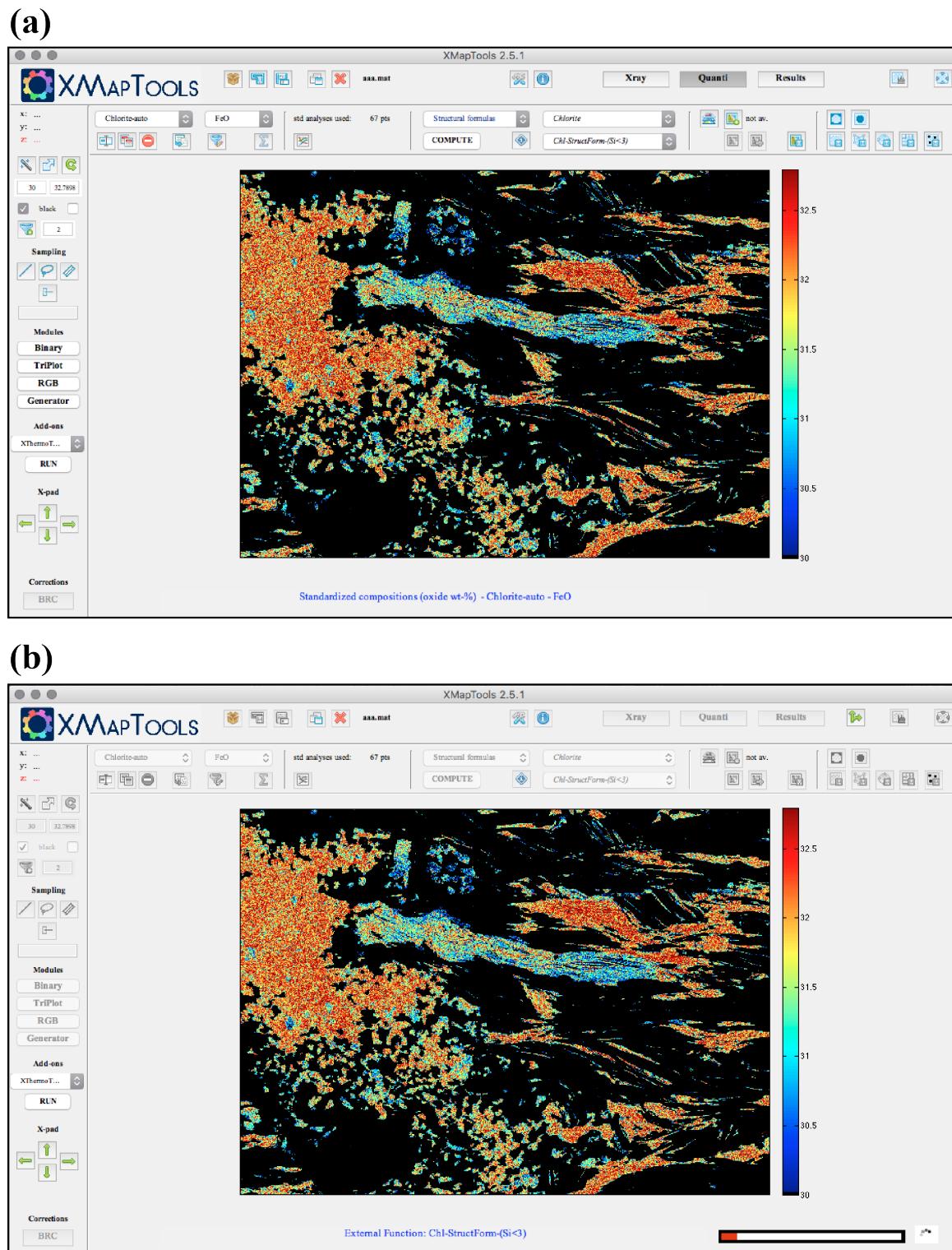


Figure 5.1 – XMAPTOOLS main interface: (a) normal (b) busy

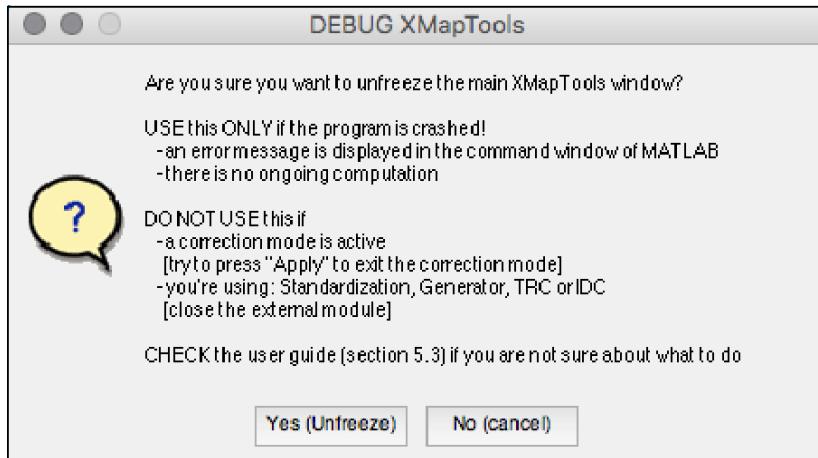


Figure 5.2 – Warning message appearing when the button unfreeze the interface has been pressed

- The GENERATOR module is in use. Solution: close the module.
- The *Import tool* or the *standardization tool* module is in use. Solution: close the module.
- XMAPTOOLS is waiting for the result of an external function, but the job is not accomplished yet (e.g. if the progress bar is still moving, Fig. 5.2b). In this case, wait that the function finishes his job, or click into the MATLAB[®] *Command Window* and hit *Ctrl + C* to kill the job first; then, and only then press the button *unfreeze the interface* .

XMAPTOOLS ADD-ONS

6

6.1 INTRODUCTION

You can add new functionality to XMapTools by installing one of the official extensions. Add-ons have been introduced in XMAPTOOLS 3.3

- Add-ons stand as separate programs
- They can be called from the XMapTools interface at any step to perform extra computations
- Add-ons have access via the API to the data generated by XMapTools
- Developers can create their own add-on

The up-to-date list of add-ons is available at: <https://www.xmaptools.com/add-ons/>

6.2 ADD-ON MANAGEMENT SYSTEM

6.2.1 Download add-ons

Several add-ons are provided in the official XMapTools package. They also can be downloaded directly via the XMAPTOOLS interface using the Extension manager.

Warning: You must use the Extension manager to get the add-ons if you updated to XMAPTOOLS 3.3.1 or more recent versions via MATLAB®(i.e. without downloading the full package).

1. Open MATLAB®, set the working directory and open XMAPTOOLS
2. In menu, select File > Add-Ons > Manage Extensions
3. In the Extension manager, select one add-on in the menu located on the top left
4. If you do not have this add-on, press the button Download
5. If you already have a version of this add-on and you want to update, press the button Delete & Download.
6. This operation will download the last version of the add-on available on the server
7. Note: Some add-ons require an additional setup. Simply open the add-on from the XMAPTOOLS interface and follow the instructions.

Note: Some add-ons have an auto-update functionality directly implemented in the extension. The add-on checks for update every time it is opened. Add-ons without update system should be updated manually following the procedure given above.

6.2.2 Disable or Remove Add-Ons

Follow these steps if you want to remove an add-on:

1. Navigate to the folder `/MyDocuments/MATLAB/XMapTools/Addons/`
2. Simply delete the folder containing the add-on

6.3 XMAPTOOLS API FOR DEVELOPERS

The application programming interface (API) is intended to simplify the implementation and maintenance of XMAPTOOLS' add-ons.

XMAPTOOLS performs the following checks before calling an add-on:

1. Call the add-on installer (e.g. the program `AOTest_Install.m` for an add-on `AOTest`) and sends as input variable the absolute path of the add-on. XMAPTOOLS proceeds further only if the generic answer 1 is received
2. Call the add-on update program (e.g. `AOTest_Update.m`) and sends as input variable the absolute path of the add-on. Depending on the update state XMAPTOOLS stops or continues further (see below). The developers can decide to make the update mandatory or not (can be skipped)
3. Call the add-on gateway (e.g. `AOTest.m`)

6.3.1 Step 1: Create the add-on folder and files

1. Create a new folder having the add-on name (case-sensitive) in `/MyDocuments/MATLAB/XMapTools/Addons/`. For an add-on called `AOTest`, the add-on directory would be `?/XMapTools/Addons/AOTest/`
2. In this directory, create three MATLAB®m-files based on the add-on name (here `AOTest`): `AOTest.m`; `AOTest_Install.m`; `AOTest_Update.m`. Those files are required for allowing XMAPTOOLS to properly interact with the add-on.

6.3.2 Step 2: Add-on installer

A template for the setup function (in this example `AOTest_Install.m`) is provided below.

```
function [OKrun] = AOTest_Install( Path )
%
% Add any installation code here...
%
OKrun = 1;
return
```

Code 6.1 – Creation of the add-on installer

If the variable *OKrun* is not set to 1, XMAPTOOLS will prevent the add-on to be used and displays the following warning message: The add-on is not correctly installed and cannot be called by XMAPTOOLS.

6.3.3 Step 3: Add-on updater

A template for the update function (in this example *AOTest_Update.m*) is provided below.

```
function [ UpdateState ] = AOTest_Update( varargin )
%
% This is the update for the program
%
% Output varibale "UpdateState" (from XMapTools ...):
% [-1]      No update system           Continue
% [0]      Server cannot be reached   Continue
% [1]      This add-on is up-to-date   Continue
% [2]      An update has been installed Continue
% [3]      An update is available but skiped Stop
% [4]      An update is available but skiped Continue
% [5]      Abord the call             Stop

UpdateState = -1;
return
```

Code 6.2 – Creation of the add-on updater

The value of *UpdateState* controls the behavior of XMAPTOOLS. If there is no update system, the value should be -1 . Other options are given in the comment of the code above.

6.3.4 Step 3: Add-on gateway

It is strongly recommended to use the program with the add-on name (in this example *AOTest.m*) as a gateway to the add-on interface (e.g. *VER_AOTest.m* and *VER_AOTest.fig*). A simple example is provided below.

```
ffunction varargout = AOTest(varargin)
% AOTest runs the program VER_AOTest
%     AOTest is a MATLAB-based graphic user interface used
%     to illustrate the XMapTools add-on system
%

% Step 1: Get data from XMapTools
Infos = varargin{1};          % State of XMapTools
RawData = varargin{2};         % Data from the X-ray workspace
MaskFile = varargin{3};        % Data from the mask files in X-ray
Quanti = varargin{4};          % Data from the Quanti workspace
Results = varargin{5};         % Data from the Result workspace
ColorBar = varargin{6};        % Data of the active colour palette

% Step 2: Check if the add-on can be called (EXAMPLES...)
if ~isequal(Infos.Mode,1)
    warndlg('AOTest is only available from the workspace "Xray" ... ', 'Warning');
    return          % i.e. the add-on does not open
end

if ~iscell(Infos.Xray.ListMaps) || length(Infos.Xray.ListMaps) < 2
```

```
Text{1} = 'AOTest can not be called because there is no map';
warndlg(Text,'Warning');
return          % i.e. the add-on does not open

end

% If we passed all the tests made above...
VER_AOTest(RawData);      % i.e. call the add-on
                          % in this example only the data in X-ray are used by the
                          % add-on
                          % Other variables (e.g. MaskFile) can be sent to
                          % VER_AOTest

return
```

Code 6.3 – *Creation of the add-on gateway*

6.3.5 Step 4: Add-on GUI

The add-on interface can be generated using the GUIDE environment of MATLAB

Note: At the moment it is not possible to send data back via the API; files should be created instead and then imported via the XMAPTOOLS interface.

TUTORIAL 1: EPMA DATA PROCESSING (CENTRAL ALPS - 2013)

7

7.1 INTRODUCTION

A set of X-ray maps is provided as an example with XMAPTOOLS. In this chapter I describe how to use the XMAPTOOLS to import X-ray maps, standardize them and calculate the P-T conditions of crystallization. If you are using XMAPTOOLS for the first time, it is strongly suggested to read first the previous chapters (1, 2) before you begin this tutorial. For example the setup procedure discussed in chapter 2 is not described here and this step must be achieved before to begin the tutorial. The chapter ?? provides a comprehensive description of the functions used in this tutorial.

X-ray images used in this example were measured at the University of Lausanne (UNIL) using a electron probe micro-analyzer JEOL JXA 8200 Superprobe. The studied sample comes from Garvera outcrop, Urseren zone in the Central Alps. This sample has been studied in details by [Janots et al. \(2008\)](#), [Bernier \(2011\)](#), [Gardonio \(2012\)](#).

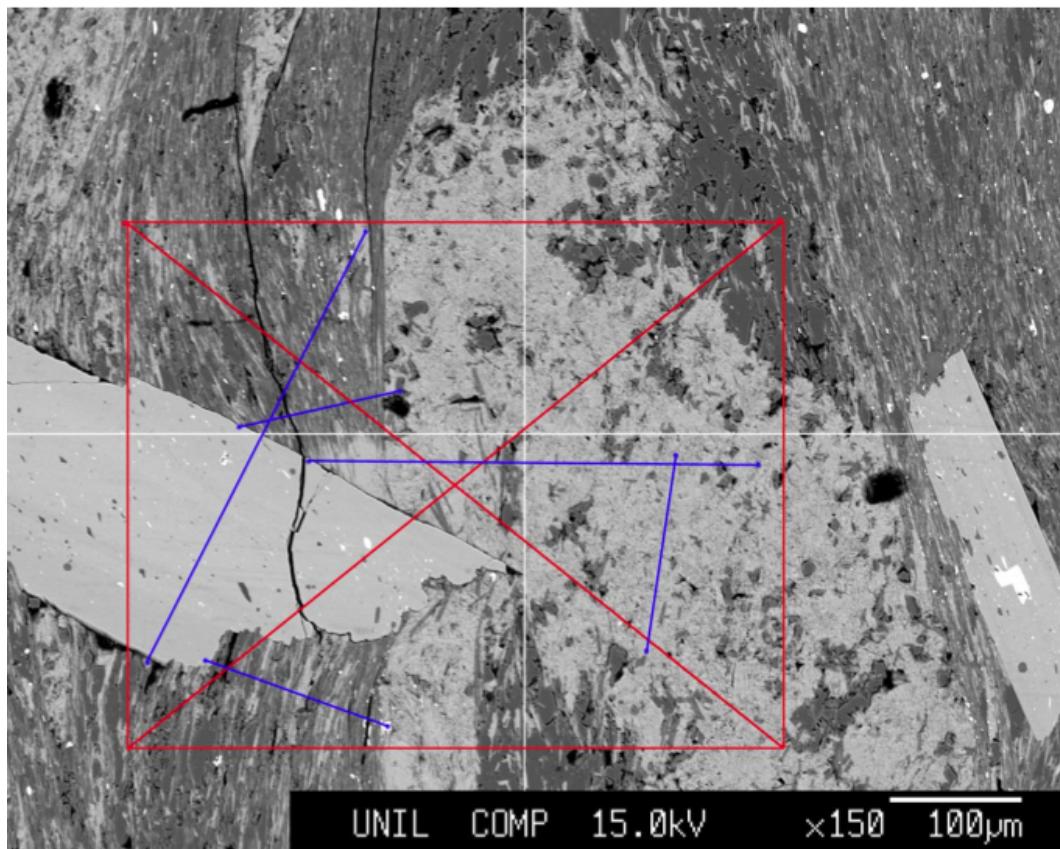


Figure 7.1 – BSE image of the studied area (red rectangle) with transect of spot analyses (blue lines) from [Bernier \(2011\)](#).

7.1.1 How to get started

XMAPTOOLS is a software that can only be executed from the MATLAB environment. The following steps explain how to use XMAPTOOLS in your computer.

(1) Open MATLAB

(2) Go to the data example repertory using the *Current Folder* window in the MATLAB window. This step is critical as many files will be generated by XMAPTOOLS and stored in the working directory. Make sure that the current path is .../Example as in Figure 7.2a.

(3) Open XMAPTOOLS using the command: » **XMapTools** (case sensitive, example in Fig. 7.2a)

(4) Information such as software version and attached files are reported in the MATLAB command window (Fig. 7.3b) XMAPTOOLS main window appears after few seconds (Fig. 7.3)

As discussed in Introduction, XMAPTOOLS is organized in three workspaces: *X-ray*, *Quanti* and *Results*. The next sections described the corresponding operations of data processing.

7.2 X-RAY WORKSPACE

7.2.1 Add new data

(1) Import new maps via the menu: *File, Import, Add Map(s)*, or using the button  (arrow in Fig. 7.4).

(2) A dialog box opens in which files can be selected (7.4a). Select all the files together (i.e. Al.txt, Ca.txt, Fe.txt, K.txt, Mg.txt, Mn.txt Na.txt and Ti.txt) using the *maj* button. Press the button *open* and XMAPTOOLS reads and imports the selected files.

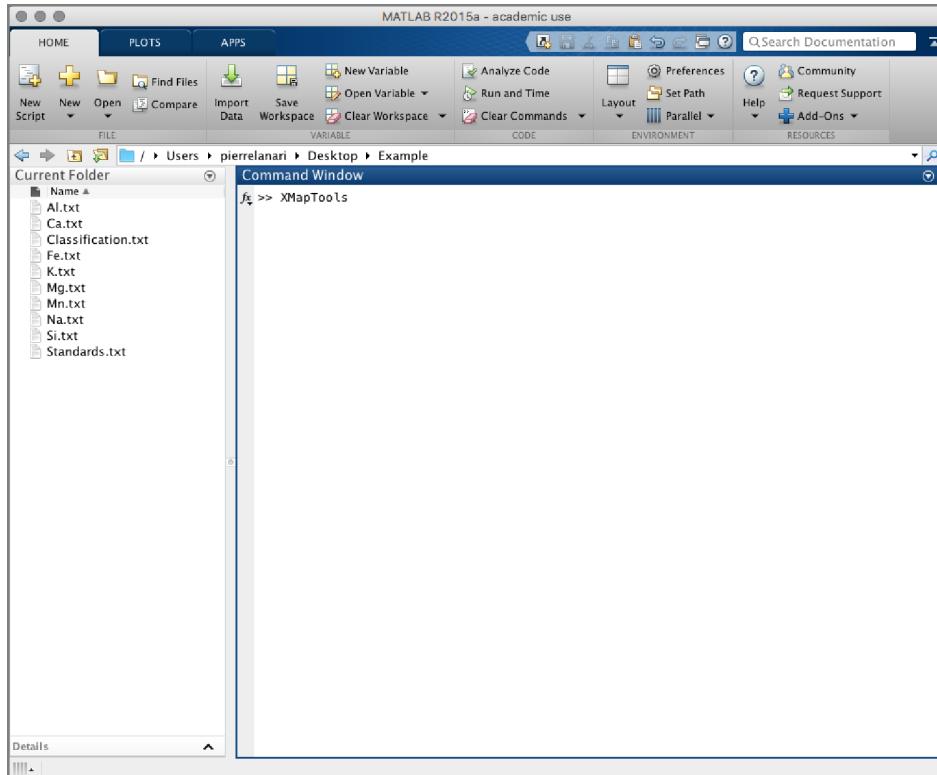
(3) The program loads each file and search the corresponding element in the database. When this is done, it opens the *Import Tool* (Fig. 7.4b).

(4) In the *Import Tool*, activate the dead time correction; a dwell time of 200 ms and a dead time of 300 ns were used (Fig. 7.4b) for this project. When this is completed, press *Apply Corrections* to correct the WDS maps for dead time and import all the maps in the main XMAPTOOLS user interface.

Warning: Do not apply any transformation such as rotation to EPMA maps, otherwise the map coordinates defined in the file *Standard.txt* will not work anymore. The rotation correction should only applied to standardized maps such as LA-ICP-MS data.

(6) When all the corrected files have been imported, XMAPTOOLS displays the first map in the main figure area (Fig. 7.5). The details about the maps and the corrections are displayed in the MATLAB *Command Window* (see insert 7.1).

(a)



(b)

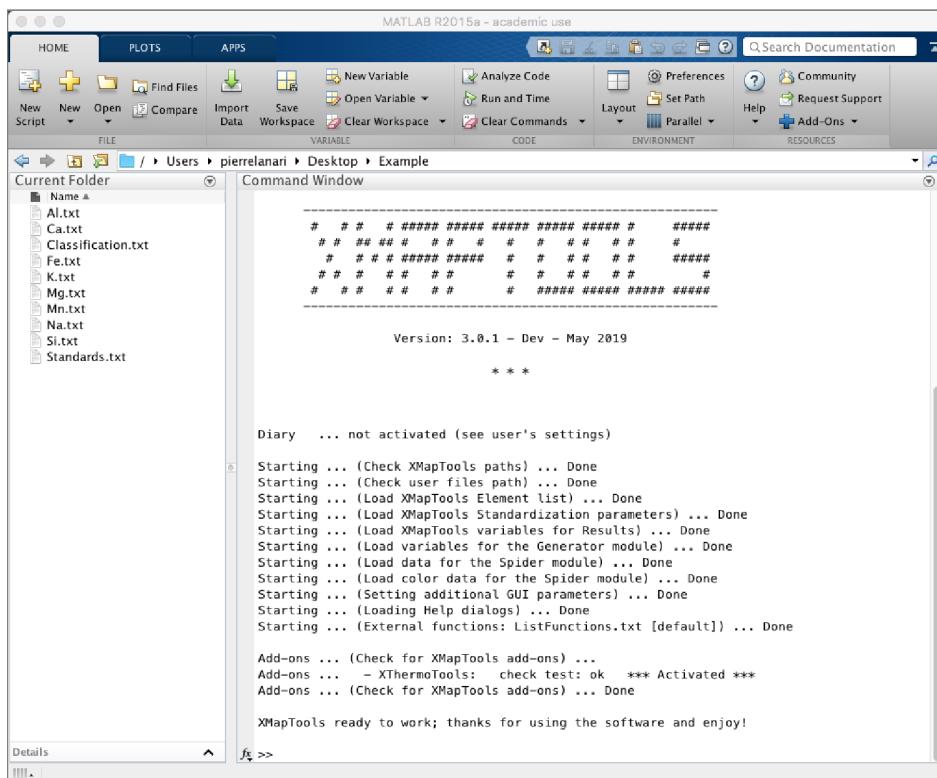


Figure 7.2 – Procedure to open XMAPTOOLS from the MATLAB command window

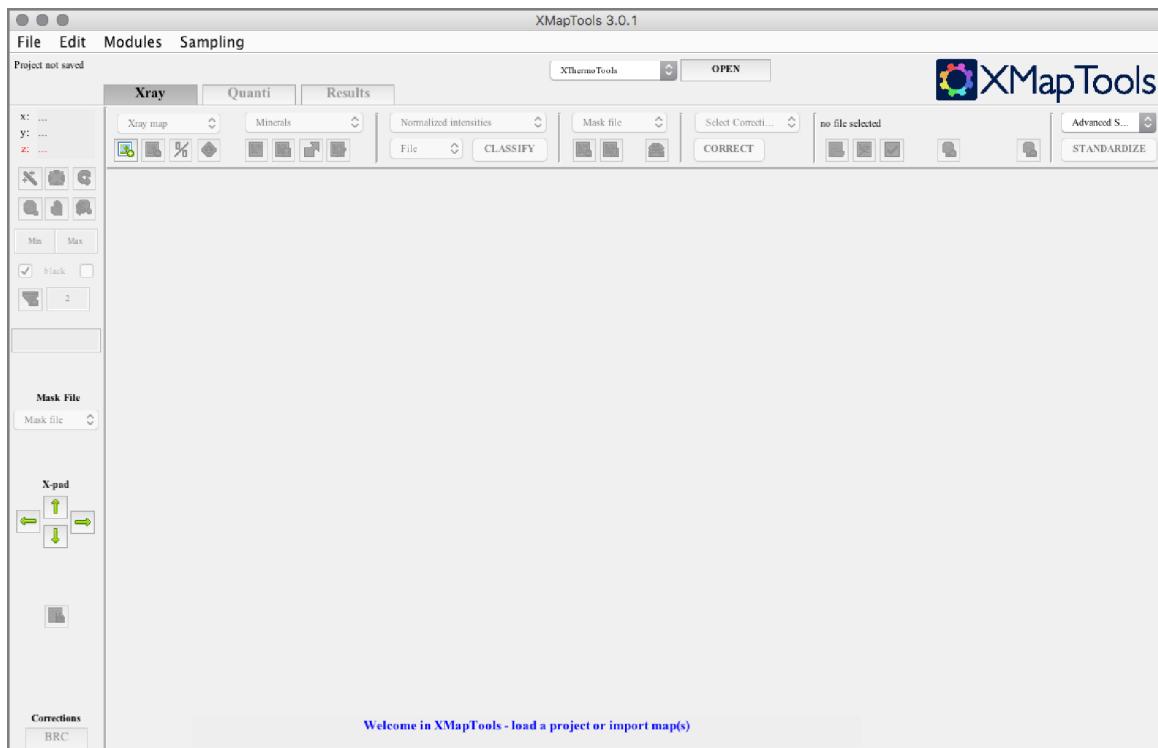


Figure 7.3 – XMAPTOOLS main Graphical User Interface

```

Import Tool ... (apply corrections) ...
  - Map: Al      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Ca      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Fe      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: K       [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Mg      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Mn      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Na      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
  - Map: Si      [type: 1]
    * Dead time correction applied: DwellT(200); DeadT(300)
Import Tool ... (Saving Import.txt) ... OK

```

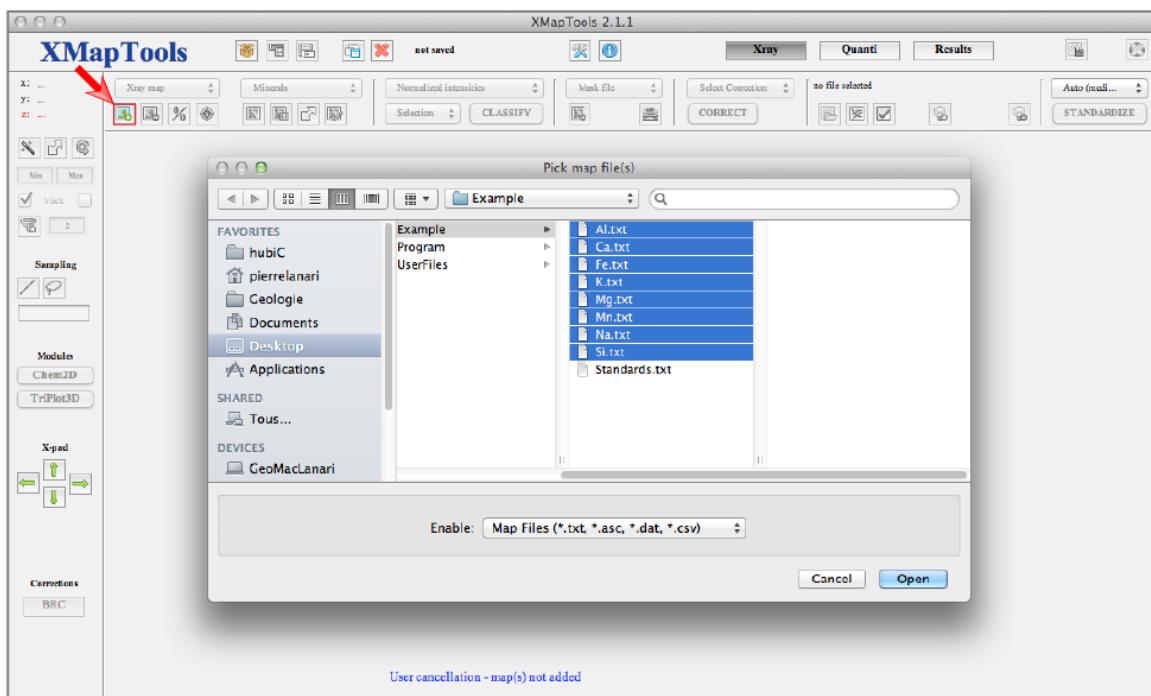
Code 7.1 – Import Tool

7.2.2 Display X-ray images

X-ray images can be displayed using the X-ray menu (red arrow in Fig. 7.5). Use this menu and select a new map. The figure is automatically updated and the new map displayed.

NB: The color bar *lower* and *upper* values are fixed as the min and max values of the displayed image (corresponding to *min* and *max* intensity values for raw X-ray data). In order to change this values, figure options must be used (see below).

(a)



(b)

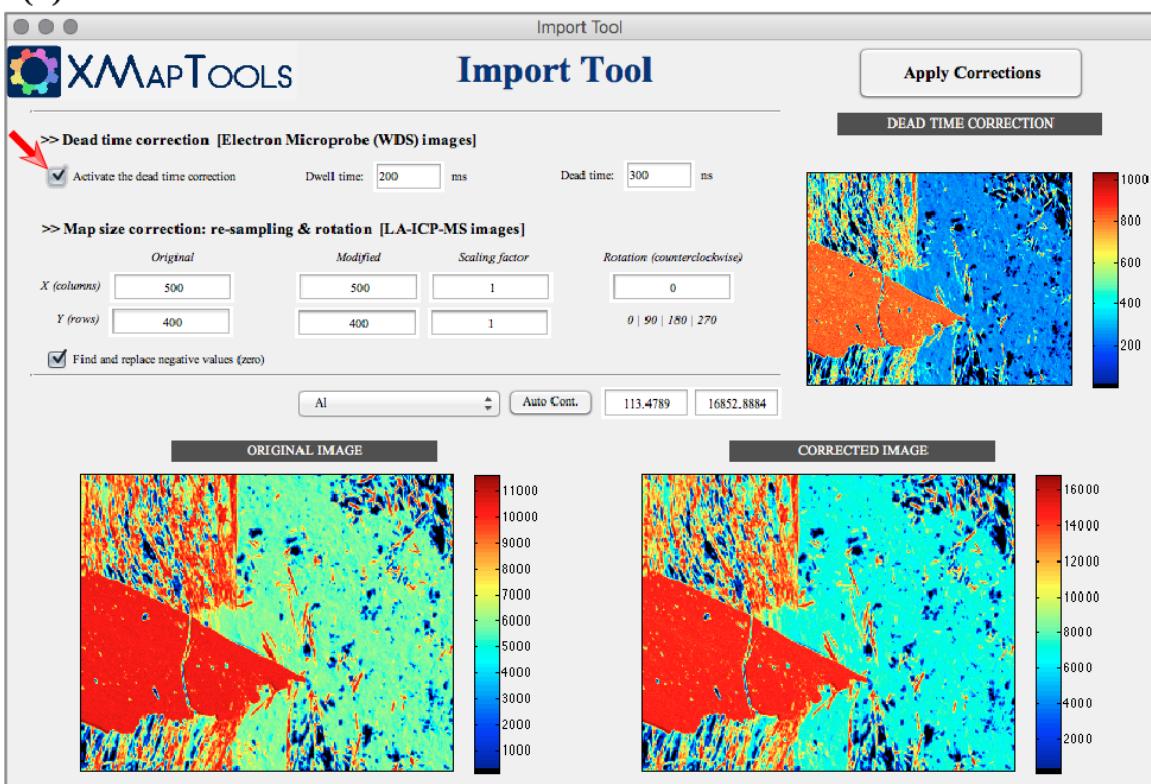


Figure 7.4 – Add new X-ray map(s) and Import Tool

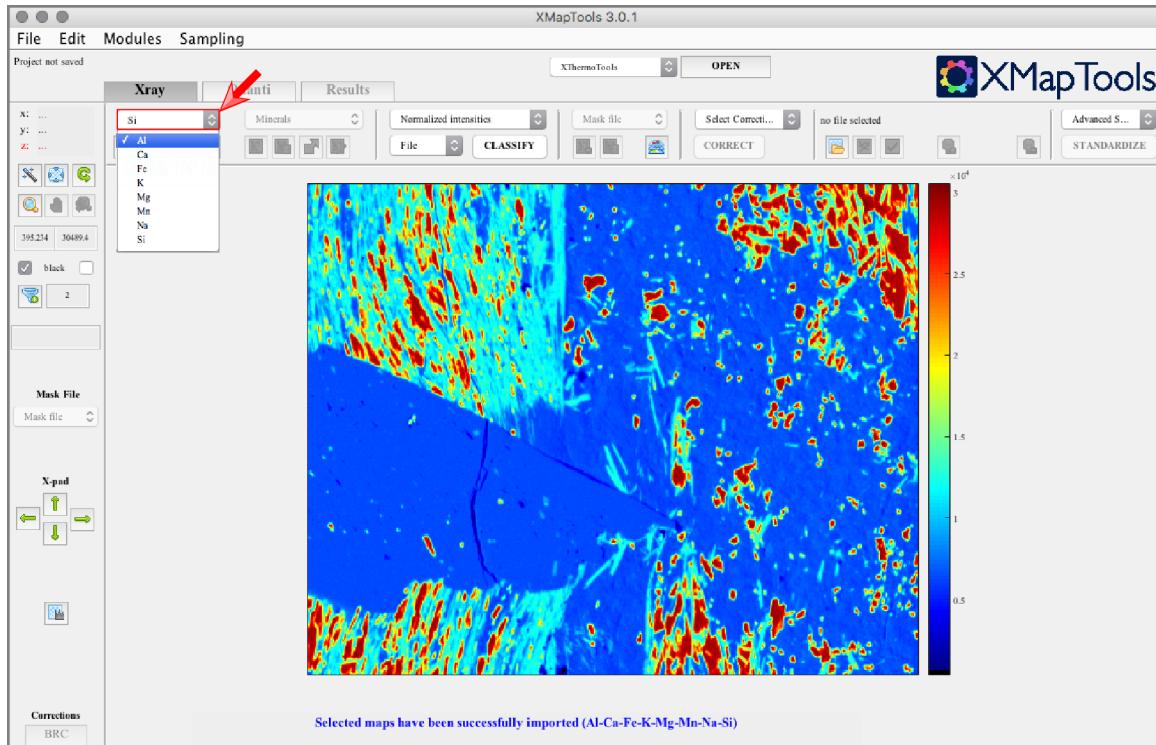


Figure 7.5 – X-ray menu is available to display X-ray images

7.2.3 Figure options

The window allowing to manage Figure options is available on the left part of the main XMAPTOOLS GUI (Fig. 7.6a).

7.2.3.1 Live coordinates

- (1) Display the map *Al* using the X-ray menu (red arrow in Fig. 7.5, first map)
- (2) In the figure option window, the live coordinate screen displays X, Y and Z coordinates corresponding to the mouse position on the X-ray map. The Z value is the value of the overflow pixel located at (X,Y) position. Try to displace your mouse above the map in order to get Z values, here corresponding to the number of recorded counts, of minerals.

The porphyroblast colored in red shows for instance an average intensity of 10,200 counts for Al. The greenish matrix on the right part of the map exhibits an average intensity of 5,700 counts.

NB: This feature is available in all the workspaces.

7.2.3.2 Image contrast

- (3) The contrast of the image (i.e. lower and upper limits of the color bar) can be automatically adjusted using the button *auto-contrast* . Press this button and the min and max values of text areas with the values of the color bar are optimized (Fig. 7.6b).
- (4) If the auto-contrast mode is active the lower and upper limits are fixed by XMAPTOOLS. You can switch back to min-max values for the contrast using the same button *auto-contrast* .

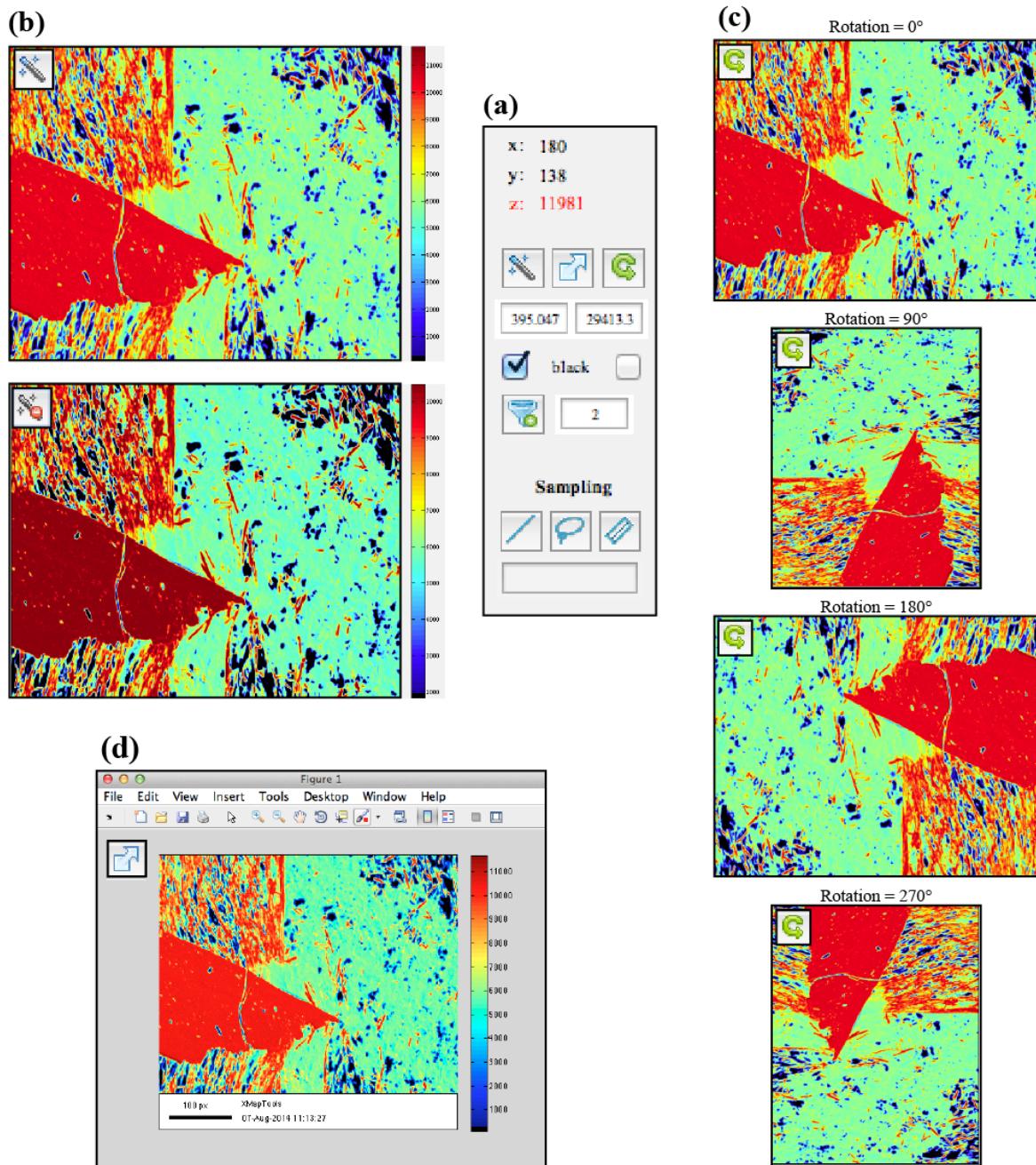


Figure 7.6 – Display options. (a) Display option menu; (b) auto-contrast mode activated (down), unactivated (up); (c) rotation mode for different rotation angles.

NB: In this example, the displayed image does not change significantly (7.6b). The usefulness of the auto-contrast function can be demonstrated with the Ca map.

(5) Display the map *Ca* using the X-ray menu (red arrow in Fig. 7.5, second map)

(6) Activate the auto-contrast mode using the button *auto-contrast* 

(7) Unactivate the auto-contrast mode using the button *auto-contrast* 

(8) Check all the maps with the auto-contrast mode

7.2.3.3 Image rotation

(9) Image orientation can be changed using the button *rotate* . Press this button to rotate the image of 90° (counterclockwise). Four positions corresponding to 0°, 90°, 180° and 270° are available (Fig. 7.6c).

NB: The image coordinates displayed in the live coordinate screen are coordinates in the original system that correspond to 0° rotation, i.e. the coordinates of an object are exactly the same in all the rotation modes.

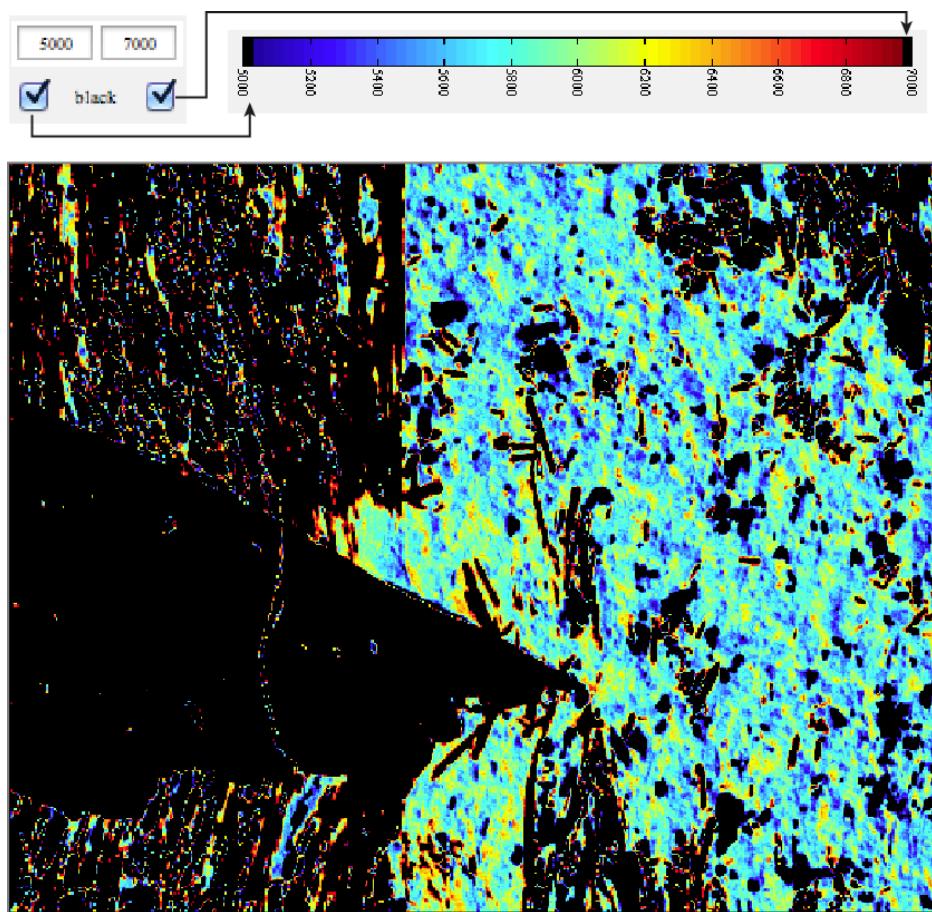


Figure 7.7 – *Display options. (a) Display option menu; (b) auto-contrast mode enabled (down), disabled (up); (c) rotation mode for different rotation angles.*

7.2.3.4 Export and save image

(10) The Image displayed in the figure area can be exported by via the menu *File, Export Image*. The image is opened in a new MATLAB figure (Fig. 7.6d). Use the button *save* to save the figure in common image formats (pdf; png; tif). The format PDF is recommended for the figure to be editable in Adobe Illustrator.

Note that it is also possible to copy the figure as vectorized object to the clipboard using the menu *Edit* and the item *Copy Figure*.

7.2.3.5 Black layers in color bar

- (1) Display the map *Ca* using the X-ray menu (red arrow in Fig. 7.5, second map)
- (2) Manually adjust the color bar limits to: lower = 5000 and upper = 7000 (Fig. 7.7)
- (3) Black colors can be added to the color bar in order to hide the pixels with intensities higher and lower than the max and min values. The black layer for the min value (left in Fig. 7.7) is automatically activated.
- (4) Enable the upper black color by selecting the second checkbox (right in Fig. 7.7). All the pixels with intensities higher than 7000 are displayed in black.

NB: These settings are saved by XMAPTOOLS and will be applied to any other map displayed in the main figure window.

- (5) Disable the upper black color by deselecting the second checkbox (right in Fig. 7.7). All the pixels with intensities higher than 7000 are displayed in the last red color of the color bar (normal mode).

7.2.3.6 Median Filter

- (1) Display the map *Fe* using the X-ray menu (third map)
- (2) Adjust manually the color bar limits using the values: min = 4000 and max = 5200 (Fig. 7.8a).
- (3) Press the button *median filter*  A rectangular median filter is applied to the displayed map (Fig. 7.8b).
- (4) Turn off the median filter by pressing the button *median filter* .
- (5) Edit the size of the median filter (in pixel) to 5 and turn on the median filter. The new filter is applied to the displayed map (Fig. 7.8c).
- (6) Turn off the median filter by pressing the button *median filter* .

NB: The median filter may be used to remove the noise and to extract chemical composition trends. This is only a display option, the data stored in the program are not altered.

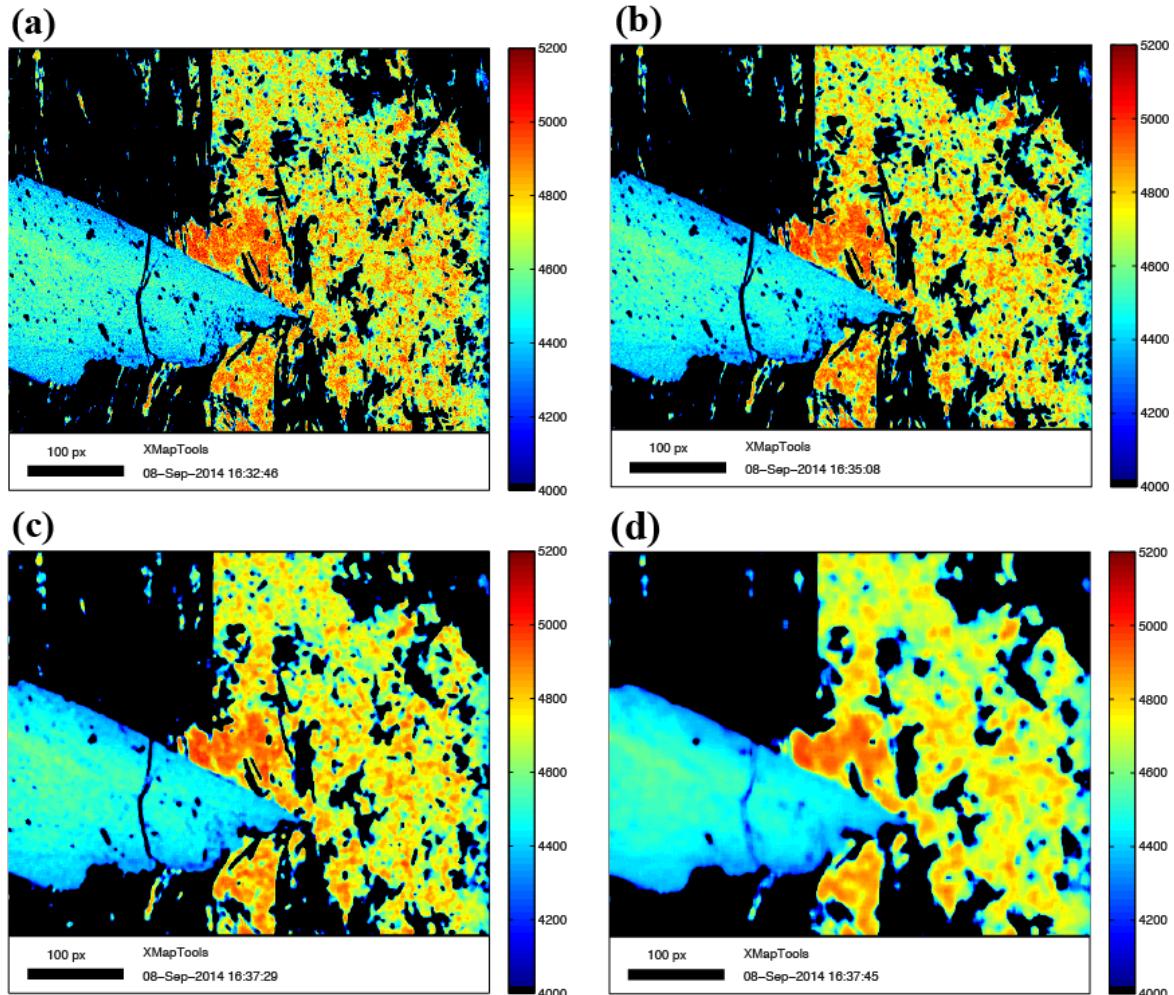


Figure 7.8 – Median Filter. (a) not used; (b) size = 2; (c) size = 5; (d) size = 10;

7.2.3.7 Sampling

- (1) Display the map Mg using the X-ray menu (fifth map) and apply the auto contrast using the button *auto-contrast*
- (2) In the menu, select *Sampling* and then *Line* and define two points of a transect going across the porphyroblast (see points 1 and 2 in Fig. 7.9a). The program opens a new figure window with the diagram *distance (in pixel)* against *chemical composition*.

If the sampling option *Save data* is selected in the sampling menu, the save the data in a text file as well as the map showing the transect line. The figure files *.fig can be opened with MATLAB and converted to PDF. In this example the diagram is distance in pixel (180 pixel units) against Fe intensity (in counts).

NB: The transect is always displayed from the point 1 (left in chemical diagram) to the point 2 (right in chemical diagram).

- (3) In order to delete the points and the transect displayed on the main figure, Select again the map Mg using the X-ray menu and apply the auto contrast using the button *auto-contrast* . If the option

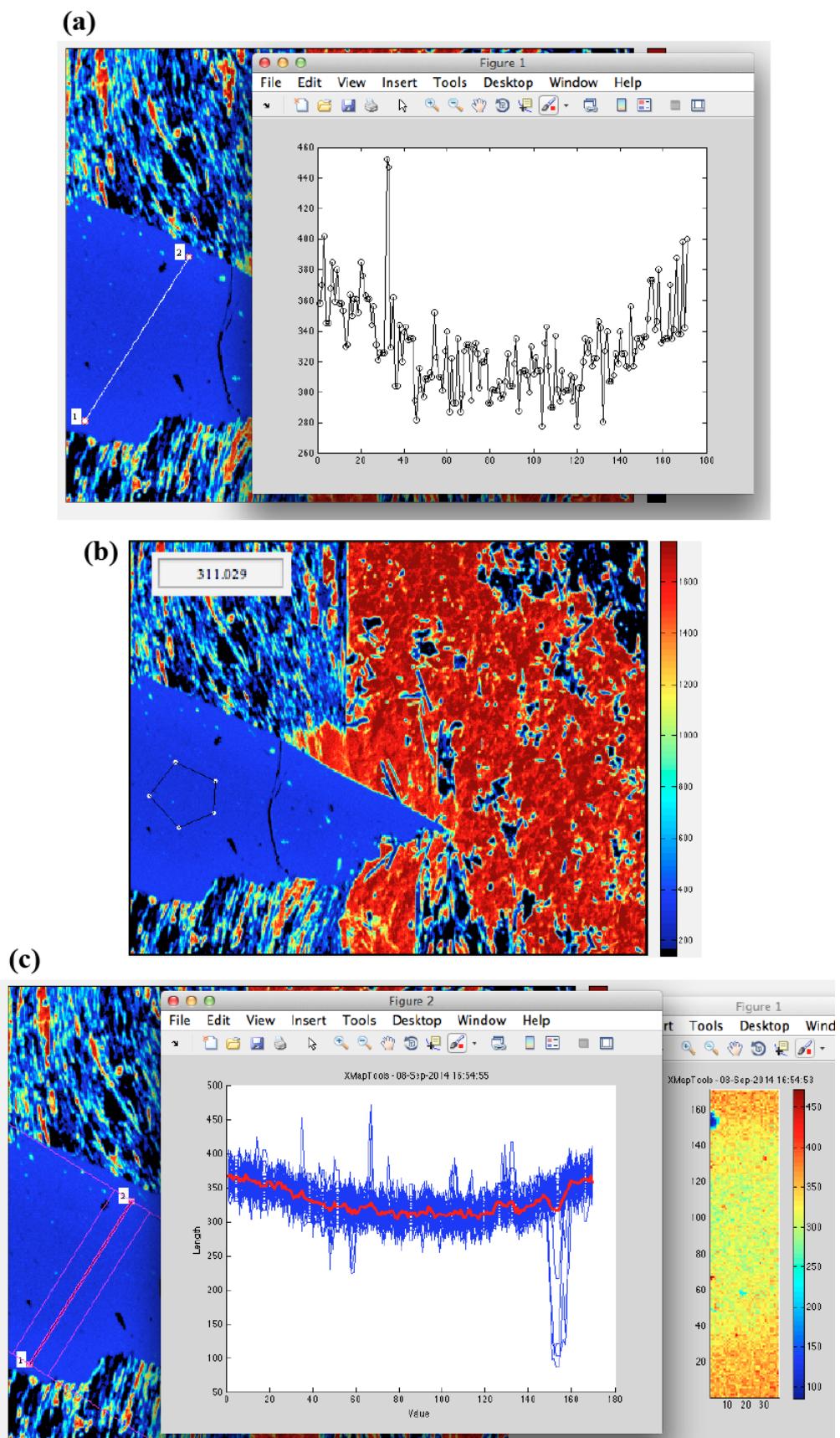


Figure 7.9 – Sampling functions. (a) mode: line; (b) mode: area (c) mode: integrated lines.

Clean Figure is selected in the sampling function, the figure will be cleaned every time a sampling function is used.

(4) In the menu, select *Sampling* and then *Area* and select an area in the same porphyroblast (Fig. 7.9b). The program display the mean composition (and standard deviation) of this area in the box located in the figure option window. In this example the mean intensity of Fe is 311 ± 18 counts (1σ).

(5) In the menu, select *Sampling* and then *Integrated lines* and select two points across the porphyroblast and one additional point to define the half-width of the rectangle along which the transect lines will be integrated (see points 1 and 2 in Fig. 7.9c). The program open a new figure with the map of the integrated area (labeled *Fig. 1* in 7.9c). Then a new figure window is opened with the diagram *distance in pixel* against *chemical composition*. The lines in blue are all the transects and the red curve is the mean transect.

NB: In all the sampling mode, XMAPTOOLS can save the results in ASCII files and export the figures if the option *Save Data* is selected in the sampling menu.

NB: In all the sampling mode, XMAPTOOLS can export data from several maps if the mode *Multiple Maps* is selected in the sampling menu.

7.2.4 X-ray images options

7.2.4.1 Precision map

(1) Display the map *Al* using the X-ray menu (first map) and apply the auto contrast using the button *auto-contrast* 

(2) Press the button *Display precision map*  (Fig. 7.10a) to generate a precision image (in % 2σ) that opens in a new window (Fig. 7.10b). This precision image reflects the random error from the detector estimated using counting statistics (Lanari et al. 2014b). More detailed explanations are provided in section 1.6.1.2.

(3) Set the precision image as the current active figure by selecting the window.

(4) In the MATLAB command window, set the color axis range of the figure to 1-11% using the following command. The result is displayed in figure 7.10c.

```
caxis ([1 11])
```

Code 7.2 – *caxis* function may be used to set the min and max values of the color bar of a figure

(5) Set the color axis range of the figure to 1.5-3.5%. The result is displayed in figure 7.10d. The analytical error on Al is 2% for chloritoid and phengite, 2.5% chlorite and 12% for quartz.

(6) The precision image generated may be saved using the menu *File* and *Save as ...*

7.2.4.2 X-ray info

(1) Display the map *Al* using the X-ray menu (first map) and apply the auto contrast using the button *auto-contrast* 

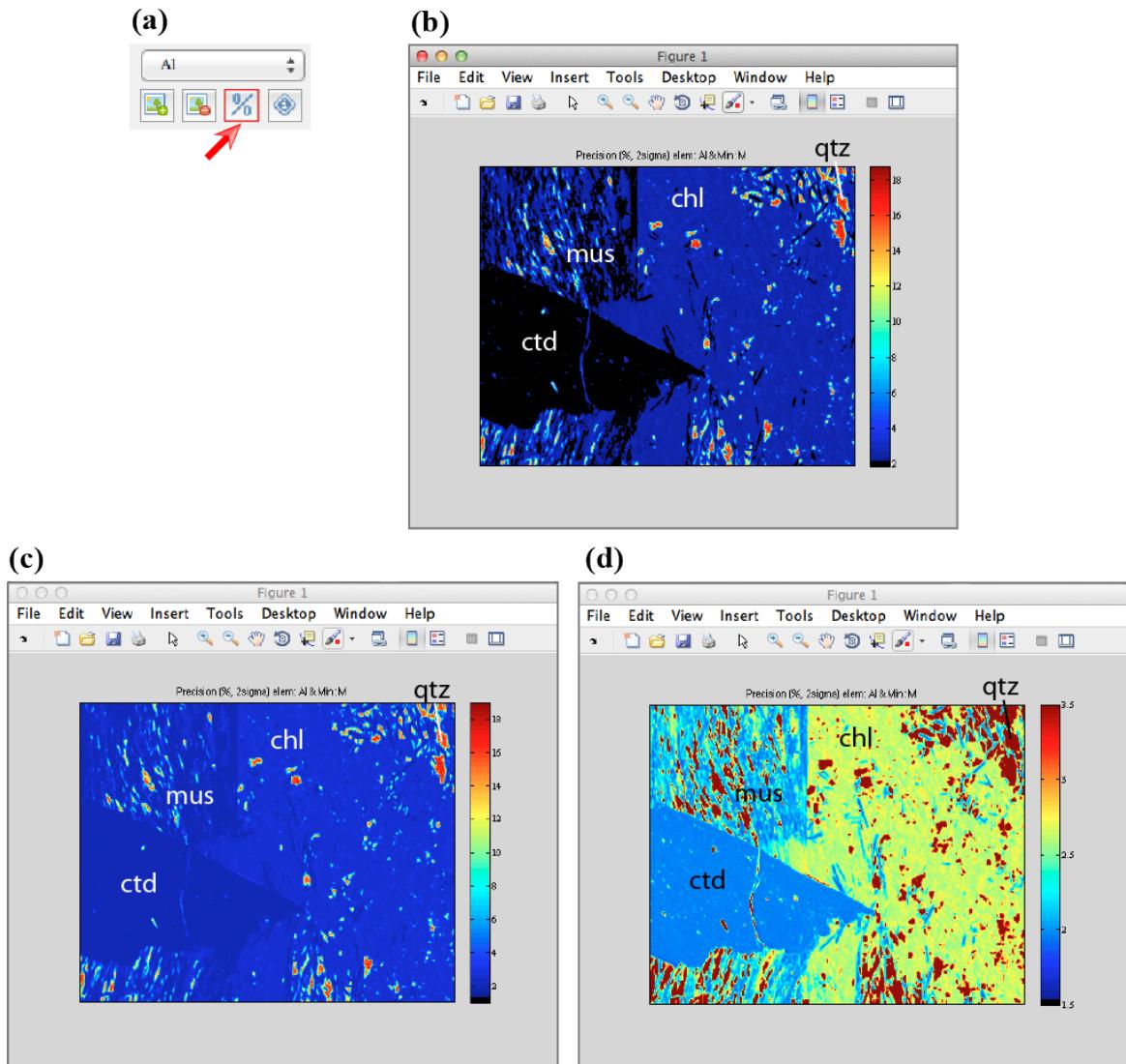


Figure 7.10 – Precision image in % calculated from the X-ray map of Al. (b), (c) and (d) are the same data (precision image for Al in %) plotted with different color bar axis values (see text)

- (2) Display the *X-ray info* window using button *X-ray info*
- (3) The resulting info window is displayed in Fig. 7.11 and the text reported in the box 7.3

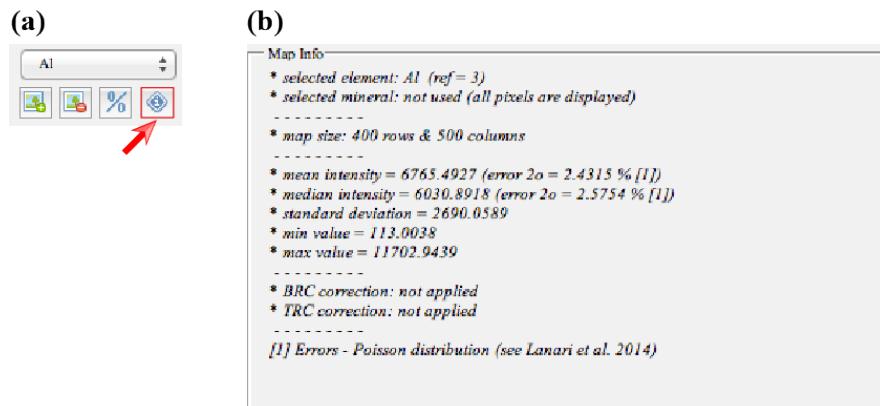


Figure 7.11 – Info button (a) and window (b) available into the workspace X-ray

```

Map Info
* selected element: Al (ref 3)
* selected mineral: not used (all pixels are displayed)
-----
* map size: 400 rows & 500 columns
-----
* mean intensity = 6765.4927 (error 2o = 2.4315 \% [1])
* median intensity = 6030.8918 (error 2o = 2.5754 \% [1])
* standard deviation = 2690.0589
* min value = 113.0038
* max value = 11702.9439
-----
* BRC correction: not applied
* TRC correction: not applied
-----
[1] Errors - Poisson distribution (see Lanari et al. 2014)

```

Code 7.3 – Text printed in the info window

In this example, the selected element is Al (the XMAPTOOLS reference of this map is the number 3). Mask are not yet created and all the displayed pixels are used to calculate the following values: mean intensity and median intensity, standard deviation, min and max values. The precision is calculated for both mean and median intensities. In this example BRC and TRC correction are not used.

7.2.5 Classification

The classification function generates masks corresponding to entities identified in the map (e.g. mineral, mineral boundaries, fractures). This function allocates each individual pixel of the image to one of the minerals phases defined by the user. This step is crucial because each mineral must be individually proceeded through the next steps.

The mask creating function uses the statistical analysis method K-means clustering to distribute the pixels into groups of similar compositions ([Lanari et al. 2014b](#)).

Two approaches are available in XMAPTOOLS: the *normalized* and the *classical* approaches. Both of them use a K-means clustering approach, but with different X-ray intensities inputs. In the *normalized* function, X-ray intensities of each element are normalized to their mean values, with the result that all

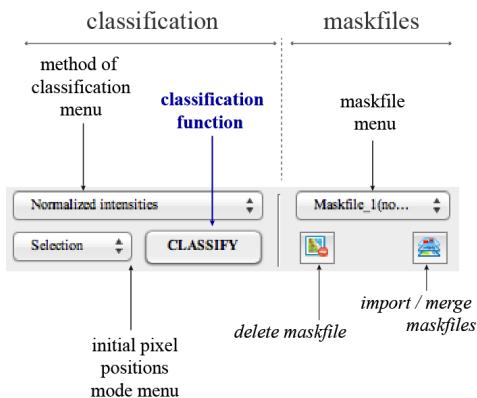


Figure 7.12 – Classification and mask file menus and buttons

elements have the same weight and only the variances are compared. In contrast, the X-ray intensities of each element in the *classical* method depend on the absolute concentration in each element. This *classical* method is therefore more appropriate for elements present in high concentration. These two automatic approaches are intensively discussed in the next section (7.2.5.1).

A manual classification is available in XMAPTOOLS and will be discussed later (see section 7.2.5.3).

7.2.5.1 Automatic classification (normalized and classical modes)

- (1) Display the map *A1* using the X-ray menu (first map) and in the classification window, select *Normalized intensities* and the mode *selection* (see Fig. 7.12). If *selection* is active the user will have to select the input pixels during the classification. The number of points clicked is interpreted by the program as the number of phases in which the pixels are classified.
- (2) Press the button *CLASSIFY* (Fig. 7.12)
- (3) Select all the X-ray maps for the classification and press *OK*
- (4) Select the following pixels (by clicking on the map, see Fig. 7.13a) to define the phases: chloritoid: $x = 66$ $y = 242$; chlorite: $x = 210$ $y = 203$; phengite: $x = 186$ $y = 119$; quartz: $x = 481$ $y = 85$ and use a right-click within the image to continue.
- (5) Set the name of the standardization to: *Maskfile_1(norm)*
- (6) The masks are generated and the mask image is automatically displayed in the main figure window (Fig. 7.13b). In this example the function fails to distinguish the pixels of quartz and the corresponding compositions are allocated to the phase 3. Pixels allocated to phase 4 are mineral boundaries between chlorite and phengite and a small mineral on the top and in inclusion in the chloritoid. In this example, the problem is due to the initial coordinates given for the phase quartz that does not have a pure quartz composition but contains Ca. This mask corresponds to a distinct phase that has been classified, indicating that a new phase must be defined for quartz. Information regarding the classification are printed out in the Command Window (Code 7.4).

```

Mask creating ... (Maskfile_1(norm)) ...
Mask creating ... (Selected maps: Al Ca Fe K Mg Mn Na Si)

```

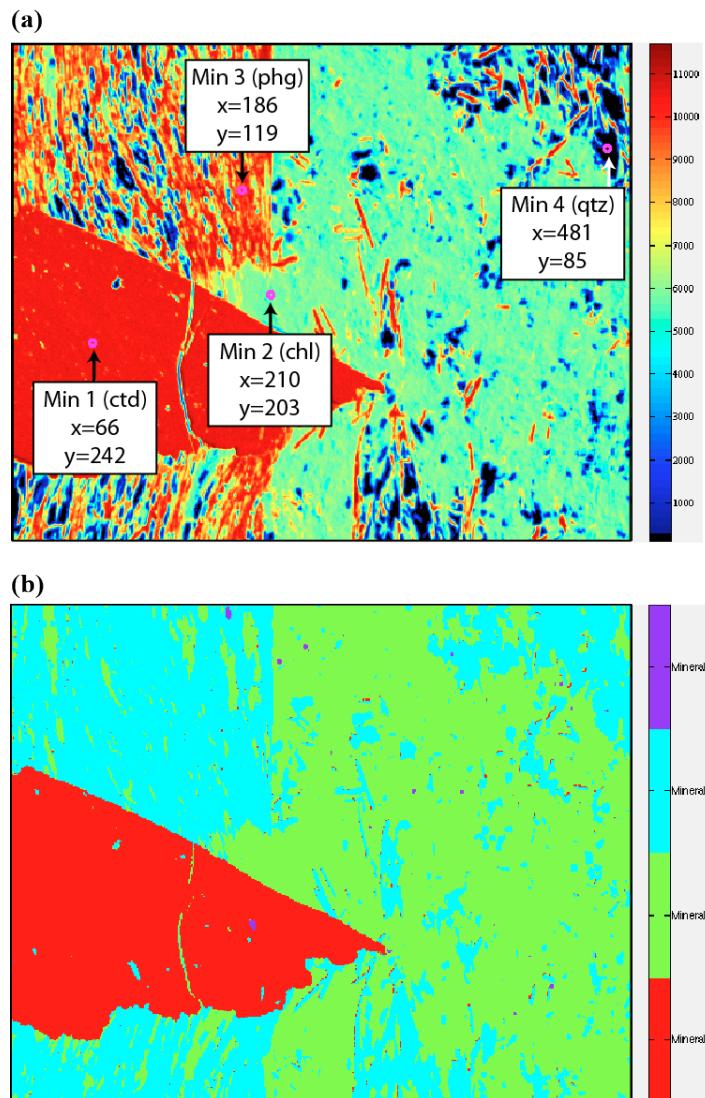


Figure 7.13 – Classification: (a) Coordinates and position of the input pixels selected by the user in order to define the compositions of the minerals (map: Al in number of counts). (b) Mask image generated using the mode Normalized intensities and the mode Selection (see [6])

```

Mask creating ... (Nb Masks: 4)
Mask creating ... (Selected Pixels: 1 Coordinates: 66/242
Mask creating ... (Selected Pixels: 2 Coordinates: 210/203
Mask creating ... (Selected Pixels: 3 Coordinates: 186/119
Mask creating ... (Selected Pixels: 4 Coordinates: 481/85
Mask creating ... (Method: Normalized intensities)
Mask creating ... (Phase: 1 name: Mineral1 < 18.9325\% >
Mask creating ... (Phase: 2 name: Mineral2 < 48.054\% >
Mask creating ... (Phase: 3 name: Mineral3 < 32.9255\% >
Mask creating ... (Phase: 4 name: Mineral4 < 0.088\% >
Mask creating ... (Maskfile_1(norm)) ... Ok

```

Code 7.4 – Text printed in the command window during the classification

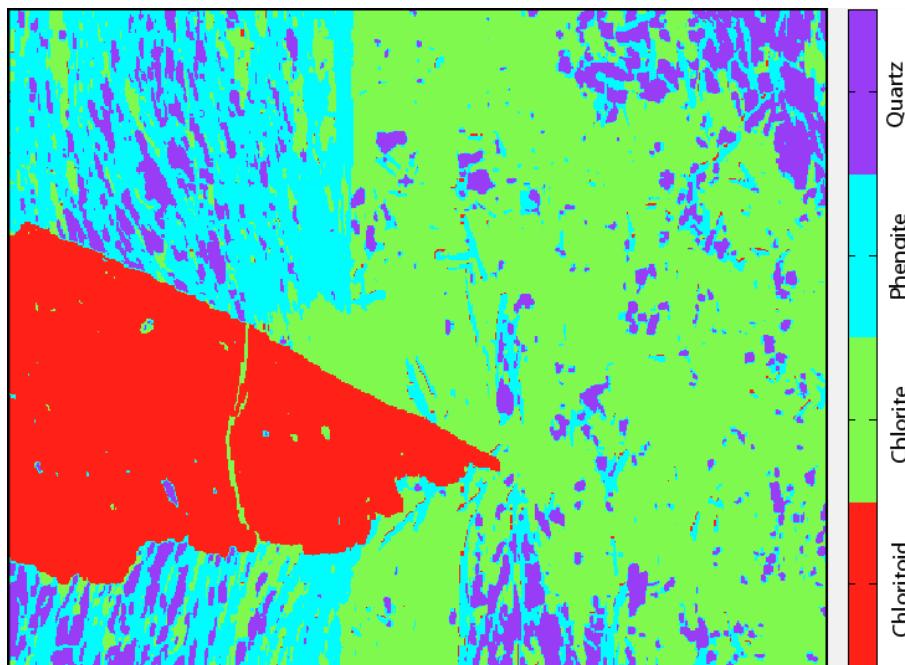


Figure 7.14 – Classification: Mask image generated using the mode Classical computation and the mode File (see [8])

- (7) The name of the phases may be edited using the function *rename phases*. Press the button (Fig. 7.12) and define the new names for each phase. In this example, phase 1 belongs to chloritoid, phase 2 chlorite, phase 3 phengite+quartz and phase 4 is a Ca-rich phase (see inclusion in chloritoid).
- (8) In your data example repertory, open the file *Classification.txt*. The names of the phases and the corresponding pixel coordinates are listed below the keyword *>1*. These names must be defined as one string chain without space.
- (9) Calculate a new mask file called *Maskfile_2(Classic)* with the mode *Classical computation* and the mode *File*. The result is displayed in figure 7.14. In this second example quartz pixels were correctly classified (note that the coordinates in the file *Classification.txt* for quartz have been edited compare to the previous example).
- (10) As the first mask file *Maskfile_1(norm)* does not distinguish quartz from chlorite, it can be deleted using the function *delete maskfile*. Select the mask file *Maskfile_1(norm)* in the *maskfile menu*. Press the button (Fig. 7.12) to delete it.

7.2.5.2 Display X-ray images of a specific phase

Once the classification is achieved a mask file is active. The menu *phase (masks)* (Fig. 7.15b) is available and the first line *none* is automatically selected. This means that all the pixels of the selected X-ray image are displayed.

- (1) Display the map *Mg* using the X-ray menu and keep *none* selected in the mask menu. Adjust the contrast by pressing the button *auto-contrast* . The result is reported in figure 7.15a. All the pixels are displayed.

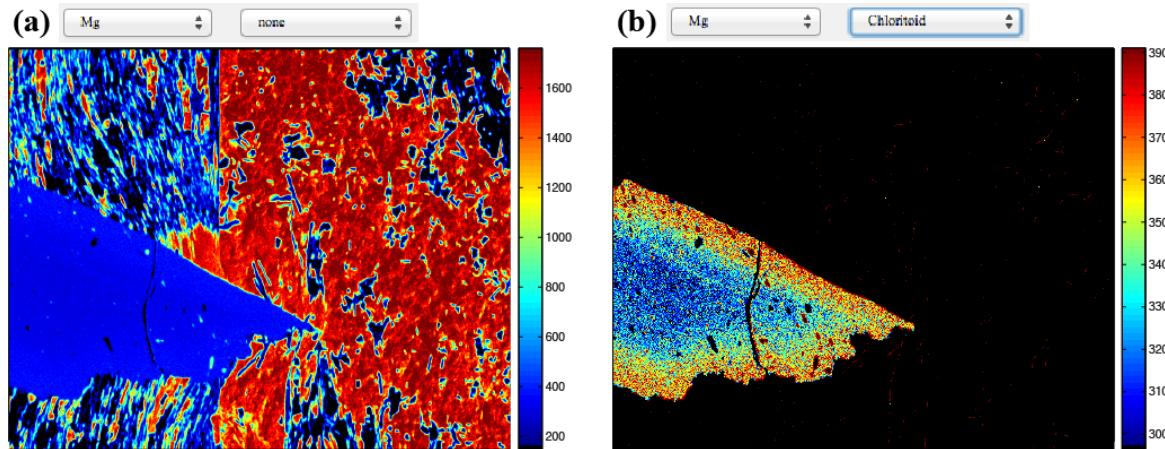


Figure 7.15 – Display X-ray image Mg (a) with none selected in the mask menu and (b) with chloritoid selected in the mask menu. The auto-contrast function has been used before to generate the images.

- (2) Select the phase *chloritoid* in the mask menu. Adjust the contrast by pressing the button *auto-contrast* . The result is reported in figure 7.15b. In this case, only the pixels that belong to the mask *chloritoid* are displayed.

7.2.5.3 Manual classification using Binary and TriPlot3D modules

The manual classification option has been developed in the framework of XMAPTOOLS 2. This method consists of defining groups of pixels (i.e. masks) for each phase by delimiting area-of-interest in chemical diagrams. The two modules *Binary* and *TriPlot3D* can be used to generate these mask files. The masks are then imported and merged in XMAPTOOLS to create a new mask file (see 7.2.5.1). This section contains the description of the procedure used to generate mask files with the *Binary* module. The module *TriPlot3D* is described later on in the tutorial.

- (1) In the workspace *X-ray*, select the map *Al* using the *X-ray* menu (first map) and the phase *none* in the mask menu.
- (2) Send the maps to the chemical module by pressing the button *Binary*.
- (3) Plot *Fe* vs *Mg* using the menus *X* and *Y* (see Fig. 7.16).

In the diagram displayed in figure 7.16, the blue dots correspond to X-ray intensity of the selected pixels. In this example, three groups of pixels can be easily identified in the *Fe* vs *Mg* diagram (Fig. 7.17). The first group enriched in Fe and Mg belongs to chlorite. The second group shows high Fe and low Mg contents belongs to chloritoid. The last group showing both low- Fe and Mg contents contains the pixels of phengite and quartz. Mixing analyses are visible between the group chlorite and the group phengite+quartz (Fig. 7.17).

One of the most important tool of *Binary* module is the *Identify pixels* function. User can select groups of pixel compositions in the binary diagram by defining a region-of-interest and display the location of the corresponding pixels in the map. In the following the mode *Single group: quick (rectangle)* of the function *Identify pixels* is used. In this mode, compositions are selected using a rectangle defined by two points.

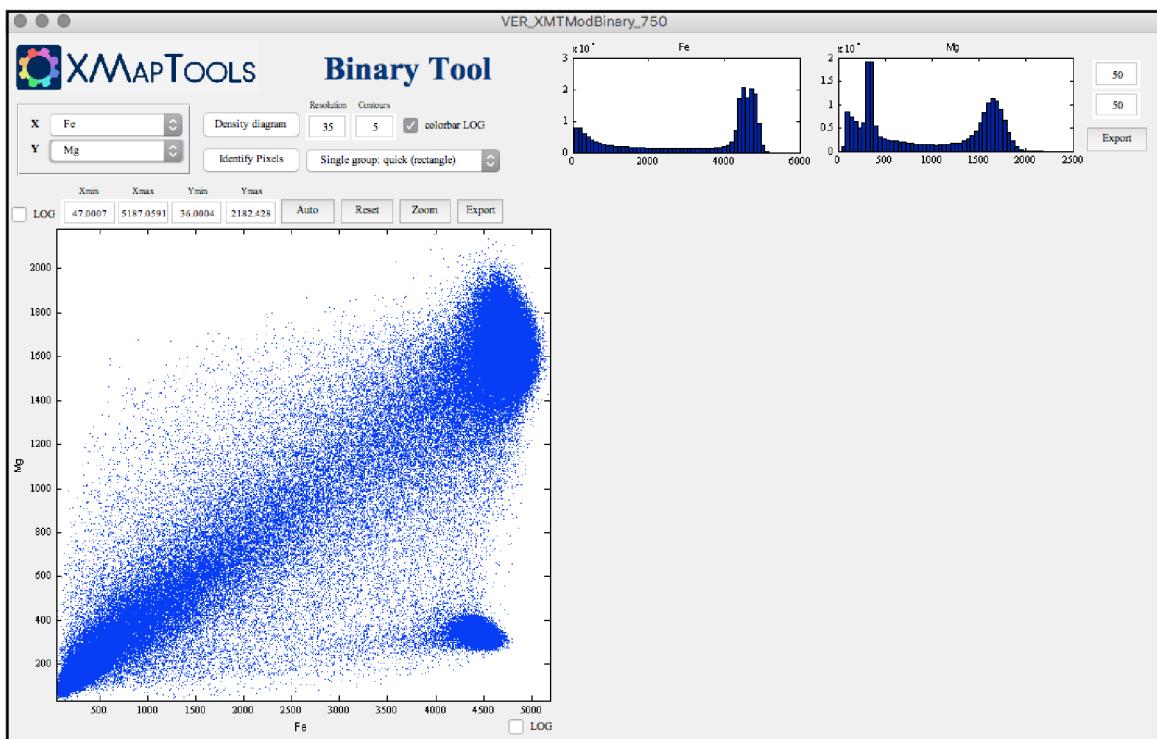


Figure 7.16 – Binary module (diagram Fe vs Mg)

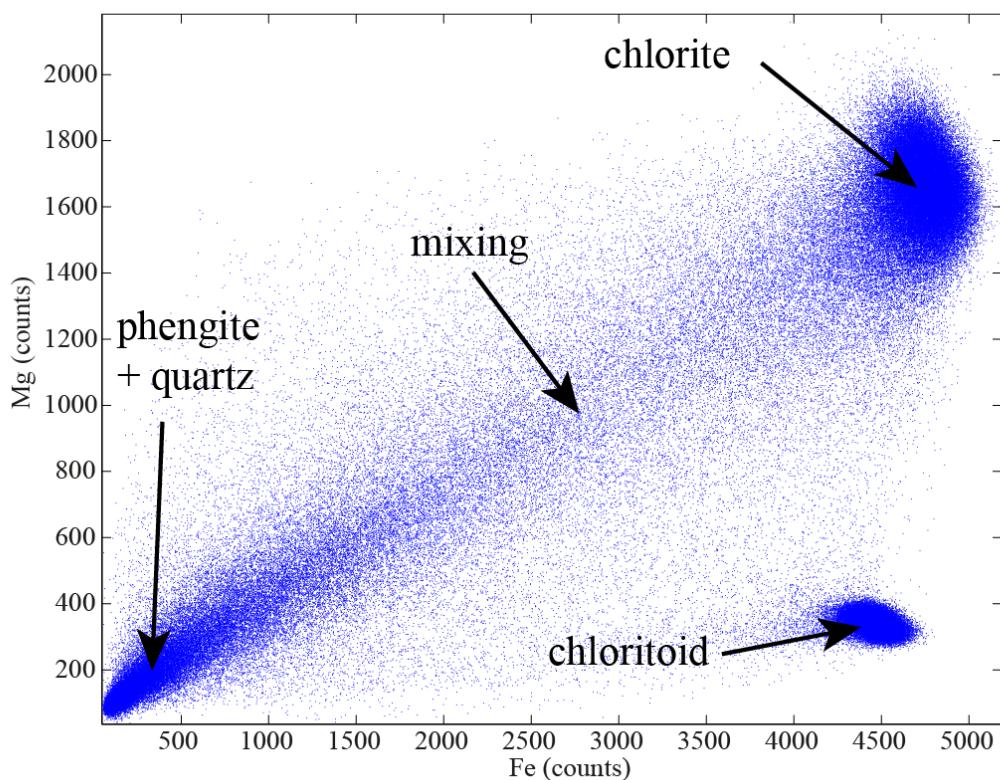


Figure 7.17 – Chemical diagram Fe vs Mg exported from the Binary diagram

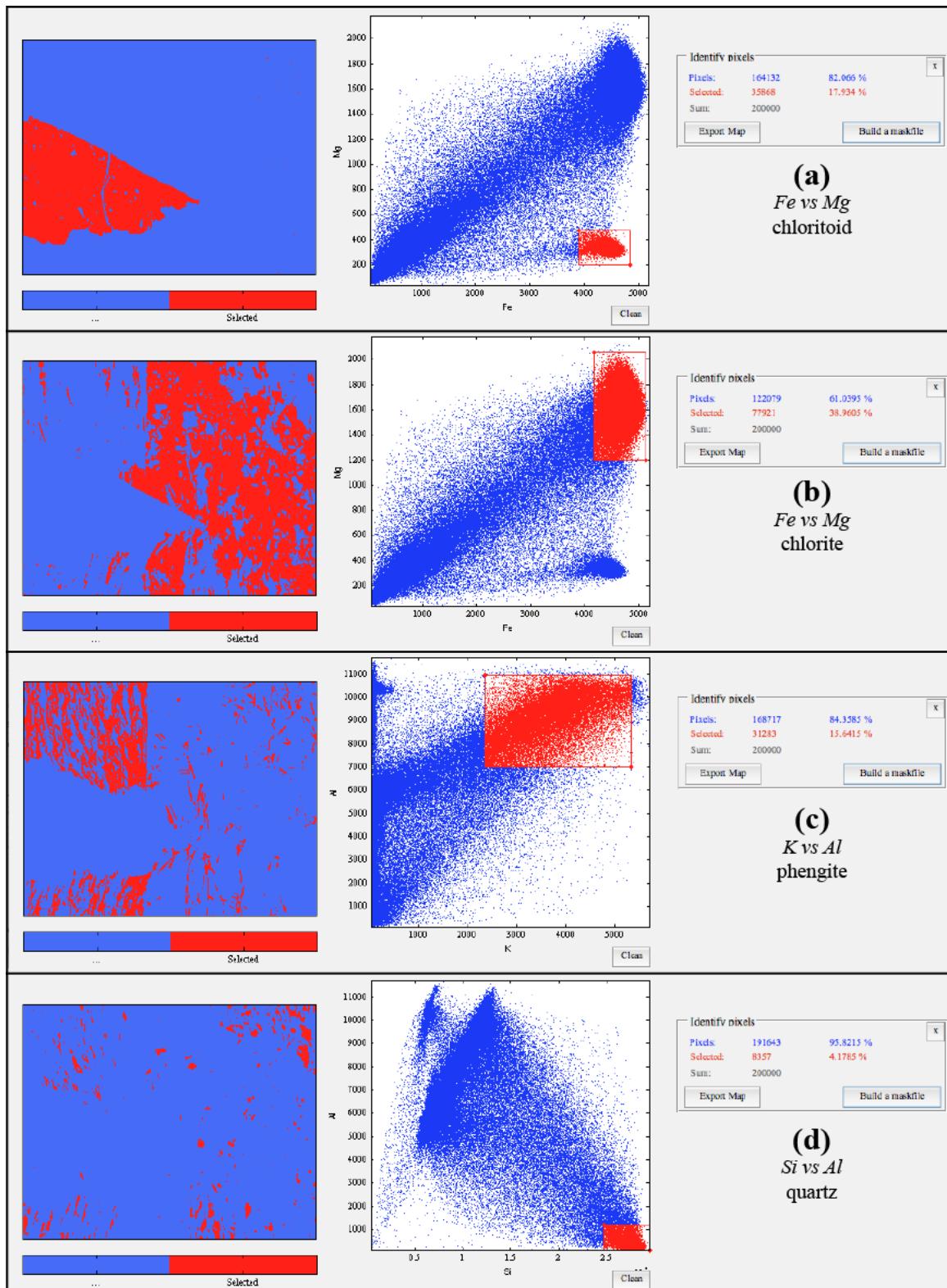


Figure 7.18 – Function identify pixels in the Binary diagram

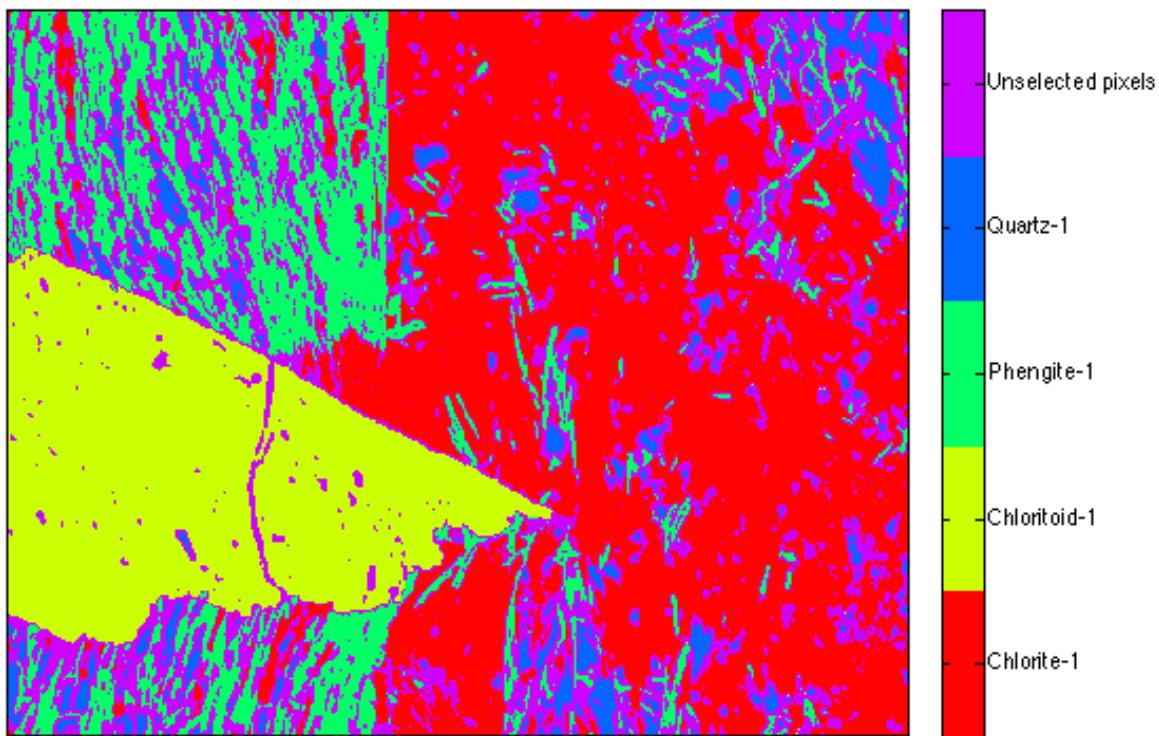


Figure 7.19 – Mask image of the mask file: *Merged-Maskfile*

- (4) Select the points belonging to the group chloritoid using the function *Identify pixels* and the mode *Single group: quick (rectangle)*. The corresponding pixels are displayed in red in a new map (Fig. 7.18a).
 - (5) Press the button *build a maskfile* and save a Mask file named *Chloritoid.txt*. NB: The file created is automatically saved in the folder *MaskFiles/*.
The same procedure is repeated for the phases identified above.
 - (6) In a diagram *Fe vs Mg* select the points belonging to the group chlorite and generate a mask file named *Chlorite.txt* (Fig. 7.18b).
 - (7) In a diagram *K vs Al* select the points belonging to the group phengite and generate a mask file named *Phengite.txt* (Fig. 7.18c).
 - (8) In a diagram *Si vs Al* select the points belonging to the group quartz and generate a mask file named *Quartz.txt* (Fig. 7.18d).
- Individual or merged Mask files can be imported in XMAPTOOLS.
- (9) Close the *Binary* module.
 - (10) In XMAPTOOLS, press the button *import and merge maskfiles* and import the mask files: *Chlorite.txt*; *Chloritoid.txt*; *Quartz.txt* and *Phengite.txt*. The new mask file is named *Merged-Maskfile*. The result is displayed in figure 7.19.

(11) Look at carefully the difference between the two mask files (automatic and manual procedures). Then select the mask file *Merged-Maskfile* and press the button *Delete maskfile*  to delete it. *Maskfile_2(Classic)* will be used in the following.

7.2.5.4 Display and export the mask image

The normal export function does not work properly with mask images. In order to display the selected mask image in a new window, press the button *Export mask image* (the one in the horizontal menu of the X-ray workspace) .

7.2.6 Corrections

The full description of all corrections available in XMAPTOOLS is provided in the section [3.8.4](#).

Work in progress.

7.2.7 Standardization

When all required steps are accomplished it is possible to process to the analytical standardization, i.e., to transform each phase X-ray maps into maps of weight percentage oxide concentration. More details about the process are given in XMAPTOOLS' papers of [Lanari et al. \(2014b\)](#) and [Lanari et al. \(2019\)](#).

7.2.7.1 Importing spot analyses

The spot analyses to be used for the analytical standardization are stored in the file *Standards.txt*. The method used to create such file is detailed in section [2.7.6](#) and is not discussed in the tutorial.

- (1) In the *X-ray workspace*, display the map *Al* and select the phase *none*.
- (2) Use the function *import standard file* to open the standard file (Fig. [7.20a](#)).
- (3) As a file *Standards.txt* exists in the working directory, XMAPTOOLS suggests to open that file (Fig. [7.20b](#)). Press *yes*.
- (4) The spots analyses stored in *Standards.txt* have been imported and are plotted in the map displayed in the main window (Fig. [7.20d](#)). The group of buttons for internal standards has also been updated (Fig. [7.20c](#)).
- (5) Hide the spots analyses using the function *hide standards* and display them again using the function *display standards*

7.2.7.2 Position of spot analyses and SPC correction

- (1) Display the map *Si* and select the phase *none*.
- (2) Display the spot analyses using the function *display standards*
- (3) Use the function *display intensity vs composition chart* to compare the spectra of *Si* (counts) and *SiO₂* (wt-%). The result is reported in figure [7.23](#) (case: original position). The correlation coefficient between the two spectra is 0.78 (see Code [7.5](#)).

```
Standards testing ... (Element: Si) ...
Standards testing ... (Correlation: 0.77956)
Standards testing ... (Element: Si) .... Ok
```

Code 7.5 – Text printed in the command window by the function *display intensity vs composition chart*

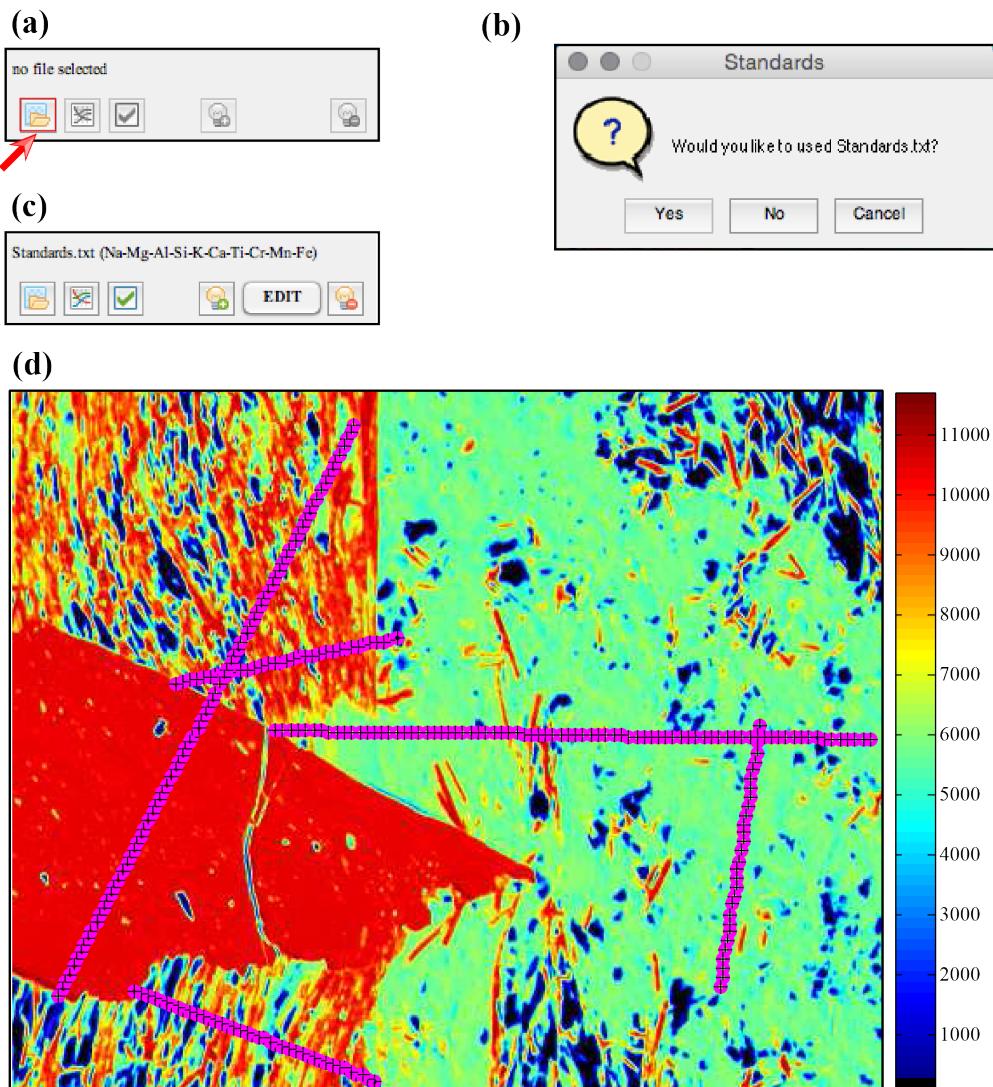


Figure 7.20 – Procedure to load standards. (a) Group of buttons for internal standards (no standard file) (b) If a file Standards.txt exists in the working directory, the program proposes to open that file. (c) Group of buttons for internal standards (standard file loaded). (d) Map of Al with the spot analyses that are used as internal standards.

- (4) Use the function *check quality of std/maps positions* to test the position of the internal standard analyses and the X-ray maps. Use X and Y shifts of 10 pixels each (Fig. 7.21).

The spots analyses are displaced from (-10,-10) to (+10,+10) and a correlation coefficient is calculated for each position. The result is a map of 20×20 pixels for which the center pixel (0,0) is the original position of the spot analyses (marked by a black star in Fig. 7.22).

The function display in new figures windows: (1) the correlation map for all the selected elements and (2) the image of the sum of square of correlation coefficients. In case of good correlation, the second map is likely to indicate the best position of the spot analyses. In this example, it comes out that the spot analyses are shifted of $X = -1$ and $Y = +2$.

- (5) Select the correction *SPC* in the correction menu and press *activate* to activate the correction mode. Press *No*, because you do not need to check again the quality of std/maps positions (see step

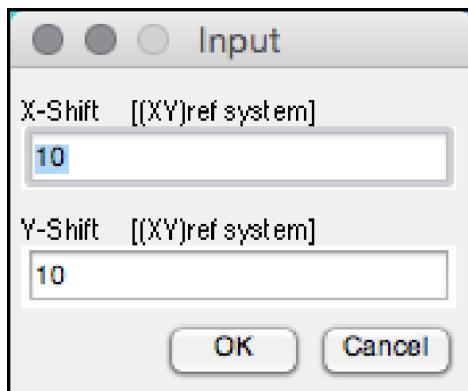


Figure 7.21 – Window to define X and Y shifts

4). Use the X-pad navigator (left hand side) to move the spot analyses of *one* pixel rightward and *two* pixels downward. Please wait for figure update before to press again on of the arrow button.

(6) Press *Apply* button located below the X-pad navigator in order to apply the correction. The correction is printed in the MATLAB Command Window (see Code 7.6).

```
SPC ... [ Standard Position Correction ]
SPC ... X correction of 1 pixels applied ... OK
SPC ... Y correction of 2 pixels applied ... OK
SPC ... Done
```

Code 7.6 – Text printed in the command window by the standard position correction function (SPC)

(7) Use the function *check quality of std/maps positions* to test again the position of the internal standard analyses and the X-ray maps. As before, use X and Y shifts of 10 pixels each (Fig. 7.21). The results are reported in figure 7.23 (case: corrected positions).

The new correlation coefficient between Si and SiO₂ spectra is 0.94.

(8) Save the project.

The new positions of spot analyses are saved. If you want to retrieve the original positions, you must load again the file *Standards.txt* or apply a inverse correction.

7.2.7.3 Select/unselect internal standards: chloritoid

In order to select or unselect spot analyses of chloritoid, repeat the following strategy as many times as necessary:

- (1) Display the map *Si* and select the phase *chloritoid*.
- (2) Display the spot analyses using the function *display standards*

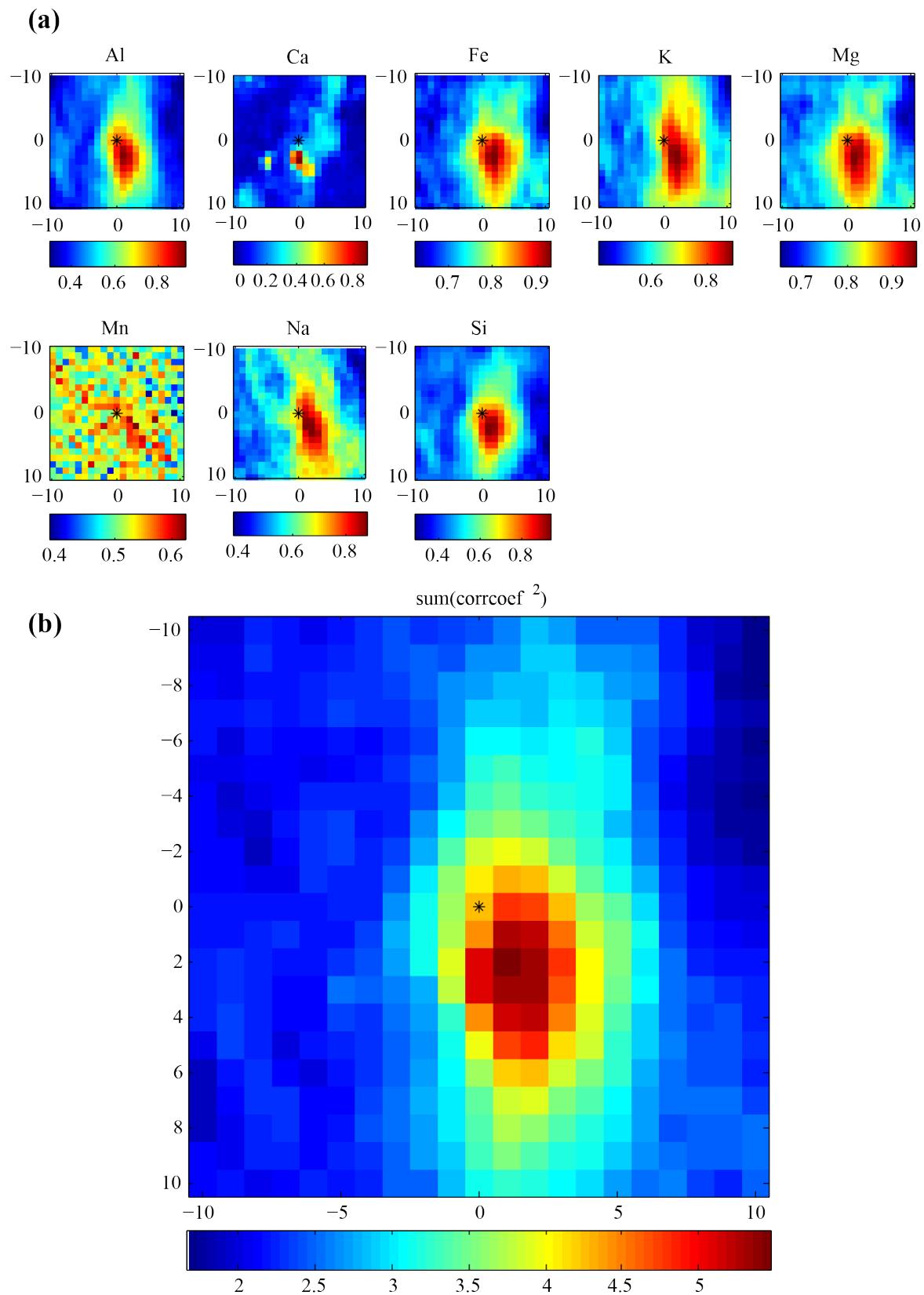


Figure 7.22 – Results of the check quality of std/maps positions

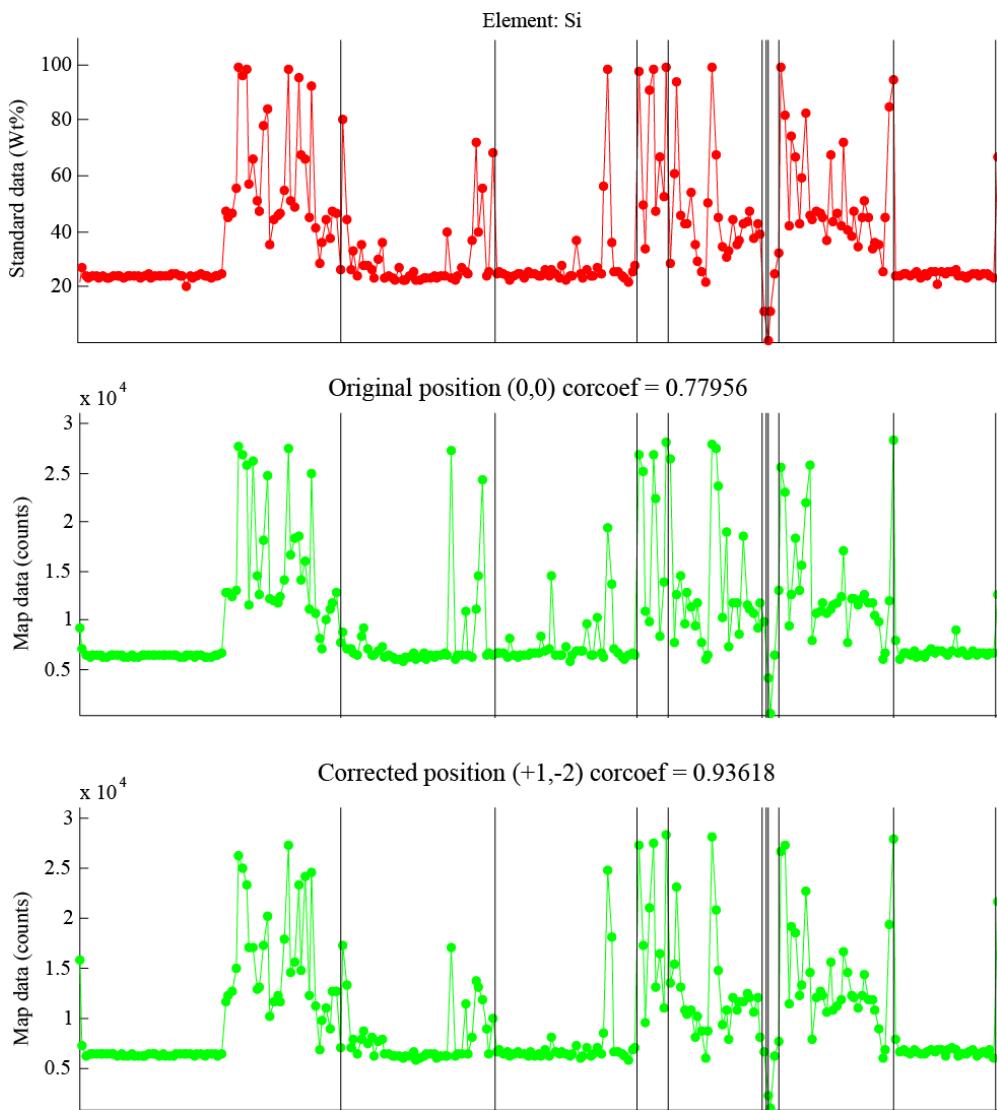


Figure 7.23 – Results of display intensity vs composition chart for the original and corrected positions

- (3) Use the zoom tool to restrict the view to an area of interest (Nb: The zoom option is deactivated during the selection mode). To use the zoom, click on the image and drag the mouse to define a rectangle, or just click onto the image to zoom in.
- (5) Press the button *select/unselect standard (Edit)* to activate the selection mode
- (6) selected/unselected spot analyses (internal standards) by clicking directly on the map close to the spot. Please wait for the figure update before to select/unselect the next spot. In this example it is necessary to delete the spot analyses located near the grain boundaries (Fig. 7.24).
- (9) Display the spot analyses using the function *display standards*
- (10) Save the project.

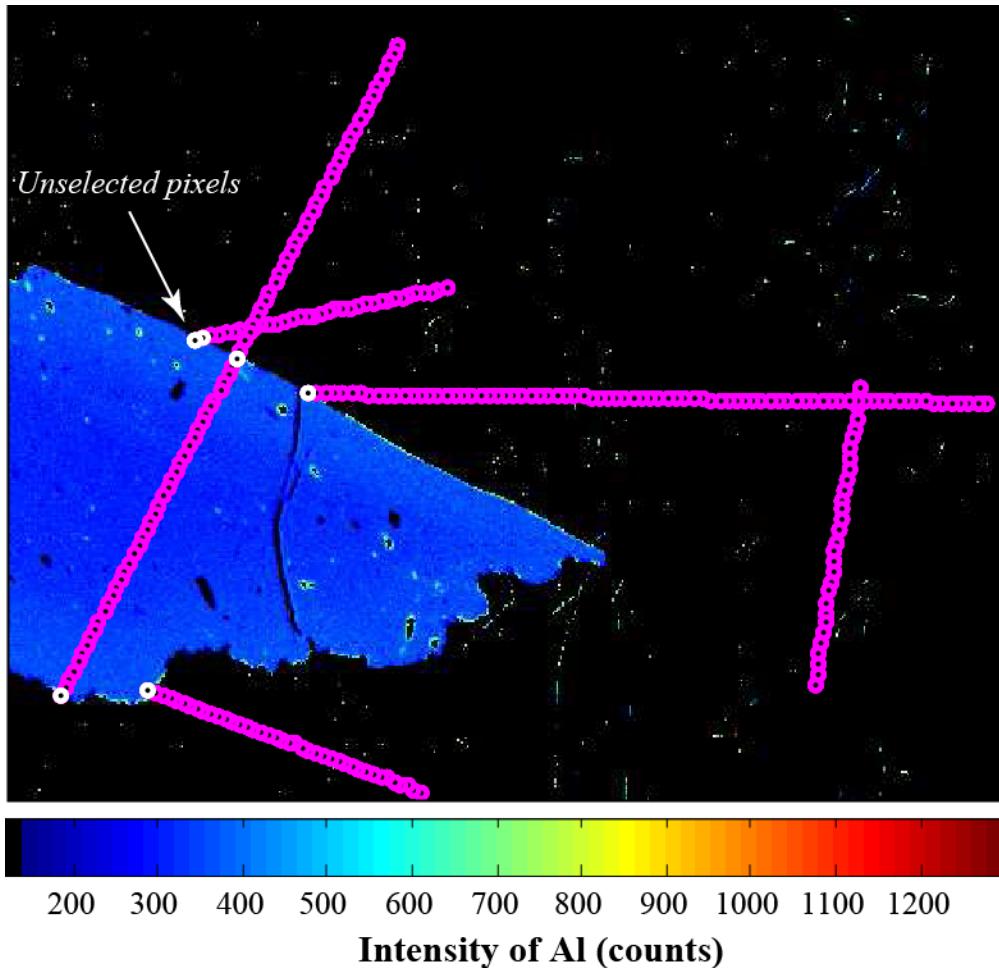


Figure 7.24 – Internal standards for chloritoid. Note that the spot analyses near the grain boundaries are unselected (white circles)

7.2.7.4 Select/unselect internal standards: chlorite

In order to select or unselect spot analyses of chlorite, repeat the following strategy as many times as necessary:

- (1) Display the map *Si* (or alternatively *Fe* or *Ca*) and select the phase *chlorite*.
- (2) Display the spot analyses using the function *display standards*
- (3) Use the zoom tool to restrict the view to an area of interest (Nb: The zoom option is deactivated during the selection mode)
- (5) Press the button *select/unselect standard (Edit)* to activate the selection mode
- (6) selected/unselected spot analyses (internal standards) by clicking directly on the map close to the spot. Please wait for the figure update before to select/unselect the next spot. In this example it is necessary to delete the spot analyses located near the grain boundaries (Fig. 7.25).

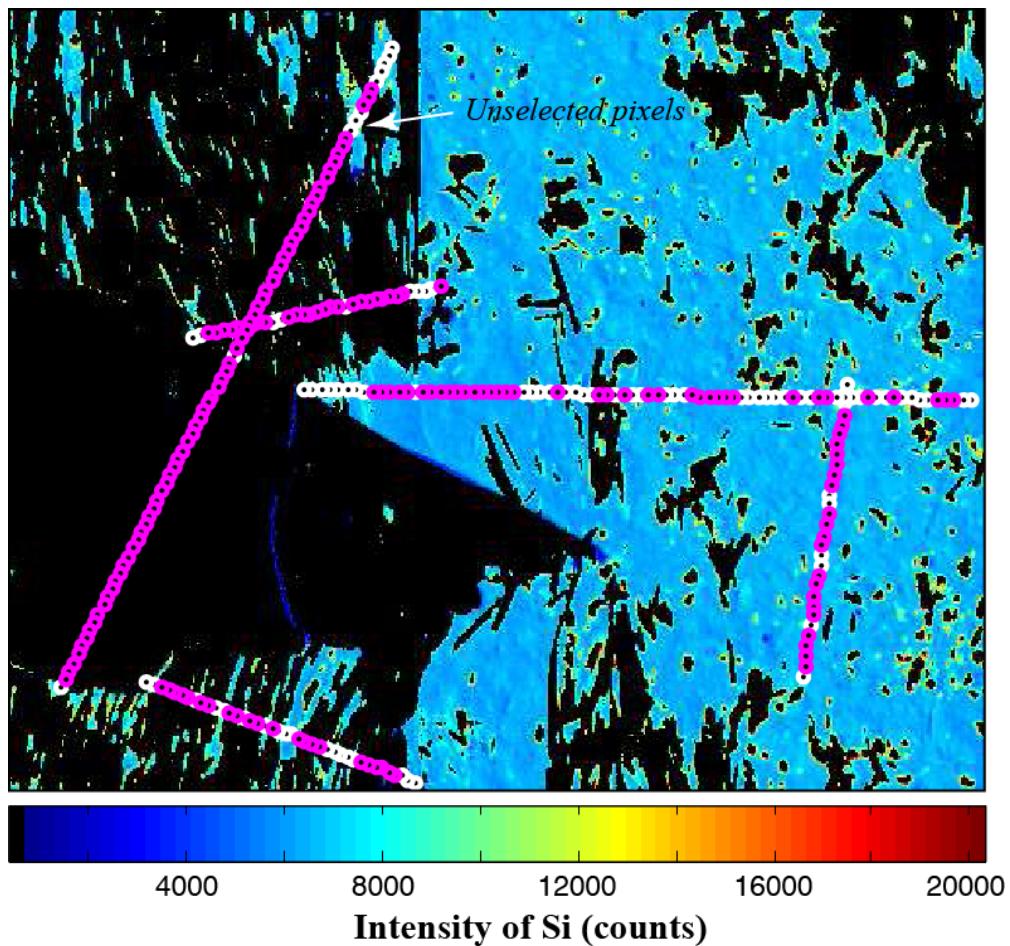


Figure 7.25 – Internal standards for chlorite. Note that the spot analyses near the grain boundaries are unselected (white circles)

- (7) Display the spot analyses using the function *display standards*
- (8) Save the project.

7.2.7.5 Advanced standardization: chloritoid

Many spot analyses have been measured for this map and it is important to unselect the analyses located near grain boundaries or mineral inclusions before proceeding to the analytical standardization (see §7.2.7.3 for chloritoid).

- (1) Select the phase *chloritoid*, the standardization method *Advanced Standardization* and press the button *STANDARDIZE*. Note that this button is only available when a phase is selected. Use the name proposed by the program for the standardized phase; Select all the elements to be standardized.
- (2) The advanced standardization module opens (see Fig. 7.26). The element can be selected in the main menu. The standards concentrations (wt-%) are plotted against the intensities of the corresponding pixels in the standardization diagram (upper right diagram). The automated background detection diagram shows (left) shows the evolution of the residuals (square root of the sum of

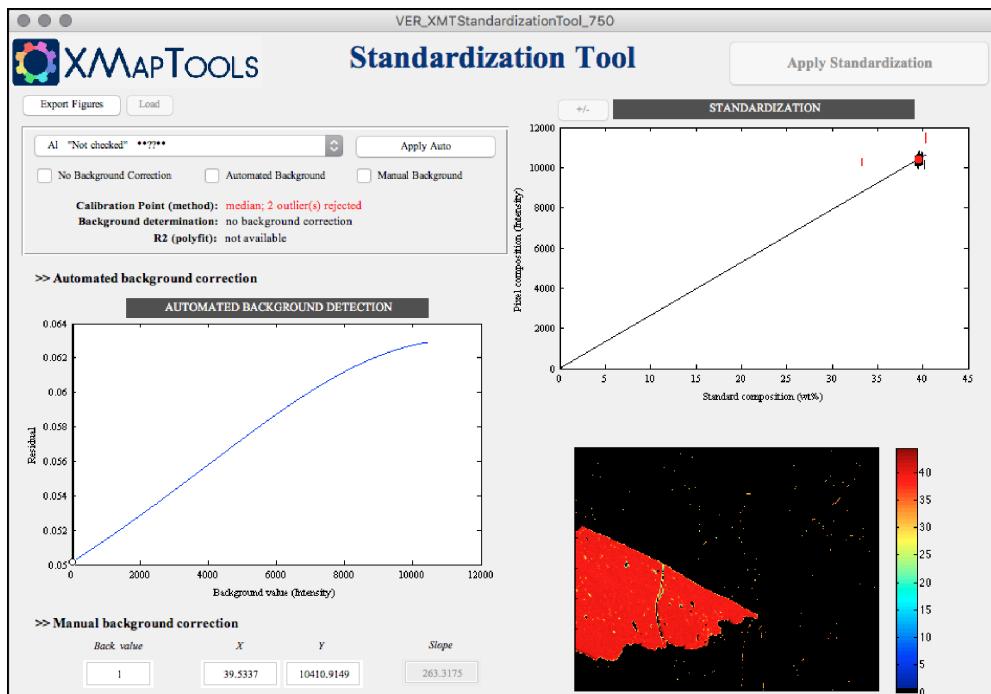


Figure 7.26 – Advanced standardization tool

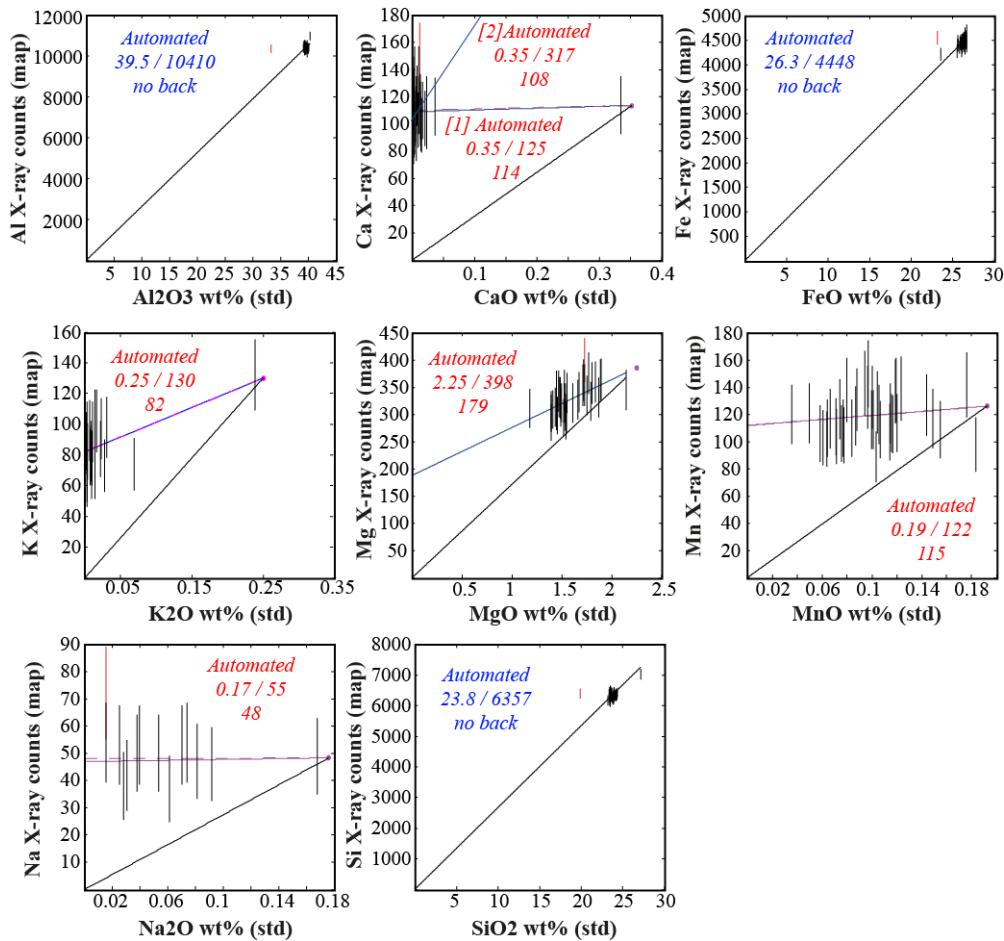


Figure 7.27 – Standardization diagrams for chloritoid

the square of distances between the curve and the model) with the background value. The map on the lower right panel shows the calibrated map for the corresponding oxide of the selected element.

(3) Select the first element Al and press the button *Apply Auto*. The program calculate the best standardization curve and update the display located below the menu. In this example, there is no background correction and the calibration curve is defined by the point $X = 39.53$ wt%; $Y = 10410$ counts (Figs. 7.26 & 7.27). Note that the figures can be slightly different if a different set of spot analyses are used.

(4) Select the next element Ca and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point $X = 0.35$ wt%; $Y = 125$ counts; a background value of 114 counts is estimated ([1] in Fig 7.27). A warning message is displayed as there are 3 pixels with concentration of CaO above 110 %. This is unrealistic for this example and it suggests that the spot analysis with a concentration of $CaO = 0.32$ wt% is an outlier. Press the button $+/-$ and click onto this point. The new calibration curve is defined by the point $X = 0.35$ wt%; $Y = 317$ counts; a background value of 108 counts is estimated ([2] in Fig 7.27). This is more realistic and the highest concentration of CaO shown in the map has changed to 7 wt%.

(5) Select the next element Fe and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point $X = 26.3$ wt%; $Y = 4448$ counts; no background correction needed (Fig. 7.27).

(6) Select the next element K and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point $X = 0.25$ wt%; $Y = 130$ counts; a background value of 82 counts is estimated (Fig 7.27). The K_2O composition of a few mixing pixels in the matrix is between 10 and 13 wt% (see the map in the *Standardization tool*). These values are realistic for pixels of phengite that might have been misclassified.

(7) Apply the automated technique to define the calibration curves of the next elements (Mg, Mn, Na, Si) and compare the results with those shown in Figure 7.27.

The analytical standardization of Si, Al and Fe do not required any background correction because of the high intensity-to-background ratios (Lanari et al. 2019). The spot analyses used as internal standards are indeed already corrected for background and the background effects on the calibration curve are negligible. On the contrary, the elements with a low intensity-to-background ratios such as Mg and Mn requires a background correction to obtain an accurate calibrated map (Fig. 7.27). In this example, the calibration curves for Ca, Na and K are almost horizontal indicating that those elements were below detection limit for the mapping conditions (Lanari et al. 2014b).

(8) Once all the calibration curves haven been defined, press the button *Apply Standardization* (Fig. 7.26).

(9) Export the standardization parameters. The file *Chloritoid_advanced_DATE_TIME.txt* (with DATE and TIME the current date and time) will be stored in the folder .../Standardization/.

(10) The program applies the calibration to the X-ray maps and generate a map of oxide weight percentage that is then shown in the workspace *Quanti*.

(11) Save the project.

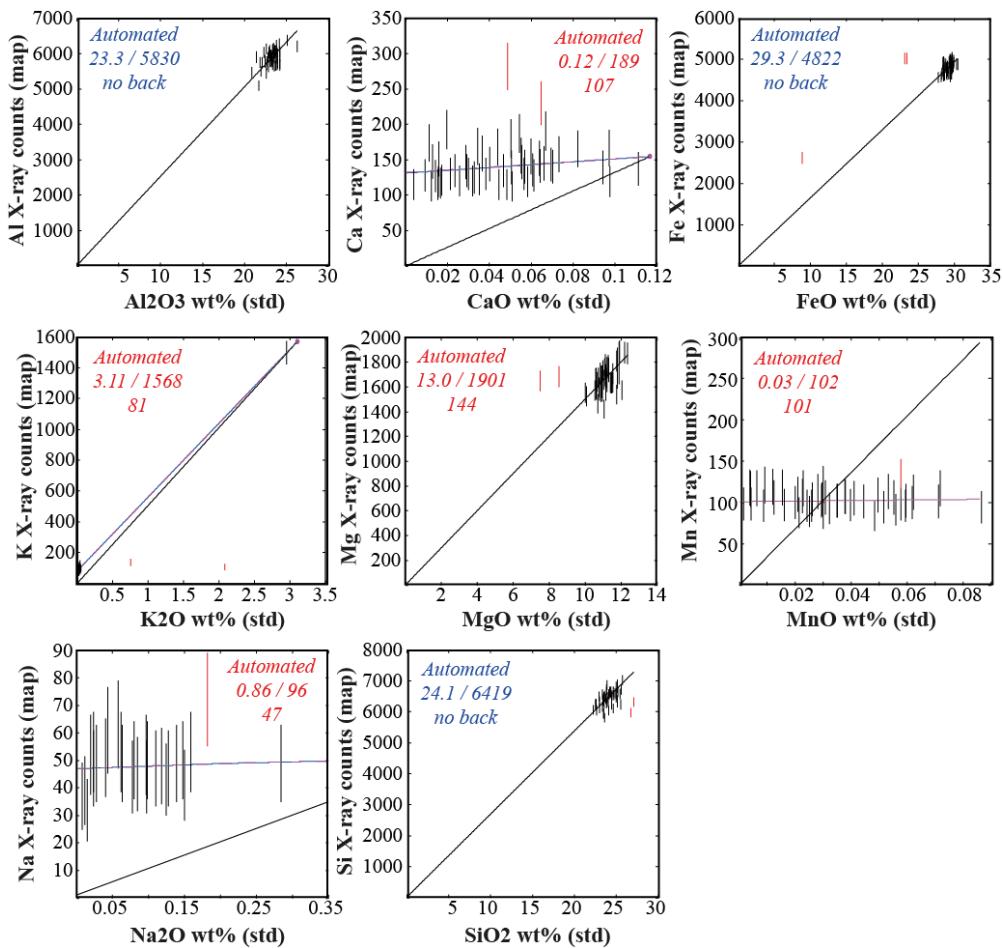


Figure 7.28 – Standardization diagrams for chlorite

(12) Check the quality of standardization using the function *Generate the oxide wt% sum map* Σ

7.2.7.6 Advanced standardization: chlorite

- (1) In the workspace *X-ray*, select the phase *chlorite*, the standardization method *Advanced Standardization* and press the button *STANDARDIZE*. Use the name proposed by the program for the standardized phase; Select all the elements to be standardized.
- (2) Use the automated procedure to define the calibration curves of all the elements and compare the results with Figure 7.28.
- (3) Once all the calibration curves have been defined, press the button *Apply Standardization* (Fig. 7.26) and save the standardization parameters.
- (4) Check the quality of standardization using the function *Generate the oxide wt% sum map* Σ
- (5) Save the project.

7.2.7.7 Manual (homogeneous phase) standardization: quartz

- (1) In the workspace *X-ray*, select the phase *quartz*, the standardization method *Manual (homogeneous phase)* and press the button *STANDARDIZE*. Use the name proposed by the program for the standardized phase; Select all the elements to be standardized.
- (2) In the input windows, set a value of 100 (wt%) for SiO_2 and press *OK*.

The program used a calibration point of $X = 100$ (wt%), $Y = 24123$ counts (median value of the Si for the mask quartz) and a background of 0 to calibrate the map. Note that this value can be obtained using the function *Display "Info" window*  in the workspace *X-ray*.

The problem in this example is that the interiors of the quartz grains exhibit significantly higher intensity of 28500 counts. In the standardized map of quartz the SiO_2 concentration of these interiors is overestimated by 5-10 %. To solve this issue we are going to lower the calibration value of quartz.

- (3) Delete the standardized map *Quartz-homog* using the function *Delete Quanti file* 
- (4) Come back to the workspace *X-ray*, select the phase *quartz*, the standardization method *Manual (homogeneous phase)* and press again the button *STANDARDIZE*. Use the name proposed by the program for the standardized phase; Select all the elements to be standardized.
- (5) In the input windows, set a value of 85 (wt%) for SiO_2 and press *OK*.
- (6) In the workspace *Quanti*, check the concentration of SiO_2 in quartz.
- (7) Save the project.

7.2.7.8 The problem of white mica

In this example, it is not possible to standardize the maps of white mica. The reasons are the following:

- The potassium in white mica was volatilized during the acquisition of the spot analyses, as they were measured with a current of 20 nA and a beam size too small ($1 \mu m$). In the file *Standards.txt*, the values of K_2O range between 4 and 6 wt% whereas they should be around 10 wt%. The map cannot be accurately standardized if the internal standards are not accurately measured.
- The compositional zoning in white mica occurs on a very small scale ($< 2 \mu m$) and the position of the spot analyses measured along the transects is not accurate enough to ensure a good standardization. In this case it is important to use BSE images to locate a few spot analyses in specific areas inclusion free and showing more homogeneous composition.

Try to filter the spot analyses in phengite (see §7.2.7.3) to obtain a cluster in the standardization tool. This is not possible.

For the following sections of the tutorial, the phengite pixels are ignored.

7.3 QUANTI WORKSPACE

7.3.1 How to generate concentration maps and extract local bulk compositions?

When all the phases have been standardized, it is possible to merge the *Quanti* files to obtain maps of mass concentration in oxide weight percentages. Local bulk compositions can be extracted from specific area, provided that the maps are corrected for density [Lanari and Engi \(2017\)](#).

7.3.1.1 Merge function

- (1) Press the button *merge standardized phases*  [B2401] to merge *Quanti* files. Select the three *Quanti* files available in this example (see Fig. 7.29a). While the button *OK* is pressed, standardized map containing the pixel compositions (in oxide weight percentage) for all the selected phases is generated.

Nb: The function *merge standardized phases* [B2401] sums up the selected standardized phases. This functions does not check if the same phase is selected twice, e.g. same phase calibrated using two different standardization methods. If the composition of a given pixel is provided twice or more, the result will simply show the sum of compositions.

7.3.1.2 Quanti files of specific areas

- (1) Duplicate the *Quanti* file *Merged_Map* using the button *Duplicate Quanti file*  [B2106] (Fig. 7.30a). A new *Quanti* file labeled *Merged_Map_copy* is created (Fig. 7.30b).
- (2) Use the function *select and area and delete the pixels inside*  [B2410] (Fig. 7.30c) to remove pixels of any domain that is not in the area-of-interest from which you want to extract the local bulk composition. In this example we want to remove the pixels of the two domains containing the phengite (areas 1 and 2 in Fig. 7.30d). It is important to keep in this layer only the pixel compositions to be averaged to estimate the local bulk composition as the function applying the density correction needs to evaluate the average density of the selected domain ($\rho_{mixture}$ in Eq. 3.24).

7.3.1.3 Density map and density correction

As discussed in [Lanari and Engi \(2017\)](#), it is necessary to apply a density correction prior exporting any local bulk composition. Note that the functions described below use the mask file selected in the workspace *X-ray* to apply this density correction.

- (1) The average density of each mineral phase can be defined in the file *Classification.txt* as shown in the example 7.8 below. Density of phengite is set to zero as phengite pixels are not used in this example. The density values are taken from the website *webmineral*. Minor density variations with P and T and within a given solid solution are neglected. The order must be the same as the one used to define the mineral phases below the keyword *>1*. Each row should contain a single number.

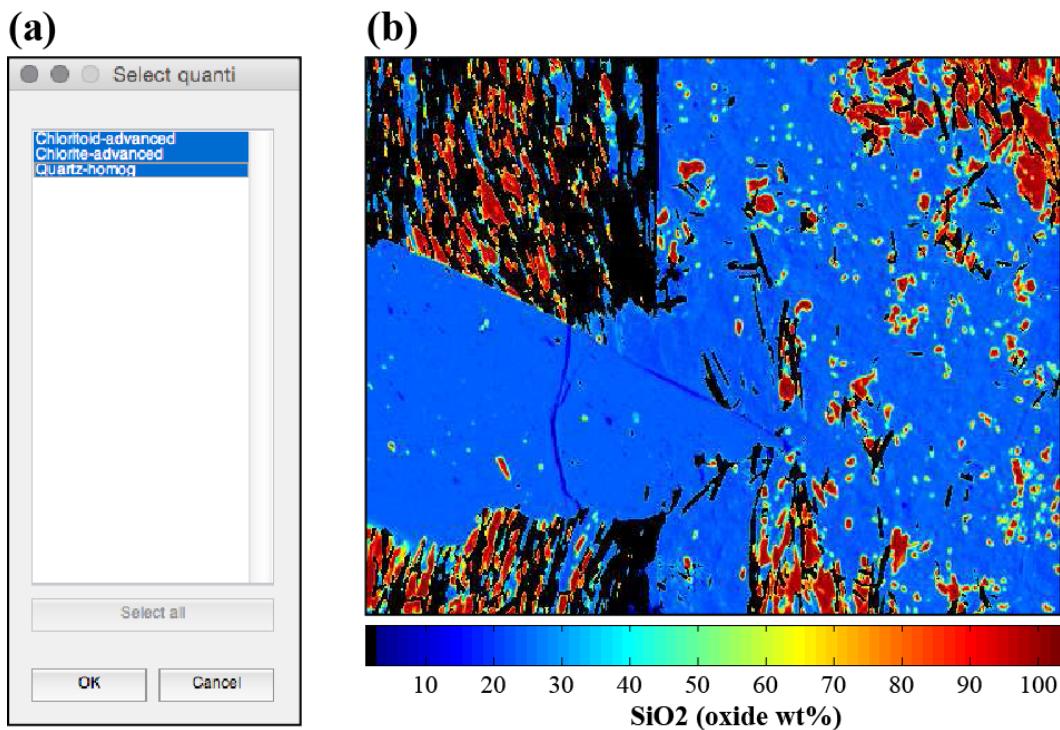


Figure 7.29 – Merge 'Quanti' files. (a) Select the maps. (b) map of silica

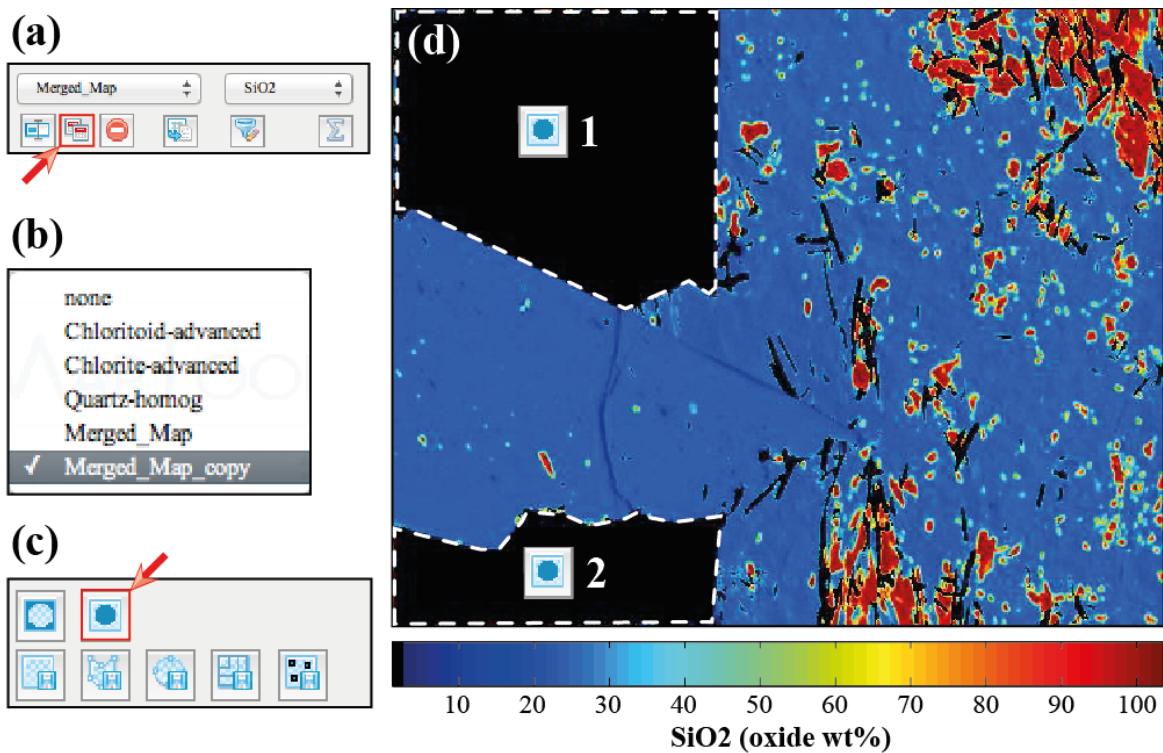


Figure 7.30 – (a) Duplicate the Quanti file 'Merged_map'. (b) The 'Quanti' file 'Merged_Map' has been duplicated. (c) Function used to delete the selected pixels of an area. (d) The pixels of two domains (labeled 1 and 2) have been deleted, i.e. they will not be used to extract the local bulk composition.

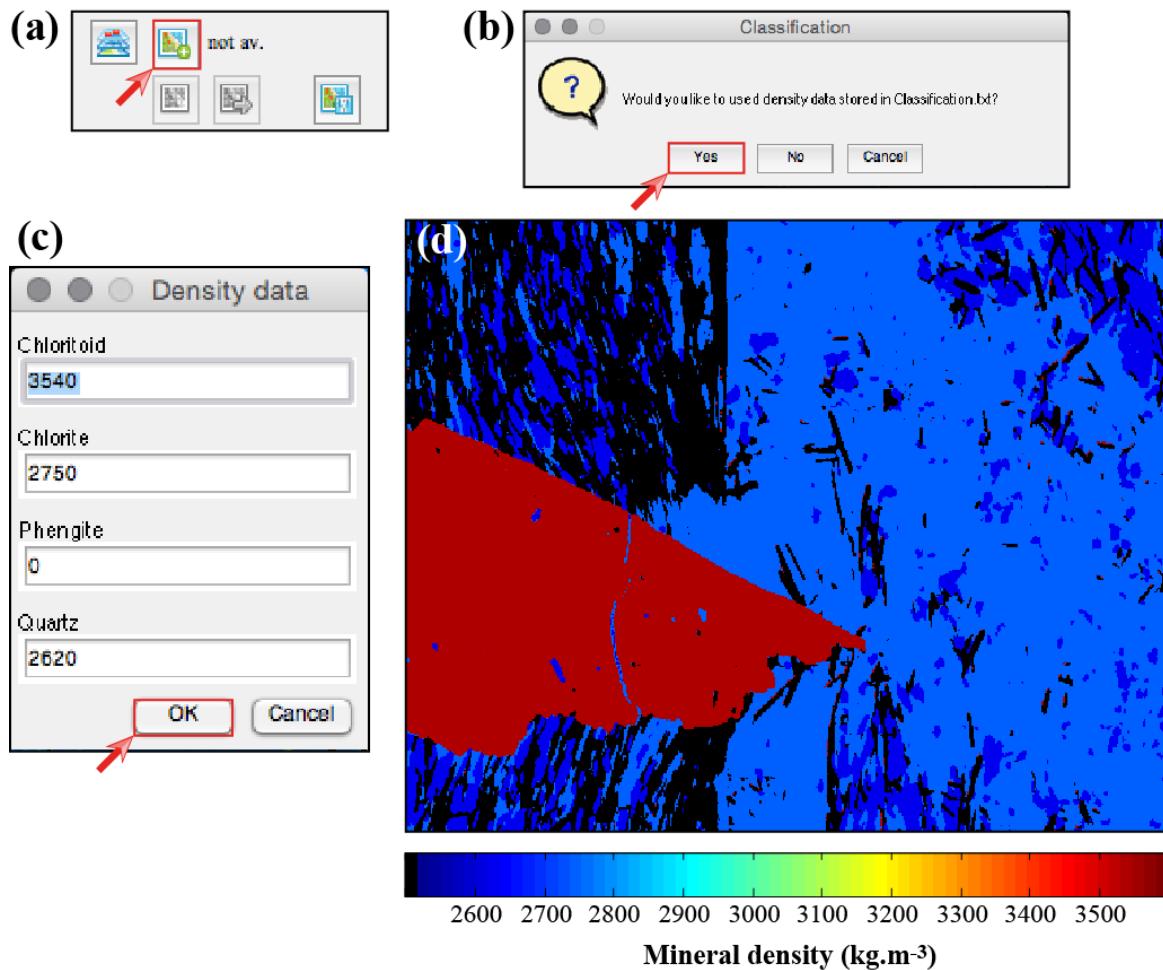


Figure 7.31 – (a) Define a new density map (b) Read the density data stored in the file Classification.txt. (c) Density values for each phase. (d) Density map used to apply the density corrections.

```
>1 Put below the list of | Mask_Name | X | Y | ...
Chloritoid    66    242
Chlorite      210   203
Phengite      186   119
Quartz        480   78

>2 density of phases taken from webmineral (same order as >1)
3540
2750
0
2620
```

Code 7.7 – Density of the mineral phases listed in the file Classification.txt. Note that the mineral order must be the same as in the one of the first block

- (2) Generate a density map from the mask file selected in *X-ray* (the correct mask must be selected in the workspace *X-ray* as there is no mask menu in the workspace *Quanti*; important!) using the function *generate a density map (from selected mask file)* [B2406] (Fig. 7.31a). The program reads the density data stored in *Classification.txt*, provided that this option is activated (Fig. 7.31b). The density values can be edited in the input dialog-box shown in Figure 7.31c.

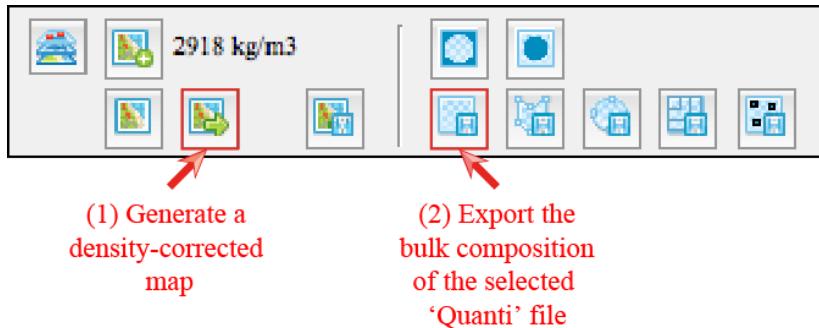


Figure 7.32 – Buttons to apply the density correction and export local bulk compositions

- (3) You can display the density map any time (Fig. 7.31d) by pressing the button *display the density map* [B2407].

7.3.1.4 Density-corrected maps and local bulk composition

- (1) Generate a density-corrected map *DCM_Merged_Map_Copy using the function *compute a density-corrected oxide map* [B2408].

Note: This map should only be used to export local bulk compositions because each pixel is multiplied by $\frac{\rho_i}{\rho_{mixture}}$. The sum is not anymore 100 wt-%. The name of this Quanti file begins with *DCM- to remember you to not use it for other purpose. There is a warning if you try to use this density-corrected map for structural formula. It is strongly recommended to delete this map after exporting the bulk composition.

- (2) The composition of this specific domain may be exported using the function *export local composition: map* [B2402] (Fig. 7.32).

7.3.1.5 Local bulk composition and effects of the density correction

- (1) Export the local bulk composition from the following maps: *DCM_Merged_Map_Copy and Merged_Map_Copy using the function *export local composition: map* [B2402].

The results are shown in the insert 7.8. If no density correction is applied for this example, the Al contained in the chloritoid is significantly underestimated.

Elem .	DCM	noDCM
Al ₂ O ₃	25.7	22.8
CaO	0.36	0.32
FeO	24.3	22.4
K ₂ O	0.29	0.28
MgO	6.73	6.57
MnO	0.07	0.07
Na ₂ O	0.52	0.48
SiO ₂	30.8	29.4

Code 7.8 – Comparisons between local bulk composition determined for *DCM_Merged_Map_Copy (DCM) and Merged_Map_Copy (noDCM).

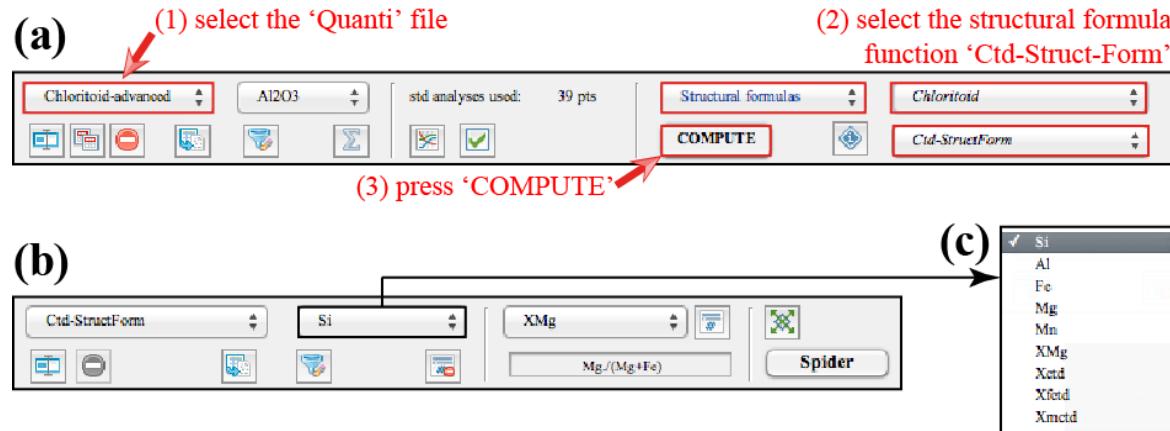


Figure 7.33 – Computation of structural formula maps: chloritoid. (a) select the ‘Quanti’ file and the external function Ctd-Struct-Form. (b, c) Buttons and menu of in the workspace Results.

7.3.2 Structural formulas and thermobarometry

When all the phases have been standardized, it is possible to compute maps of structural formulas (in atoms per formula units; apfu) or pressure and temperature maps based on empirical and semi-empirical thermobarometers.

7.3.2.1 Structural formula of chloritoid

(1) Select the *Quanti* file *Chloritoid-advanced* in the workspace *Quanti* (Fig. 7.33a).

The external functions are grouped among several categories:

- Structural formulas
- P-T / map mode
- P-T / spot mode
- General functions
- Density functions
- Transfer to results

(2) Select the category *Structural formulas*, the phase *Chloritoid* and the function *Ctd-StructForm* (Fig. 7.33a).

(3) Press the button *COMPUTE* (Fig. 7.33a).

(4) XMAPTOOLS opens the workspace *Results* and display the first element of the structural formula, here Si (in apfu, see Fig. 7.33b,c).

(5) Display the variable *XMg* (corresponding to $\frac{Mg^{2+}}{Mg^{2+} + Fe^{2+}}$) using the menu shown in Figure 7.33c.

Additional variables can be generated in the workspace *Quanti* (see section 7.4.1 below).

7.4 RESULTS WORKSPACE

7.4.1 How to generate additional variables?

Use the GENERATOR module to generate new variables (see [3.11.5](#)).

TUTORIAL 2: EPMA DATA PROCESSING
(HIMALAYA - 2020)

8

8.1 INTRODUCTION

This tutorial will guide you through the main process of EPMA data reduction using XMAPTOOLS. A description of the tutorials available is provided in chapter 1.5. If you are using XMAPTOOLS for the first time, it is strongly suggested to read first the previous chapters (1, 2) before you begin this tutorial. For example the setup procedure discussed in chapter 2 is not described here and this step must be achieved before to begin the tutorial. The chapter 3 provides a comprehensive description of the functions used in this tutorial.

The X-ray maps and spot analysis data used in this tutorial were acquired at the Institute of Geological Sciences, University of Bern, using a electron probe micro-analyzer JEOL JXA 8200 Superprobe. The studied sample is described in [Lanari and Duesterhoeft \(2019\)](#).

The same dataset is used in chapter 9 for the tutorial on XTHERMOTOOLS & BINGO-ANTIDOTE.

8.1.1 How to get started

- (1) Open MATLAB and navigate to the tutorial directory (usually */User/MyDocuments/MATLAB/Xray_Data/Tutorial2/*)
- (2) Double check that you are in the right directory (see Fig. 8.1)
- (3) Open XMAPTOOLS using the case-sensitive command: » **XMapTools**
- (4) In the main menu, navigate through *Files* » *Import* » *Add Map(s)* and select the map files available in the working directory: *_Ce.txt*; *_La.txt*; *_Ni.txt*; *_P.txt*; *_S.txt*; *_Zr.txt*; *Al.txt*; *Ca.txt*; *Fe.txt*; *K.txt*; *Mg.txt*; *Mn.txt*; *Na.txt*; *SEI.txt*; *Si.txt*; *Ti.txt*; *TOPO.txt*

Warning: Do not select the files *Classification.txt* and *Standards.txt*; these are not valid map files (see recommended format in sections 2.7.1 and 2.7.4)

The maps *_Ce.txt*, *_La.txt*, *_Ni.txt*, *_P.txt*, *_S.txt*, *_Zr.txt* were measured by EDS, the other one (except SEI and TOPO) by WDS. Underscore (_) in front of the element name is used by XMAPTOOLS to detect EDS maps (see section 2.7.4).

- (5) In the *Import Tool* (Fig. 8.2), activate the dead time correction (option to be selected), set the dwell time to 150 ms and press the button *Apply Corrections*

Note: the dead time correction is only applied to WDS maps.

- (6) Display each map using the first menu in the workspace *X-ray*. Eventually adjust the color contrast using the auto-contrast button  Note that the lower and upper limits of the color bar are set to min and max values every time a map is selected in the menu.

- (7) Save the project as *aaa.mat*; in the menu navigate to *Files* » *Save as ...*. Note that after closing you can restart your session by using the following command in the working directory: » **XMapTools open aaa**

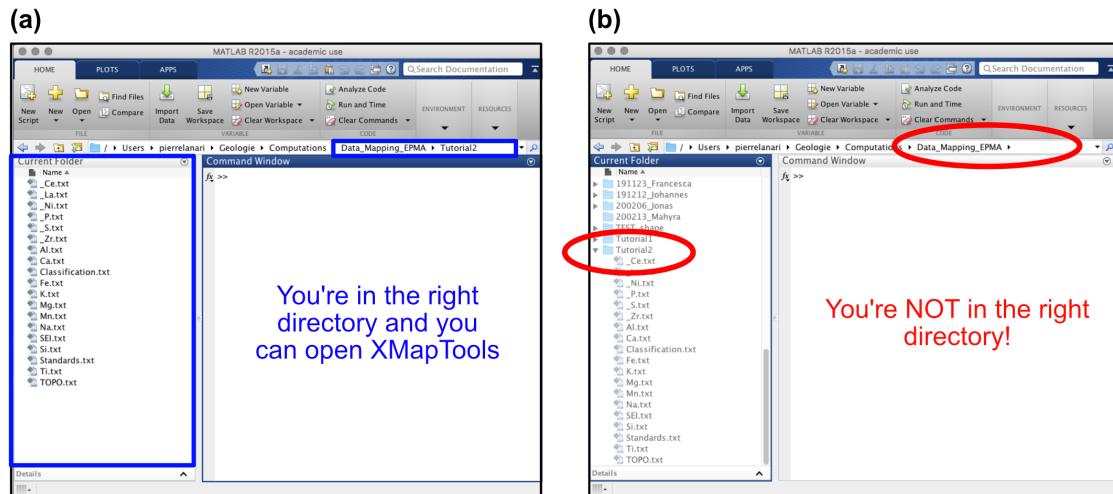


Figure 8.1 – Directory check to be performed before to open XMAPTOOLS. (a) the directory containing the maps is opened in MATLAB®; (b) the path is not correct: double-click the folder name in Current Folder (left ellipse) to open it.

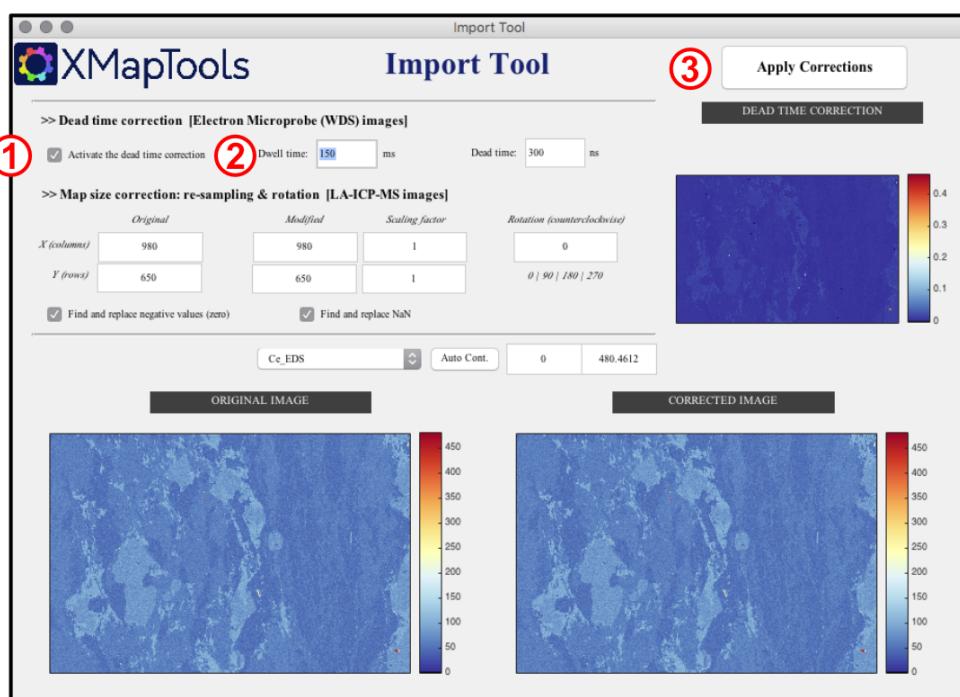


Figure 8.2 – Main steps in the Import Tool: (1) activate the dead time correction; (2) set the dwell time to 150 ms; (3) press the Apply Corrections

8.1.2 Classification

- (1) Open in MATLAB the file *Classification.txt* and provide under the keyword *>1* a name and the coordinates of a reference pixel for each phase for the classification.

The following maps can be deleted as they will not be used for classification:

- *La_EDS*: only present in rutile and ilmenite; slightly higher intensities observed in biotite, but this information is not required to classify these pixels
- *Ni_EDS & P_EDS*: Below detection limit; variations in intensity between phases are mainly caused by background variations (matrix effect) or interferences
- *S_EDS*: Grains are too small to be classified
- *SEI & TOPO*: Not required for classification

Note that these maps can be re-imported at any time (see step 1 in section 8.1.1).

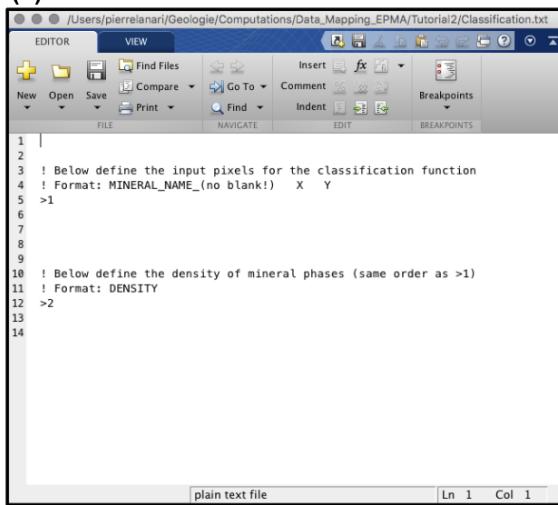
The following mineral phases can be recognized from the maps. The coordinates shown in the examples were obtained in XMAPTOOLS by moving the mouse pointer over the main figure and reporting the *X* and *Y* coordinates displayed above *Plot Options*

- *Garnet*: using the Fe map (intensity \sim 2500 counts)
- *Biotite & K-feldspar*: using the K map (intensity \sim 2800 counts for biotite and \sim 3600 counts for K-feldspar)
- *Sillimanite*: using the Al map (intensity \sim 5000 counts)
- *Plagioclase*: using the Na map (intensity \sim 480 counts)
- *Quartz*: using the Si map (intensity \sim 10,000 counts)
- *Rutile & ilmenite*: using the Ti map (intensity \sim 4800 counts for rutile and \sim 2800 counts for ilmenite); use the zoom to zoom in on the single rutile grain located in the center of the map
- *Zircon & apatite & monazite*: using the Zr map (intensity \sim 1200 counts for zircon, \sim 900 counts for apatite (you can also zoom in and then select the Ca map) and \sim 560 counts for monazite); note that there is a strong overlap between the Zr and P lines in EDS and that both are measured on the Zr map in this example

<i>>1</i>		
Garnet	213	372
Biotite	117	426
K-feldspar	20	420
Sillimanite	83	238
Plagioclase	52	73
Quartz	164	275
Rutile	419	181
Ilmenite	233	353
Zircon	88	326
Apatite	536	425
Monazite	945	590

Code 8.1 – Pixel coordinates used in the tutorial for the classification (to be copied to Classification.txt)

(a)



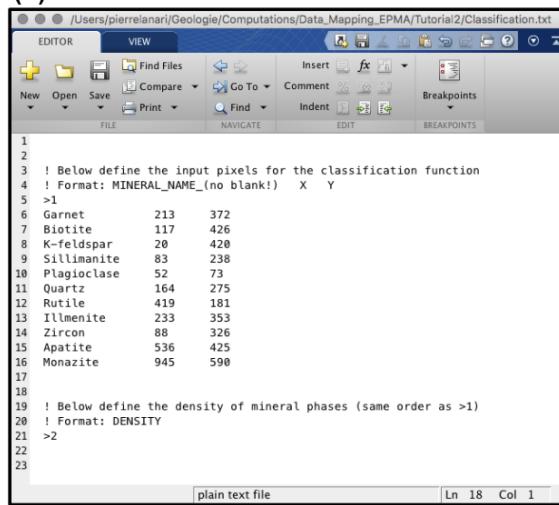
```

EDITOR      VIEW
New Open Save Find Files Compare Go To Comment fx Breakpoints
FILE NAVIGATE EDIT BREAKPOINTS
1
2
3 ! Below define the input pixels for the classification function
4 ! Format: MINERAL_NAME_(no blank!) X Y
5 >1
6
7
8
9
10 ! Below define the density of mineral phases (same order as >1)
11 ! Format: DENSITY
12 >2
13
14

```

plain text file | Ln 1 Col 1

(b)



```

EDITOR      VIEW
New Open Save Find Files Compare Go To Comment fx Breakpoints
FILE NAVIGATE EDIT BREAKPOINTS
1
2
3 ! Below define the input pixels for the classification function
4 ! Format: MINERAL_NAME_(no blank!) X Y
5 >1
6 Garnet      213    372
7 Biotite     117    426
8 K-feldspar   20     420
9 Sillimanite  83     238
10 Plagioclase 52     73
11 Quartz      164    275
12 Rutile       419    181
13 Ilmenite    233    353
14 Zircon       88     326
15 Apatite      536    425
16 Monazite    945    590
17
18
19 ! Below define the density of mineral phases (same order as >1)
20 ! Format: DENSITY
21 >2
22
23

```

plain text file | Ln 18 Col 1

Figure 8.3 – File Classification.txt (a) empty file; (b) with the phase definition.

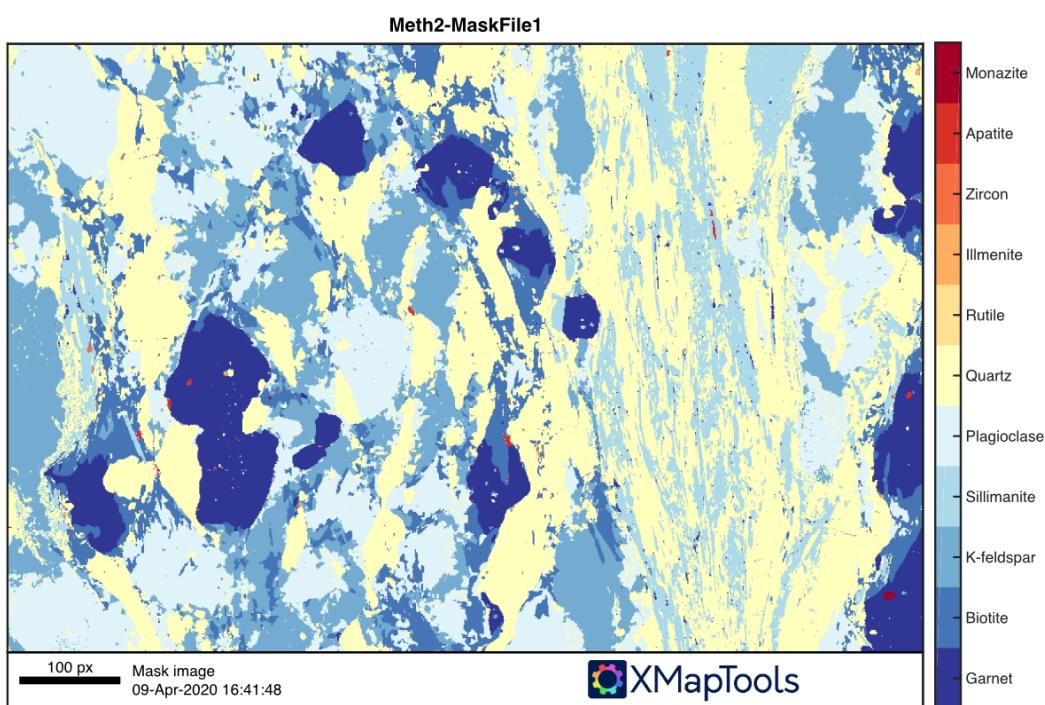


Figure 8.4 – Mask image. The pixel size is 20 μm ; In the scale bar, 100px corresponds to a distance of 2mm

- (2) Add the coordinates to the file *Classification.txt* (Fig. 8.3). Save the file. In XMAPTOOLS, select the method *Normalized intensities*, the option *File* and press the button *CLASSIFY*.
- (3) The mineral distribution map (mask image) can be exported via the menu *File* » *Export Mask Image*. The result is shown in Figure 8.4.
- (4) The compositional zoning of minerals can be displayed using the X-ray maps and the mask of each phase. Example: Select the element *Ca*, the mineral *Garnet* and press the button *Apply auto-contrast* 

8.1.3 Standardization

This section contains a description on how to convert the X-ray intensity data of every phase into compositions expressed in weight percentage of oxide. Detailed information regarding the standardization methods can be found in section 3.8.6.

8.1.3.1 Internal standards: importing the file Standards.txt

The file *Standards.txt* contains the map coordinates and the spot analyses used as internal standard.

- (1) Import the standard data in XMAPTOOLS using the the button *Import Standard File ...* 
- (2) Delete the maps that cannot be calibrated: Ce_EDS, S_EDS, Zr_EDS; Select each map in the map menu and delete it using the button *Delete map ...* 
- (3) Save the project; in the menu navigate to *Files* » *Save*.

8.1.3.2 Internal standards: check and correct the spot positions

The projection quality can be evaluated by using the tool *Check quality of std/maps positions*

- (1) Press the button *Check quality of std/maps positions* 
- (2) Adjust the position of the spots of *one pixel left* and *one pixel down* using the SPC correction tool. Select *SPC* in the correction menu and press the button *ACTIVATE*. Use the arrows available in the left panel to move the spot positions by *one pixel left* and *one pixel down*. Press the button *APPLY* to save the modified positions.

```
SPC ... [ Standard Position Correction ]
SPC ... X correction of -1 pixels applied ... OK
SPC ... Y correction of 1 pixels applied ... OK
SPC ... Done
```

Code 8.2 – Results of the SPC correction displayed in the MATLAB Command Window

- (3) Save the project; in the menu navigate to *Files* » *Save*.

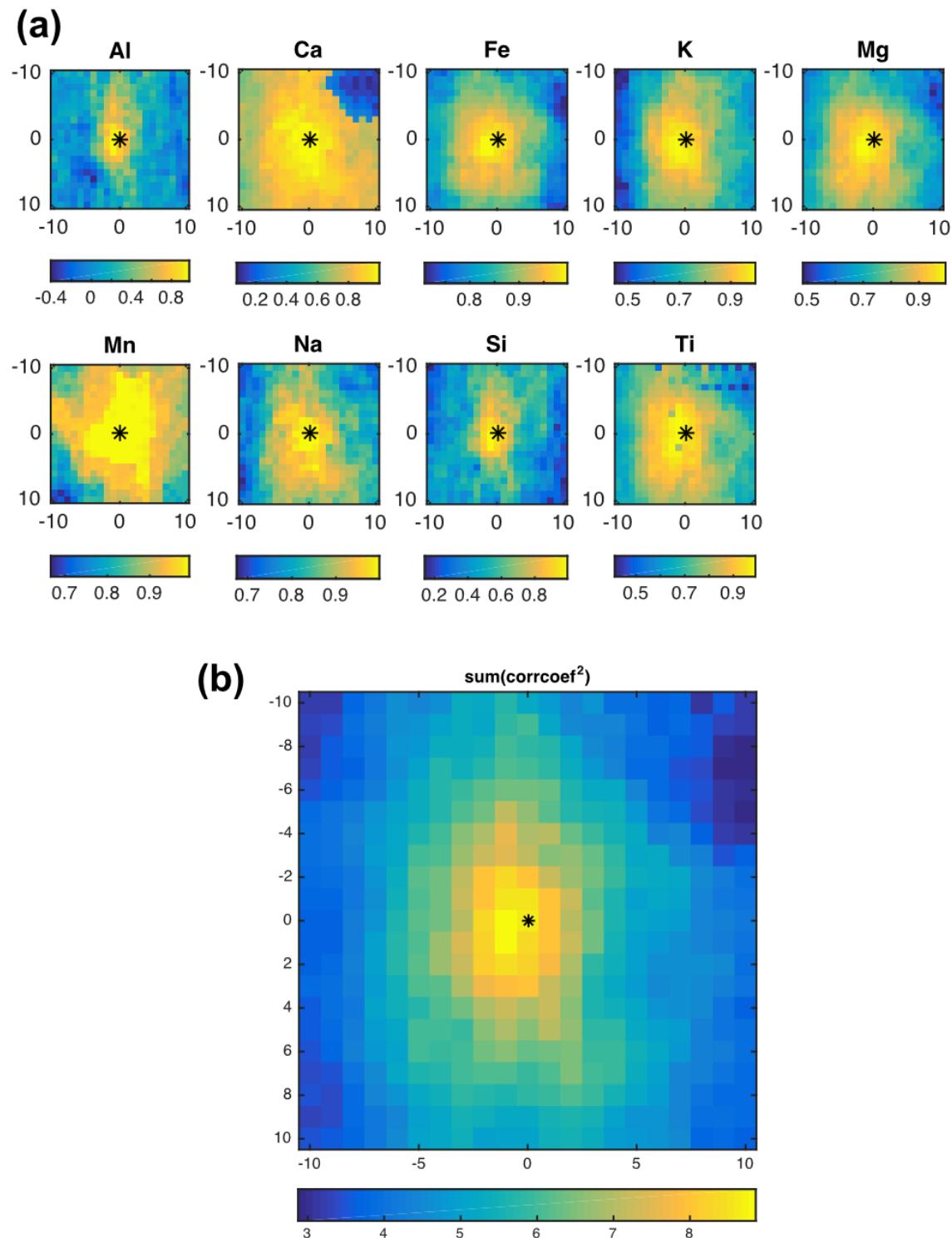


Figure 8.5 – Result of the projection check. (a) Correlation coefficient map obtained by moving the standards over the maps using a 21×21 grid centered on the original position (star). (b) Correlation map showing the sum of the square of the correlation coefficient maps shown in (a).

Element	No back.	Auto Poly.	Auto LS	Man.	Back.	X	Y
Al	x				1	21.43	1477
Ca		x			48	2.121	539.8
Fe	x				1	30.39	2592
K		x			37	0.022	39.41
Mg	x				1	6.830	340.2
Mn			x		87	1.100	421.3
Na		x			7	0.068	10.78
Si	x				1	38.57	3163
Ti		x			15	0.041	19.91

Table 8.1 – Parameters used for the advanced standardization of garnet

8.1.3.3 Standardization: Garnet (advanced standardization)

- (1) Select the mineral *Garnet* in the menu, the method *Advanced standardization* and press the button *STANDARDIZE*. Select all the elements available in the list displayed by the standardization function.
- (2) In the *Standardization Tool* window, select each element one-by-one and press the button *Apply Auto*. Check the calibration curve and, if required, adjust the calibration manually (see section 3.8.6). Note that the predictive routine implemented for standardization works successfully for the standardization of garnet in this example. The calibration details are provided in Table 8.1.
- (3) Press the button *APPLY STANDARDIZATION*

Two files are saved:

- **LOD_Garnet-advanced.txt** in the folder *LOD* containing the limit of detection for each element (see section 3.8.6.3 for details).
- **Garnet_advanced_DATE_TIME.txt** in the folder *Standardization* containing the calibration data for each element. This file can be provided as Supplementary Material in publications ([Lanari et al. 2019](#)).

8.1.3.4 Standardization: Biotite, K-feldspar, Plagioclase (advanced standardization)

- (1) In the workspace *X-ray*, select the mineral *Biotite* in the menu, the method *Advanced standardization* and press the button *STANDARDIZE*. Check the calibration curve for each element and, if required, adjust the calibration manually (not required in this example).
- (2) In the workspace *X-ray*, select the mineral *K-feldspar* in the menu, the method *Advanced standardization* and press the button *STANDARDIZE*. Check the calibration curve for each element and, if required, adjust the calibration manually (not required in this example).
- (3) In the workspace *X-ray*, select the mineral *Plagioclase* in the menu, the method *Advanced standardization* and press the button *STANDARDIZE*. Check the calibration curve for each element and, if required, adjust the calibration manually (not required in this example).

8.1.3.5 Standardization: Quartz, Sillimanite (manual standardization)

(1) In the workspace *X-ray*, select the mineral *Sillimanite* in the menu, the method *Manual (homogeneous phase)* and press the button *STANDARDIZE*. Select all the elements available in the list displayed by the standardization function. Enter the following reference composition for sillimanite: $Al_2O_3 = 62.92\text{ wt\%}$ and $SiO_2 = 37.08\text{ wt\%}$.

(1) In the workspace *X-ray*, select the mineral *quartz* in the menu, the method *Manual (homogeneous phase)* and press the button *STANDARDIZE*. Use the following reference composition for quartz: $SiO_2 = 100.0\text{wt\%}$ and $Al_2O_2 = 0.01\text{ wt\%}$. If zero is set for Al_2O_3 in quartz, these pixels will not be considered by the sampling functions (see below). The value of 0.01 wt% is small enough not to affect the determination of local bulk compositions.

8.1.3.6 Standardization: Accessory minerals

The accessory phases ilmenite, rutile, zircon apatite and monazite are not calibrated in this tutorial. The grain size of ilmenite and rutile is too small in this example. The calibration of zircon apatite and monazite would require spot analyses including Zr and P, which is not the case here.

8.1.4 Local bulk composition

The goal of this section is to extract local bulk composition (LBC) for thermodynamic modeling. Theoretical considerations are given in section 1.7.1 based on [Lanari and Engi \(2017\)](#).

8.1.4.1 Bulk composition of the mapped area

- (1) In the workspace *Quanti*, create a new map *Merged-Map* by merging the calibrated map of each phase. Press the button *Merge Quanti Files*  and select all the maps.
- (2) Add average density values for each phase in the file *Classification.txt*. Open the file and add the density values in the second bloc > 2 (see 8.3). Note that the order should match the order of the first bloc > 1 (see 8.1). Save the file *Classification.txt*.

```
>2
4.13
3.09
2.56
3.24
2.68
2.62
0
0
0
0
0
```

Code 8.3 – Input of average density for the minerals in *Classification.txt*

- (3) In XMAPTOOLS, press the button *Generate a density map (from selected mask file)* 

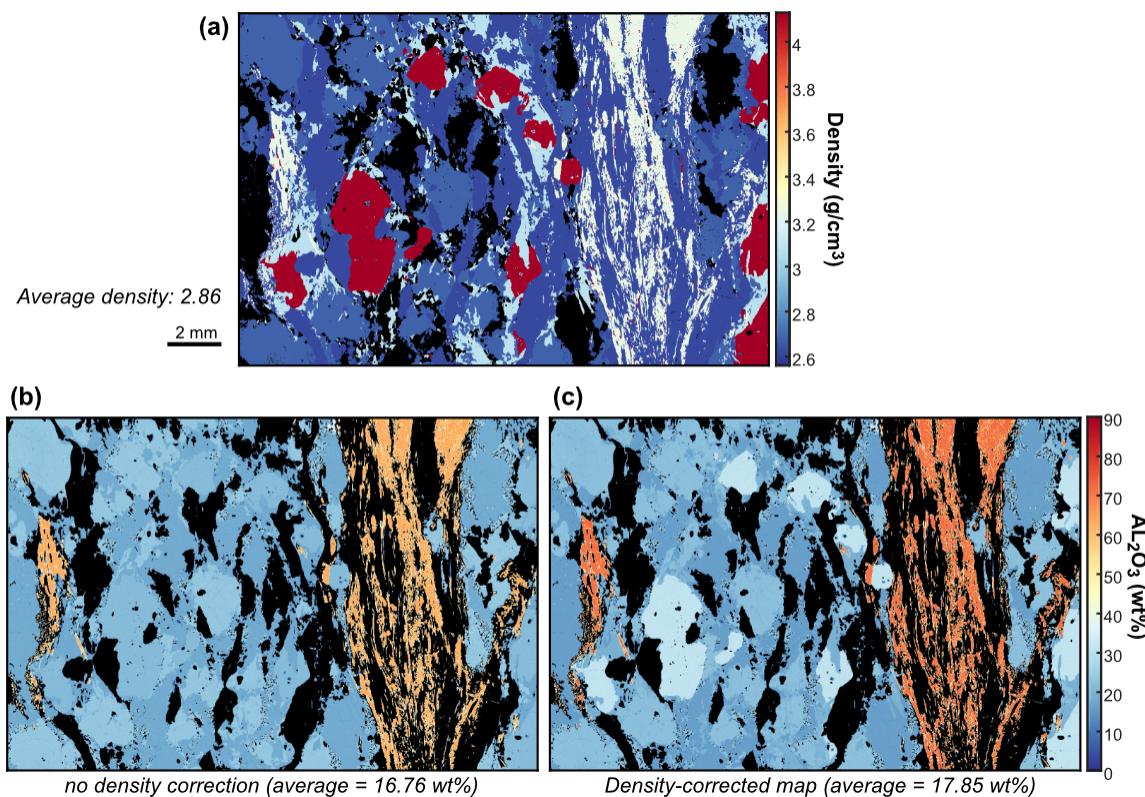


Figure 8.6 – Example of density correction for alumina. (a) density map. (b) Merged map of Al_2O_3 uncorrected for density. (c) Merged map of Al_2O_3 after density correction (see text)

- (4) Select the map *Merged-Map* and generate a density-corrected map by pressing the button *Compute a density-corrected oxide map*
- (5) Select the map *Merged-Map* and export the average composition (file name: *Merged.txt*) using the tool *Export local composition: map*
- (6) Select the map **DCM-Merged-Map* and export the average composition (file name: *Merged_DCM.txt*).

The results are shown in Figure 8.6 and Table 8.2.

The density map obtained from the density data reported in 8.3 is shown in Figure 8.6a. The effects of the density correction are illustrated based on the map of Al_2O_3 . The bulk composition of alumina calculated without any density correction (assuming that the volume fraction of a single-pixel of garnet in this domain is equal to its weight fraction) is 16.76 wt% (Fig. 8.6b). By contrast, the bulk composition of alumina after density correction is higher at 17.85 wt% (Fig. 8.6c). The absolute difference between these two estimates is 1.09wt% (corresponding to 6% relative) and is likely to affect any thermodynamic model based on local bulk compositions. The density correction consists of the multiplication of the composition of each pixel by $\frac{\rho_{\text{mineral}}}{\rho_{\text{domain}}}$; in this example, $\rho_{\text{domain}} = 2.86 \text{ g.cm}^{-3}$.

Oxide	Uncorrected map	Density corrected map	Domain 1
SiO_2	69.66	67.25	66.05
TiO_2	0.441	0.474	0.636
Al_2O_3	16.77	17.85	15.13
FeO	4.030	5.274	6.802
MnO	0.116	0.161	0.201
MgO	1.496	1.815	2.376
CaO	1.221	1.207	1.644
Na_2O	2.105	1.968	2.703
K_2O	3.233	3.060	3.943
<i>Total</i>	99.07	99.07	99.49

Table 8.2 – Comparison of the LBC determined for the entire map using uncorrected maps and density-corrected maps. Note that Domain 1 is a density-corrected LBC (see text)

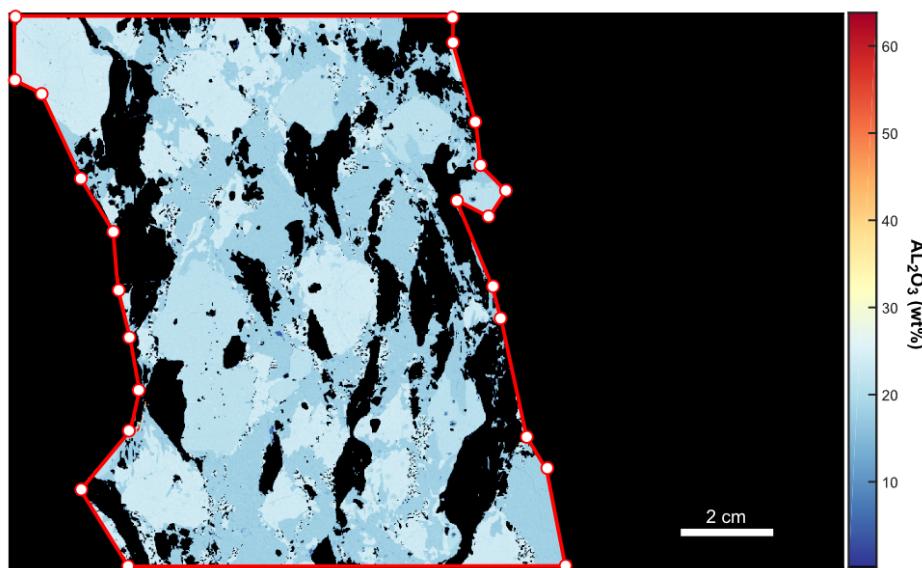


Figure 8.7 – Example of area-of-interest for LBC calculation in the sillimanite-absent domain

8.1.4.2 Bulk composition of a domain

The goal of this section is to extract the local bulk composition of a sillimanite-absent domain. The density correction should be applied to the pixels of this domain only as ρ_{domain} can be different.

- (1) In the workspace *Quanti*, select the map *Merged-Map*. Press the button *Duplicate Quanti file* to duplicate the map. The name of the new map is *Merged-Map_copy*
- (2) In this map, select an area-of-interest and eliminates pixels outside. Press the button *Select an area and eliminate pixels outside* and select an area-of-interest in the sillimanite absent domain (see example in Figure 8.7). Select spots that define a polygon by clicking on the figure. Selection mode is disabled using right-clicking and the polygon is closed without taking into account the right clicking position.
- (3) Select the map *Merged-Map_copy* and generate a density-corrected map by pressing the button *Compute a density-corrected oxide map*

(4) Select the map **DCM-Merged-Map_copy* and export the average composition (file name: *Merged_Domain1.txt*). You can save the corresponding figure.

(5) Save the project.

The corresponding local bulk composition is reported in Table 8.2. The bulk composition of domain 1 is enriched in FeO , MgO and depleted in Al_2O_3 .

8.1.4.3 Imagine spatial variations in local bulk composition

A couple of methods to visualize spatial heterogeneities in local bulk compositions are presented in this section. The density-corrected map of Al_2O_3 is used as an example. The comparison of two local bulk compositions obtained for the sillimanite-absent and the sillimanite-bearing domains shows an absolute increase in Al_2O_3 of 6 wt% (between 18 and 24 wt%).

(1) In the workspace *Quanti*, select the map **DCM-Merged-Map* and the oxide Al_2O_3 . In the menu *Sampling*, activate the option *Dave Data*. In the same menu *Sampling*, click on *Integrated Line (Strip)* and define a horizontal profile centered vertically starting in the sillimanite-absent domain (left) and going to the sillimanite-quartz domain (right, see Fig. 8.8). Save the result as *Strip1_Al2O3.txt*. The result shows that there is a difference in local bulk Al_2O_3 composition between the two domains. However the absolute values are spread due to the local heterogeneities in each vertical profile used for integration.

(2) Select again the map **DCM-Merged-Map* and the oxide Al_2O_3 . In the menu *Sampling*, click on *Sliding Window* and define a vertically elongated window starting in the sillimanite-absent domain (left) and going to the sillimanite-quartz domain (right, see Fig. 8.9). Save the result as *Window1_Al2O3.txt*. In this case, the variation Al_2O_3 is centered on the absolute values of 18 wt% in the sillimanite-absent domain and 24 wt% in the sillimanite-bearing domain.

8.1.5 Structural formula, chemical modules and thermobarometry

8.1.5.1 Structural formula of garnet and biotite

(1) In the workspace *Quanti*, select the map *Garnet-advanced*. In the external function menu, select *Structural Formulas*, *Garnet* and *Grt-StructForm-Fe3* and press the button *COMPUTE*. Note that the program switches to the workspace *Results* once the computation is achieved.

(2) Display the map of the grossular fraction (X_{grs}), adjust the color contrast automatically using the auto-contrast functionality 

(3) Export this map. In the menu, select *File* » *Export Image*. The image opens in a new window. Here the image can be copied to the clipboard (menu: *Edit* » *Copy Figure*) or saved (menu: *File* » *Save As ...*)

(4) Navigate back to the workspace *Quanti*, select the map *Biotite-advanced*. In the external function menu, select *Structural Formulas*, *Biotite* and *Bio-StructForm-Fe3* and press the button *COMPUTE*.

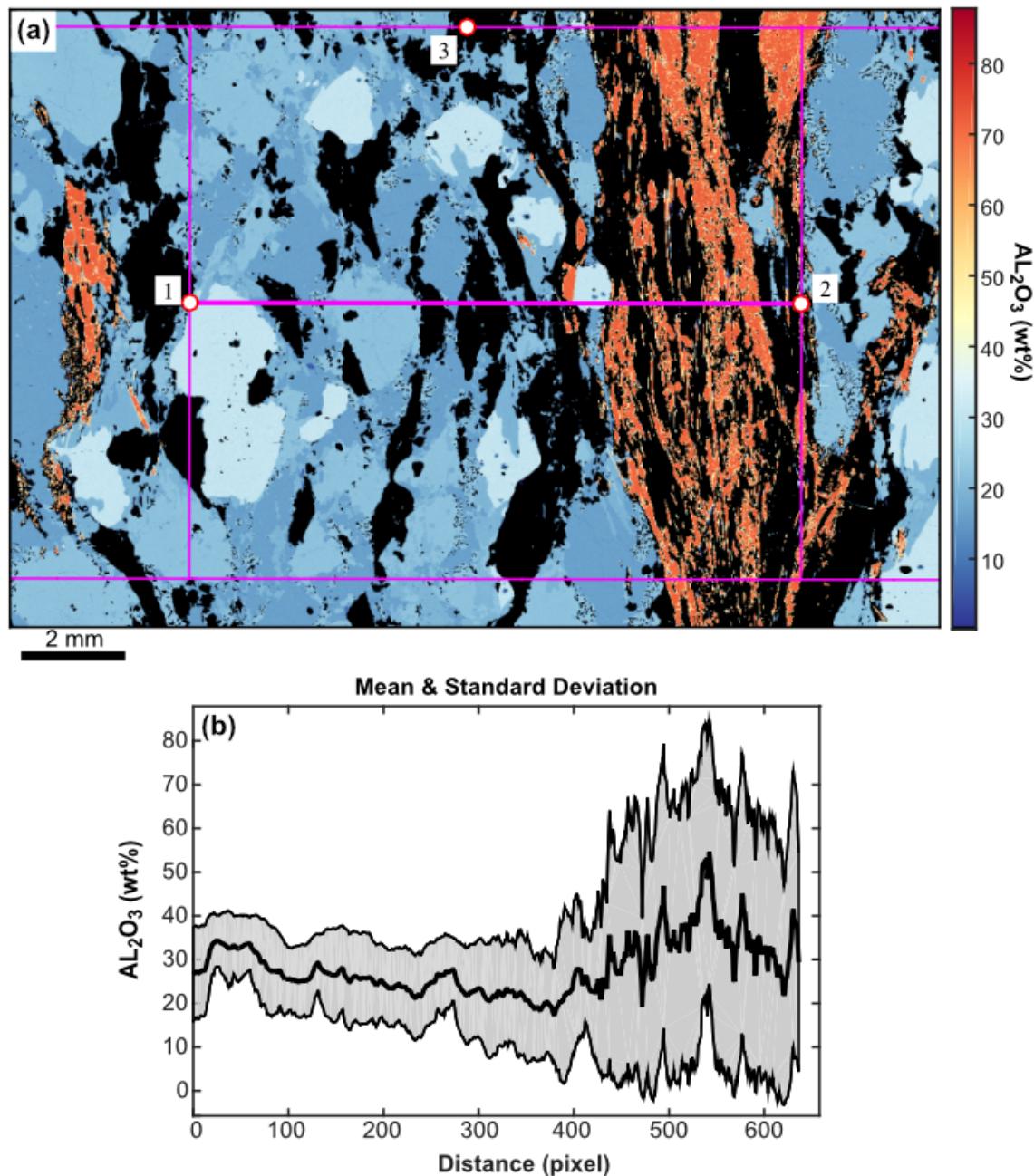


Figure 8.8 – Example of sampled profile using the tool Integrated Line (Strip). (a) map showing the three points (1-3) used to define the strip. (b) profile showing the mean and standard deviation

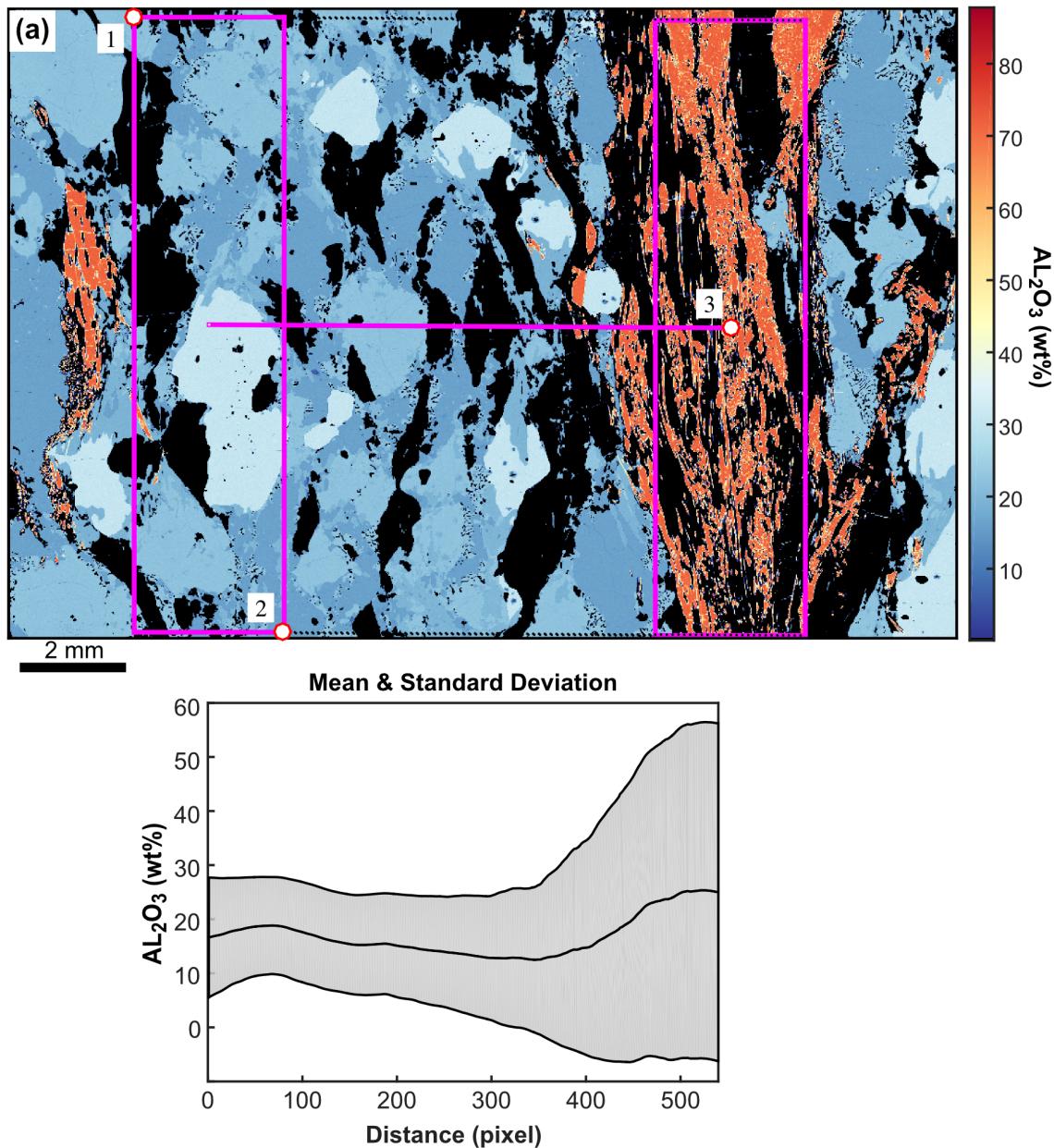


Figure 8.9 – Example of sampled profile using the tool Sliding Window. (a) map showing the three points (1-3) used to define the window (1-2) and the trajectory (3). (b) profile showing the evolution of the mean and standard deviation of each window

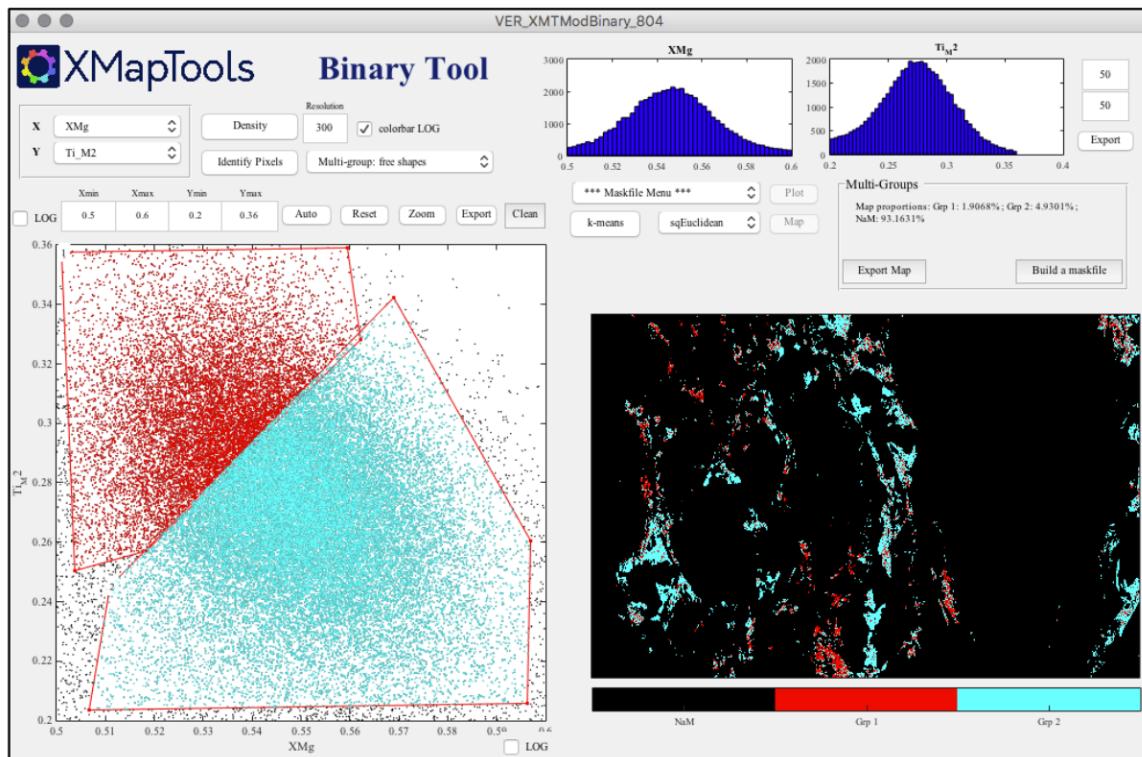


Figure 8.10 – *Binary module* (Ti vs XMg) and selection of two groups (1 in red and 2 in cyan) using the option *Multi-group free shape*

(5) Display the map of XMg in biotite. Export the image (do not close it) and display the map of Ti_M2 in biotite. The biotite grains enriched in Ti exhibit lower XMg values and are located far away from the garnet porphyroblasts.

(6) Select the result *Bio-StructForm* and navigate in the menu to *Modules* » *BInary*. Select XMg as X and Ti_M2 as Y variables. Adjust the display to $Xmin = 0.5$, $Xmax = 0.6$, $Ymin = 0.2$ and $Ymax = 0.36$. Use the tool *Identify Pixels* and the mode *Multi-group: free shapes* to select two groups as shown in Figure 8.10. A description of the Binary module is provided in chapter 3.11.2. This tool allows you to check the correlation between two compositional variables. The other modules available in XMAPTOOLS are described in chapter 3.11.

(7) Close the *Binary* module and save the project

8.1.5.2 Semi-empirical thermobarometry

(1) Navigate to the workspace *Quanti*, select the map *Biotite-advanced*. In the external function menu, select *P-T, map mode*, *Biotite* and *Bio-T Henry et al. 2005* and press the button *COMPUTE*. Display the map of formation temperature of biotite and adjust the color contrast manually.

(2) In the main menu select *Modules* » *Histogram*. Adjust the min value to 720 and the max value to 780; press the button *Auto* to optimize the number of bins and press the button *Map* to display the map view. The spatial variation of T (between the Ti-poor and Ti-reach biotites) that is visible in the map view is not easily identified in the histogram. In this case it would be judicious to show the data rather as a map of formation temperature.

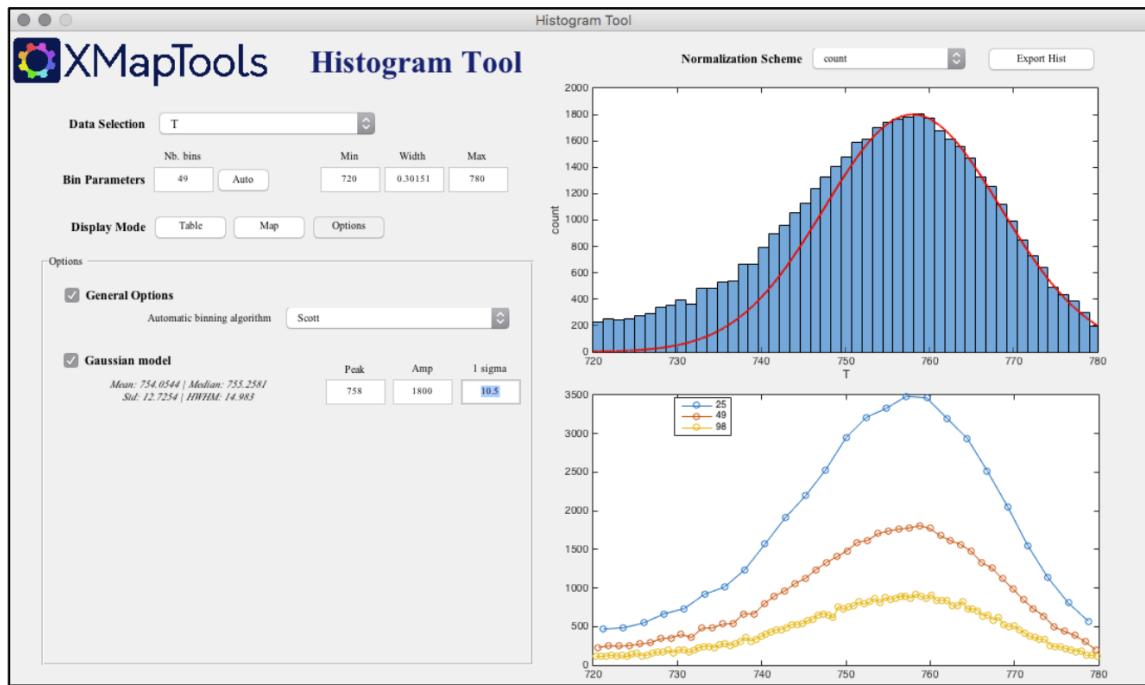


Figure 8.11 – Histogram module showing the distribution of T in biotite

(3) In the *Histogram* module, select the tabulation *Options*, activate the *Gaussian model* and adjust the peak position to 758, the amplitude to 1800 and the standard deviation to 10.5. In this example the distribution cannot be fully modeled using a Normal (Gaussian) distribution suggesting the presence of several peaks (Fig. 8.11).

(4) Close the *Histogram* module and save the project

TUTORIAL 3: ITERATIVE THERMODYNAMIC MODELING (XTERMOTOOLS, BINGO-ANTIDOTE)

9.1 INTRODUCTION

This tutorial will guide you through a simple example of iterative thermodynamic model using BINGO-ANTIDOTE implemented in the add-on XTHERMOTOOLS 1.2 using a small selection of the dataset published in [Lanari and Duesterhoeft \(2019\)](#).

This tutorial follows the previous one (chapter 9), but it can also be followed independently as the project file is provided.

The documentation of XTHERMOTOOLS is available via the menu *File » Help & Documentation*

9.2 HOW TO GET STARTED

- (1) Open MATLAB and XMAPTOOLS using the command: » *XMapTools*
- (2) In the main menu, select *Help » Download Tutorial Data*
- (3) Select *Tutorial 3* and press the button *Download*; save the files to */User/MyDocuments/MATLAB/Xray_Data/*
- (4) In the menu, select *File » Open Project* and select the project file *aaa.mat* in the folder *Tutorial3_BingoAntidote*
- (5) Navigate to the workspace QUANTI, select the map *Merged-Map* and the mask file *Meth2-MaskFile1* (left menu)
- (6) In the add-on menu, select XTHERMOTOOLS and press the button *APPLY*
- (7) *Optional.* Follow the instructions to install the add-on on your computer. Select *Yes*; Press on the button *Select THERIAK directory*; Note that compatible versions of THERIAK-DOMINO are provided in the folder *XThermoTools/XTT-Programs/*
- (8) If you are opening *XThermoTools* for the first time, a warning message is displayed as the thermodynamic database JUN92 is not available in this directory. Select *Yes* and the program will copy this file to the working directory.

XTHERMOTOOLS runs a diagnostic on the data sent by XMAPTOOLS and prints a report in the MATLAB Command Window (see Code 9.1). In this case 921 pixels are not considered (rejected) including those belonging to rutile (25 pixels), ilmenite (165), Zircon (273), apatite (366) and monazite (92). This is because these phases were not calibrated in the present example.

The option file *OptionsXTT.txt* does not exist yet and default values were taken (see Code 9.1).

```

-> rejected pixels: 921/637000 (0.14%)
    Rutile      25/637000 (0.00%)
    Ilmenite    165/637000 (0.03%)
    Zircon      273/637000 (0.04%)
    Apatite     366/637000 (0.06%)
    Monazite    92/637000 (0.01%)

-> options:          default (OptionsXTT.txt not found)
    opt1        H(1)O(?)
    opt2        *
    opt3        500
    opt4        10000
    opt5        100
    opt6        40
    opt7        8,500
    opt8        2
    opt9        300:10:700
    opt10       2000:500:25000

```

Code 9.1 – Information displayed in the Command Window while XThermoTools starts

9.3 GENERAL SETTINGS

(1) In the menu, select *Initialize* » *Generate OptionsXTT.txt* and adjust the following options (see also Fig. 9.1):

- *Default PT conditions for Bingo*: 700 °C and 5000 bar
- *P-T window*: 600 to 900 °C with a step of 10 °C
- *P-T window*: 2000 to 12000 bar; after fixing the temperature range, press the button *Apply* to adjust the step for the Y-axis and set a squared grid

(2) Press the button *Generate Options XTT*. The program generates *OptionsXTT.txt*. Note that the values of these settings can be updated either via the interface (step 1 above) or directly in the file without breaking the format.

(3) In XHERMOTOOLS, select the database *JUN92.bs* using the drop-down menu

(4) Press the button *Set* to define the chemical system. In the new window (Fig. 9.2), exclude the elements Ti and Mn by clicking on their names and then press *APPLY*

9.4 LOCAL BULK COMPOSITION

The first drop-down menu in *Bulk Composition* lists all the minerals defined in the mask file. Mineral can be excluded by pressing the button *Reject phases*. This is not required in the tutorial as the pixels belonging to rutile, ilmenite, zircon, apatite and monazite were not calibrated.

(1) In the menu, select *Bulk* » *Add Bulk* and select a large rectangular area-of-interest by clicking into the map. Select 4 points (see example in Fig. 9.3) and press right-click to validate the selection. The shape closes automatically.

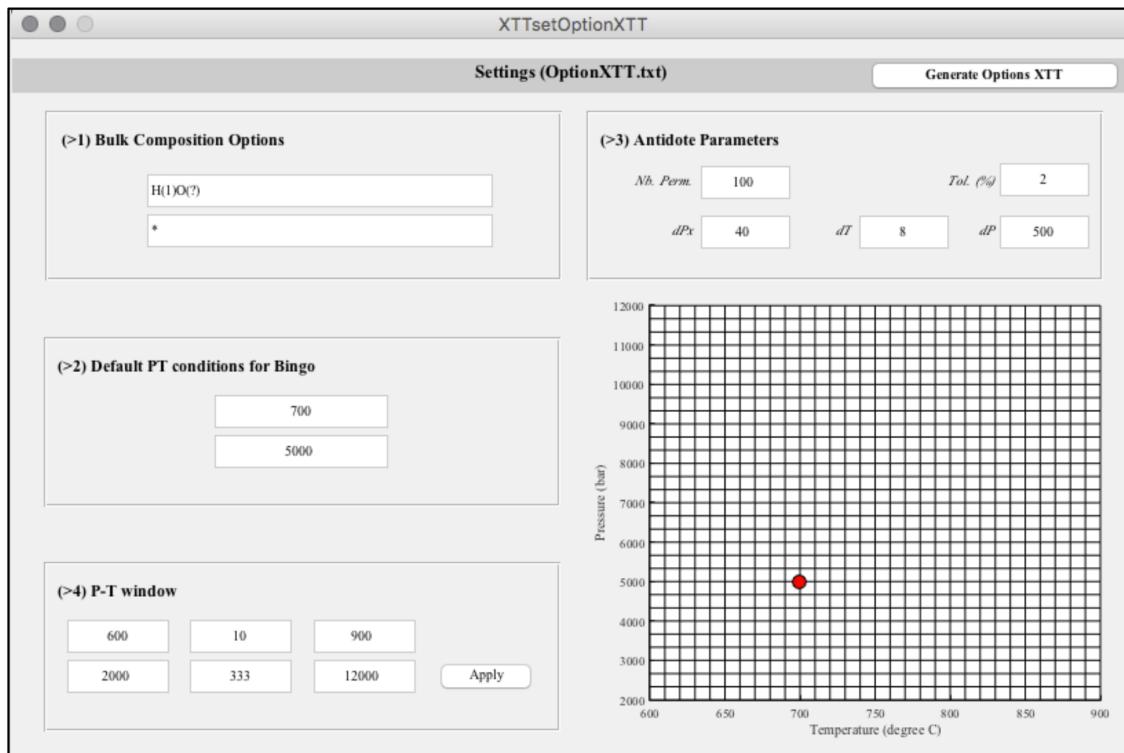


Figure 9.1 – Adjusted parameters for OptionsXTT.txt

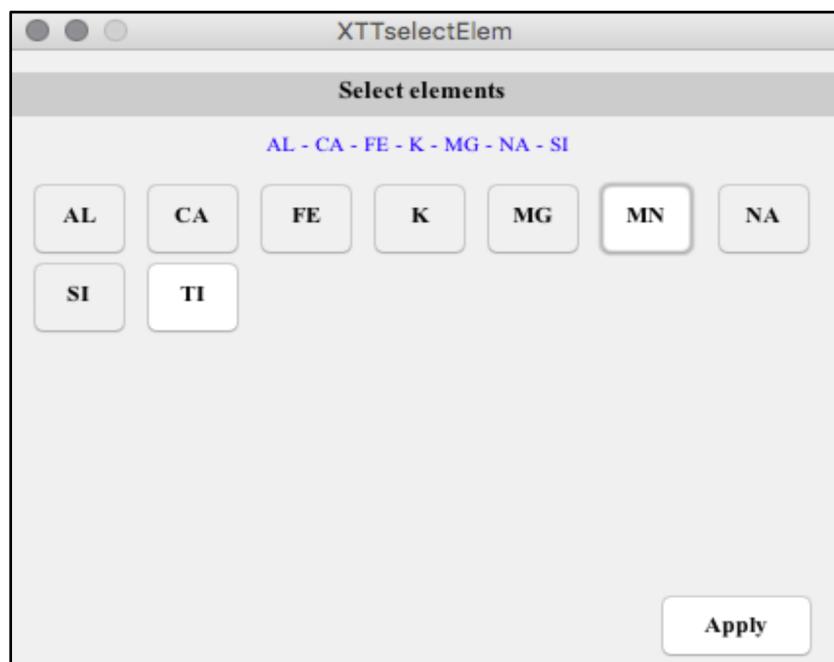


Figure 9.2 – Selection of the chemical system (here: Al-Ca-Fe-K-Mg-Na-Si)

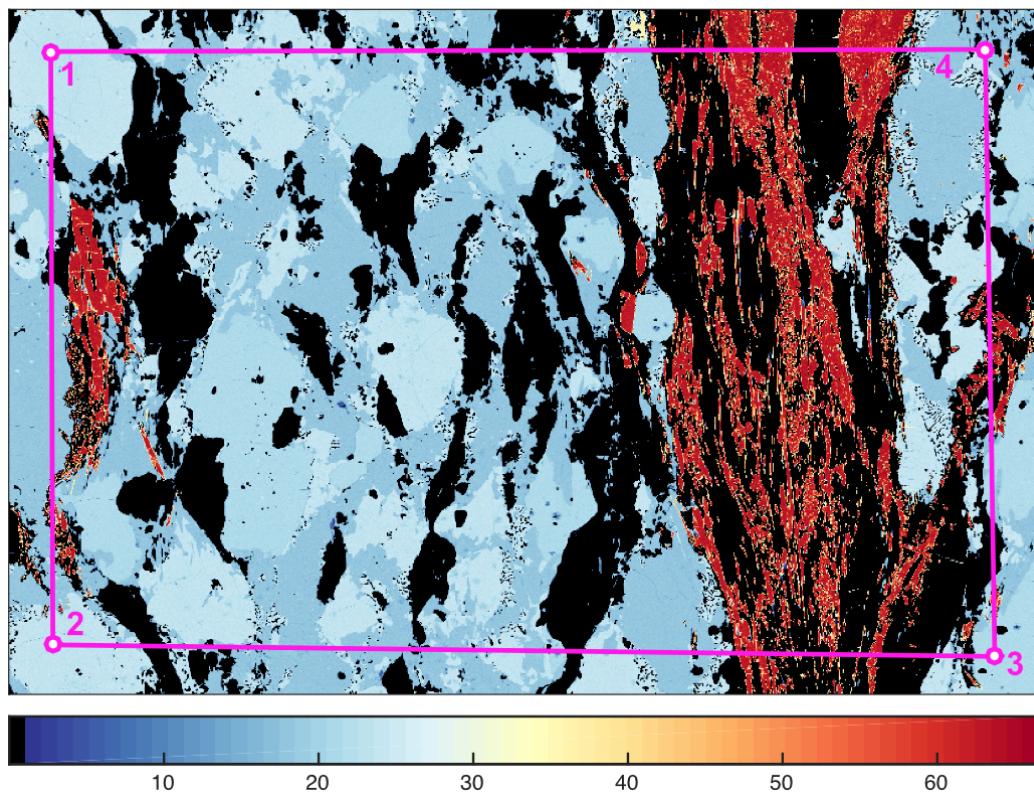


Figure 9.3 – Points selected to define a rectangular area-of-interest used to calculate a local bulk composition (LBC)

(2) Once the shape has been selected a new window appears. In this case the single fluid specie *Fluid_H2O* will be controlled controlled by the amount of H available in the bulk. In this case, we keep first the amount of H to 1 mol. Press *Apply* to validate and close this window.

The corresponding local bulk composition (LBC) is displayed in the MATLAB Command Window as oxide weight fraction of oxide (Code 9.2) and in the THERIAK format in the bulk field of XTHERMOTOOLS (Code 9.3).

----- NEW BULK COMPOSITION (LB_2) -----						
AL2O3	CAO	FEO	K2O	MGO	NA2O	SIO2
17.691	1.134	4.949	2.928	1.720	1.853	68.156

Code 9.2 – Local bulk composition expressed in weight percentage of oxide

0 AL(0.34703)CA(0.020224)FE(0.068892)K(0.062164)MG(0.042667)NA(0.059806)SI (1.1343)H(1)O(?) * LB_2

Code 9.3 – Local bulk composition in number of moles of elements (Theriaik format)

(3) In the menu, select *Bulk* » *Save Bulk Configuration* and in the new window simply press the button *Save*. These settings are saved in the folder *Bingo* and we keep the default name *BIN_Bulk.xtt*.

Is it critical to save the selected area-of-interest (bulk file) before to close the program as there is no project file in XTHERMOTOOLS. It will be necessary to reload the bulk data every time the program

will be used. Only the selection is saved and the program recalculates the bulk composition for the selected chemical system every time.

Example of restart:

- (4) Close XTHERMOTOOLS
- (5) In XMAPTOOLS, select the add-on and press *APPLY* to restart XTHERMOTOOLS. Note that this time the settings are imported from *OptionsXTT.txt*
- (6) Select the database *JUN92.bs* using the drop-down menu
- (6) Set the chemical system (exclude Mn and Ti) and validate
- (7) In the menu select *Bulk* » *Load Bulk Configuration* and click *Yes* to load the area-of-interest saved in *BIN_Bulk.xtt*. Note that if you changed the name of the file, you need to click *No* to select an other file. Press *Apply* to validate the settings of the fluids melts and gases.

You are back to the same point as (3) above.

9.5 PHASE SYNCHRONIZATION AND MINERAL COMPOSITIONS

Each mineral to be included in the computation of quality factors needs to be synchronized with either a pure phase or a solid solution of the thermodynamic database. For example the mask *garnet* in this example corresponds to the solid solution *GARNET* in the database Jun92.bs. The reference composition known as *Observed composition* and its relative uncertainties are then defined as the average and standard deviation of composition for a group of pixels taken over a small area considered as homogeneous.

9.5.1 Garnet

- (1) Select *Garnet* in the drop-down menu below the item *Phase definitions*
- (2) In the menu, select *Phase Matching* select *Synchronize Garnet*; the name of the corresponding solution model is displayed in the field located right of the drop-down menu (GARNET in Jun92.bs)
- (3) In the *Map* panel (top-right) press the button *Element* and select *CAO*; press the button *Auto* to adjust the color contrast as in XMAPTOOLS
- (4) Click on the map and drag the mouse to zoom on the elongated grain located on the left.
- (5) In the menu, select *Phase Matching* and *Add Group* and select a small area in the Ca-rich part of the grain (see Figure 9.4a).

The average mineral composition is displayed in the MATLAB Command Window (see Code 9.4). The pixels within the area of interests are checked to detect possible outliers. The average composition is reported in oxide weight percentage (first row) with the standard deviation (second row); The structural formula (average and standard deviation) is also given.

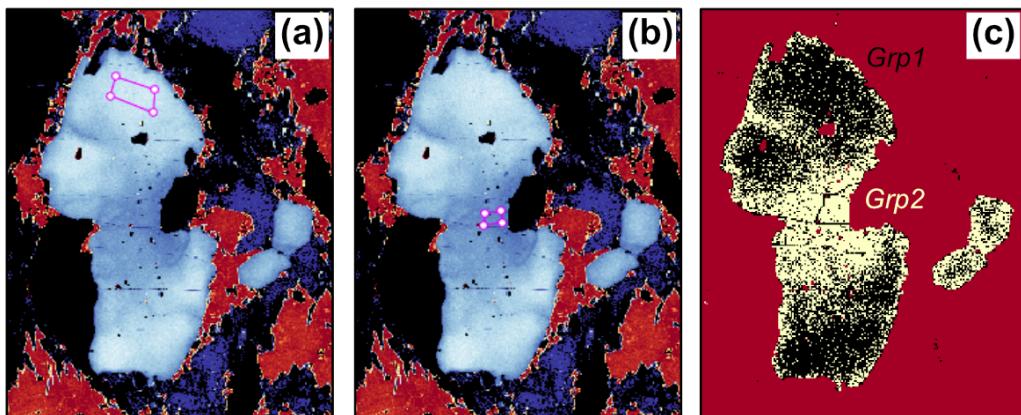


Figure 9.4 – Definition of the compositional groups of garnet: (a) Group 1; (b) Group 2; (c) Result of a pixel classification using the compositions of Grt1 and Grt2

Mineral: Garnet Grp: 1						
AL	1/444 (0.22523 %) of the pixel(s) rejected					
CA*	0/444 (0 %) of the pixels are outliers – ALL PIXELS SELECTED					
FE	2/444 (0.45045 %) of the pixel(s) rejected					
K*	0/444 (0 %) of the pixels are outliers – ALL PIXELS SELECTED					
MG*	0/444 (0 %) of the pixels are outliers – ALL PIXELS SELECTED					
NA*	0/444 (0 %) of the pixels are outliers – ALL PIXELS SELECTED					
SI	1/444 (0.22523 %) of the pixel(s) rejected					
AL2O3	CAO	FEO	K2O	MGO	NA2O	SIO2
21.37	2.10	29.85	0.04	6.68	0.02	38.46
0.72	0.12	1.13	0.04	0.42	0.03	1.00
AL	CA	FE	K	MG	NA	SI
1.99	0.18	1.97	0.00	0.79	0.00	3.04
0.08	0.01	0.08	0.00	0.05	0.00	0.10

Code 9.4 – Mineral composition and standard deviation for Grt1 (in oxide and apfu). Note that the outlier rejection subroutine applies a 6 sigma test with a 5% cut-off threshold (not displayed here)

- (6) In the menu, select again *Phase Matching* and *Add Group* and select a small area in the Ca-poor part of the grain (see Figure 9.4b).

The average composition and standard deviation of the second group is shown below (Code 9.5).

AL2O3	CAO	FEO	K2O	MGO	NA2O	SIO2
21.55	0.92	30.26	0.04	7.31	0.02	39.19
1.18	0.08	1.50	0.04	0.42	0.03	3.30
AL	CA	FE	K	MG	NA	SI
1.98	0.08	1.98	0.00	0.85	0.00	3.06
0.14	0.01	0.13	0.00	0.06	0.00	0.29

Code 9.5 – Mineral composition and standard deviation for Grt2 (in oxide and apfu)

The result of a pixel classification based on the compositions of Grt1 and Grt2 is shown in a new figure (9.4c). This result should reflect the repartition of each group and is used to approximate the modes.

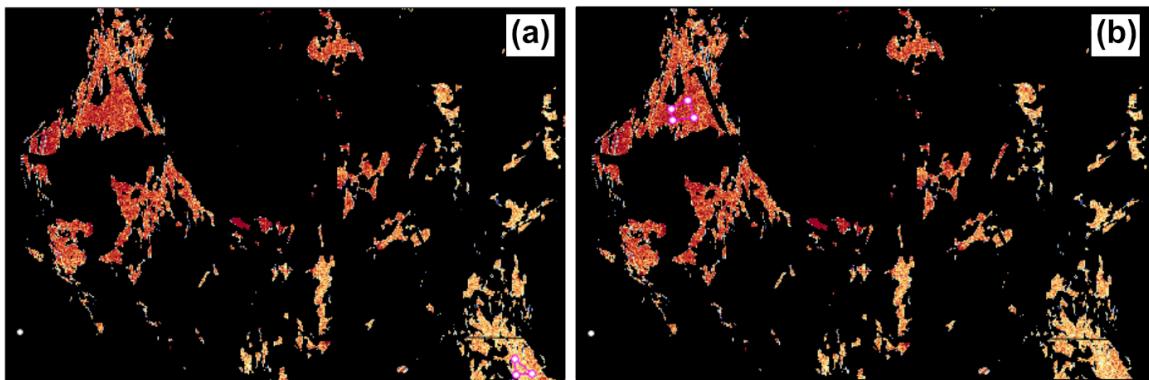


Figure 9.5 – Definition of the compositional groups of biotite: (a) Group 1, Mg-poor biotite; (b) Group 2, Mg-rich biotite

- (7) Right-click on the map and select the option *Reset to Original View* to reset the zoom.

9.5.2 Biotite

- (1) Select *Biotite* in the drop-down menu below the item *Phase definitions*
- (2) In the menu, select *Phase Matching* select *Synchronize Biotite*; the name of the corresponding solution model is displayed in the field located right of the drop-down menu (BIOTITE in Jun92.bs)
- (3) In the *Map* panel (top-right) press the button *Element* and select *MGO*
- (4) Press the button *Sel. phases display*; in the new window, click *None*, then select *Biotite* and press *Apply*; press the button *Auto* to adjust the color contrast. Two populations of biotite can be recognized: Mg-rich in the vicinity of garnet and Mg-poor in the matrix far from the garnet porphyroblasts.
- (5) Click on the map and drag the mouse to zoom on the bottom left quarter.
- (6) In the menu, select *Phase Matching* and *Add Group* and select a small area in the Mg-poor biotite (see Figure 9.5a).
- (7) Set a second group using pixels within the Mg-rich biotite (see Figure 9.5a).
- (8) Reset the zoom and display all the phases in the map

9.5.3 K-feldspar

- (1) Select *K-feldspar* in the drop-down menu
- (2) In the menu, select *Phase Matching* select *Synchronize K-feldspar*; the name of the corresponding solution model is displayed in the field located right of the drop-down menu (FSP2 in Jun92.bs). Note that as two feldspar can be stable at the same time in this sample, the model detects the K-rich felspar in using the name *FSP2_Kfs*.

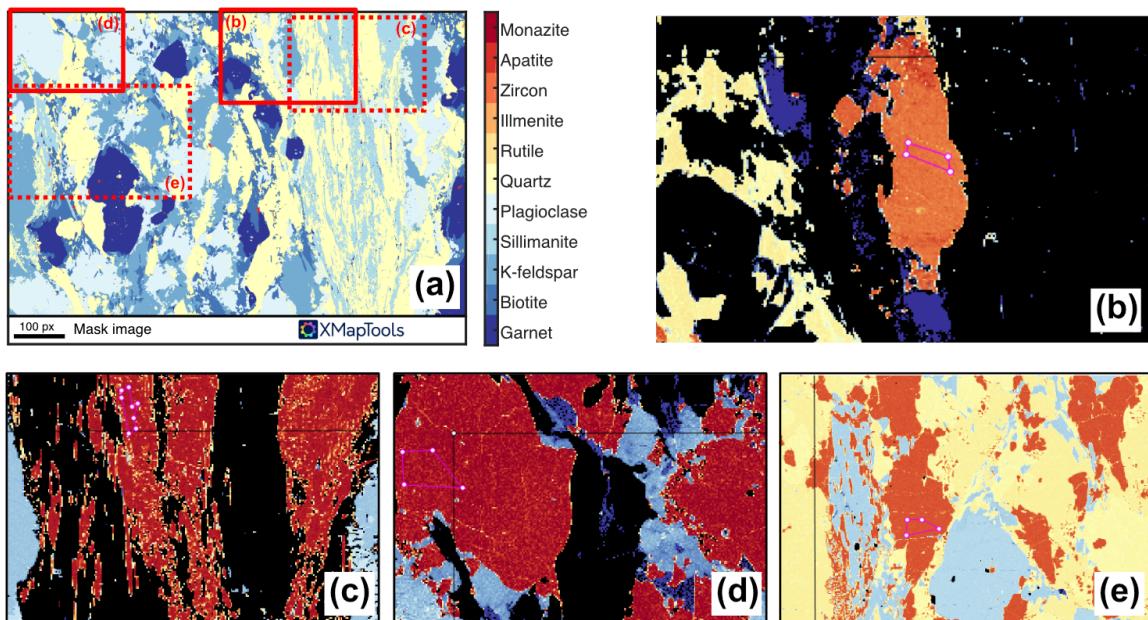


Figure 9.6 – Definition of the compositional groups of : (b) K-feldspar, (c) Sillimanite, (d) Plagioclase and (e) Quartz

- (3) In the *Map* panel (top-right) press the button *Element* and select *K2O*
- (4) Use the zoom option to adjust the view and select a small area (e.g. Figure 9.6) to define the K-feldspar composition (select *Phase Matching* and *Add Group*). A single group of K-feldspar is used in this tutorial.

9.5.4 Sillimanite

- (1) Select *Sillimanite* in the drop-down menu
- (2) In the menu, select *Phase Matching* select *Synchronize Sillimanite*; the name of the corresponding phase is displayed in the field located right of the drop-down menu (SILLIMANITE in Jun92.bs).
- (3) In the *Map* panel (top-right) press the button *Element* and select *AL2O3*
- (4) Use the zoom option to adjust the view (top right corner is a good spot, see Figure 9.6) and select a small area to define the sillimanite composition (select *Phase Matching* and *Add Group*). A single group of sillimanite is used in this tutorial.

9.5.5 Plagioclase

- (1) Select *Plagioclase* in the drop-down menu
- (2) In the menu, select *Phase Matching* select *Synchronize Plagioclase*; the name of the corresponding solid solution is displayed in the field located right of the drop-down menu (FSP2 in Jun92.bs).

(3) In the *Map* panel (top-right) press the button *Element* and select *NA2O* and adjust the color contrast automatically

(4) Use the zoom option to adjust the view and select a small area (e.g. Figure 9.6) to define the plagioclase composition (select *Phase Matching* and *Add Group*) in the grain located in the top right corner. A single group of plagioclase is used in this tutorial.

9.5.6 Quartz

(1) Select *Quartz* in the drop-down menu

(2) In the menu, select *Phase Matching* select *Synchronize Quartz*. As there is no correspondence in the database a menu containing all the solid solutions and phases available is displayed. Select *B-quartz* and press *Ok*

(3) In the *Map* panel (top-right) press the button *Element* and select *SIO2*

(4) Use the zoom option to adjust the view (e.g. Figure 9.6) and select a small area to define the quartz composition.

9.6 CALCULATING PHASE PROPORTIONS AND SAVING MINERAL DEFINITIONS

Phase proportions can be calculated once the synchronization is accomplished provided that at least one compositional group has been created for each phase. All the phases considered for modeling should be synchronized before calculating phase proportions.

(1) Select one of the synchronized phase via the drop-down menu (e.g. *Garnet*)

(2) In the menu *Phase Matching* select *Validate Phase Definitions*

The volume fraction of the selected phase in the selected area-of-interest is displayed below the solution name.

(3) Phase definitions can be saved via the menu *Phase Matching* and *Save Phase Configuration*. The file is saved as *BIN_Phases_JUN92.bs_.xtt*. It is important to keep the name of the database in this file as the phase definition including the solution model names are database dependent.

A phase definition file should be saved for each database used, optimally using the same mineral compositions. Note that it is possible to change the database and save a new file.

Several files containing phase definition can be generated for a given map, for example if two assemblages represent two distinct P-T stages.

To load saved condition, navigate to the menu *Phase Matching* and *Load Phase Configuration*. The mineral compositions are recalculated for the selected chemical system and displayed in the MATLAB Command Window.

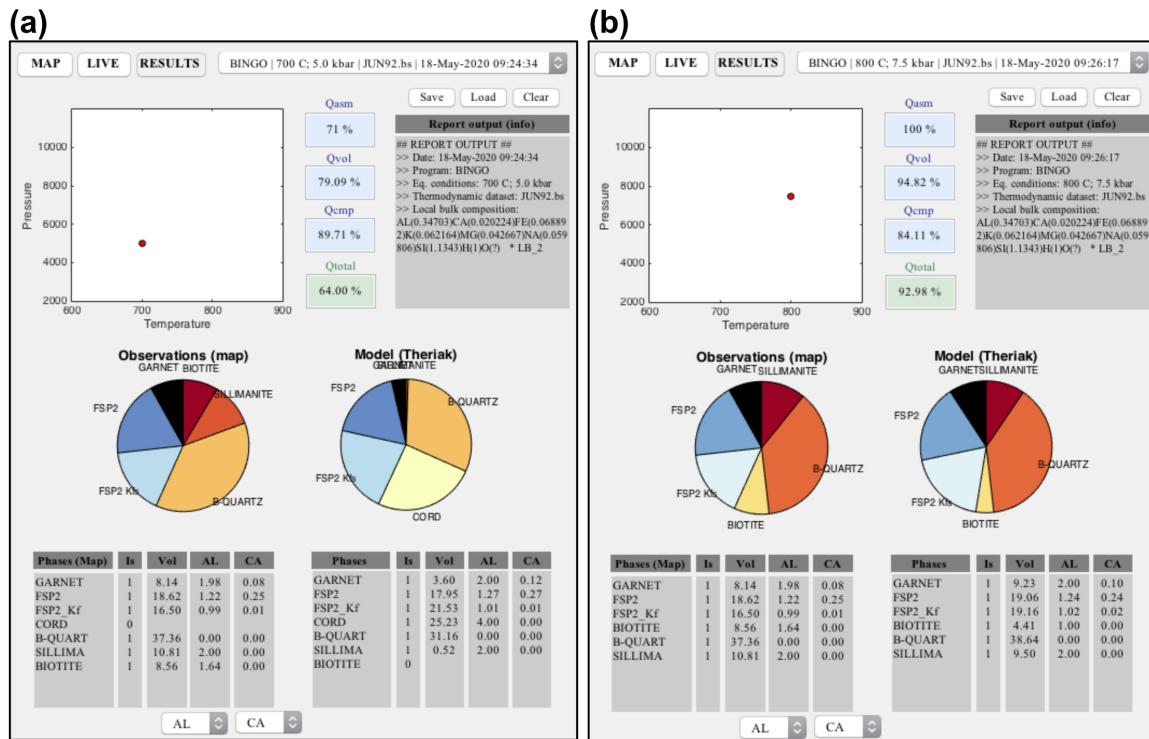


Figure 9.7 – Results of Bingo: (a) at 700 °C and 5000 and (b) 800 °C and 7500

9.7 BINGO

Once all the required steps are accomplished (database, bulk, fluid and solid definitions) the BINGO part of XHERMOTOOLS becomes available.

Note: As the selected area-of-interest used to calculate the local bulk composition is different for each user the results might slightly vary. However, no significant differences are expected for minor variations in local bulk composition (Lanari and Engi 2017).

9.7.1 Description of the first Bingo's output

(1) Set the P - T conditions to 700 °C and 5000 bar in the corresponding text boxes below the item BINGO and press the button BINGO

- The panel on the right switches to the workspace *Results* and displays the comparison between mode and observations (Fig. 9.7a). The following information is displayed:
- P-T diagram* showing the P - T conditions at which the comparison was performed by BINGO
 - Model quality factors*, Q_{asm} (assemblage); Q_{vol} (mineral modes); Q_{cmp} (mineral compositions); Q_{total} (global evaluation factor as defined in the options)
 - Report output* containing the date, program used, thermodynamic dataset and local bulk compositions. These data can be saved using the button *Save*.
 - Visual comparison between observations (map) and model (Theriaik)* using pie charts. The names of phases and solution models are used in these plots (database dependent) for a quick evaluation of potential synchronization issues. The same color scheme is used in both plots

- *Table of mineral modes and composition* to quickly display the differences between observed and modeled modes or mineral compositions. The two displayed elements can be changed via the two drop-down menus available below the table

A report containing all the information used in the calculation of the quality factor is shown in the MATLAB Command Window every time Bingo is used. An example is shown and described below.

```
----->>> New BINGO Run: 18-May-2020 09:54:06 <<<
----->>>

Bulk          1   AL(0.34703)CA(0.020224)FE(0.068892)K(0.062164)MG(0.042667)NA(0.059806)SI(1.1343)H(1)O(?) * LB_2
Database      JUN92.bs
P(bar)       5000
T(C)         700

##### Evaluation criterion (1) ASSEMBLAGE #####
Phases:    GARNET        FSP2        FSP2_Kfs      CORD        B-QUARTZ     SILLIMANITE   BIOTITE
THER:      1.000000     1.000000     1.000000     1.000000    1.000000    1.000000    0.000000
XMAP:      1.000000     1.000000     1.000000     0.000000    1.000000    1.000000    1.000000

n =       6
m =       6
l =       5
Qasm =   71.43
-----

##### Evaluation criterion (2) VOLUME FRACTIONS #####
Phases:    GARNET        FSP2        FSP2_Kfs      CORD        B-QUARTZ     SILLIMANITE   BIOTITE
THER:      0.036024     0.179548     0.215310     0.252311    0.311631    0.005177    0.000000
XMAP:      0.081400     0.186234     0.164987     0.000000    0.373601    0.108131    0.085648
abs(D):   0.045376     0.006686     0.050323     0.252311    0.061970    0.102954    0.085648

Qvol = 79.09
-----

##### Evaluation criterion (3) PHASE COMPOSITIONS #####
-
GARNET
Els:      O           AL           CA           FE           H           K           MG
NA        SI
THER:    12.000000   2.000000   0.117953   2.530194   0.000000   0.000000   0.351853
        0.000000   3.000000
XMAP:    12.000000   1.982995   0.077062   1.975278   0.000000   0.004047   0.851149
        0.003155   3.059209
abs(D):  0.000000   0.017005   0.040891   0.554916   0.000000   0.004047   0.499296
        0.003155   0.059209

Els:      CA           MG           FE           MN*
THER:    0.117953   0.351853   2.530194   0.000000
XMAP:    0.077062   0.851149   1.975278   0.000000
-
UNC:     0.010000   0.062561   0.133713   0.000000
DIFFab:  0.040891   0.499296   0.554916   0.000000
DIFF2:   0.030891   0.312807   0.421204   0.000000
-
QUALs:   0.341193   0.000000   0.029896   0.000000
-
Qcmp = 12.3696 %

-
FSP2
Els:      O           AL           CA           FE           H           K           MG
NA        SI
THER:    8.000000   1.274898   0.274898   0.000000   0.000000   0.056701   0.000000
        0.668401   2.725102
XMAP:    8.000000   1.221469   0.252098   0.002122   0.000000   0.026917   0.001555
        0.745961   2.762792
abs(D):  0.000000   0.053429   0.022800   0.002122   0.000000   0.029784   0.001555
        0.077560   0.037690

Els:      SI           AL           NA           CA           K
THER:    2.725102   1.274898   0.668401   0.274898   0.056701
XMAP:    2.762792   1.221469   0.745961   0.252098   0.026917
-
UNC:     0.061954   0.034636   0.037717   0.010386   0.010000
DIFFab:  0.037690   0.053429   0.077560   0.022800   0.029784
DIFF2:   0.000000   0.018793   0.039843   0.012414   0.019784
-
QUALs:   1.000000   0.770032   0.673029   0.705881   0.587313
-
Qcmp = 74.7251 %

-
FSP2_Kfs
Els:      O           AL           CA           FE           H           K           MG
NA        SI
```

THER:	8.000000	1.009285	0.009285	0.000000	0.000000	0.781519	0.000000
	0.209196	2.990715					
XMAP:	8.000000	0.985530	0.007593	0.001944	0.000000	0.795165	0.003574
	0.199307	3.005679					
abs (D) :	0.000000	0.023755	0.001692	0.001944	0.000000	0.013646	0.003574
	0.009889	0.014964					
Els :	SI	AL	NA	CA	K		
THER:	2.990715	1.009285	0.209196	0.009285	0.781519		
XMAP:	3.005679	0.985530	0.199307	0.007593	0.795165		

UNC:	0.051126	0.024618	0.018941	0.010000	0.016973		
DIFFab:	0.014964	0.023755	0.009889	0.001692	0.013646		
DIFF2:	0.000000	0.000000	0.000000	0.000000	0.000000		

QUALs:	1.000000	1.000000	1.000000	1.000000	1.000000		
Qcmp = 100 %							
---	Phase: CORD has been skipped by BINGO ---						
-							
B-QUARTZ							
Els :	O	AL	CA	FE	H	K	MG
	NA	SI					
THER:	2.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	1.000000					
XMAP:	2.000000	0.000118	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.999912					
abs (D) :	0.000000	0.000118	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000088					
Els :	SI						
THER:	1.000000						
XMAP:	0.999912						

UNC:	0.014279						
DIFFab:	0.000088						
DIFF2:	0.000000						

QUALs:	1.000000						
Qcmp = 100 %							
-							
SILLIMANITE							
Els :	O	AL	CA	FE	H	K	MG
	NA	SI					
THER:	5.000000	2.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	1.000000					
XMAP:	5.000000	1.997003	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	1.002248					
abs (D) :	0.000000	0.002997	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.002248					
Els :	AL						
THER:	2.000000						
XMAP:	1.997003						

UNC:	0.043705						
DIFFab:	0.002997						
DIFF2:	0.000000						

QUALs:	1.000000						
Qcmp = 100 %							
---	Phase: BIOTITE has been skipped by BINGO ---						

Phase	GARNET	FSP2	FSP2_K	CORD	B-QUAR	SILLIM	BIOTIT
Evaluated	Yes	Yes	Yes	No	Yes	Yes	No
Qual (%)	12.37	74.73	100.00	0.00	100.00	100.00	0.00
v_norm	0.05	0.24	0.29	0.00	0.42	0.01	0.00
v	0.04	0.18	0.22	0.25	0.31	0.01	0.00
Qcmp_vn =	89.71						
Qcmp_v =	67.07						
Qcmp =	89.71						

##### CHEMICAL POTENTIAL OF COMPONENTS #####							
Oxide	mm (J)						
CAO	-808344						
MGO	-688732						
AL2O3	-1761530						
FEO	-359917						
K2O	-935768						
SiO2	-966534						
NA2O	-864996						
H2O	-375634						
O2	-492382						
##### STABLE ASSEMBLAGE (THERIAK) #####							
Phase (solids)	Volume (%)	Density (kg.m^-3)					

```

GARNET      3.60      4147
FSP2       17.95     2623
FSP2_Kfs   21.53     2543
CORD        25.23     2593
B-QUARTZ   31.16     2551
SILLIMANITE 0.52      3235

Phase (fluid) XH2O    XCO2    Density (kg.m^-3)
STEAM       1.000   0.000     756

>>> End BINGO Run: 18-May-2020 09:54:06 <<<
-----
```

Code 9.6 – Report of Bingo displayed in the Command Window

The report includes (see Code 9.6 above):

- *Model information* listing the bulk composition, database, T and P conditions
- *Evaluation criterion (1) ASSEMBLAGE* showing the list of observed and modeled phases and if they are present in model (THER) and/or observations (XMAP)
- *Evaluation criterion (2) VOLUME FRACTIONS* showing the volume fraction of each phase in model (THER) and observations (XMAP)
- *Evaluation criterion (3) PHASE COMPOSITIONS* listing the mineral composition of each phase in model (THER) and observations (XMAP) for the matching phases. The non-matching phases are ignored as they are *skipped by Bingo*. The first table contain the mineral composition for each element of the chemical system. The second table contains only the compositions and their uncertainties for the elements used to calculate Q_{cmp} . A summary of each individual Q_{cmp} values is also provided including the volume fractions used to estimate the value of Q_{cmp} for the model
- *CHEMICAL POTENTIAL OF COMPONENT* listing the chemical potential of each component. These values are relevant only of the chemical potential is buffered for the system under consideration (not checked here)
- *STABLE ASSEMBLAGE (THERIAK)* shows the mineral assemblage predicted to be stable the volume fractions (in percent) and the density of each phase. It also shows the fluid phases if present. If a fluid phase is present the model is fluid-saturated, otherwise it is fluid under-saturated.

9.7.2 Manual P-T investigation using Bingo

(1) Adjust the P - T conditions manually in the corresponding text boxes below the item BINGO and press the button *BINGO* to try to improve the value of Q_{asm} to 100 %; this corresponds to finding the mineral assemblage in a phase diagram.

(2) Set the P - T conditions to 800 °C and 7500 bar in the corresponding text boxes below the item BINGO and press the button *BINGO*.

The result is shown in Figure 9.7b. At these P - T conditions, the value of Q_{asm} is 100 %, Q_{vol} approximately 95 % and Q_{cmp} is lower at 84 %. The global evaluation parameter Q_{total} (here Q_{total1}) is of to 93 %.

In the following, the P - T conditions of the "optimal model" are derived using ANTIDOTE.

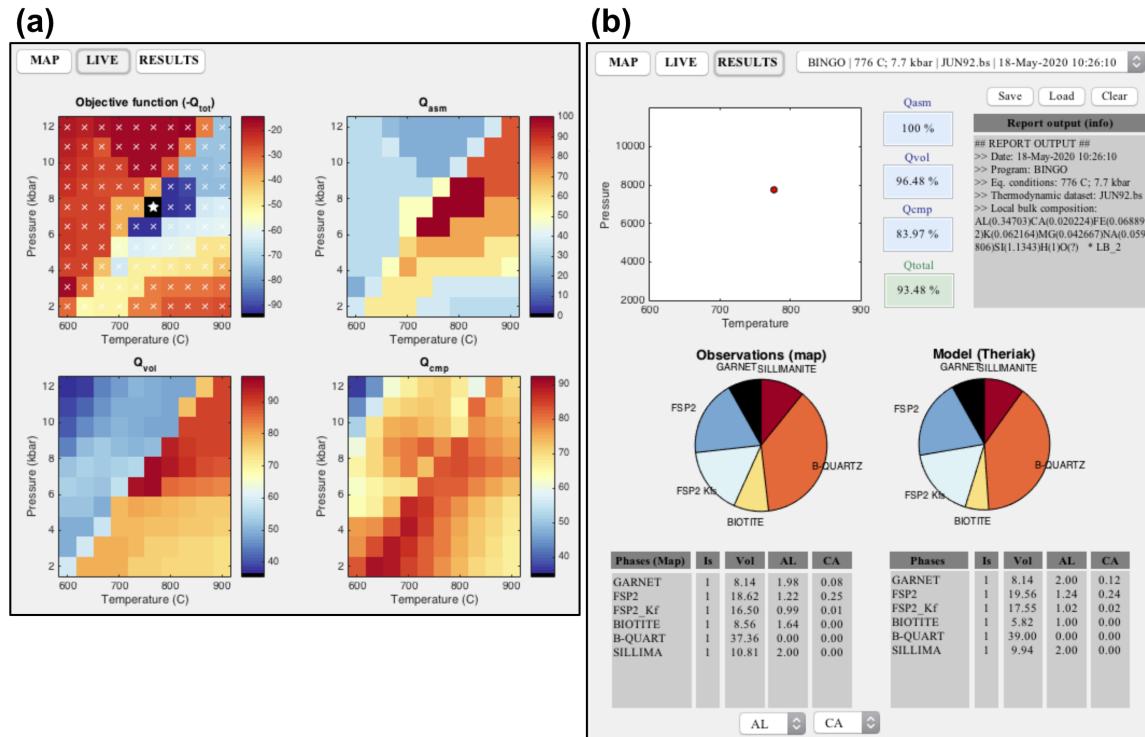


Figure 9.8 – Results of Antidote, recipe 1 (find optimal P-T conditions)

9.8 ANTIDOTE

The main functionalities of ANTIDOTE are illustrated in the example below. The proposed strategy is general and can be easily transposed to other examples.

9.8.1 Recipe 1: find optimal P-T conditions

- (1) Select the first recipe *find optimal P-T conditions* in the antidote menu and press the button *ANTIDOTE*.

The results are shown in Figure 9.8 and the report in Code 9.7.

The minimization of the objective function $-Q_{total}$ in the P-T space involves two steps of optimization:

- *Exploratory P-T scanning (10 x 10)*. During this first stage, the objective function is mapped using a regular grid of 10 x 10 steps. The minimal value of $-Q_{total}$ is taken as the starting point for the second step of optimization. The corresponding P-T conditions (here 676 °C and 7550 bar) are shown using a white star in the figure (Fig. 9.8a). Note that the grid size can be changed in settings (via the menu *File » Preferences*); this parameter is important for catching small P-T stability fields.
- *Final P-T Optimization* is a gradient iterative optimization starting at the the P-T conditions with the lower value of $-Q_{total}$. The iterations are displayed in the MATLAB Command Window (e.g. Code 9.7)

```

-----  

>>> New ANTIDOTE job: 18-May-2020 10:25:38 <<<  

Antidote      [ Recipe 1] Find optimal P-T(-X)  

Bulk          1 AL(0.34703)CA(0.020224)FE(0.068892)K(0.062164)MG(0.042667)NA(0.059806)SI(1.1343)H(1)O(?) * LB_2  

Database     JUN92.bs  

##### Exploratory P-T scanning (10 x 10) #####  

** WARNING **  

The component H2O is "saturated" for 100/100 P-T couples  

-> This may cause convergence to local minima if H is part of the optimization  

Further warning messages related to this issue will be displayed below  

RESULTS (Exploratory P-T scanning)  

X0(1)    P(bar)   7550  

X0(2)    T(C)      767  

CPU time       23.0195  

##### Final P-T Optimization (from: 766.6667 bar; 7550 C) #####  

Method:        Simplex  

Equation:      Classic [E4 = -1/3*(E1 + (E1/100)*E2 + (E1/100)*E3)]  


| Iteration | Func-count | min f(x) | Procedure       |
|-----------|------------|----------|-----------------|
| 0         | 1          | -93.3434 |                 |
| 1         | 3          | -93.3434 | initial simplex |
| ...       |            |          |                 |
| 27        | 51         | -93.483  | contract inside |

Optimization terminated:  

the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-04  

and F(X) satisfies the convergence criteria using OPTIONS.TolFun of 1.000000e-04  

RESULTS (Final P-T optimization)  

X(1)    P(bar)   7727  

X(2)    T(C)      776  

CPU time       6.6016  

>> ANTIDOTE calls BINGO ---->

```

Code 9.7 – Report of Antidote recipe 1 (find optimal P-T conditions) displayed in the Command Window

Once the optimization is done, ANTIDOTE calls BINGO and the display switches to the result tab (Fig. 9.8b).

It is interesting to go through the details for this result:

- At the P - T conditions of 776 °C and 7.7 bar, the value of Q_{asm} is 100 %, Q_{vol} 96.5 % and Q_{cmp} is 84 %. The global evaluation parameter Q_{total} (here Q_{total1}) is of to 93.5 %. These values are largely similar to the results obtained with BINGO at 800 °C and 7500 bar. This shows that the quality factors do not change significantly within the stability field of the peak assemblage. Yet the "optimal solution" from a statistical point of view is at 776 °C and 7.7 bar.
 - None of the mineral composition is matching the observations and the model quality factors are systematically lower than 100 % (see Code 9.9). The Q_{cmp} value of biotite is only 11 % reflecting stark differences in Al, Mg contents (check the output of BINGO).

- (2) Select *Biotite* in the drop-down menu below the item *Phase definitions* and switch to *Grp1* corresponding to the biotite composition of grains far away from garnet.

(3) Press the button BINGO and check the Q_{cmp} value of biotite. The result has improved (46 %), but is still far from the optimal value of 100 %.

	GARNET	FSP2	FSP2_K	BIOTIT	B-QUAR	SILLIM
Evaluated	Yes	Yes	Yes	Yes	Yes	Yes
Qual (%)	88.58	72.15	70.72	11.21	100.00	100.00
v_norm	0.09	0.19	0.19	0.04	0.39	0.09
v	0.09	0.19	0.19	0.04	0.39	0.09
Qcmp_vn =	84.11					
Qcmp_v =	84.11					
Qcmp =	84.11					

Code 9.8 – Partial report of Bingo obtained at the P-T conditions of 776 °C and 7.7 bar using biotite Bt2

	GARNET	FSP2	FSP2_K	BIOTIT	B-QUAR	SILLIM
Evaluated	Yes	Yes	Yes	Yes	Yes	Yes
Qual (%)	76.19	74.05	78.99	49.31	100.00	100.00
v_norm	0.08	0.20	0.18	0.06	0.39	0.10
v	0.08	0.20	0.18	0.06	0.39	0.10
Qcmp_vn =	86.35					
Qcmp_v =	86.35					
Qcmp =	86.35					

Code 9.9 – Partial report of Bingo obtained at the P-T conditions of 776 °C and 7.7 bar using biotite Bt1

(4) Save the phase definitions via the menu *Phase Matching* and *Save Phase Configuration* to update the selection of the biotite group (overwrite *BIN_Phases_JUN92.bs_.xtt*)

(5) Select the first recipe *find optimal P-T conditions* in the antidote menu and press the button *ANTIDOTE* to optimize P-T using the composition of Bt1 (*Grp1*).

In this example, the optimal conditions are obtained at similar P-T conditions of 775.6 °C and 7720 bar (it was 776.3 °C and 7727 bar with biotite Bt2), but the maximal value of Q_{cmp} raised to 86 % and Q_{total} to 94.3 %. According to the model, this biotite composition is more likely in equilibrium with the other phases at these conditions.

(6) Save the optimal P-T conditions. In the menu, navigate to *Initialize* and *Generate OptionsXTT.txt*. Input the optimal P-T conditions reported in BINGO as default values with the same number of significant figure. Note that the optimal result can be very close to a reaction boundary and rounding could result in a shift to a different stability field. Press the button *Generate OptionsXTT.txt* to close the window, apply the parameters and save the file.

(6) Save the corresponding result of BINGO using the button *Save* located in the *Results* panel.

9.8.2 Recipe 2: P-T map of Q factors

(1) Select the second recipe *P-T map of Q factors* in the antidote menu and press the button *ANTIDOTE*.

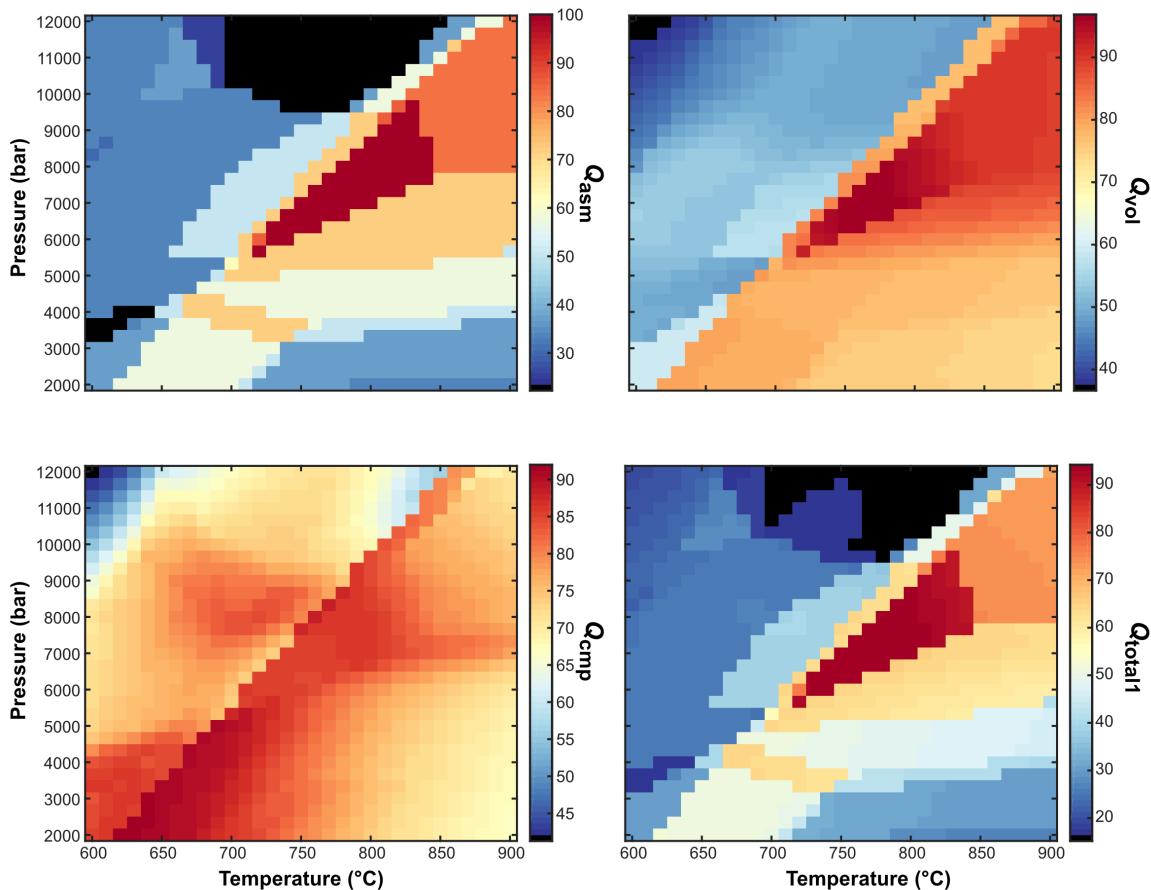


Figure 9.9 – Results of Antidote, recipe 2 (P-T map of Q factors)

This recipe produces P-T maps of each quality factor including Q_{cmp} of each phase as well as other quantities (e.g. volume fractions) using the P-T window (and step) defined in the settings (OptionsXTT.txt). Results are saved in `/Antidote/Recipe2_DATE_TIME/`

This operation takes between 2 and 10 minutes with the selected database and map resolution. The figures are then saved one-by-one; be patient!

Warning: Do not change the working directory in MATLAB while opening the figures for visualization. Use the small arrows located left of the folder in the Current Folder window!

9.8.2.1 Maps of quality factors for the assemblage

- (1) Navigate to the folder `/Antidote/Antidote_Recipe2_DATE_TIME/` (do not change the working directory in MATLAB, see the warning above) and open the maps of quality factors

The results of the four quality factors are shown in Figure 9.9. The observed mineral assemblage (garnet, biotite, sillimanite, k-feldspar, plagioclase and quartz) is modeled in a stability fields between 700 and 850 °C, and between 6000 and 9000 bar (Q_{asm} of 100 %). The value of Q_{vol} is above 85 % in this stability field. The pattern of Q_{cmp} is different with maxima outside the stability field. Note that Q_{cmp} is calculated only for the matching phases, so the values should be compared only within a single stability fields.

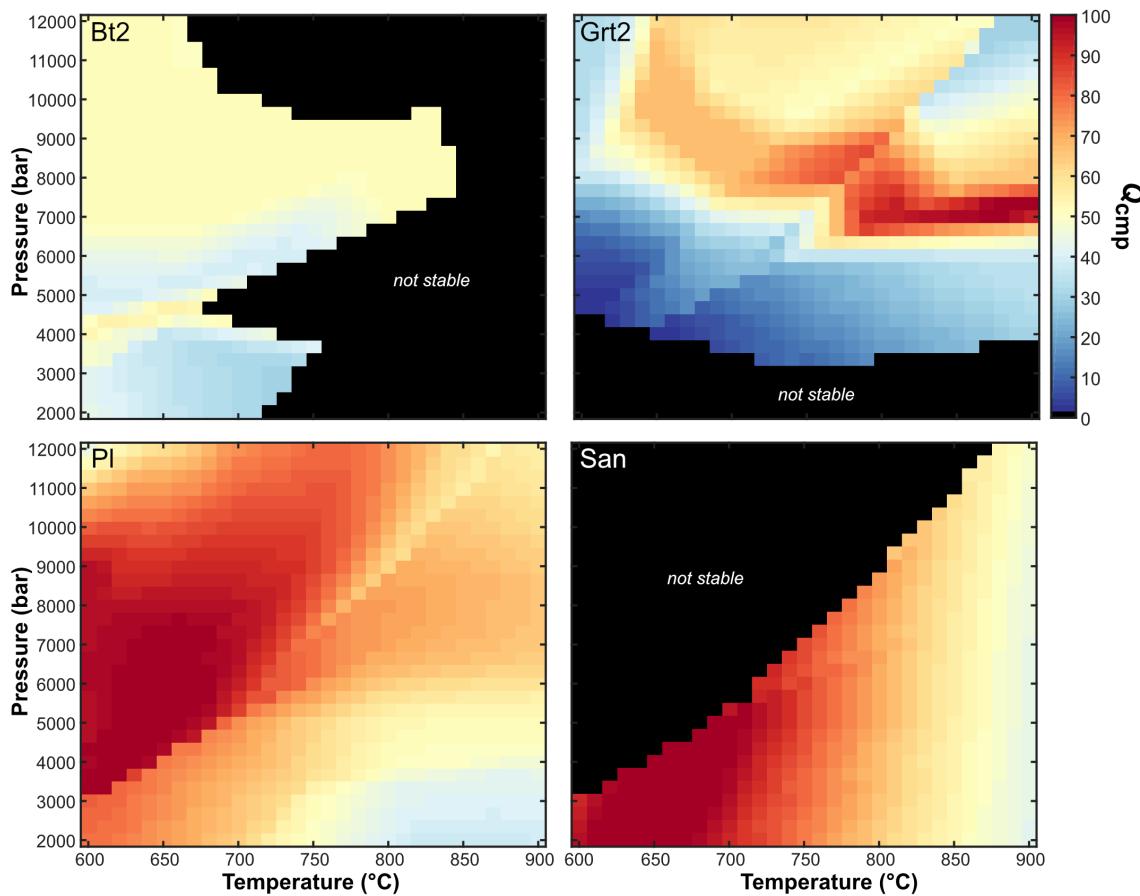


Figure 9.10 – Results of Antidote, recipe 2: P-T map of Q_{cmp} for minerals

9.8.2.2 Maps of quality factor for each mineral

- (1) Open the file `5_Qcmp_BIOTITE.fig` in the folder `/Antidote/Antidote_Recipe2_DATE_TIME/` (do not change the working directory in MATLAB, see the warning above). Click on the figure and change the color contrast using the command: » `caxis([0 100])` in the MATLAB Command Window. The results of the Q_{cmp} maps of each minerals are shown in Figure 9.10. These results indicate that both plagioclase and K-feldspar formed at lower P - T conditions (600 - 700 °C).

Note that the maps of quality factors in [Lanari and Duesterhoeft \(2019\)](#) were generated with a different database including a melt model while fixing the amount of H. This last change reduced the stability of white mica at the expense of k-feldspar. This scenario is explored below.

9.8.3 Recipe 14: Scanning H (fixed P-T)

This recipe evaluates the model quality factors at fixed P - T conditions and fixed bulk composition except for the amount Hydrogen (H). The amount of H in the model can be adjusted manually or automatically. Both strategies are described below.

9.8.3.1 Adjusting manually the amount of H in bulk

- (1) Restore the optimal P - T conditions previously determined in the BINGO input fields and press the button *BINGO*. Note that these conditions can be restored by applying the settings saved in the

OptionXTT file. Navigate to *Initialize*, *Generate OptionsXTT.txt* and press the button *Generate OptionXTT.txt*

A fluid phase is predicted to be stable at these conditions. This information is given in the BINGO report displayed in the Command Window (see Code 9.10).

#stable assemblage (theria)		
Phase (solids)	Volume (%)	Density (kg.m ³)
GARNET	8.10	4039
FSP2	19.57	2622
FSP2_Kfs	17.50	2551
BIOTITE	5.87	2970
B-QUARTZ	39.01	2559
SILLIMANITE	9.96	3238
Phase (fluid)	XH2O	XCO2
STEAM	1.000	0.000
		Density (kg.m ³)
		839

Code 9.10 – Partial report of Bingo obtained at the P-T conditions of 776 °C and 7.7 bar for 1 mol of H

- (2) In the menu *Additional Elements*, select the item *Set Fluids, Melts and Buffers*. Change the amount of H to 0.5 mol and press the button *Apply*. Note that the bulk composition was updated.
- (3) Run BINGO again and check if a fluid phase is predicted to be stable. In this case, the same result as shown in Code 9.10 is obtained. The model is still saturated in fluid at these conditions.
- (4) Change the value to 0.05 mol of H (via the menu *Additional Elements* and *Set Fluids, Melts and Buffers*) and check the BINGO's output. The model is still saturated in fluid.
- (5) Change the value to 0.01 mol of H and check the BINGO's output. In this case there is no fluid predicted to be stable at 776 °C and 7.7 bar and the values of the model quality factors changed.

9.8.3.2 Optimizing the amount of H in bulk using Recipe 14

- (1) In the menu, navigate to *Additional Elements* and *Set Fluids, Melts and Buffers*. Select the option *Optimize N fluid* and set the range of H value to 0.0001 to 0.06. In this example, the upper limit was selected in the saturated region. Press *Apply* to close the option window

Note that the value of H in the bulk was set to the central value of 0.03005 which correspond to saturated conditions (can be checked using BINGO).

- (2) Select the recipe 14 *Scanning H (fixed P-T)* in the antidote menu and press the button *ANTIDOTE*.

The results are stored in the folder */Antidote/Antidote_Recipe14_DATE_TIME/* (do not change the working directory in MATLAB, see the warning above) and in Figure 9.11. The optimal value of Q_{cmp} is obtained for 0.16 mol of H whereas the optimal value of Q_{vol} is obtained at saturation for $H > 0.27$. An intermediate result of 0.25 mol H is selected in the following.

- (3) Open the *Set Fluids, Melts and Buffers* tool, deselect the option *Optimize N fluid*, set the amount of H to 0.025 and press *Apply*

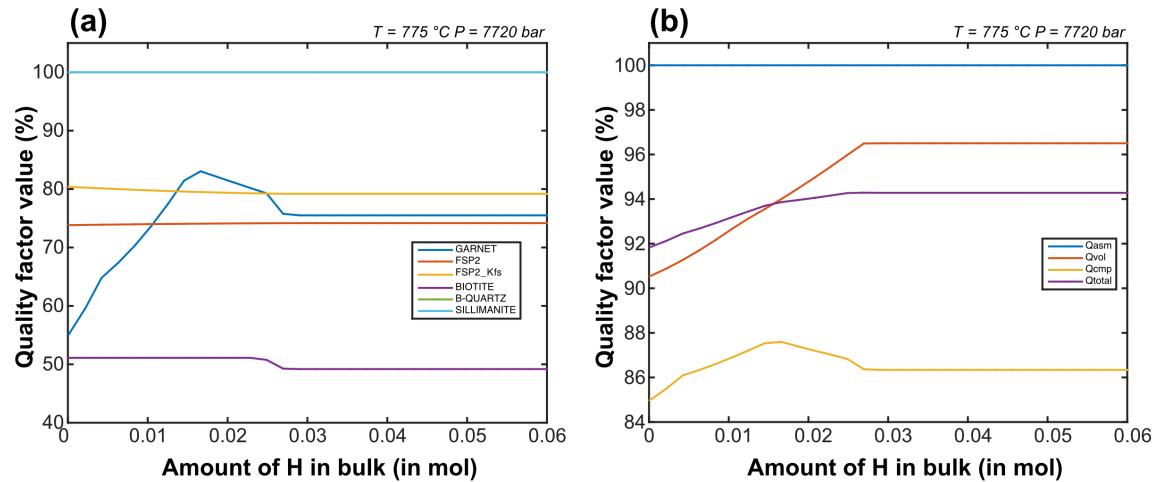


Figure 9.11 – Results of Antidote, recipe 14: Scanning H (fixed P-T)

(4) Edit the file *Generate OptionXTT.txt* (menu *Initialize* and *Generate OptionsXTT.txt*) and set the bulk composition option to $H(0.025)O(?)$. This action saves the value and automatically use as default value for H upon restart.

(5) (Optional) Recalculate the maps of quality factors using ANTIDOTE' recipe 2 and compare with the previous results and with the results reported in [Lanari and Duesterhoeft \(2019\)](#).

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