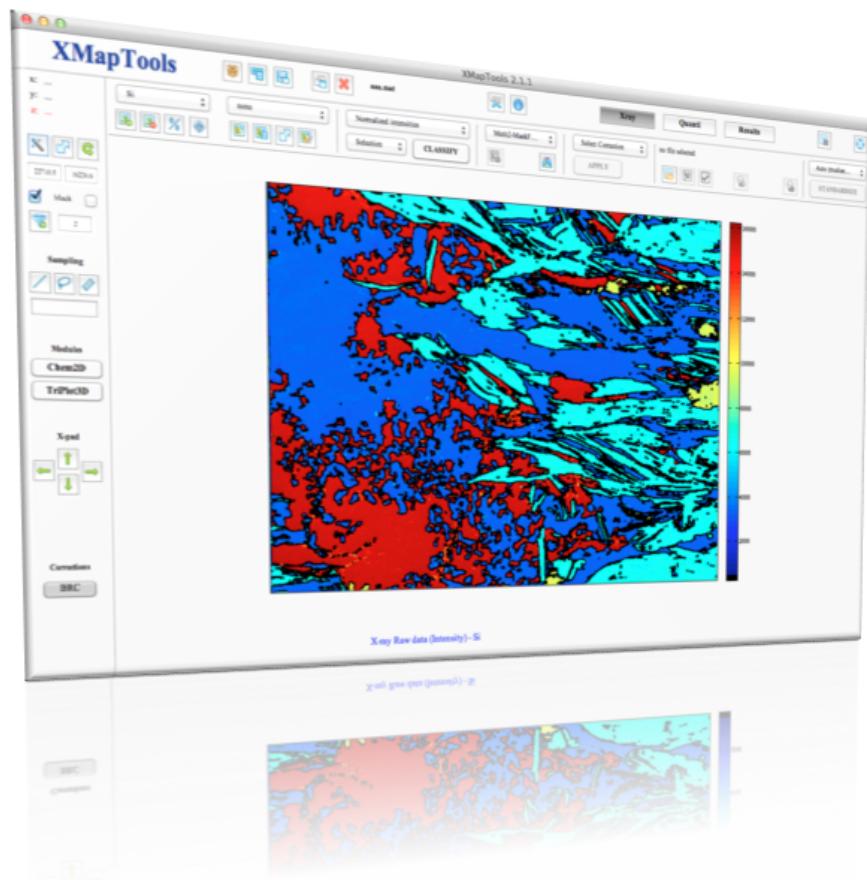


Dr. Pierre Lanari

# An introduction to XMapTools 2.6

*numerical tools for quantitative petrology*



INSTITUTE OF GEOLOGICAL SCIENCES  
UNIVERSITY OF BERN

Bern, Saturday 15<sup>th</sup> December, 2018

Dear user,

It is a pleasure to introduce you XMAPTOOLS 2.6, a software solution to process and analyze compositional maps, notably those obtained by EPMA, SEM or LA-ICP-MS. This project was initiated in 2009; the first public release was provided in late 2012. Since that time, the program has continuously been improved with numerous updates containing new functionalities and improvements. XMAPTOOLS is an active product of research that is developed on a weekly basis. These are collected and provided to you via public updates every years.

This user guide aims to assist you and to give you the better experience possible with XMAPTOOLS. However, before to go further into details and see how each part of the program works, it is important to acknowledge undergraduates, PhD students and researchers that have actively participated in testing XMAPTOOLS.

Dr. Pierre Lanari

## XMAPTOOLS HISTORY

XMAPTOOLS 2.X (2014-present) has been developed by Dr. Pierre Lanari at the University of Bern (Institute of Geological Sciences).

XMAPTOOLS 1.X (2009-2014) was developed by Dr. Pierre Lanari at the University of Grenoble (ISTerre) with support from Dr. Olivier Vidal and Dr. Éric Lewin

## ACKNOWLEDGEMENTS

I would like to thank 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 (Durham University) M. Engi, J. Hermann, D. Rubatto, M. Burn, A. Berger, M. Tedeschi, A. Vho, E. Kempf, T. Bovay and F. Giuntoli (University of Bern) 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) for help, suggestions, comments, data and/or collaborations in order 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 (<http://www.xmaptools.com>) is available and provides the latest version of the software including online updates with additional tools, user guide and a tutorial.

XMAPTOOLS software (Lanari et al. 2014b) uses a Castaing-like approach (De Andrade et al. 2006, Lanari et al. 2018) 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 et Engi 2017).

## 1.2 CITATION GUIDELINES

Please use the following citations in your publications when you refer to XMAPTOOLS. The version of the program should be specified just after the name. Example: *Mapping data were processed using XMAPTOOLS 2.6.1 (Lanari et al. 2014; 2018)*

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., (2018). Quantitative compositional mapping of mineral phases by electron probe micro-analyser. *Geological Society of London Special Publication*, DOI:10.1144/SP478.4
- 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 and density correction:

- LANARI, P., ENGI, M., 2017. Local bulk composition effects on metamorphic mineral assemblages. *Reviews in Mineralogy and Geochemistry*, 83, 55-102

### 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 et Engi \(2017\)](#), [Lanari et al. \(2017\)](#), [Raimondo et al. \(2017\)](#)

**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.

## 1.3 LICENCE

XMAPTOOLS software is distributed in an Double Regime: Academic and Commercial.

In the Academic and Public Research World, XMapTools is distributed under the terms of the [Scientific Software Open Source Academic For Free License](#). This License sets the program Gratis and Open Source, and grants Freedom to use, copy, study, modify and redistribute it. But these policies hold only within the Academic and Public Research world. Thus the Academic World can be reassured that the normal research academic policies in working with scientific software are granted by this license. And it goes even beyond GNU-GPL, since it explicitly sets GRATIS the software.

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## 1.4 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. \(2018\)](#). 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.

### 1.4.1 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.

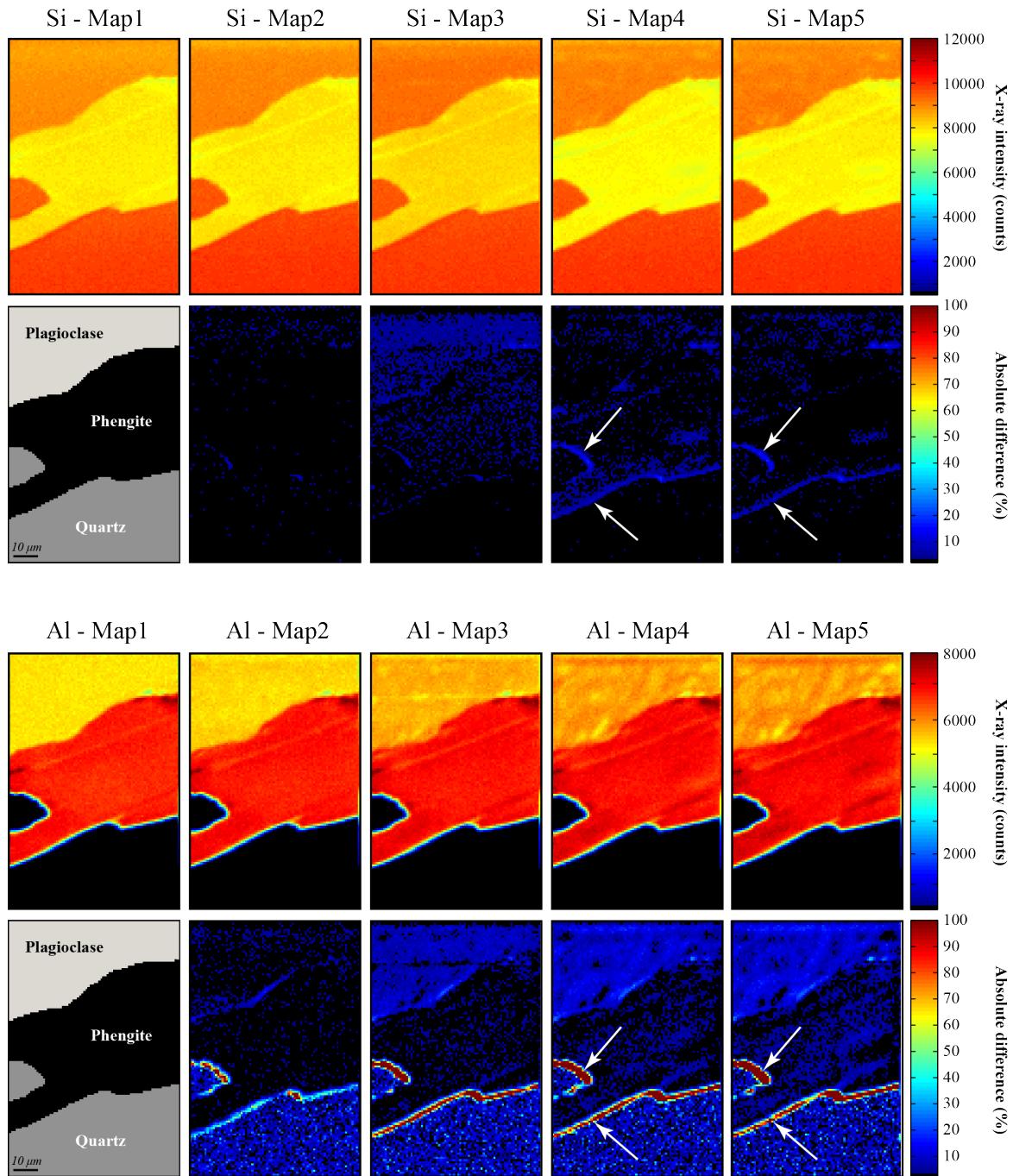


Figure 1.1 – X-ray maps Si (top) and Al (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating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

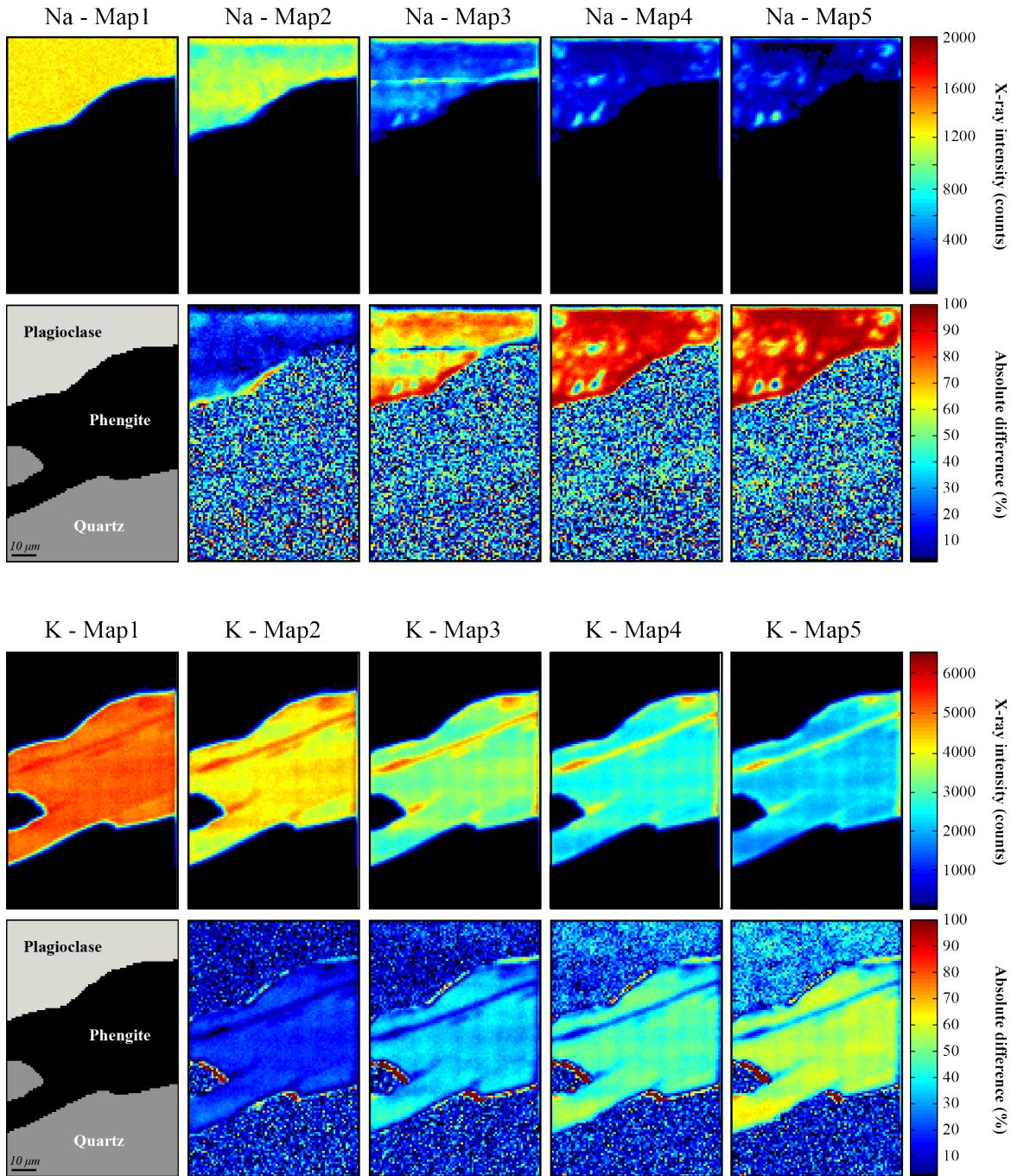


Figure 1.2 – X-ray maps Na (top) and K (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating voltage was 15 KeV, specimen current 200 nA, dwell time 200 ms and the beam size 1  $\mu\text{m}$ . 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).

#### 1.4.1.1 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  $\mu m$  will generates images of  $36 \times 35$ ,  $18 \times 17$ ,  $12 \times 11$  and  $9 \times 8$  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  $\mu m$  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  $\mu m$  (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  $\mu m$  spot size, 24 with 2  $\mu m$ , 10 with 3  $\mu m$  and 4 with 4  $\mu m$ . 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  $\mu m$  (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.

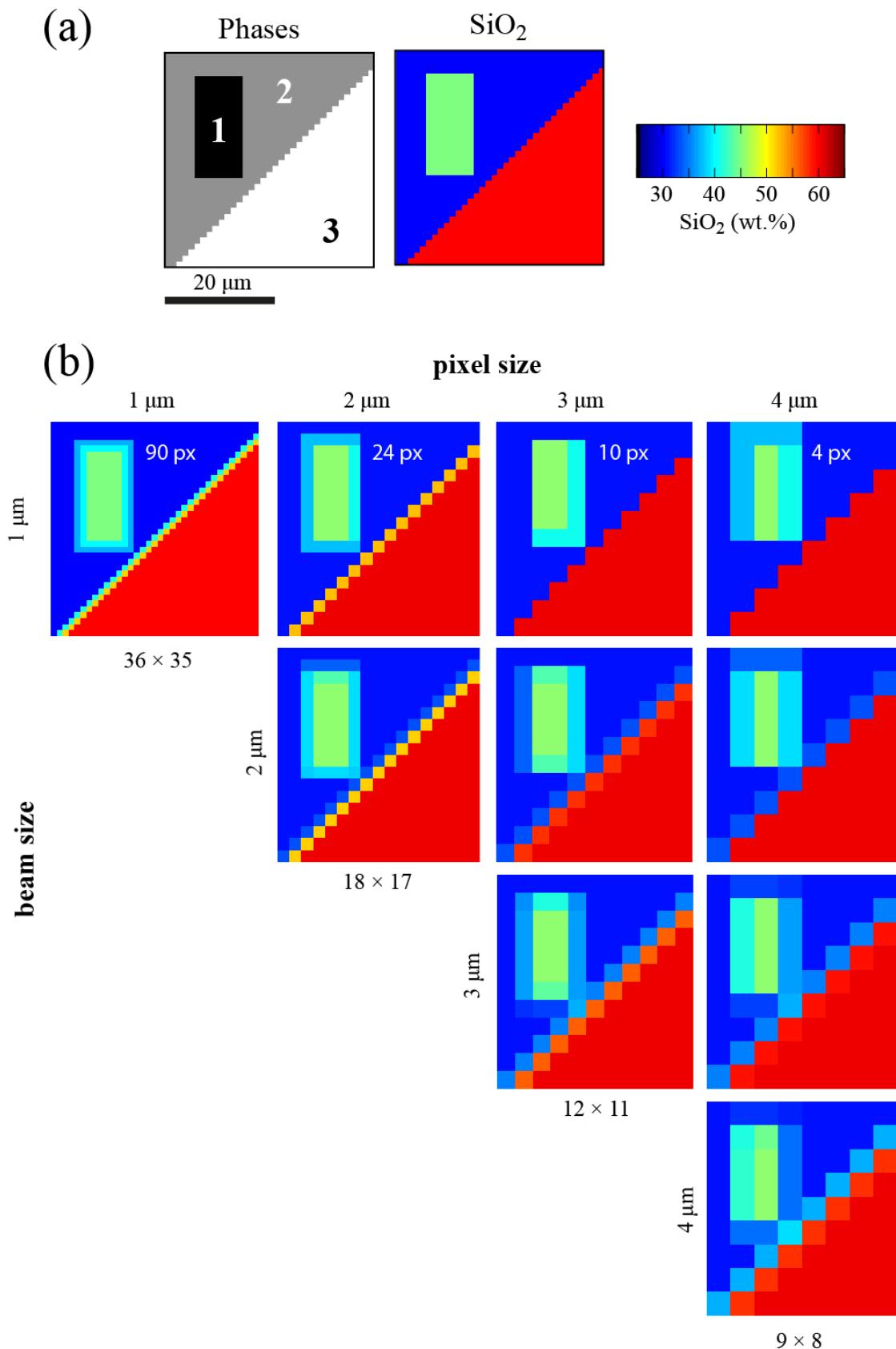


Figure 1.3 – Spatial resolution dependency to pixel size and beam size. (a) Images of the different phases (left) and compositions of  $\text{SiO}_2$  (right). The phase compositions are assumed to be perfectly homogeneous with  $\text{SiO}_2$  composition of 45 wt.%, 30 wt.% and 60 wt.% for phases 1, 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  $\mu\text{m}$  (see text for details).

### 1.4.1.2 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  $2\sigma$ ), 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% ( $2\sigma$ ), 10,000 counts for 2% ( $2\sigma$ ), and 20,000 for 1% ( $2\sigma$ ).

**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,  $100\text{ nA}$  specimen current,  $200\text{ ms}$  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. \(2014b\)](#).

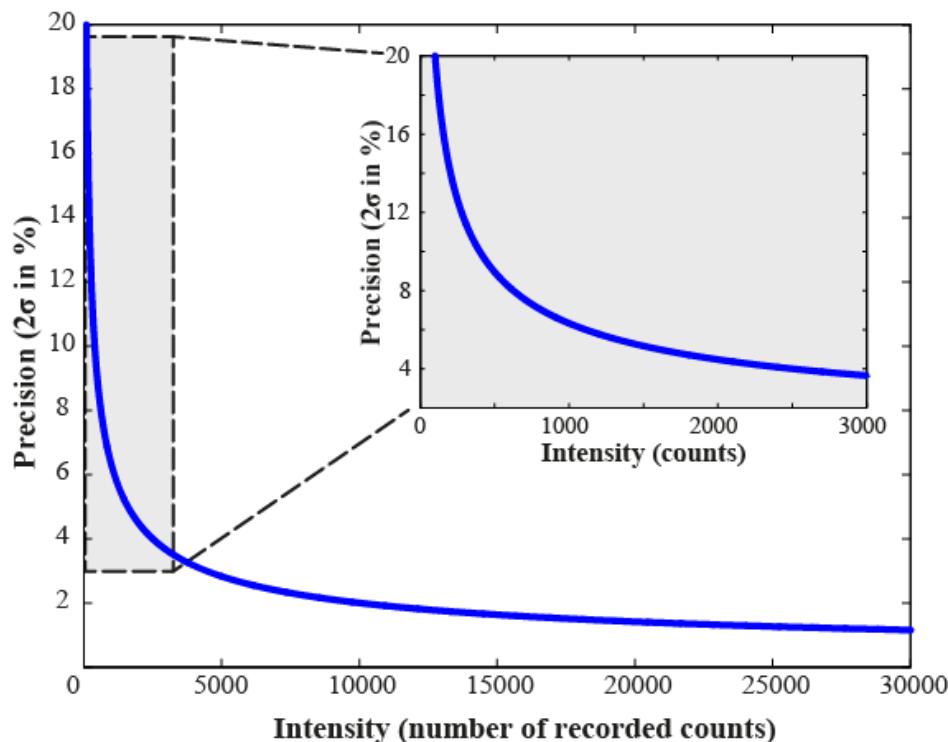


Figure 1.4 – Relation between the number of recorder counts and the analytical precision of an analysis

## 1.5 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.

### 1.5.1 How to precisely determine local bulk composition from compositional maps?

#### 1.5.1.1 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.

### 1.5.1.2 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. 3.19).

(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 3.14). 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].

### 1.5.1.3 Method evaluation

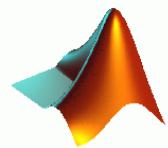
The description of this technique as well as some tests are provided in [Lanari et Engi \(2017\)](#).

HOW TO GET STARTED

2

## 2.1 REQUIREMENTS

XMAPTOOLS is a MATLAB<sup>©</sup>-based program that requires MATLAB<sup>©</sup> to be executed. **Unfortunately, there is no compiled version of XMAPTOOLS available so far and users must have a version of MATLAB<sup>©</sup> installed.** NB: For students, a cheap MATLAB<sup>©</sup> student version can be purchased in the Mathwork website ([www.mathworks.com](http://www.mathworks.com)).



XMAPTOOLS may be run with MATLAB<sup>©</sup> version 7.5 release R2007b or more recent releases. It has been developed on a MacBook Pro using MATLAB<sup>©</sup> R2012a and it has been intensively tested on MATLAB<sup>©</sup> R2014b and on Windows 10 with MATLAB<sup>©</sup> R2014b.

XMAPTOOLS 2.6.1 seems to be fully compatible with MATLAB<sup>©</sup> R2017b on OSX. The program checks which MATLAB<sup>©</sup> version is used and run the recommended GUI: *VER\_XMapTools\_750* from MATLAB<sup>©</sup> 2009b to MATLAB<sup>©</sup> 2014a and *VER\_XMapTools\_804* from MATLAB<sup>©</sup> 2014b and recent versions. This compatibility check ensures a better compatibility of XMAPTOOLS with the recent versions of MATLAB<sup>©</sup> in which a new graphical engine has been deployed.

XMAPTOOLS does not require any additional MATLAB<sup>©</sup> toolbox such as *Statistic*, *Image Processing* toolboxes. However, we strongly recommend to have such toolboxes that may provide useful functions if you want to go further than what XMAPTOOLS does.

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**Warning:** Starting at the next major release (probably XMAPTOOLS 2.7), MATLAB<sup>©</sup> R2014b or a more recent version will be required. XMAPTOOLS will not longer receive updates if used within old MATLAB<sup>©</sup> environments (pre-R2014b). Please consider upgrading your MATLAB<sup>©</sup> to ensure full compatibility with the most advanced version of XMapTools!

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## 2.2 UPGRADE PROCEDURE FOR PREVIOUS USERS (FROM XMAPTOOLS 1.6.5 TO XMAPTOOLS 2.1.X)

If you have been using XMAPTOOLS 1.6.5 or a previous version on your computer, it must be deactivated before to install XMAPTOOLS 2.

- (1) Run MATLAB<sup>©</sup>
- (2) In the MATLAB<sup>©</sup> 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 2.3).

**NB:** The installation directory of XMAPTOOLS must be stored in the pathdef file of MATLAB<sup>©</sup>. 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<sup>©</sup> 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.

## 2.3 INSTALLATION PROCEDURE (DOWNLOAD, SETUP AND FIRST CONFIGURATION)

### 2.3.1 Download XMapTools package

The XMAPTOOLS package is required for a first installation of XMAPTOOLS (release 2.1.X and later) in your computer.

XMAPTOOLS package includes the programs *XMapTools.p* *Install\_XMapTools.p*, which is a program used to install and configure XMAPTOOLS.

The package is available at: [www.xmaptools.com](http://www.xmaptools.com) in the section RESSOURCES and *Download*.

Registration on the website is mandatory before to download XMAPTOOLS package. To register, users must provide an user name together with an 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 2.X]
- (3) Download the XMAPTOOLS package using the button **download**.

*By downloading or using XMAPTOOLS, you accept the terms of the software license agreement (available in 1.3). 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*

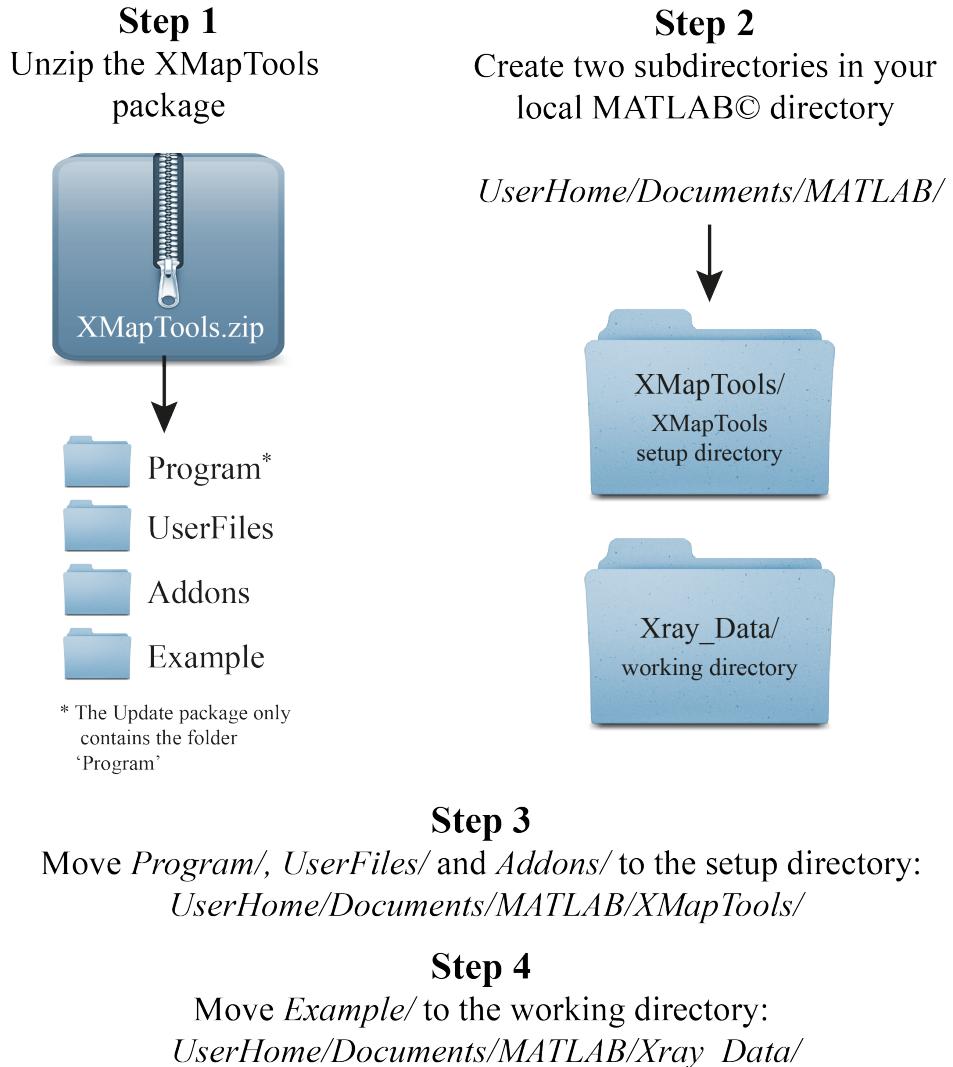


Figure 2.1 – Description of XMAPTOOLS files and repertories. The setup package contains four folders: Program, UserFiles, Addons and Example. The user data must be stored in a different directory (e.g. Xray\_Data).

### 2.3.2 Install XMapTools

#### 2.3.2.1 XMapTools package

(1) Unzip the archive file *XMapTools-2.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 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 program files and should not be modified. *UserFiles* contains user's additional functions and codes. The use of this functionality is explained in details in section 4.3 and is reserved to advanced users. *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 6).

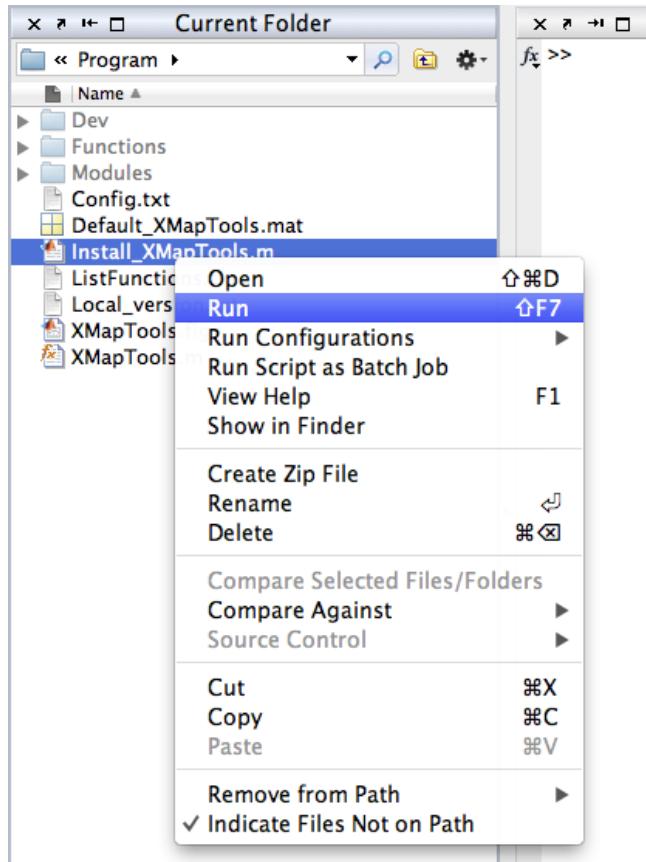


Figure 2.2 – XMAPTOOLS setup. Make a right-click on *Install\_XMapTools.p* and press run to install XMapTools on your computer.

- (2) Create two subdirectories in your local MATLAB<sup>©</sup> 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 data or projects files are stored into the folder *XMapTools/Program/*, they will be deleted during the automatic update. A warning message is displayed if the user attempts to run XMapTools from the setup directory.

### 2.3.2.2 Installation using *Install\_XMapTools.p*

- (1) Run MATLAB<sup>©</sup>
- (2) Go to the XMAPTOOLS directory (*/Program*) using the *Current Folder* window in MATLAB<sup>©</sup>
- (3) Run the program *Install\_XMapTools.p* (see Fig. 2.2, or using in the MATLAB<sup>©</sup> 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 correctly 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 go to the next section 2.3.3.

**Case 2: Setup is not completed** (see message in Fig. 2.3c). This message is displayed if XMAPTOOLS was not correctly installed in your computer. To solve this problem, try one of the two solutions below (5a and 5b):

(5a) In the main MATLAB<sup>©</sup> window, select the menu *File* and *Set Path...*. Use the button *Add folder* to add your XMAPTOOLS folder in your favourite paths. Use the button *Save* to save the favourite path file that will be loaded when MATLAB<sup>©</sup> is launched.

(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.

### 2.3.3 Run XMapTools

XMAPTOOLS may be executed only from the MATLAB<sup>©</sup> environment. The following steps explain how to run the program in your computer from the MATLAB<sup>©</sup> command window.

**Warning:** after setup or update, close MATLAB<sup>©</sup> and run it again. On some computers, XMAPTOOLS graphic user interface seems to not always launch after the setup. This problem is easily solved by restarting MATLAB<sup>©</sup>.

(1) Run MATLAB<sup>©</sup>

(2) Set the MATLAB<sup>©</sup> directory to your XMapTools working directory where are stored the X-ray maps: .../*UserHome/Documents/MATLAB/Xray\_Data/ProjectX/*. It is vitally important to set the MATLAB<sup>©</sup> path to the working directory containing the maps and then to run XMAPTOOLS (see the warning below). During the processing the program generates a lot of files that are automatically stored into the working directory. Go to the data directory (see Fig. 2.1) using the *Current Folder* window in the MATLAB<sup>©</sup> main window.

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

**WARNING:** Before running XMAPTOOLS check that you are in your working directory (See Fig. 2.4)

### 2.3.4 Run XMapTools and automatically open an existing project

A project can be loaded when you run 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**

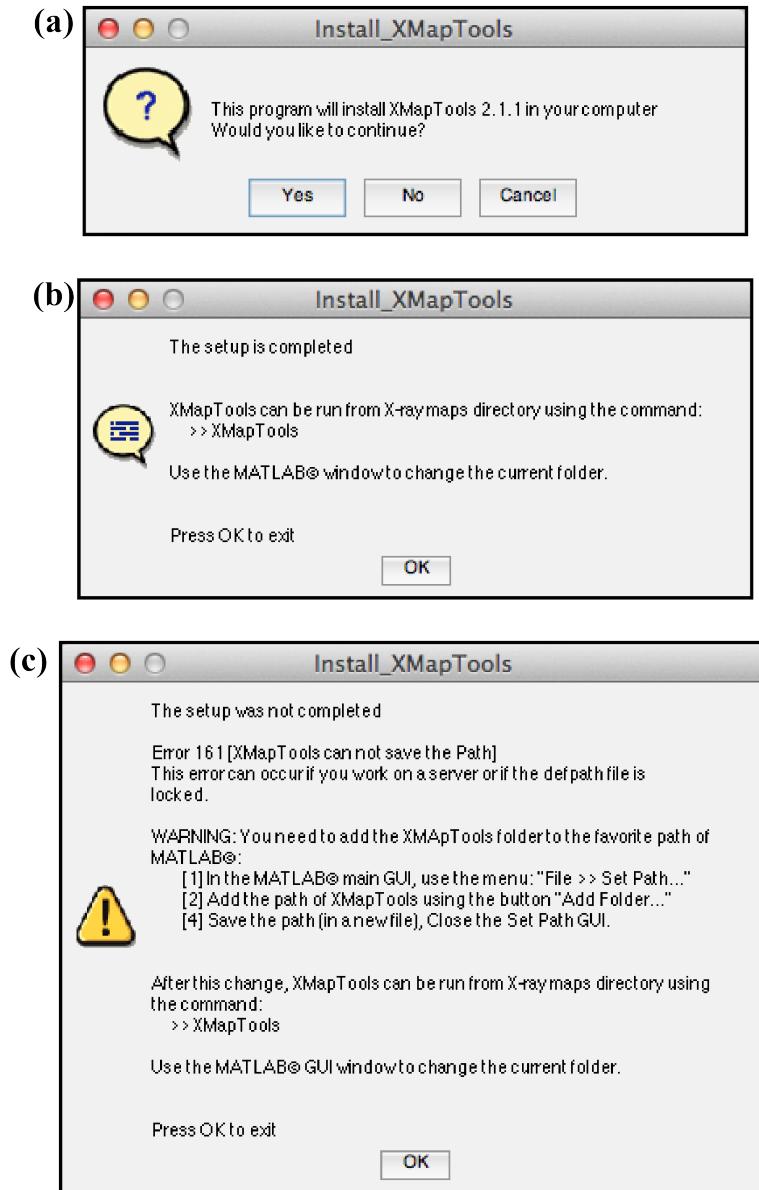


Figure 2.3 – XMAPTOOLS setup dialogue boxes

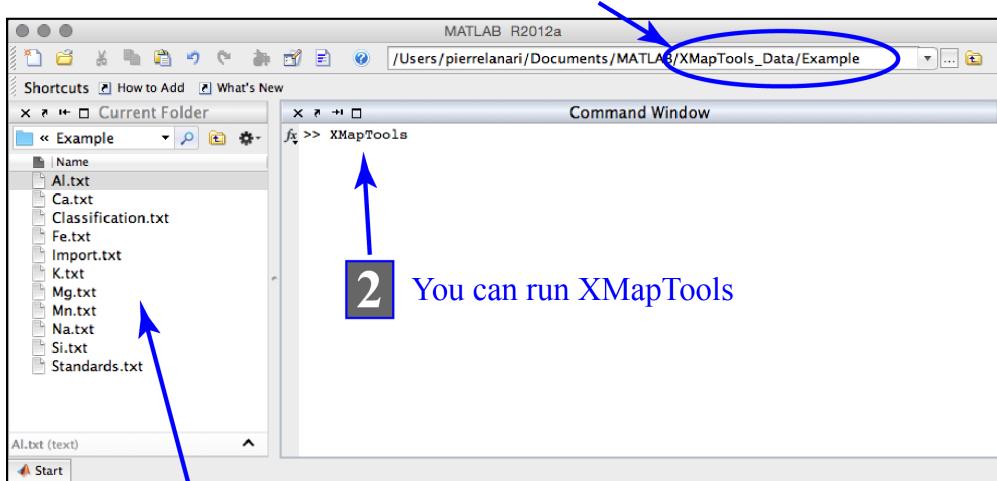
**Note:** If the MATLAB<sup>©</sup> path is not set to the working directory (see above 2.3.3), or if the project *aaa.mat* does not exist, XMAPTOOLS starts normally and do not load any project.

## 2.4 UPDATE XMAPTOOLS

A system that automatically check for updates is included in XMAPTOOLS (release 2.1.X and more recent). If a new release is available and if the computer is connected to Internet, XMAPTOOLS displays a dialog box when starting (Fig. 2.5). The user can decide to use the automatic update system (press *Update now*) or to install manually the new release (press *Remind me later*). The main features of the new release may be displayed by pressing the button *Info*.

In the last stable release XMapTools 1.6, troubles have been encountered caused by to problems with

**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

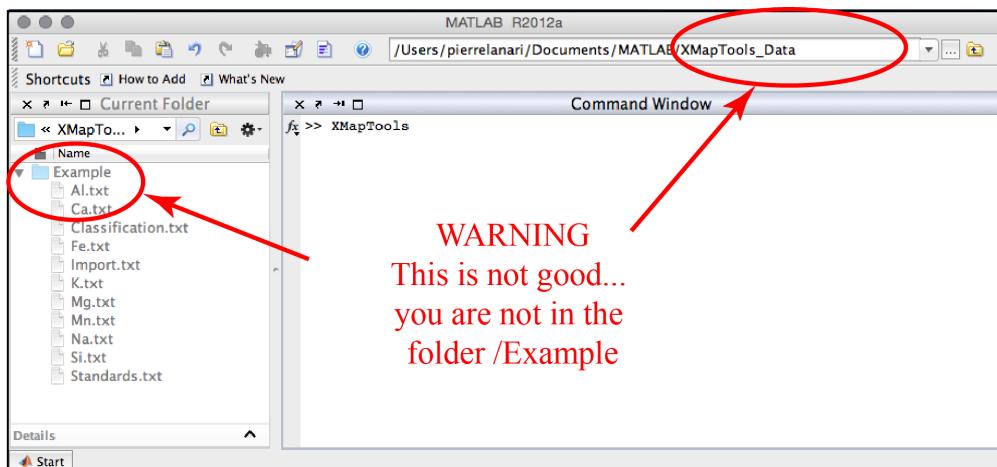


Figure 2.4 – Directory check before to run XMapTools

the FTP connection used to download the new package. This problem has been fixed in XMapTools 2 and the automatic update is expected to work in all cases.

This new automatic update system uses simple web connection to automatically download the latest version of the software from the website (see details in section 2.4.1). The folder *Program* stored in the XMAPTOOLS setup directory is updated. This is NOT the case for: *Examples* and *UserFiles* that are kept unchanged. The user files stored in *UserFiles* are not deleted by the automatic update (provided that *UserFiles* is not stored in *Program*).

If you do not want to use the automatic update (e.g. no internet access in your computer) an alternative procedure is also available (see section 2.4.2).

#### 2.4.1 Automatic update procedure

The automatic update may be done from any folder in your computer as soon as a new release becomes available on the website.

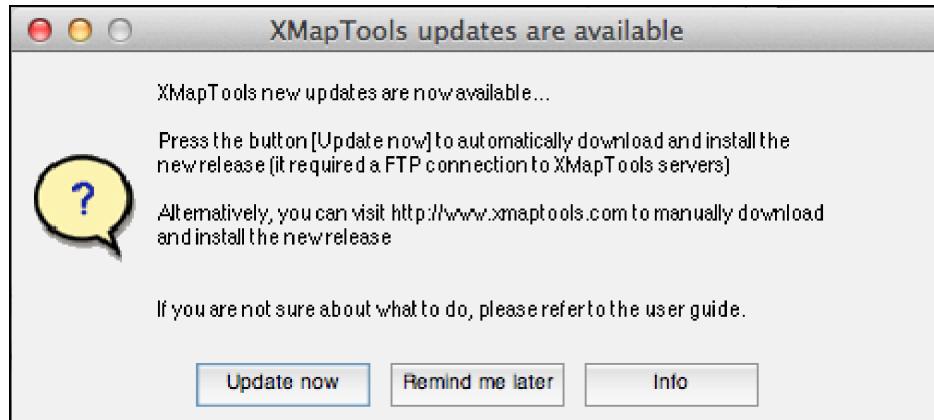


Figure 2.5 – XMAPTOOLS automatic update dialogue box

(1) Run MATLAB<sup>©</sup>

(2) Run XMAPTOOLS and press the button *Update now*.

(3) The update program ask for a second confirmation. Press *OK* to continue. The update program cleans first all the files of the folder *program*. In a second time, the new package is downloaded and unzipped at the right place. At this stage, the update program runs the normal setup procedure (see details in section 2.3.2.2; (4) and following steps).

#### 2.4.2 Manual update procedure

(1) Login to XMAPTOOLS website using you user name and password and download the new package.

(2) unzip the package in 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<sup>©</sup> and run the program *Install\_XMapTools.p* (following the procedure described in section 2.3.2.2)

## 2.5 UNINSTAL XMAPTOOLS

(1) Remove the setup repertory *Program* in which XMAPTOOLS setup files are installed. This operation removes the main program and all the functions. User's data and functions 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.

## 2.6 REQUIRED DATA

### 2.6.1 EPMA

For a given project with 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 the 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 available with the release 2.1 (see the directory *Example*).

### 2.6.2 LA-ICP-MS

For a given project with 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.*

### 2.6.3 X-ray files

X-ray files must have \*.txt, \*.asc, \*.dat or \*.csv extension, no head line and have a name compatible with the XMAPTOOLS elements names. The default list of elements is provided into 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** SiO<sub>2</sub>, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, FeO, MnO, MgO, CaO, Na<sub>2</sub>O, K<sub>2</sub>O.

**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).

## 2.6.4 Map types

The following map types can be imported into the workspace (*X-ray*) of XMAPTOOLS:

- 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 2.6.3). 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. *SiO<sub>2</sub>*, *Al<sub>2</sub>O<sub>3</sub>*, *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 3.4.6.3).
- 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 3.7.4). These maps cannot be calibrated.

Note that the corrections (see 3.4.4) cannot be applied to all the map types. All the map types can be used in the chemical modules (see 3.7). The function *info* ⓘ in the workspace *X-ray* can be used to display the type of the selected map.

## 2.6.5 File Classification.txt

This file contains the name of the different phases together with the input pixel coordinates that will be used by the classification function (see code 2.1). The input phases and the corresponding coordinates must be listed below the keyword >1. The phase names should not contain blank.

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.

```
>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*

## 2.6.6 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 in one line below the keyword >1. The oxide order must be provided below the keyword >2. **X and Y must be the two last labels and must be listed in this order.** The internal standards analyses must be listed below the keyword >3 and must respect the oxide order defined in 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*

## 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 6) 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 3.2), the display functions (section 3.3) and the processing functions (sections 3.4, 3.5 and 3.6). 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

#### **General:**

buttons - *project* [B4101] [B4102] [B4103] [B4104] [B4105] - *settings* [B4201] [B4202] - *figure options* [B4401] [B4402] [B4403]

#### **Display and corrections:**

menus: *Add-ons* [M5601]

buttons: *figure/display tools* [B5101] [B5102] [B5103] [B5104] [B5105] [B5106] [B5107] [B5108] [B5109] - *sampling tools* [B5201] [B5202] [B5203] [B5204] - *chemical modules* [B5301] [B5302] [B5303] [B5304] - *Add-ons* [B5601] - *X-pad navigator* [B5401] [B5402] [B5403] [B5404] [B5405]

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

#### **Xray:**

menus: *X-ray images display* [M1101] [M1102] - *classification* [M1201] [M1201] - *maskfiles* [M1201] - *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:**

menus: *standardized maps* [M2101] [M2102] - *external functions module* [M2301] [M2302] [M2303]

buttons: *standardized maps* [B2101] [B2102] [B2103] [B2104] [B2105] [B2106] - *info* [B2201] [B2202] - *external functions module* [B2301] [B2302] - *local compositions module* [B2401] [B2402] [B2403] [B2404] [B2405] [B2406] [B2407] [B2408] [B2409] [B2410] [B2412]

#### **Results:**

menus: *results from external functions* [M3101] [M3102]

buttons: *results from external functions* [B3101] [B3102] [B3103] [B3104] - *Other* [B3301] [B3302]

### 3.1.2 XMapTools strategy

The strategy behind XMAPTOOLS is intensively described in [Lanari et al. \(2014b\)](#) and [Lanari et al. \(2018\)](#). 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 images 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 browser buttons and display specific objects such as groups of buttons. The menu with the three buttons *Xray*, *Quanti* and *Results* enables the user to navigate between the different workspaces.

**X-ray** workspace is automatically selected during the software opening. This workspace enables to (1) add, display and manipulate raw data such as X-ray images, (2) classify the pixels, i.e. compute masks and identify minerals using a supervised multi-channel classification technique, (3) correct raw X-ray data, (4) load a standard file containing the spot analyses to be used as internal standard, (5) correct the positions of the maps and spot analyses and select/unselect the standards and (6) standardize the raw data into 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 et Engi 2017](#)), (3) calculate maps of structural formulae, (4) apply empirical to semi-empirical geothermobarometers to evaluate P-T conditions of formation ([Lanari et al. 2013](#)).

**Results** workspace allows the calculated results (mineral structural formulas, P-T maps) to be displayed, and the results to be exported.

General functions are provided in all the workspaces such as: (1) plot options, (2) filters, (3) sampling functions and (4) external modules: BINARY,TRIPILOT3D, RGB and GENERATOR.

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

XMAPTOOLS projects can be saved as \*.mat files and all the variables becomes easily accessible from the MATLAB<sup>®</sup> command window. Type in the command window ">> open MyProjectName.mat" and ">> whos" to display XMAPTOOLS variables (and data).

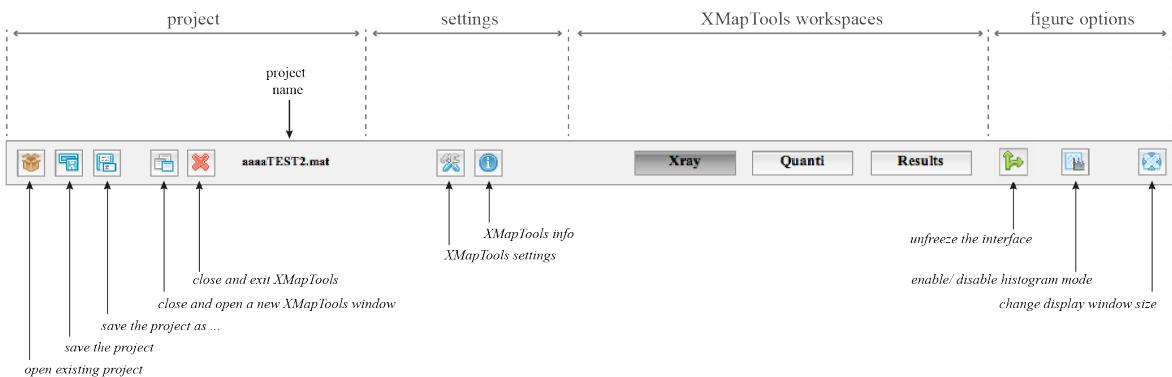
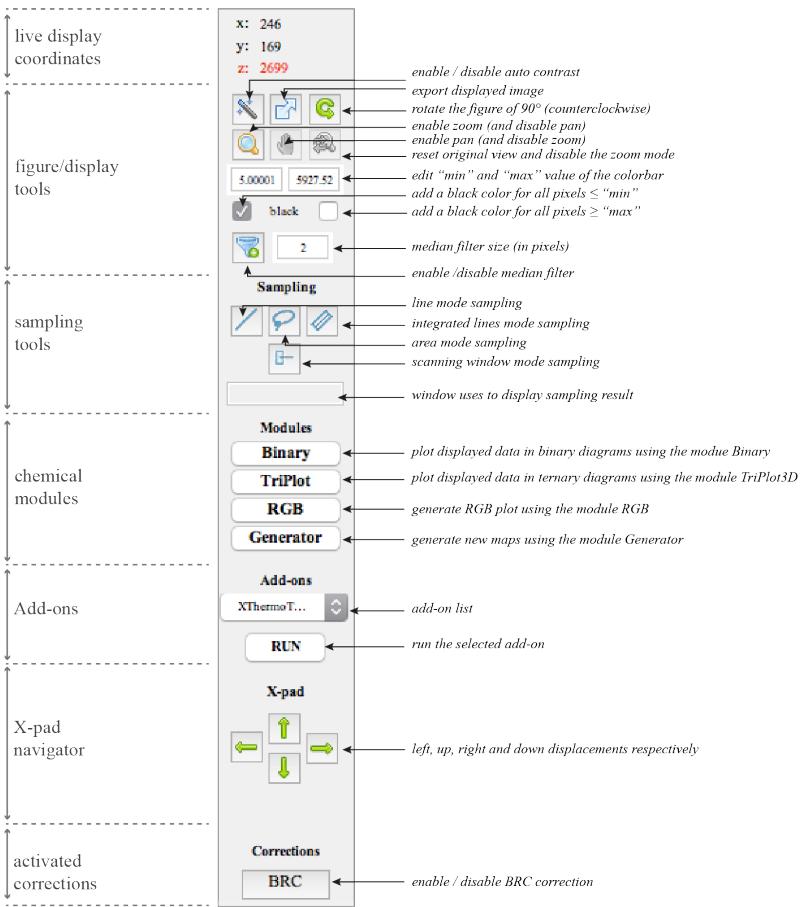
**(a) General****(b) Display and corrections**

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

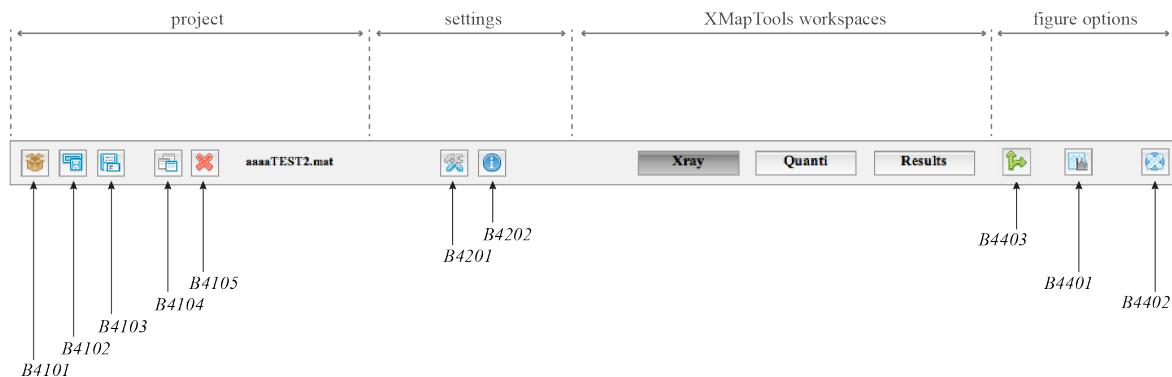
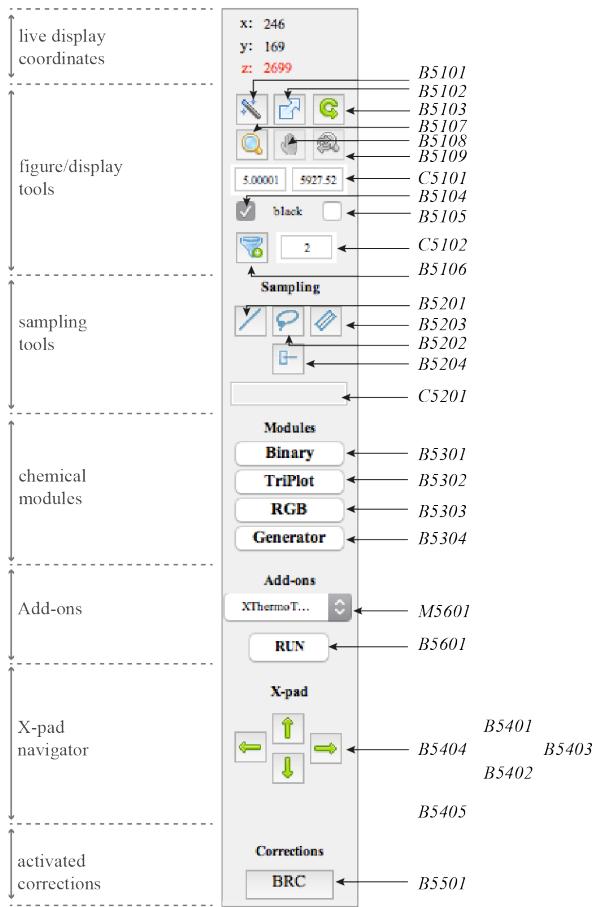
**(a) General****(b) Display and corrections**

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

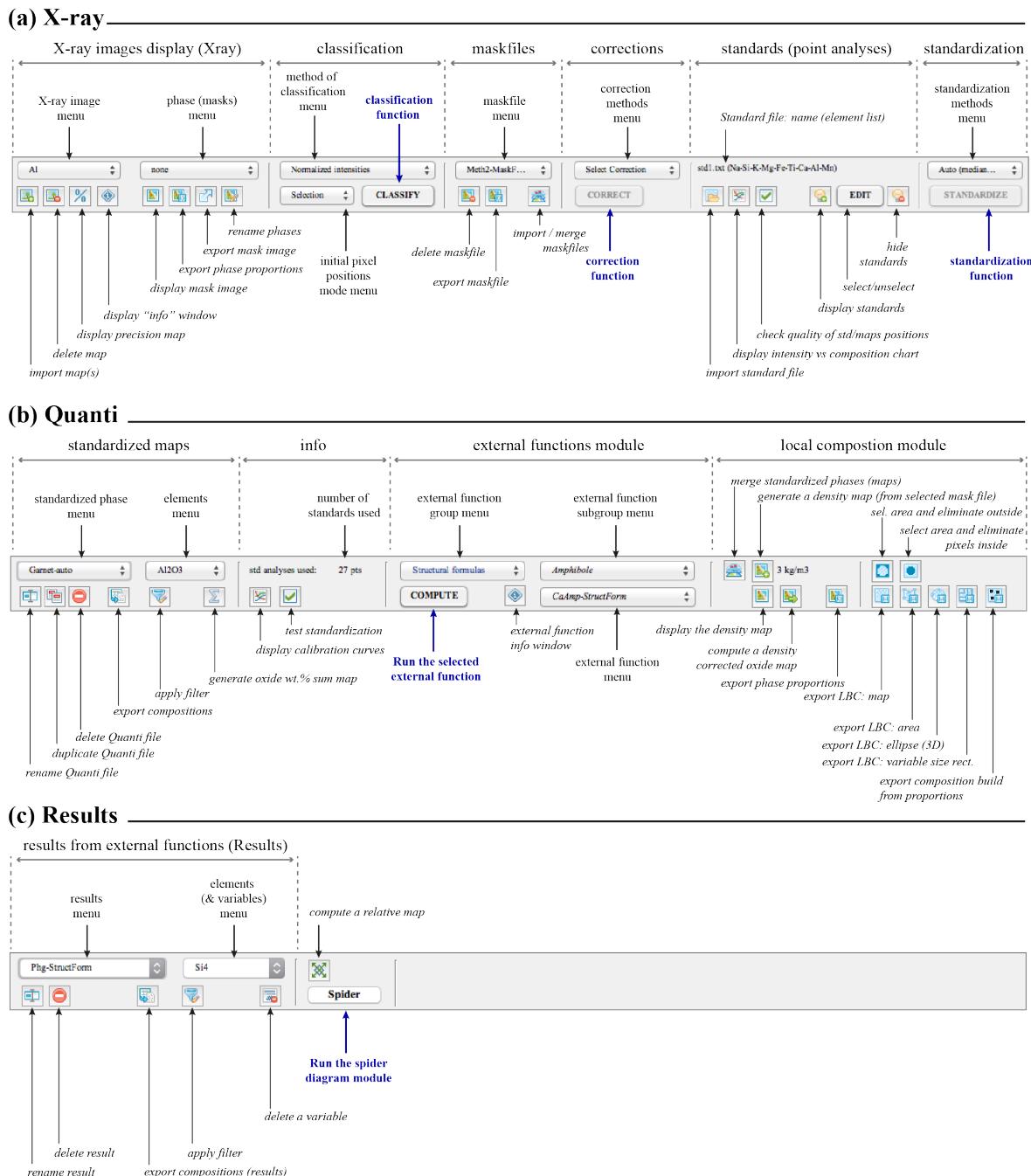


Figure 3.3 – XMapTools objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.

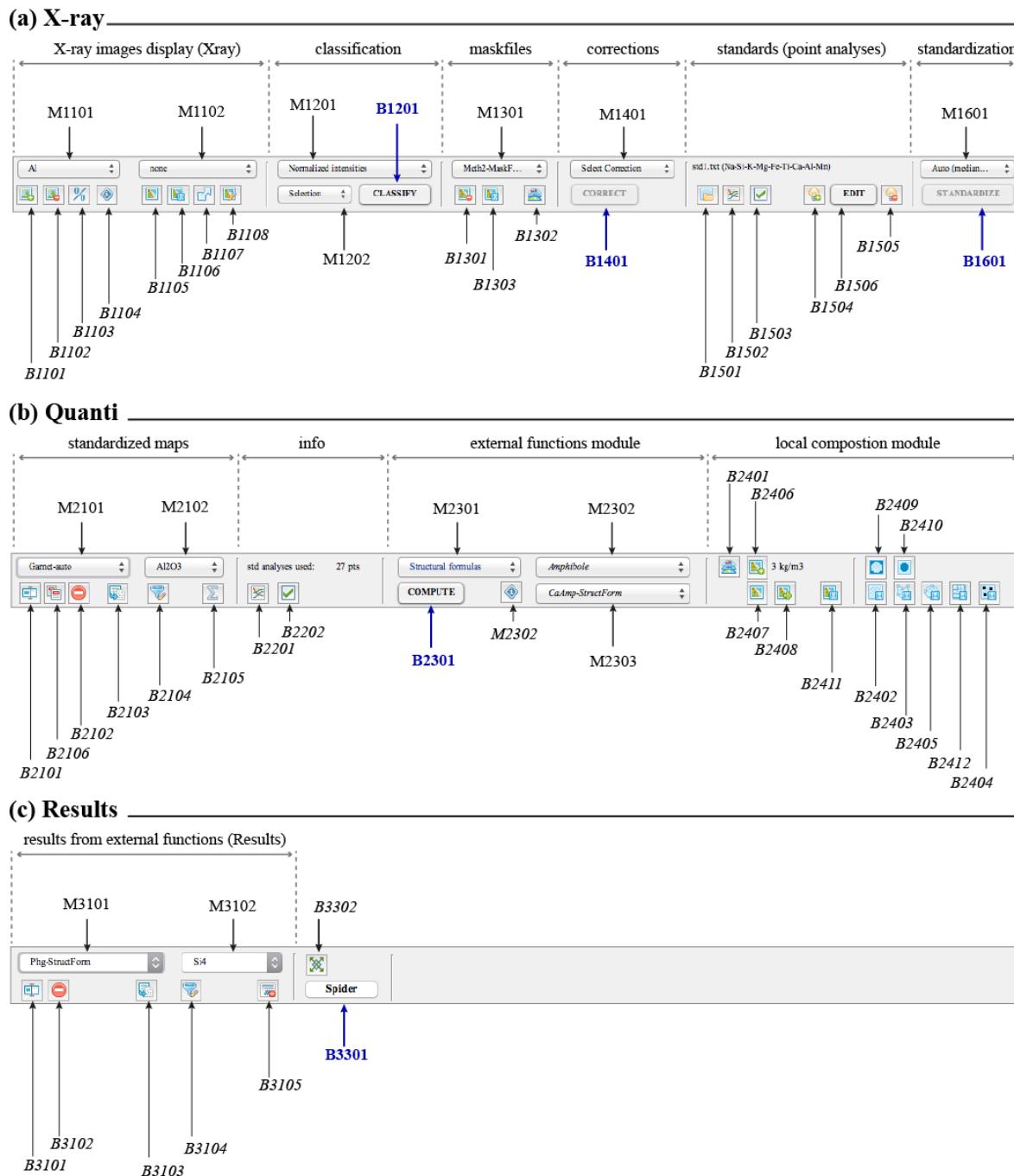


Figure 3.4 – *XMapTools objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.*

## 3.2 GENERAL FUNCTIONS

### 3.2.1 Project

**[B4101]** The button *open existing project*  enables to load a XMAPTOOLS project. The name of the selected project is displayed in the same window.

XMapTools projects are MATLAB<sup>©</sup> formatted binary file (MAT-file, extension: \*.mat). The following variables (structures): *Corrections*, *Data*, *Directory*, *ListMap*, *MaskFile*, *Profil*, *Quanti* and *Results* are stored within this file.

**NB:** The backup files are relatively heavy (about 100 Mb for a project including 10 maps, 12 standardized maps and 20 results).

**[B4102]** The button *save the project*  enables to save the selected XMAPTOOLS project. If a project file was not created before to press this button, it calls the function *save as* [B1403].

**[B4103]** The button *save the project as*  allows the XMAPTOOLS project to be saved as a new project. The user must specify the name of the new project file. The name of the saved project is displayed in the same window.

**[B4104]** The button *close and open a new window*  enables to end the current XMAPTOOLS session, clear all the variables of the workspace and start a new XMAPTOOLS session. This function may be used before to load a new project, because it cleans all the variables from the previous session.

**[B4105]** The button *close and exit*  may be used to end the current XMAPTOOLS session and to close the program.

### 3.2.2 General settings

**[B4201]** The button *XMAPTOOLS settings*  allows the settings window to be displayed or to be hidden (Fig. 3.5).

XMapTools settings options are:

- **Display help in XMAPTOOLS window [default: enabled]** display help instructions into the main window (blue text at the bottom).
- **Activate the diary [default: disabled]** enables to save all the info displayed in the MATLAB<sup>©</sup> command window in a diary file. The diary must be deactivated using the command » *diary off* if XMAPTOOLS is not closed using one of the close button.
- **Display live coordinates [default: enabled]** displays the live coordinate in the main window (top left, see description in section 3.3). This option may in some rare instances cause notable slowing down during the use of the software; it can be disabled here.
- **Figure's colormap [default: JET]** sets the figure's colormap. Available sets are: Jet (Default); ColdWarm; FreezeWarm; WYRK; Hot; Gray; HSV; Cool; Spring; Summer; Autumn; Winter; Bone; Copper; Pink.
- **Colormap resolution [default: 128]** sets the number of colors used in the colormap. Note that this option is only available to MATLAB<sup>©</sup> colormaps.



Figure 3.5 – Settings window. This window can be displayed and hidden by clicking on the button [B4201].

- **LOG scale [default: disabled]** enables to use logarithmic scale for the color bar. If this option is not selected a linear scale is used.
- **Border interpolation (merge function in Quanti) [default: unselected]** activates the border interpolation option in the function merge [B2401].

User's personal settings are saved as soon as the button *Save default* 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 automatic update will clear the personal settings; new personal settings must be redefined after each software update.

The XMapTools release number, the XMapTools setup directory and current working directories are also displayed in the settings window.

**[B4202]** The button *XMapTools info* ⓘ allows displaying some information regarding the program such as the XMAPTOOLS license policies.

### 3.2.3 Workspaces

The buttons *Xray*, *Quanti* and *Results* enable to switch between the different workspaces.

### 3.2.4 Figure options

**[B4401]** The button *enable/disable histogram mode* 📈 enables to go to the histogram mode and to return 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).

**[B4402]** The button *change display window size* 📐 allows the size of the map display window to be adjusted. Three different sizes are available (full screen, intermediate, small).

**[B4403]** The button *unfreeze the interface* 🛡️ allows the interface to be unfrozen if the program is stuck. A description is given in section 5.3.1.

### 3.3 DISPLAY FUNCTIONS

#### 3.3.1 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 3.2.2). 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.

#### 3.3.2 Figure/display tools

##### 3.3.2.1 Map display

[B5101] The button *enable auto-contrast* enables to apply an automatically 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* ) and come back to the default values. The default lower and upper values are the min and max values of the displayed image.

[C5101] The cells *edit 'min' and 'max' values of the colorbar* allow the lower and upper values of the color-scale to be manually edited.

**NB:** The use of this function switch off the auto-contrast mode.

[B5102] The button *export displayed image* can be used to export active figure. This function generates a copy of the figure displayed in the main XMapTools window (including images and user's selections, points, lines...) in a new MATLAB<sup>©</sup> 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 3.6. 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<sup>©</sup>.

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

- Orientation 1 - 0° [Default], see figure 3.7a
- Orientation 2 - 90°, see figure 3.7b
- Orientation 3 - 180°, see figure 3.7c
- Orientation 4 - 270°, see figure 3.7d

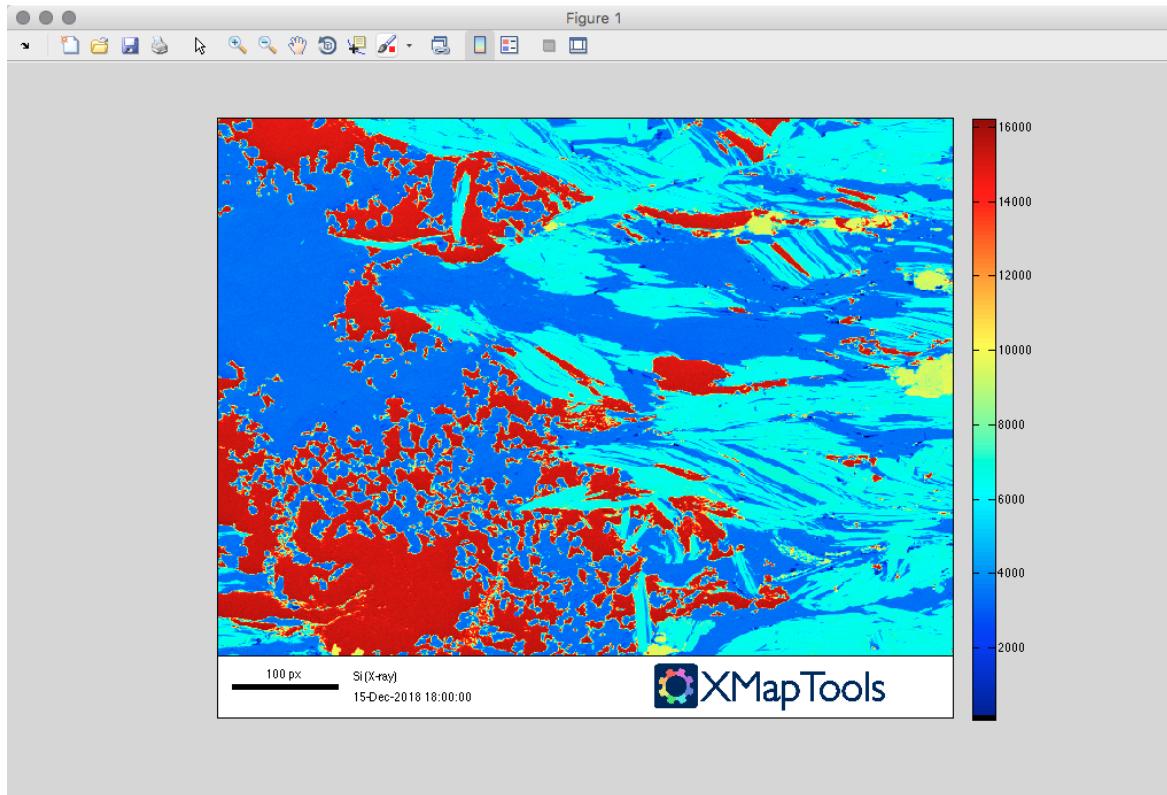


Figure 3.6 – MATLAB<sup>©</sup> Window with the exported figure (see button [B5102])

**NB:** The default orientation (1, Fig. 3.7a) is automatically set when you run XMAPTOOLS or load an existing project. Press the function *rotate the figure of 90° (counterclockwise)* to change the orientation. The selected orientation will be applied during the active session but not saved in the project file for the next sessions. Note that some functionalities are not compatible with the rotate function. In this case a warning message will be displayed inviting the user to set the reference orientation.

The coordinates reported in the *Live coordinates display window* (see section 3.3.1) 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]** The button *enable/disable median filter* is used to enable 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 entered, the median filter applied to the displayed figure is updated.

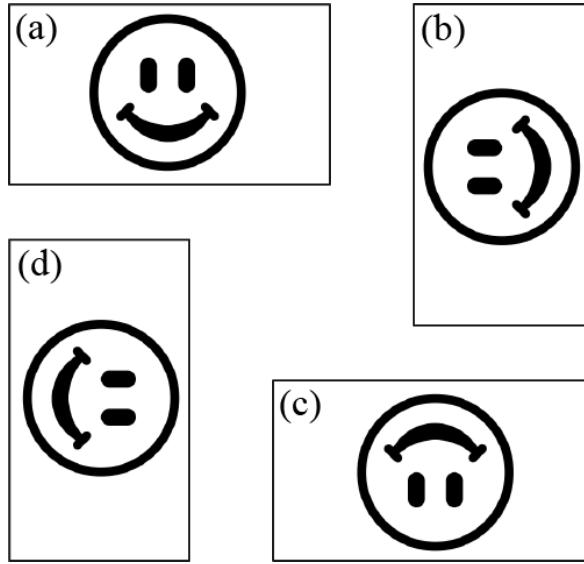


Figure 3.7 – Orientation positions available for the main figure display (see rotate function [B5103])

### 3.3.2.2 Zoom and pan

**[B5107]** The button *activate zoom mode* turns on the zoom mode. 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]** The button *activate pan mode* turns on the pan mode. 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 enabled, holding the mouse button while your cursor is within the displayed map permits panning the view of display interactively.

**[B5109]** The button *reset zoom & pan* disables both zoom and pan modes and resets the original view of the displayed image.

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



Figure 3.8 – Menu to select the sampling mode: single map (displayed) or multi-map (selected by user)

### 3.3.3 Sampling tools

**[B5201]** The button *line mode sampling* can be used to generate a compositional profile showing the evolution of the pixel compositions 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. 3.11).

This sampling function can be applied to generate compositional profiles for:

- *Single Map (color)* a color profile for the map displayed in the main window (e.g. Fig. 3.9b)
- *Multiple Map (color)* color profiles for several maps to be selected
- *Single Map (bw)* a black-and-white profile for the map displayed in the main window (e.g. Fig. 3.9c)
- *Multiple Map (bw)* black-and-white profiles for several maps to be selected

A menu allowing the sampling mode to be selected (Fig. 3.8) is displayed once the button *line mode sampling* is clicked. If the *Multiple Map* mode is selected, it will be possible to select the list of maps from which the profile are extracted. Only the maps available in the active workspace - and for the selected phase - are available.

The profiles are plotted in new window. This figure can be saved using the normal procedure described for the function export [C5102].

The data plotted can also be exported and saved as and ASCII file (in \*.txt, see Ex. 3.1). 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 selected, all the figures generated by the software are saved as both FIG and PDF files using linear and logarithmic axes in a new folder that is located in the */Export-sampling* directory. Two additional figures that contain all the elements (linear an logarithmic axes) are also saved. For a profile AB extracted from four maps (elements), twenty files are generated. In this case the data are saved as a matrix in which each column corresponds to a given element.

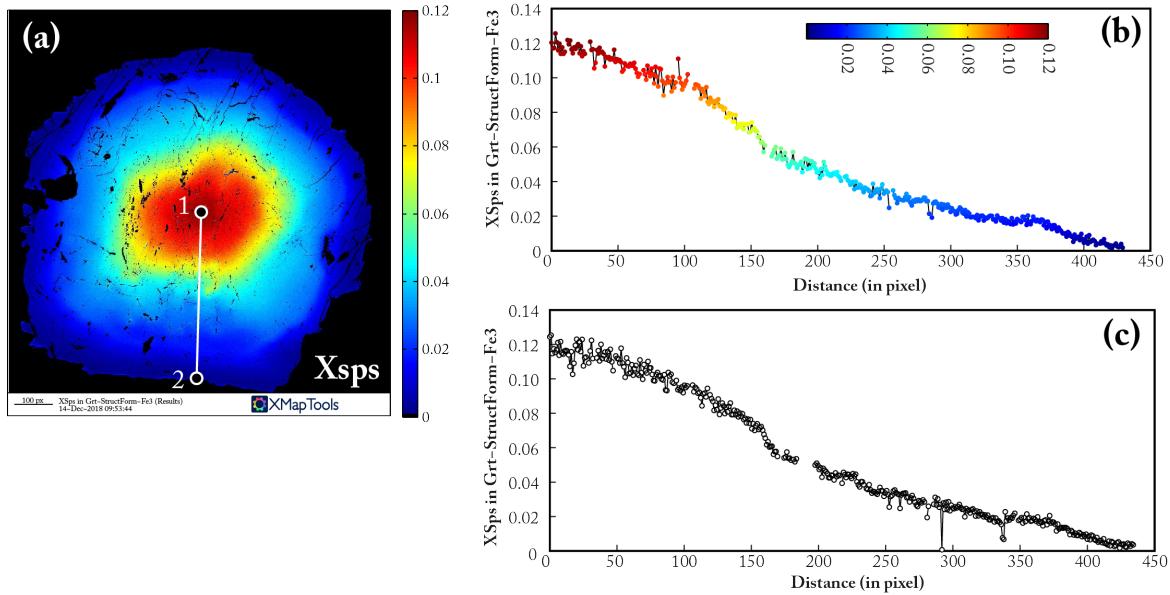


Figure 3.9 – Example of line sampling across a garnet porphyroblast using (a) the map fraction of spessartine ( $X_{Sps}$ ). (b) mode Single Map (color). note that the color of is the same as the corresponding pixel on the map. (c) mode Single Map (bw).

Sampling from XMapTools

04–May–2015

Method : Line

```

1 3372.4085
2 3365.3943
3 3327.318
4 3301.2663
5 3392.4491
6 3480.6306
7 3320.304
8 3434.5352
9 3392.4491
10 3423.5125

```

Code 3.1 – Example of exported file (sampling mode line; single map)

**[B5202]** The button *area mode sampling* enables calculating and displaying the average composition of the pixels contained in a region-of-interest. This region-of-interest is set by selecting spots that define a polygon which is converted by the program into a mask (see spots 1 to 10 Fig. 3.11b). Selection mode is disabled using right-clicking (spot 11, in Fig. 3.11b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.11b. The result is displayed in the cell [C5201]. The results including the average, the standard deviation ( $1\sigma$ ), the number of pixels and the standard error ( $1\sigma$ ) can also be exported and saved as and ASCII file (in \*.txt, see Ex. 3.2). This file is automatically stored in the repertory /Export-sampling.

For a pixel  $i$  with composition  $X_i$  from an area containing  $n$  pixels, the values shown in 3.2 are obtained using:

$$Value = \bar{x} = \frac{\sum X_i}{n} \quad (3.1)$$

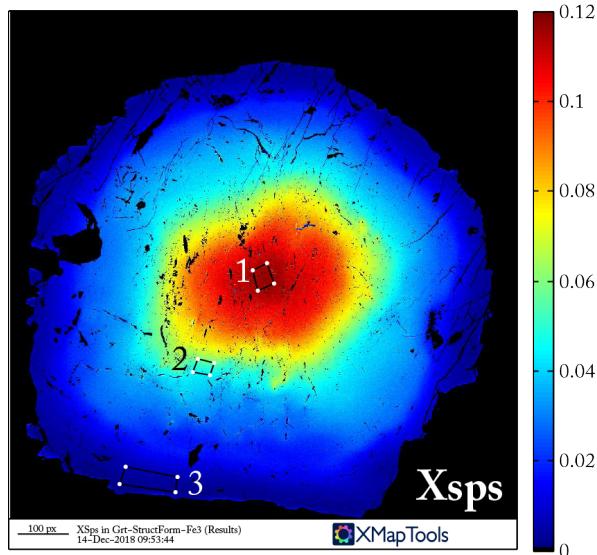


Figure 3.10 – Three areas used to export the average  $X_{Sp}$ s (see 3.2)

$$StdDev = \sigma = \sqrt{\frac{\sum(X_i - \bar{x})^2}{n}} \quad (3.2)$$

$$StdErr = \frac{\sigma}{\sqrt{n}} \quad (3.3)$$

```

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  XSp's    0.1163    0.0035  1325    0.0001

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

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

```

Code 3.2 – Example of exported file (sampling mode area, see Fig. 3.10)

**[B5203]** The button *integrated lines mode sampling* enables calculating and displaying the composition variations integrated perpendicular to a reference transect. The function plots the average values of the transects parallel to the reference transect defining a rectangle (Fig. 3.11c). For a given pixel on the reference transect, the value is calculated as the mean of the pixel compositions perpendicular to the reference transect. The rectangle is defined by three spots (see Fig. 3.11c).

Seven display options are available:

- [1] Mean + All
- [2] Mean only

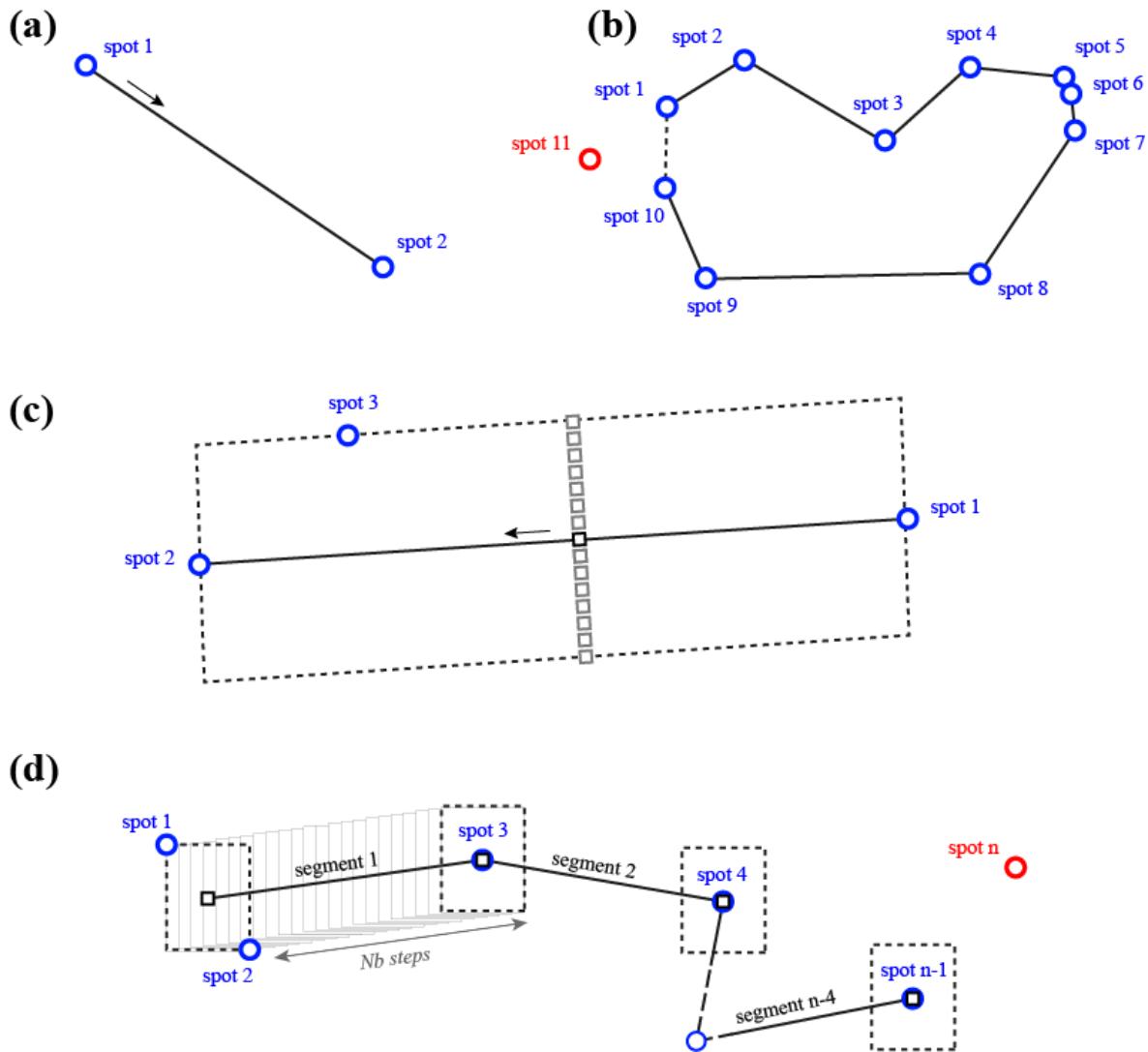


Figure 3.11 – Sampling functions: (a) line mode [C5201], (b) area mode [C5202], (c) integrated lines mode [C5203] and (d) scanning window [C5204]

- [3] Median + All
- [4] Median only
- [5] Mean + Median + All
- [7] Mean + Median
- [8] All only

All the transects are displayed in gray. The mean and median values along the reference transect are plotted in red and blue respectively. An example is given in Fig. 3.12.

The percentage of pixels used to calculate each value can also be displayed on in a new window. The results can be exported and saved as an ASCII file (in \*.txt, see Ex. 3.3).

Sampling from XMapTools 04-May-2015 Method: Integrated Area Columns: Mean   Median   Std   \% Pixels				
4667.40396858	5078.72626627	910.60390163	82.48847926	
4688.75734532	5017.54136467	863.43454482	82.48847926	
4701.61762663	5061.17299139	844.74810116	82.94930876	
4689.31515926	5040.10931113	853.34838017	82.94930876	
4648.95331479	5046.62898904	950.57552976	83.41013825	
4510.72703200	5020.04892030	1168.58539757	83.87096774	
4441.51913376	5048.63505561	1323.61199444	83.87096774	
4455.26258883	5061.67451089	1319.67582818	84.33179724	
4491.73219620	5064.68364630	1321.24794781	84.79262673	
4496.94342798	5071.70493414	1318.83308441	85.25345622	
4452.88406337	4992.46623325	1217.52367434	85.25345622	
4443.46754631	4961.87515543	1169.83159916	85.71428571	
4419.86081132	4917.24309908	1109.92131667	86.17511521	
4439.26140245	4911.22539480	1087.74223747	86.17511521	
4429.29880510	4844.02917826	1054.43698294	86.63594470	

Code 3.3 – Example of exported file (sampling mode integrated area)

[C5201] The cells *sampling results* allows to display some results of the sampling functions.

[B5204] The button *scanning window mode sampling*  enables calculating and displaying the composition variations using a moving average window (Fig. 3.13). In the given example, the rectangle is displaced from the starting point (left on Fig. 3.13-a) to the end of the path (right on Fig. 3.13-a) along 3 segments with  $3 \times 30$  steps. The average composition of the pixels for every step is calculated together with the standard deviation and they are display in a new figure window (Fig. 3.13-b).

Click two points to define the reference rectangle and successively select the location where you want to move next the center (see Fig. 3.11) to add one more segment. At least one segment must be defined (3 points in total); right-clicking ends the selection mode.

Note that in XMAPTOOLS the distance unit used is pixel. In figure 3.13 the distances have been converted from pixels to  $\mu m$ .

### 3.3.4 Chemical modules

The buttons [B5301] BINARY, [B5302] TRIPLOT3D, [B5303] RGB and [B5304] GENERATOR allow all the pixels displayed in the main figure window to be plotted into binary or ternary chemical diagrams or a RGB image to be generated. The modules can be used with data from the three workspaces. A description of the chemical modules is given in section 3.7: BINARY (3.7.1), TRIPLOT3D (3.7.2), RGB (3.7.3) and GENERATOR (3.7.4)

### 3.3.5 Add-ons

[M5601] The menu *add-on list* lists all the compatible add-ons available in .../UserHome/Documents/MATLAB/XMapTools/Addons/. The selected add-on can be called using the button [B5601] *run*.

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

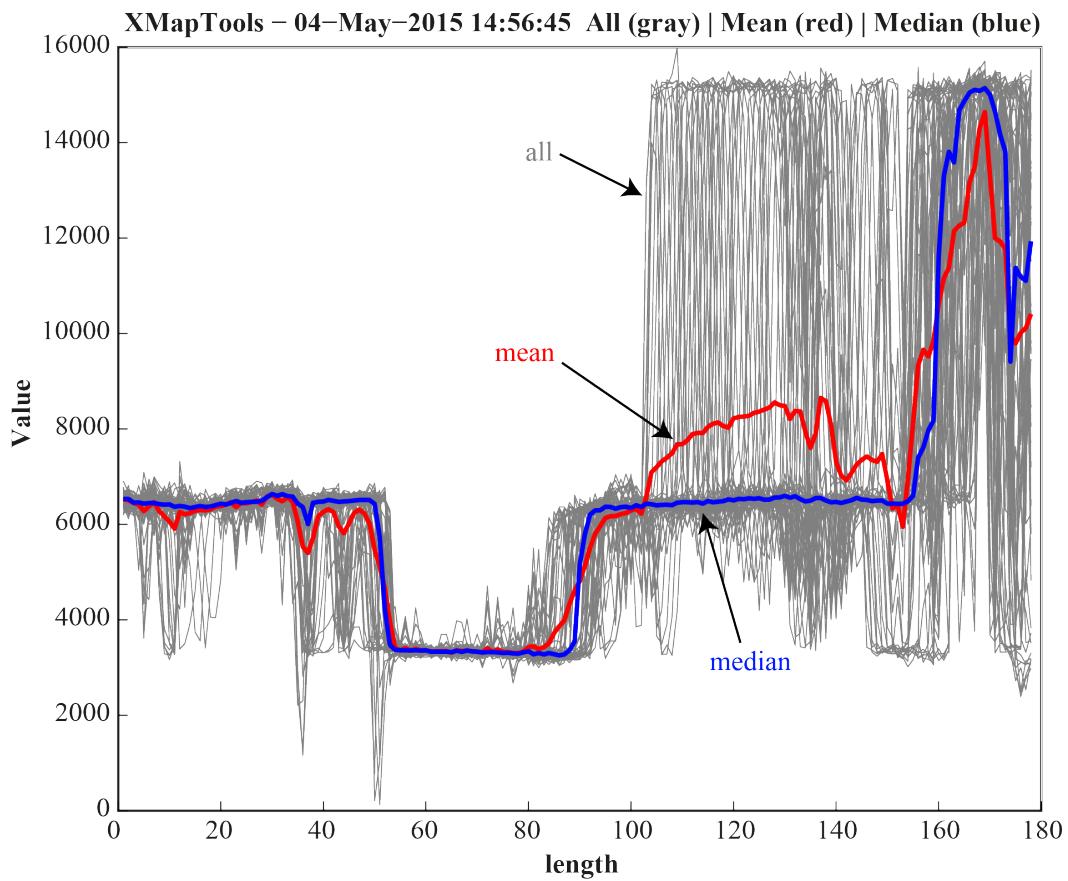


Figure 3.12 – Example of sampling integrated lines mode.

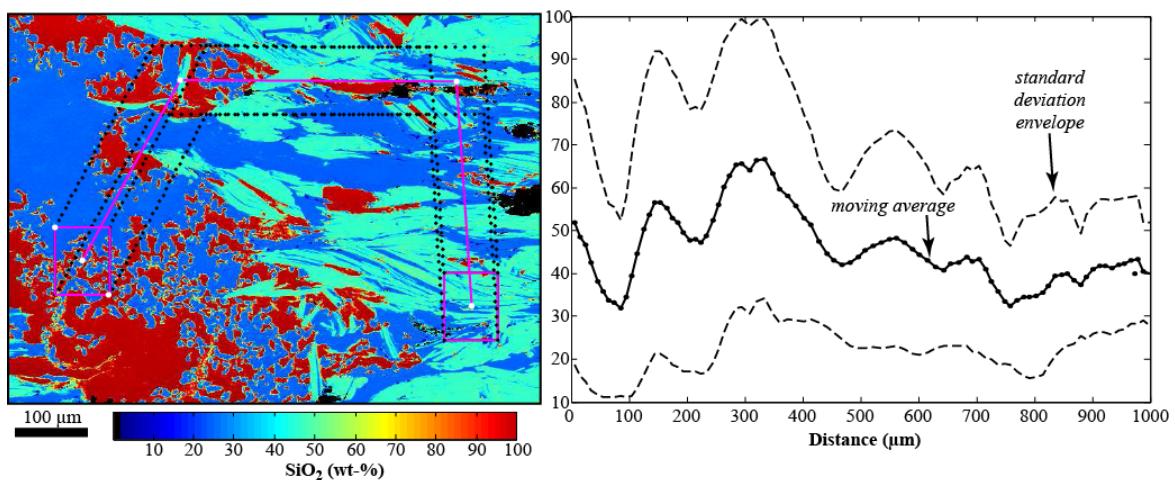


Figure 3.13 – Example of sampling using (a) a scanning window and the exported (b) the moving average and standard deviation.

### 3.3.6 X-pad navigator

**[B540X]** The buttons of the X-pad navigator - [B5401] up, [B5402] down, [B5403] right, [B5404] left - enables to move objects during the corrections. Standard position can be adjusted during the SPC correction (see section [3.4.4.4](#)) and X-ray maps during the MPC correction (see section [3.4.4.3](#)).

**[B5405]** The button *Apply* enables to exit the correction mode and apply the modifications made.

### 3.3.7 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 [3.4.4.1](#)).

## 3.4 X-RAY

### 3.4.1 X-ray images display

**[M1101]** The menu *X-ray image* enables to select the map that is displayed in the main figure window. All the maps that have been previously loaded with the function *add map(s)* [B1101] are listed in this menu.

**[M1102]** The menu *phase (mask)* enables to display only the pixels of this mask. Note that the mask is defined in the mask file selected in menu *X-ray image* [M1301]. The data of the map selected in [M1101] are displayed in the main figure window for the given phase selected in the menu [M1102]. The masks are generated during the classification. Mask can also be imported from a mask file using the button import ([B1302], see below). If *none* is selected (first choice), all the pixels of the map selected in [M1101] are displayed in the main figure window.

**[B1101]** The button *import map(s)*  allows new maps to be imported using the adding tool. All the map files may be loaded together or separately. Files must be text files and have \*.txt; \*.asc; \*.dat or \*.csv extensions with no head line (see file format in 2.6.3). Note that the *import map* function can also read single column files. In this case the program will ask for the size of the map to reshape the vector into a matrix.

The function *import map* checks the map files one by one to recognize the corresponding elements. It is possible to use an *automated indexation* technique, which scans the maps and detect the corresponding element based on the name of the file. A dialog box is displayed for the file names that does not match any entry of the database. This dialog box is displayed for all the maps if the automated indexation is not used.

The *Import Tool GUI* (Fig. 3.14) contains some correction functions to modify the maps that are imported into XMAPTOOLS. Once the corrections are set (see below) press *Apply Corrections* to send the modified data to XMAPTOOLS.

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

- *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 3.5). The following dead-time equation is used:

$$I_{corr} = \frac{I_{measured}}{1 - DT \times 10^{-9} \times I_{measured}} \quad (3.4)$$

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 expend the image by duplicating the pixels. An example of re-sampling is provided in figure 3.15.
- *All*: Find and replace negative values (zero). If this option is activated all the negative values of the images are replaced by zero.

The information regarding the corrections are printed out in the MATLAB<sup>®</sup> command window (see examples for EPMA insert 3.4 and LA-ICP-MS insert 3.5 below)

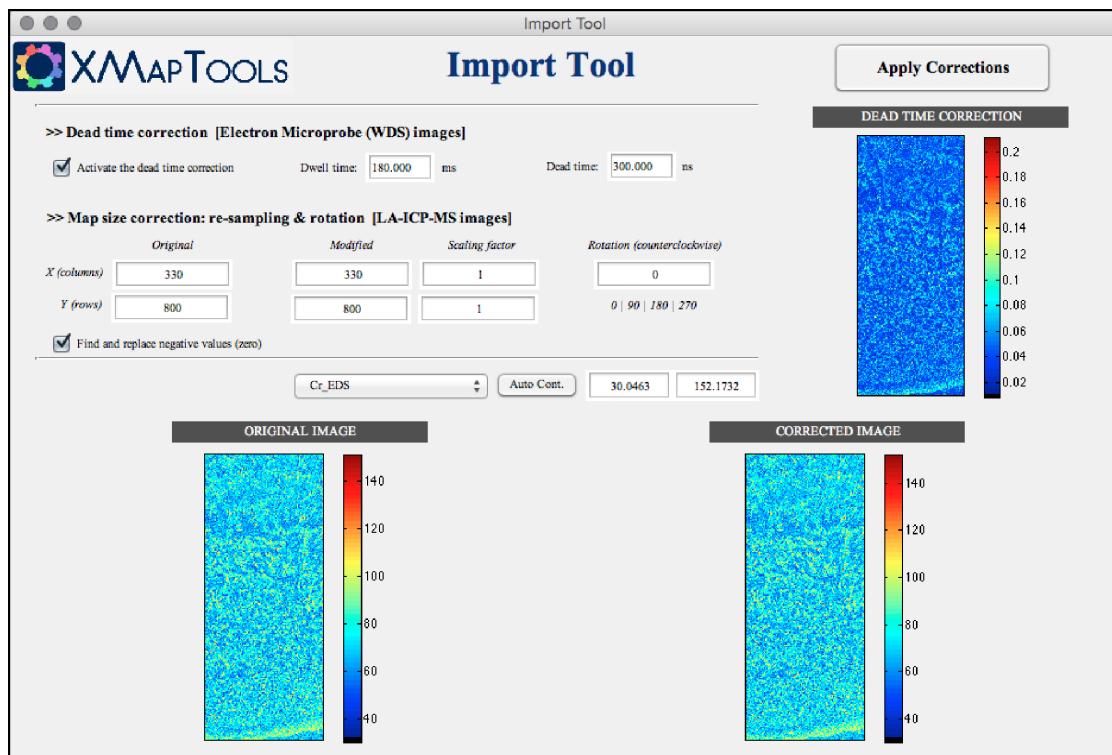


Figure 3.14 – Import module of XMapTools

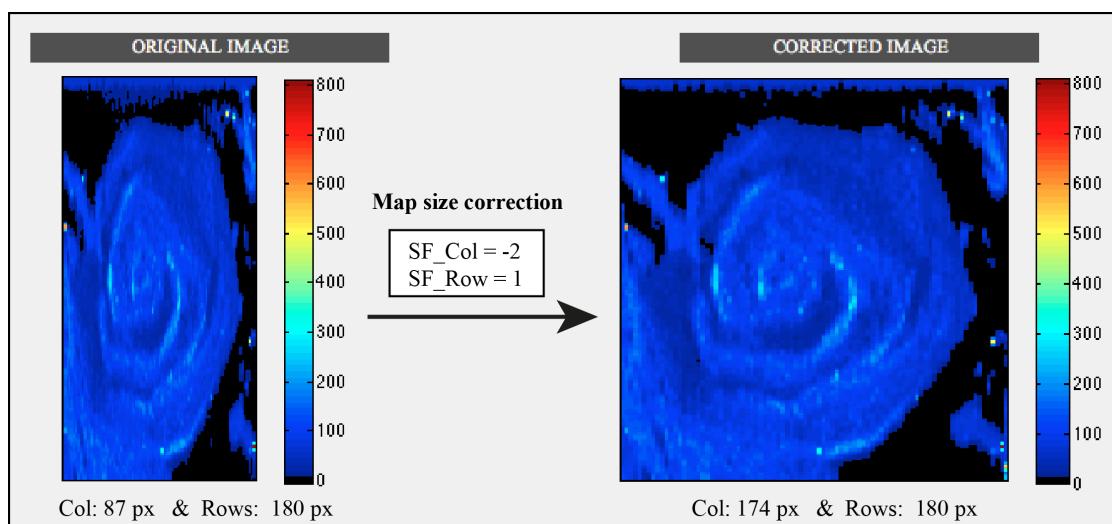


Figure 3.15 – Example of map size correction for LA-ICP-MS images

**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 3.4 – 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 3.5 – Example: Import LA-ICP-MS images and map correction

**[B1102]** The button *delete map*  enables deletion of a selected map. This button is available only if two or more maps are loaded.

**[B1103]** The button *display precision map*  allows a precision map to be generated. This map shows the precision in % at  $2\sigma$  (see general concept and equation in §1.4.1.2). 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]** The button *info*  allows a window with some information about the selected map to be displayed. This info window contains: (1) name of the selected element (with a number corresponding to the internal reference in the element database); (2) selected phase, if selected in menu [M1102]; (3) map size in pixels: format rows / columns, corresponding to Y / X; (4) mean intensity of 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  $2\sigma$ ; (5) median intensity of displayed pixels and the corresponding uncertainty at  $2\sigma$ ; (6) standard deviation; (7) lower and (8) upper intensity values; (9) BRC, (10) TRC and (11) MPC correction info (see section 3.4.4).

**[B1105]** The button *display mask image*  allows the mask image of the selected mask file (menu [M1301]) to be plotted.

**[B1106]** The button *export phase proportion*  enables exporting the phase proportions 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]** The button *export mask image*  is used to display 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. NB: the main export function ([B5102]) does not work correctly with mask images.

**[B1108]** The button *rename phases*  enables to 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 recommended to use single word phase names without blank.

### 3.4.2 Classification

**[M1201]** The menu *method of classification* enables 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. \(2014b\)](#). Different masks files could be derived using both methods depending on the magnitude of the differences between the composition of phases. For optimal results we generally recommend to try both methods.

**[M1202]** The menu *initial pixel composition mode* allows the method for defining the coordinates of the initial pixels to be selected. The compositions of these pixels will be used to define the first groups by the classification function (button [B1201]). Two options are available: *selection* and *file*. The mode *selection* enables to select by clicking pixels directly into the map during the classification. This mode requires a map on which all the mineral phases are visible. The mode *file* allows a file containing the coordinates of the initial pixels to be loaded. The format of this file is described in [2.6.5](#). If the file is named *Classification.txt* (case sensitive), then the program automatically proposes to read this file.

**[B1201]** The button *classify* calls the automated classification function, 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]). A complete description of the classification function is provided in [Lanari et al. \(2014b\)](#).

The classification function allows to select the X-ray maps that are used to classify the pixels of the image. 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 open another file.

### 3.4.3 Mask files

**[M1301]** The menu *mask file* enables 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]** The button *delete mask file*  can be used to delete the mask file selected in menu [M1301]. This button is available only if two or more mask files have been generated.

**[B1302]** The button *import / merge mask files*  enables importing mask file(s) generated with the chemical modules *Binary* and *TriPlot3D*. Users can select one (import) or more (merge) mask files stored in the folder */Maskfiles*. XMAPTOOLS generate a new mask file by merging the selected ones. Users can define the name of the new mask file.

**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<sup>®</sup> (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 3.6 – Example: Import / merge mask function (printed output)

**[B1303]** The button *Export mask file*  allows the selected mask file (in menu [M1301]) to be exported. It is possible to select which mask will be exported. Note that any unselected pixel is set to zero and will be classified as *unselected\_pixels* by the *import and merge function* [B1302].

### 3.4.4 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. 3.1. 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. 3.1) need to be validated in order to apply the correction and exit the correction mode.

Abbreviation	Name	Button string	Correction mode	Requirements
BR	Border-removing correction	APPLY	No	existing mask file
TR	Topo-related correction	SET	Yes (External GUI)	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 3.1 – Corrections available in XMapTools, modes and requirements

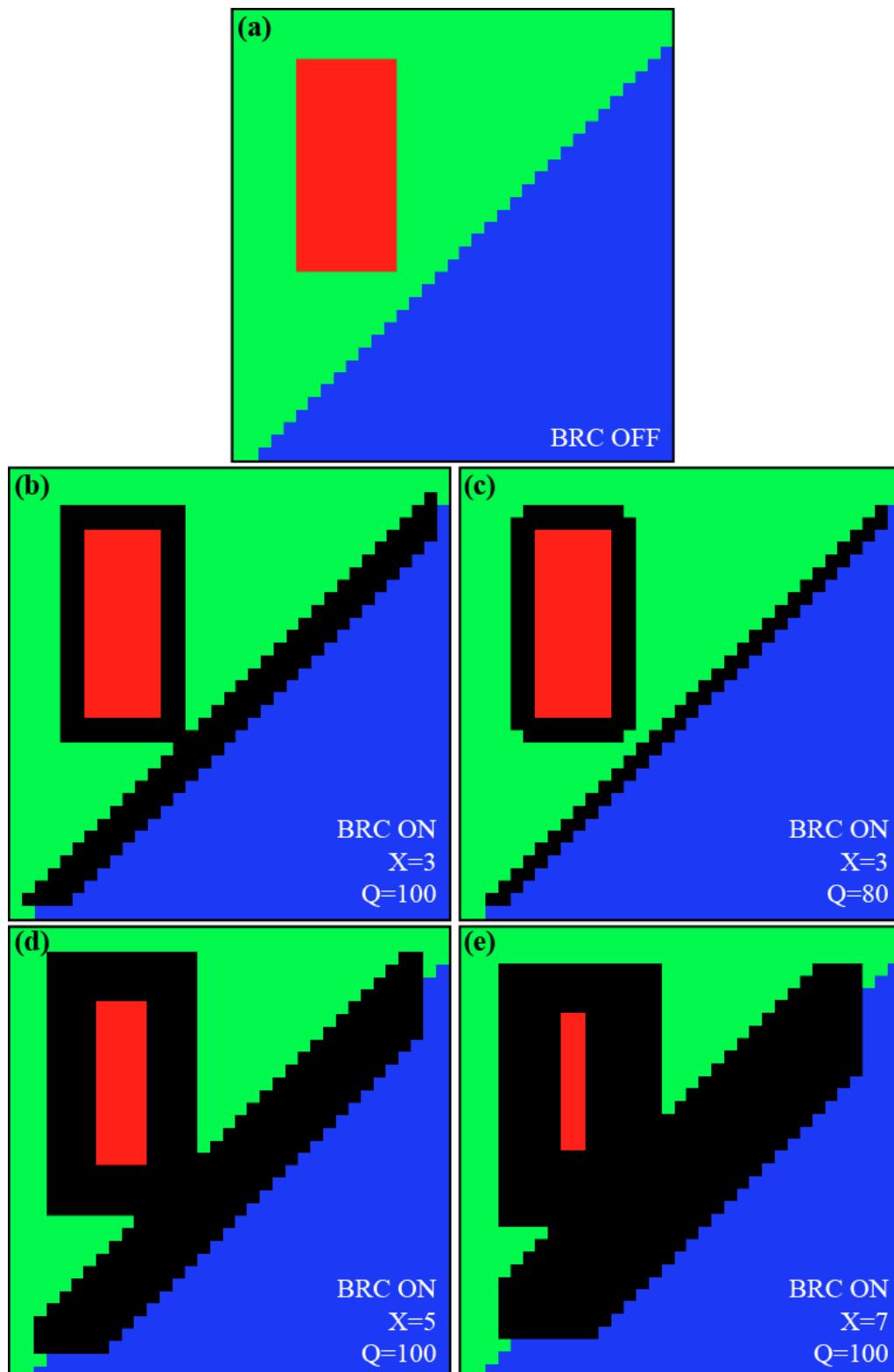


Figure 3.16 – Examples of BRC correction with various  $X$  and  $Q$  parameters. This small map ( $35 \times 35 \text{ pixels}^2$ ) exhibits three phases (Phase 1 in red; Phase 2 in green; Phase 3 in blue). Pixels removed by BRC are plotted in black. A complete description of this map can be found in Fig. 1.3.

#### 3.4.4.1 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 3.16. 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  $\geq 3$ ) 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. 3.16. Corrections are applied to a small map exhibiting three phases plotted with three colors (red, green and blue in Fig. 3.16a). Several combinations of  $X$  and  $Q$  parameters have been tested and results are reported in figs. 3.16b, 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.

#### 3.4.4.2 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. 3.17) 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.

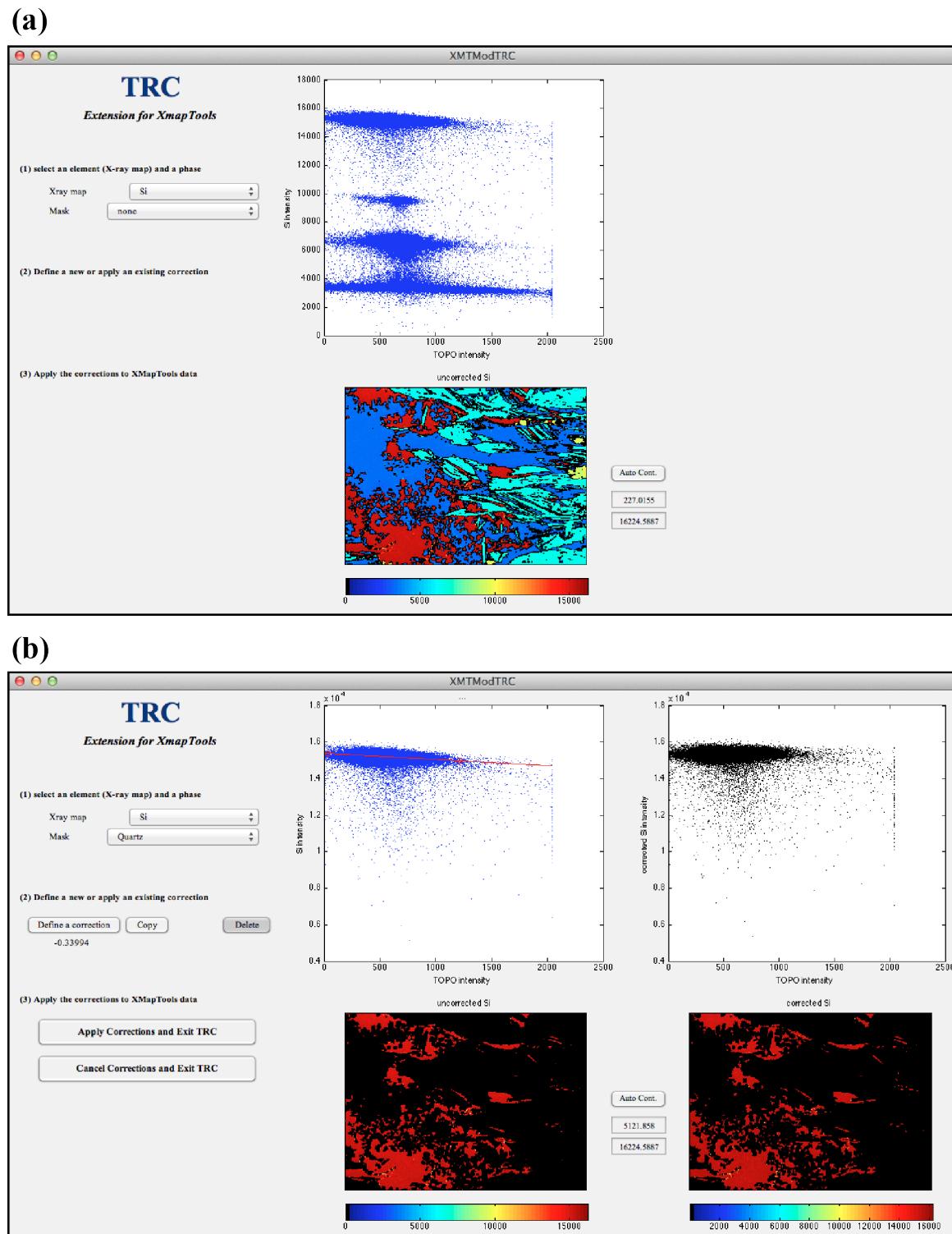


Figure 3.17 – Example of TRC correction for Si using the TRC module. In this example, BRC correction has been applied and the black contours are visible in the map in (a). In the diagram X-ray intensity against TOPO intensity, each cloud is a mineral. (a) display mode; (b) correction mode with a phase selected.

An example of *TRC* correction is given in figure 3.17. One element (e.g. Si) can be selected using the menu *X-ray maps* (Fig. 3.17a). 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 3.17b the phase quartz is selected to correct for Si. A linear relationship (red line in Fig. 3.17b) 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. 3.17b).

The correction straight line defined above may be written as:

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

with  $\Delta I$  the intensity correction and  $a$  the slope of this line.  $\Delta I$  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 XMAPTOOLS.

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.

#### 3.4.4.3 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.

#### 3.4.4.4 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.

#### 3.4.4.5 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. 3.18) 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 3.18. The measured map of Si in titanite (Fig. 3.18a) 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. 3.18) it is possible to specify the direction of acquisition, i.e. *horizontal* or *vertical* (vertical in the example shown in Fig. 3.18). 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)

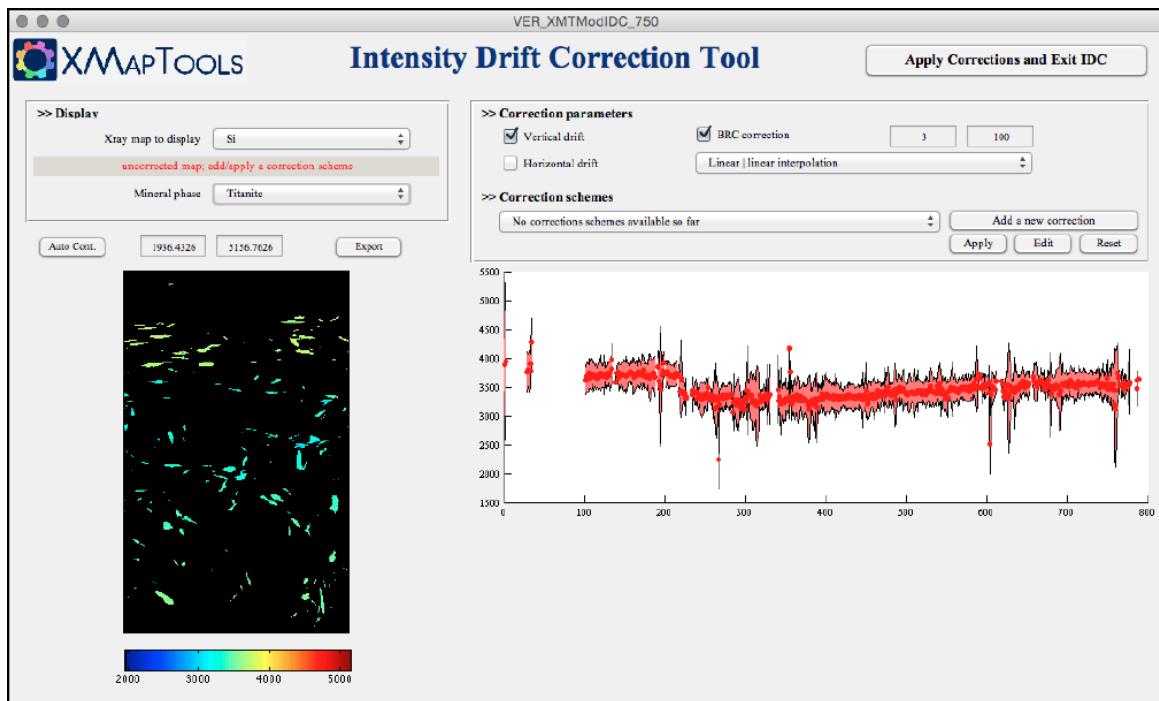


Figure 3.18 – Module to perform the IDC correction. In this example, Si in titanite is used to detect the time-dependent intensity drift (in counts) during the first scan. Note that the abrupt decrease of intensity was caused by a vacuum failure in the gun.

- *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. 3.18). The red dot show the average intensity of each line or column with the relative error and standard deviation enveloppe (at  $2\sigma$ ).

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. 3.19). 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. 3.19). The interpolation method can be changed after the selection of the points.

The correction map (see map in Fig. 3.19 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. 3.18 and Fig. 3.19).

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

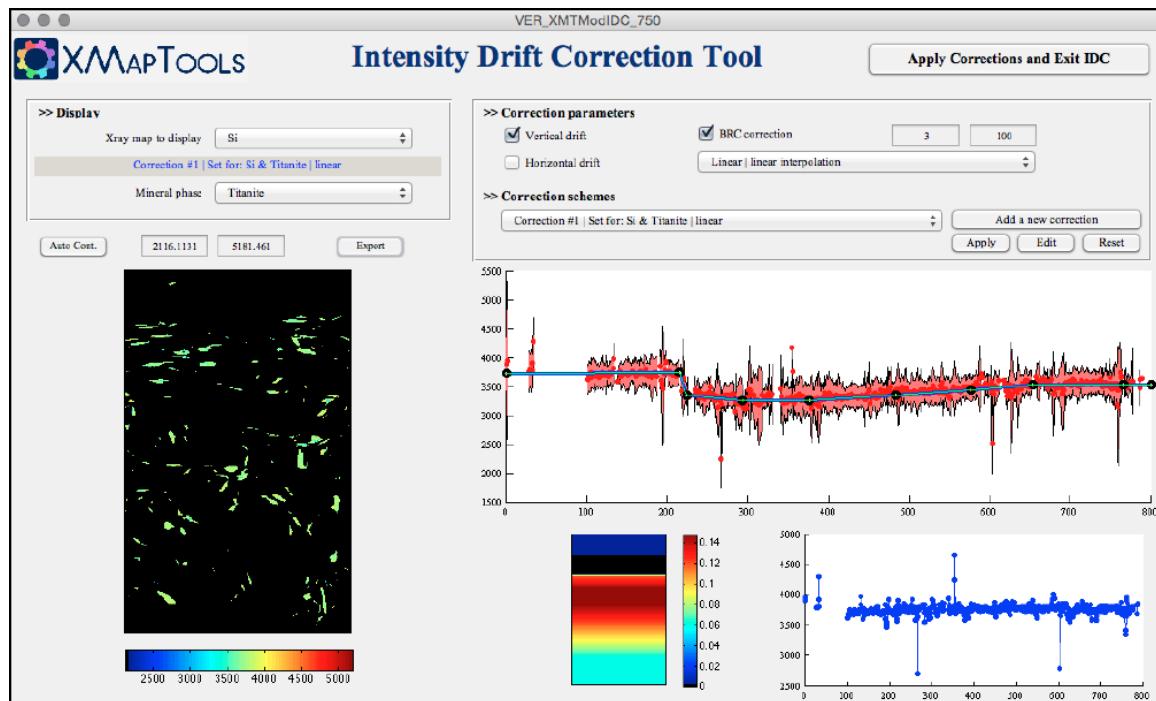


Figure 3.19 – Module to perform the IDC correction. The correction for Si in titanite has been defined in the chemical diagram.

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, 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 imported in XMAPTOOLS using the *import* function [B1101]. Be careful to not apply twice the deadtime correction.

#### 3.4.4.6 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. \(2018\)](#) to be compared with the *advanced standardization method*.

#### 3.4.4.7 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. 3.11b). the selection mode is disabled using right-clicking (spot 11, in Fig. 3.11b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.11b. 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.

#### 3.4.5 Internal standards (spot analyses)

[B1501] The button *import standard file*  enables loading a standard file. The file must have \*.txt extension and the correct format (see detailed description of the file format in section 2.6.6). The *import standard file* function (i) opens the file, (ii) reads the map coordinates, the oxide order and the data and (iii) projects the spot analysis positions onto the map coordinates.

**Example:** The file *Standards.txt* has been read. Ten oxides are provided and the corresponding elements are printed (Si, Mn, K, Na, Fe, Al, Cr, Ca, Mg, Ti). The X-ray maps that have the same names may be standardized using these standard analyses. 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 3.7 – Example: Import standard file

[B1502] The button *display intensity vs composition chart*  allows the compositions of the internal standard spot analyses to be compared with 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.%  $Al_2O_3$  in Fig 3.20a) and in the X-ray map Al (Fig 3.20b). The correlation coefficient is 0.97.

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

Code 3.8 – Example: function display intensity vs composition chart

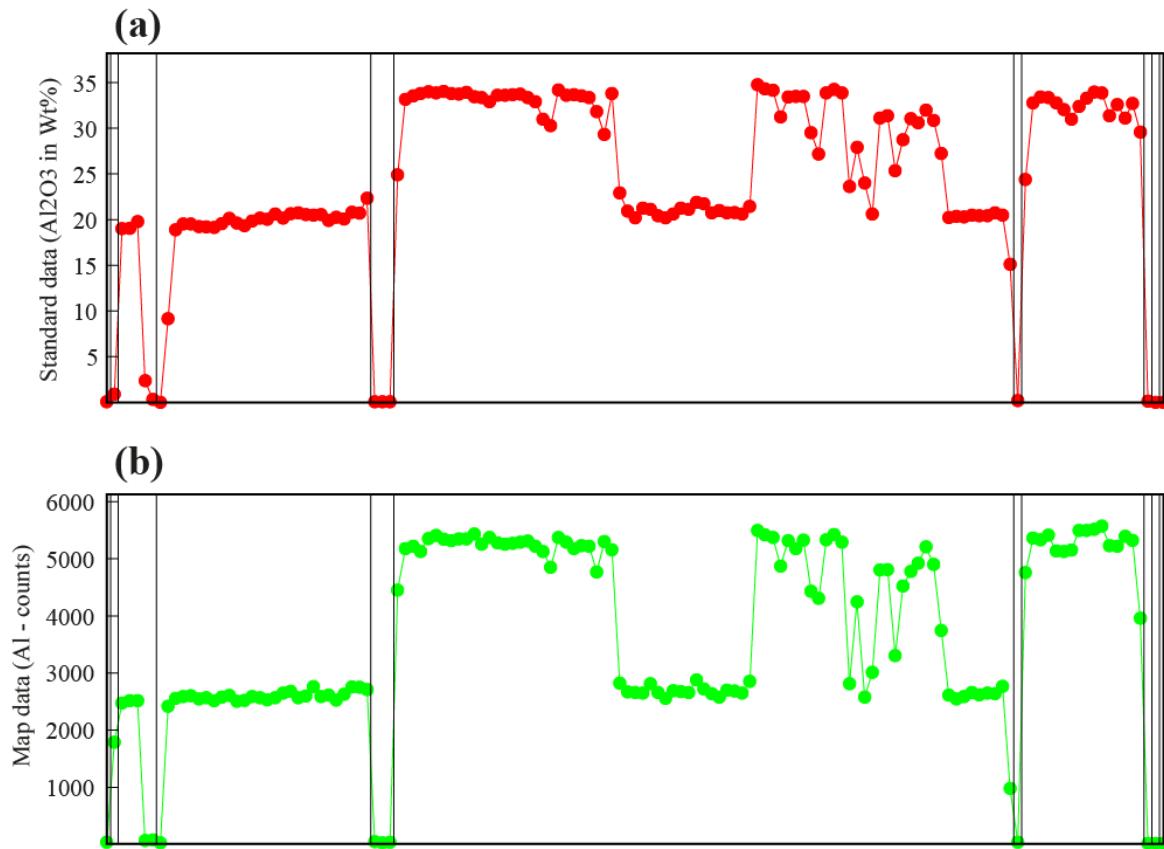


Figure 3.20 – Function display intensity vs composition chart

**[B1503]** The button *check quality of std/maps positions*  allows the positions of the internal standard analyses to be tested 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]) 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 3.9 – 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  $\Delta X$  and  $\Delta Y$  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 ( $\tau$ ) for the element  $E_{l_i}$  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  $\tau(E_{l_i})$  is a matrix with  $(2 * \Delta Y - 1)$  rows and  $(2 * \Delta X - 1)$  columns.

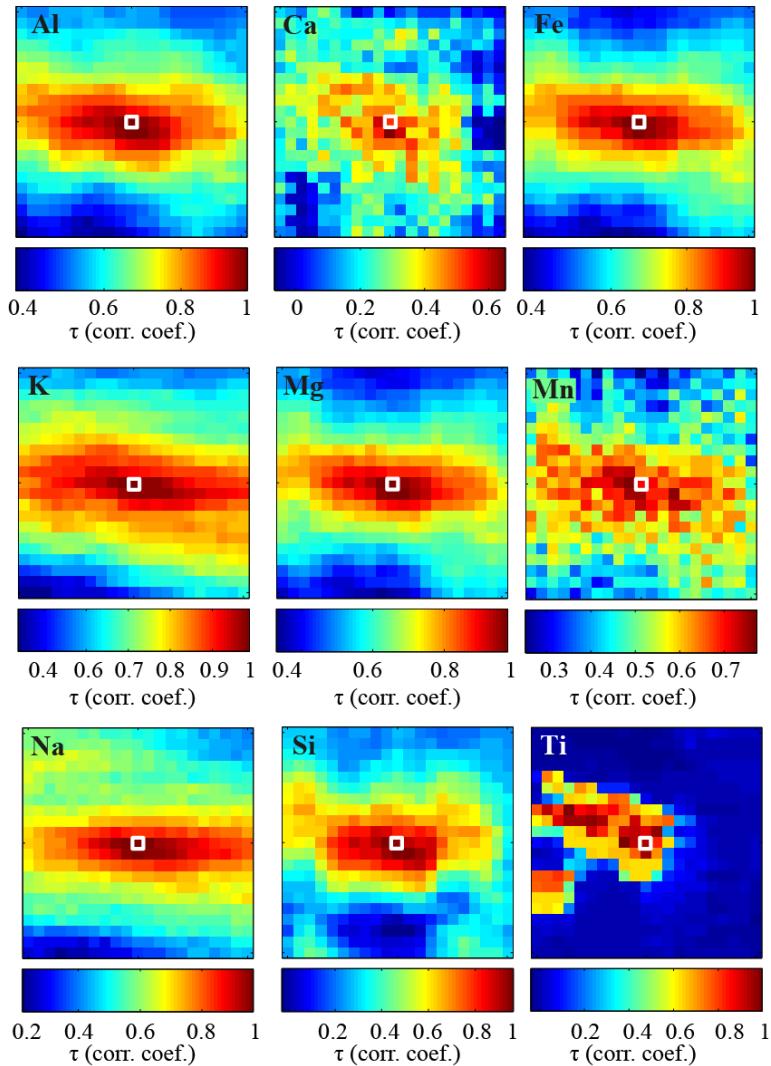


Figure 3.21 – Function: *check quality of std/maps positions*. Correlation coefficients ( $\tau$ ) maps for each element ( $El_i$ ) (see text for details)

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. 3.21). 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 3.21 and 3.22). The axis values are given in pixels from  $-\Delta X$  to  $\Delta X$  and from  $-\Delta Y$  to  $\Delta Y$ . In this example the default values  $\Delta X = 10px$  and  $\Delta Y = 10px$  are used.

The second figure 3.22 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 3.21 show contrasted  $\tau$  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  $\Delta X$  and  $\Delta Y$  might be used.

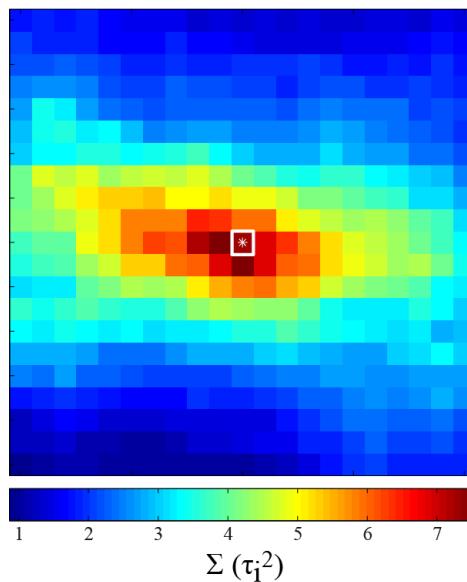


Figure 3.22 – Function: check quality of std/maps positions.  $\Sigma(\tau_i^2)$  (see text for details)

**[B1504]** The button *display standards* 🌐 allows the locations of the spot analyses to be displayed in the main figure (purple circles). The function *select/unselect standards* [B1506] is available only when the spot analyses positions are displayed.

**[B1505]** The button *hide standards* 🚫 allows the locations of the spot analyses to be hidden in the main figure window.

**[B1506]** The button *select/unselect standard (Edit)* enables to selected/unselected spot analyses (internal standards) used for the analytical standardization by selecting them directly on the map. This button is displayed (i.e. the function is available) after you pressed onto 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 switch to the editing mode.

**Why do I have to select or deselect 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.

### 3.4.6 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' papers [Lanari et al. \(2014b\)](#) and [Lanari et al. \(2018\)](#).

**[M1601]** The menu *standardization methods* is used to select the standardization method that will be apply 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. 2018](#)). The advanced standardization is applied using the module *XMTStandardizationTool* (see §3.4.6.3). 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 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. 2018](#)).
- *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 3.4.5).
- *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 povidied during calibration.

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

- *Transfert 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.

**[B1601]** The button *STANDARDIZE* enables to call the standardization function and 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 (end of the standardization function) 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 3.5).

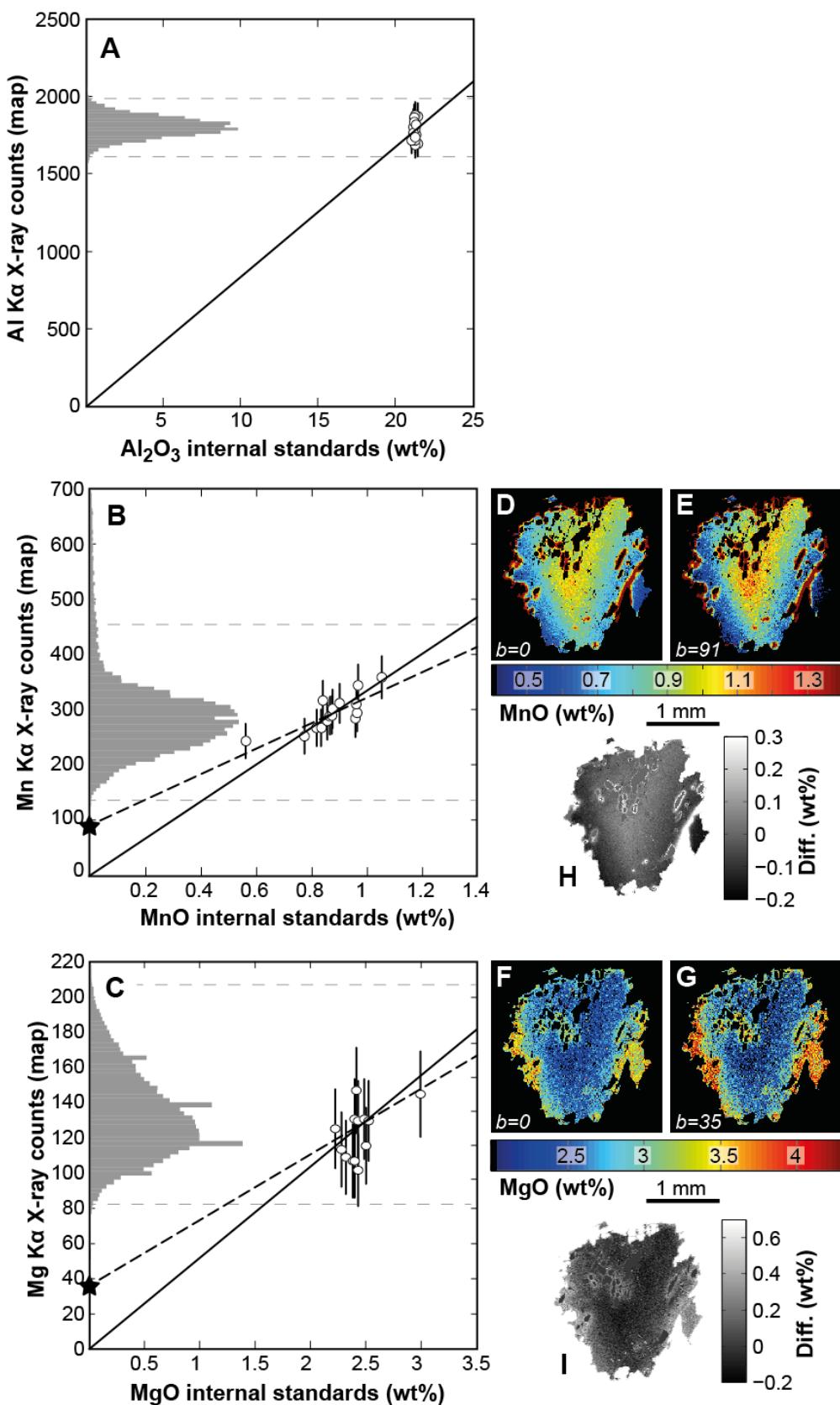


Figure 3.23 – Example of standardization for a garnet of the Central Alps after Lanari et al. (2018).

### 3.4.6.1 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:

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

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 3.23. 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. \(2018\)](#).

### 3.4.6.2 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:

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

### 3.4.6.3 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. 3.24). 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)

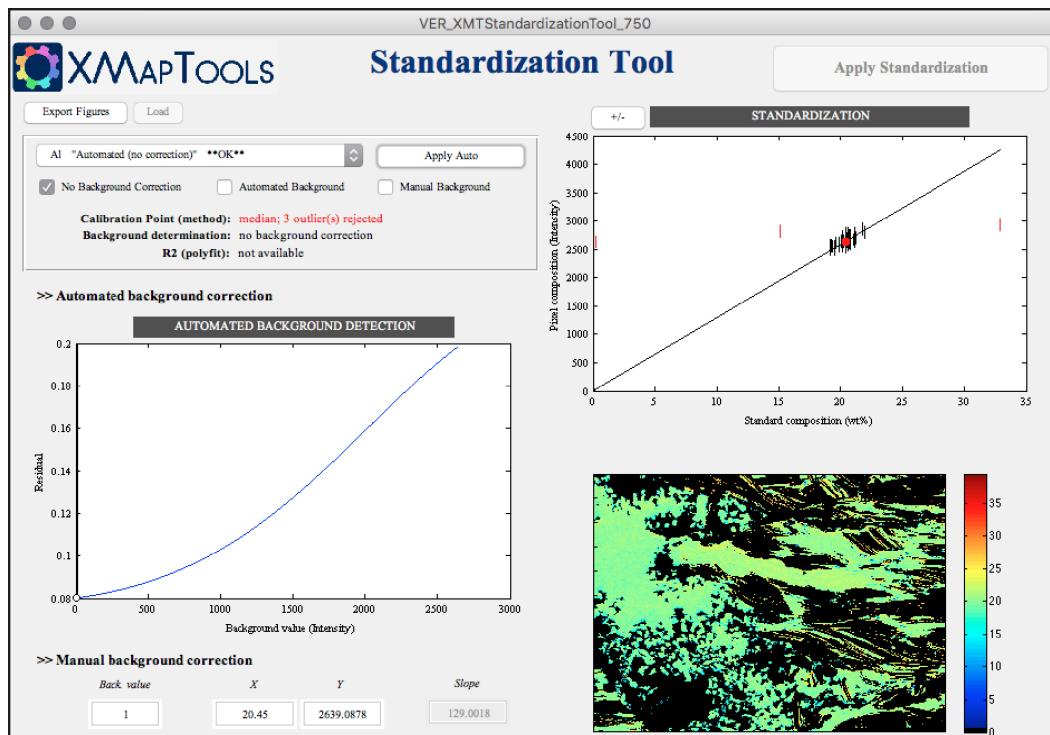


Figure 3.24 – Advanced standardization; case: automated - no background correction (here Al in chlorite)

- **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. 2018](#)).
- **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. 2018](#)).

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*,

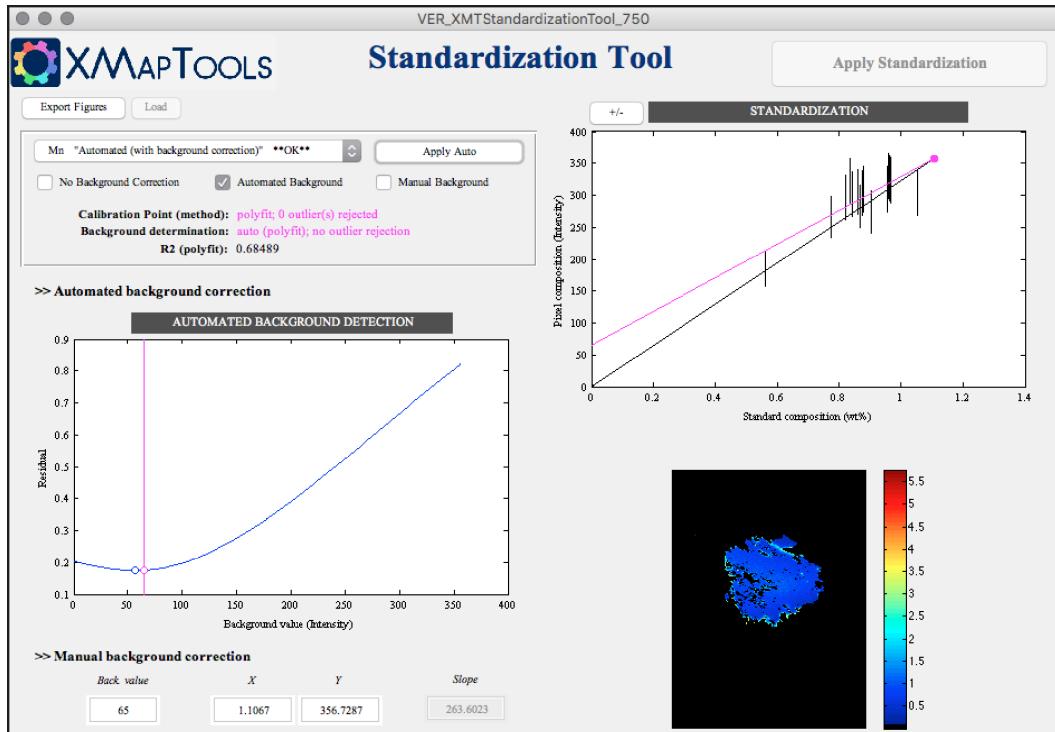


Figure 3.25 – Advanced standardization; case: automated - background correction (here Mn in garnet)

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.
- $R^2$  (*polyfit*): is displayed if the *polyfit* function has been used.

The figure *Automated background correction* show the evolution of the residuals with the background value (e.g. Fig. 3.25). 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. 3.25). 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.

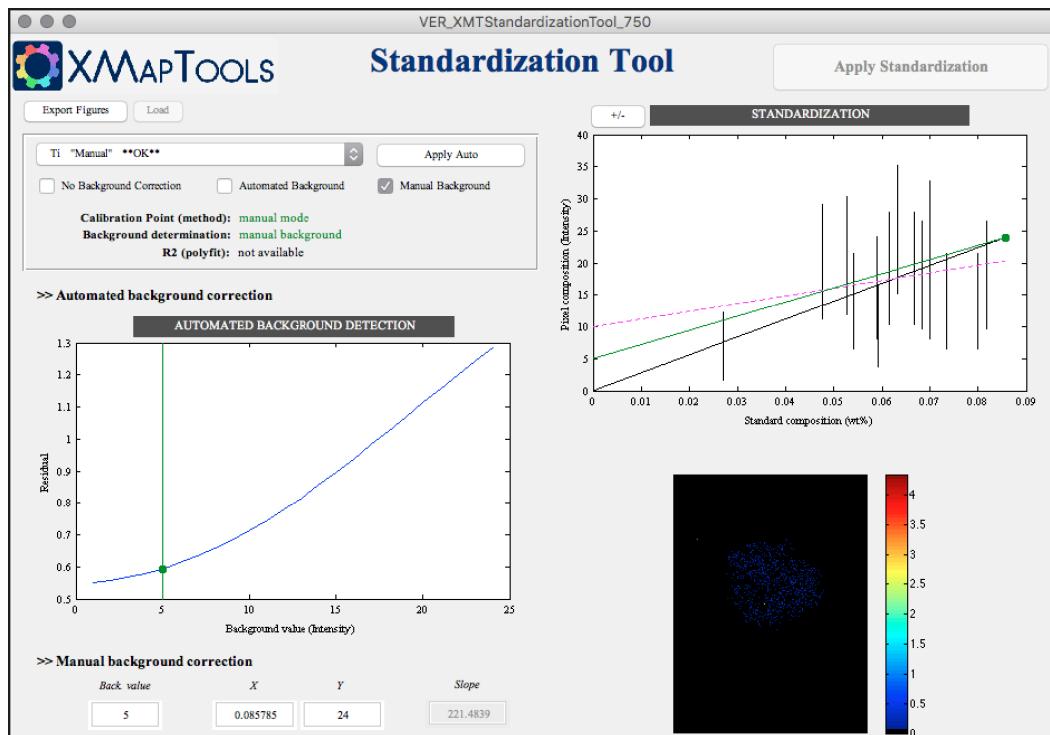


Figure 3.26 – Advanced standardization; case: manual - background correction (here Ti in garnet)

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 3.24, 3.25 and 3.26:

- (1) Automated calibration curve, method median (red dot) without any background correction (Al in chlorite, see Fig. 3.24). 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. 3.25). 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. 3.26). 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 > 95% 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 6 (see §6.2.7.6).
- 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.

## 3.5 QUANTI

### 3.5.1 Standardized maps

[M2101] The menu *standardized phase* allows the *standardized phase* (corresponding to a *standardized phase*) that is displayed in the main figure window to be selected. 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] The menu *elements* enables 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] The button *rename Quanti file*  allows the name of the *standardized phase* selected in [M2101] to be edited. This name was automatically defined during the standardization (format: *[mineral name]-[method used]*).

[B2106] The button *duplicate Quanti file*  allows the selected *standardized phase* to be duplicated.

[B2102] The button *delete Quanti file*  allows the *standardized phase* selected in [M2101] to be deleted. This button is available only if two or more *standardized phase* have been computed.

[B2103] The button *export compositions*  enables exporting oxide analyses from the *standardized phase* selected in [M2101]. The generated file is exported in the directory *Exported-Oxides*. If this directory does not exist the program makes it in the working directory. Different methods are available (see Fig. 3.27)

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. In the default order, zero values are allocated to Fe<sub>2</sub>O<sub>3</sub> and XFe<sub>3</sub><sup>+</sup>. The **format of the delimiter** may be *blank* or *tabulation*.

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

Code 3.10 – 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 3.11 – 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 TRIPLOT3D.
- [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.

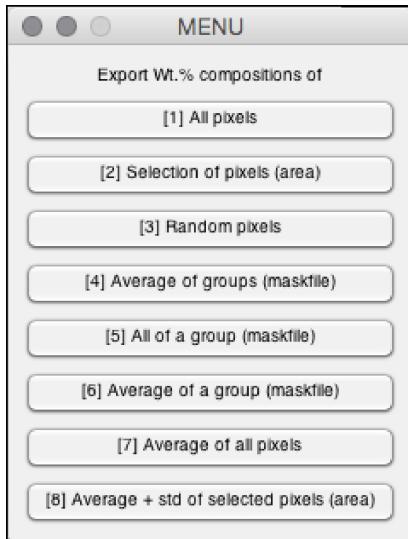


Figure 3.27 – *Menu listing the methods available to export oxide analyses from the selected Quanti file*

**[B2104]** The button *apply filter* enables creating 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 P-T study.

**[B2105]** The button *generate oxide wt-% sum map* allows the sum of the oxide wt-% compositions to be displayed. This new map can only be displayed 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]).

### 3.5.2 Standardization Info

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]** The button *display calibration curves* enables displaying a new figure with 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.

**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]** The button *test standardization* enables drawing diagrams showing the compositions of the standards (spot analyses, in oxide wt-%), against the compositions of the corresponding pixels (standardized maps, in oxide wt-%). This technique is basically used to detect the elements for which the chemical variability could be below detection limit for the mapping conditions ([Lanari et al. 2014b](#)).

### 3.5.3 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 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.
- **XThermoTools:** Thermodynamic modeling module in XMAPTOOLS to be published in a later release (work in progress).

**[M2302]** The menu *external function subgroup* lists the subgroups of external functions available in a given group set in [\[M2301\]](#).

**[M2303]** The menu *external functions* lists the external functions available in a given subgroup set in [\[M2302\]](#).

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

**[B2302]** The button *external function info window*  allows the function info window (see Fig. [3.28](#)) to be displayed. This module aims to display info regarding the external functions available in XMAPTOOLS such as:

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

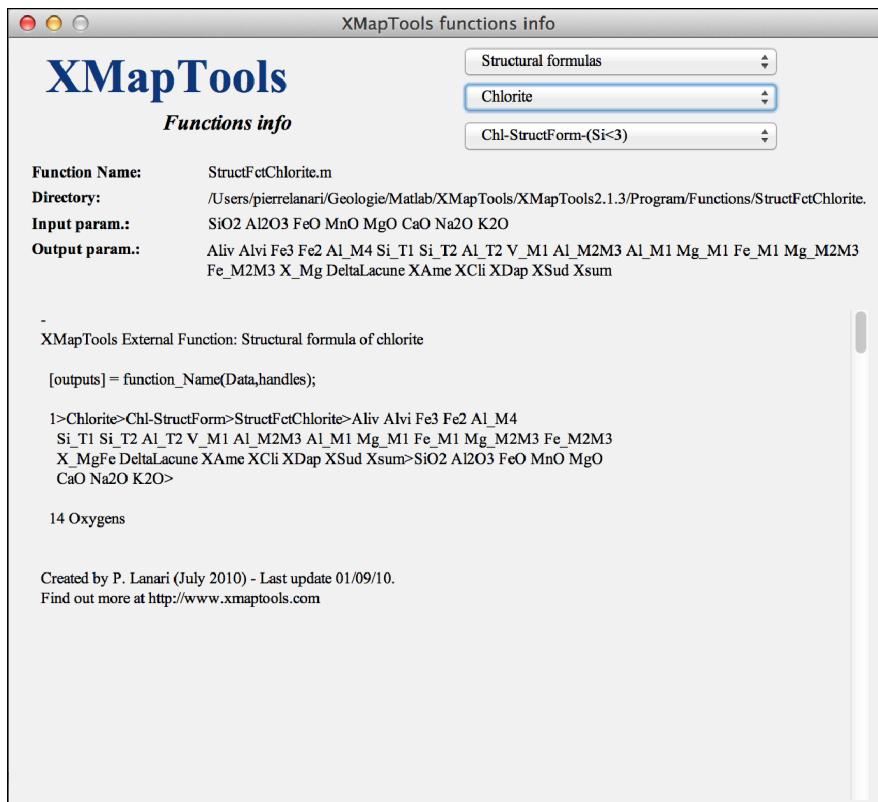


Figure 3.28 – *XMapTools function info GUI*

### 3.5.4 Local composition module

**[B2401]** The button *merge standardized phases* enables merging selected standardized phases and generating a new standardized map. The phases are selected by the user and the function generates a 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]** The button *generate a density map (from selected mask file)* allows a density map to be generated. Such density map may be used to generate a density-corrected oxide map. The procedure to export local compositions is discussed in the section 1.5.1. Density of phases may be defined in the file *Classification.txt* below the keyword >2 (see example in code 3.14). 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 3.12 – File *Classification.txt* including specific density (after the keyword >2)

**[B2407]** The button *display the density map*  allows the density map to be displayed. 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]** The button *compute a density-corrected oxide map*  enables generating a density-corrected oxide map. User can define the name of this new map. The default name begin with \*DCM abbreviation of density-corrected map. As detailed in the section 1.5.1, 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

$$DCM_i = \frac{\rho_i}{\rho_{mixture}} C_i^{wt} \quad (3.19)$$

with  $\rho_i$  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<sup>©</sup> Command Window (see code 3.13). 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 1.5.1).

```
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 3.13 – Information regarding the density-correction displayed in the MATLAB<sup>©</sup> Command Window)

**[B2409]** The button *select an area and eliminate pixels outside*  enables eliminating the 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. 3.11b). Selection mode is disabled using right-clicking (spot 11, in Fig. 3.11b). The polygon is closed without taking into

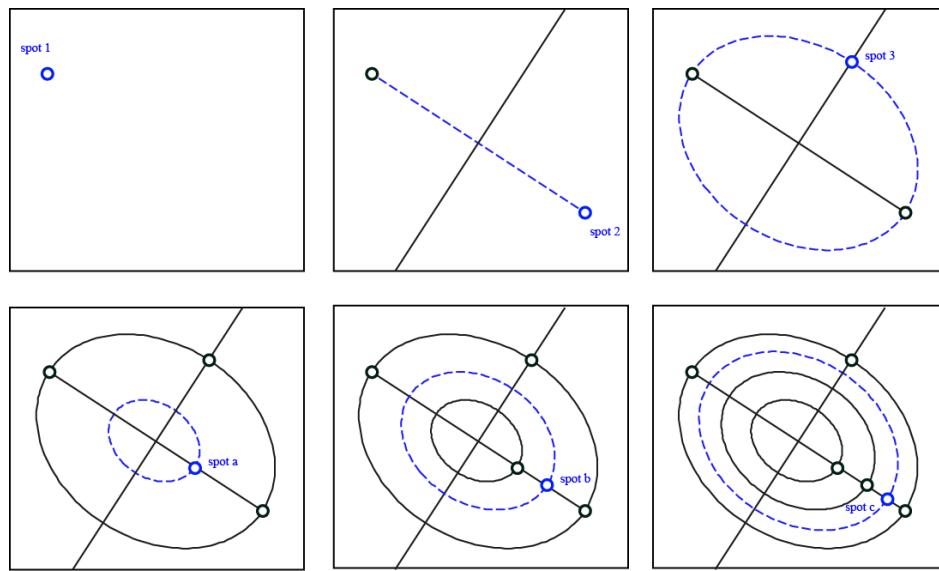


Figure 3.29 – Procedure to define an ellipse and export composition extrapolated in 3D

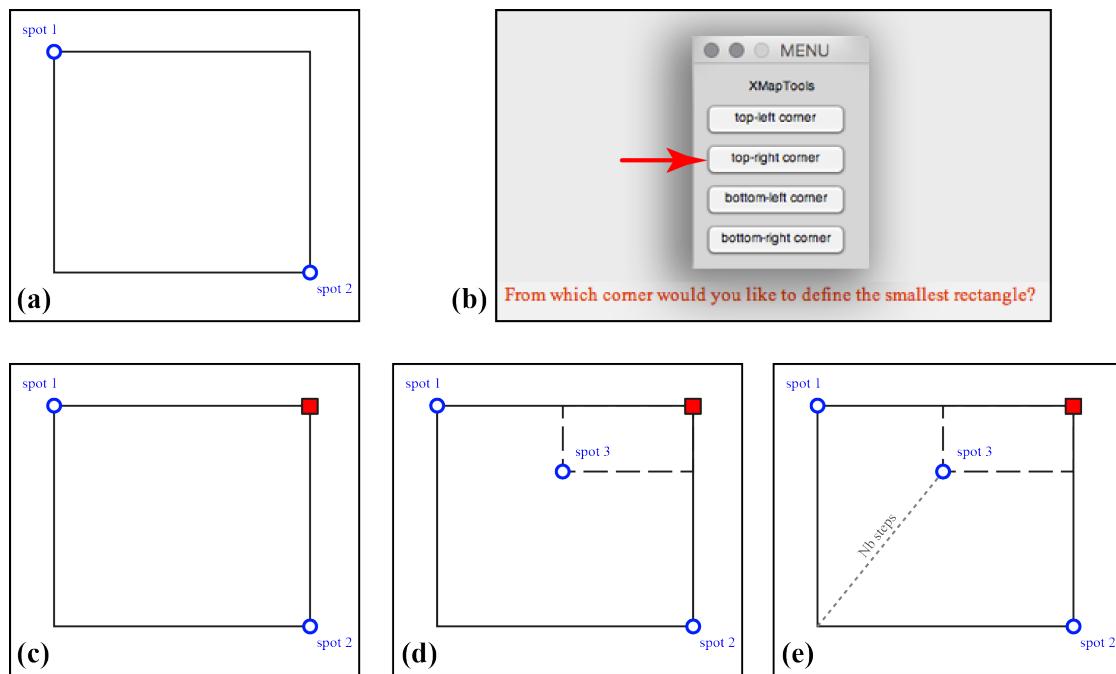


Figure 3.30 – Procedure to export compositions with a variable-size rectangle

account the right clicking position, see dashed line in figure 3.11b. For the standardized phase selected in [M2101] all pixels outside the region-of-interest are eliminated.

**[B2410]** The button *select an area and eliminate pixels inside*  enables eliminating the 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]** The button *export local composition: map*  allows the average oxide composition of the *standardized phase* or *density-corrected map* selected in [M2101] to be exported. This function has been designed to work with merged maps with or without density correction (see function [B2401]). The generated file (see code 3.14) 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	
Al2O3	24.3961
CaO	0.021694
Cr2O3	0.057805
FeO	19.6617
K2O	3.6851
MgO	6.8446
MnO	0.35621
Na2O	0.33612
SiO2	34.833
TiO2	0.18467
SUM	90.3769

Code 3.14 – Example of exported file in /Exported-LocalCompos

**[B2403]** The button *export local composition: area*  enables exporting the average oxide composition 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. 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]** The button *export local composition: ellipse (3D)*  enables exporting the average oxide composition of pixels included in ellipse defined by the user of the *standardized phase* selected in [M2101]. The composition of each small ellipse is extrapolated from 2D surface to 3D volume of an ellipsoid (e.g. code 3.15).

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. 3.29). Then integrations are defined from the center to the rim of the primary ellipse (see points a, b and c on Fig. 3.29).

Local composition (Ellipsoid) from XMapTools  
12-Nov-2015

Reference ellipse information :

Center position (X,Y)	338.86	338.86
Slope Major axis	1.89	
Radius Major axis	918.78	
Radius Minor axis	535.68	
Surface (Nb of pixels)	386429.00	
Surface (in px <sup>2</sup> )	1546191.93	

Integrations :

Number of integrations	4.00				
Integration values	0.3802	0.6565	0.8301	1.0000	
Volumes integrations (px <sup>3</sup> )	1041e6	4319e6	5475e6	8104e6	
Volumes fractions	0.0550	0.2280	0.2890	0.4279	
Nb pixels integrations	55889	110689	99739	120112	
Surface integrations (px <sup>2</sup> )	223e3	442e3	399e3	480e3	
Surface fraction (from px)	0.1446	0.2864	0.2581	0.3108	
Surface fraction (in px <sup>2</sup> )	0.1446	0.2864	0.2580	0.3108	

Compositions integrations :

Al <sub>2</sub> O <sub>3</sub>	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 <sub>2</sub> 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 <sub>2</sub> O	7.985	9.470	11.300	11.425	
TiO <sub>2</sub>	1.529	2.183	1.775	0.360	
SiO <sub>2</sub>	54.799	56.254	59.698	62.701	

Extrapolated (ellipsoid) local Compositions :

Al <sub>2</sub> O <sub>3</sub>	23.421				
CaO	0.336				
FeO	0.758				
K <sub>2</sub> O	1.439				
MgO	1.388				
MnO	0.058				
Na <sub>2</sub> O	10.754				
TiO <sub>2</sub>	1.249				
SiO <sub>2</sub>	59.928				
SUM	99.3309				

Code 3.15 – Example of exported file in /Exported-LocalCompos

**[B2412]** The function *export local composition: variable-size rectangle*  can be used to estimate the change in local bulk composition between two rectangular areas along *n* steps (Fig. 3.30 and 3.31).

The procedure consists of the following steps:

- Define the reference domain with a rectangle shape by clicking two pixels (see Fig. 3.30-a).
- Choose from which corner of this rectangle you want to define the smallest rectangle (see Fig. 3.30-b). The available options are: *top-left corner*, *top-right corner*, *bottom-left corner*, *bottom-top corner*. In the example shown in figure 3.30-c, the *top-right corner* is selected (red arrow in b).

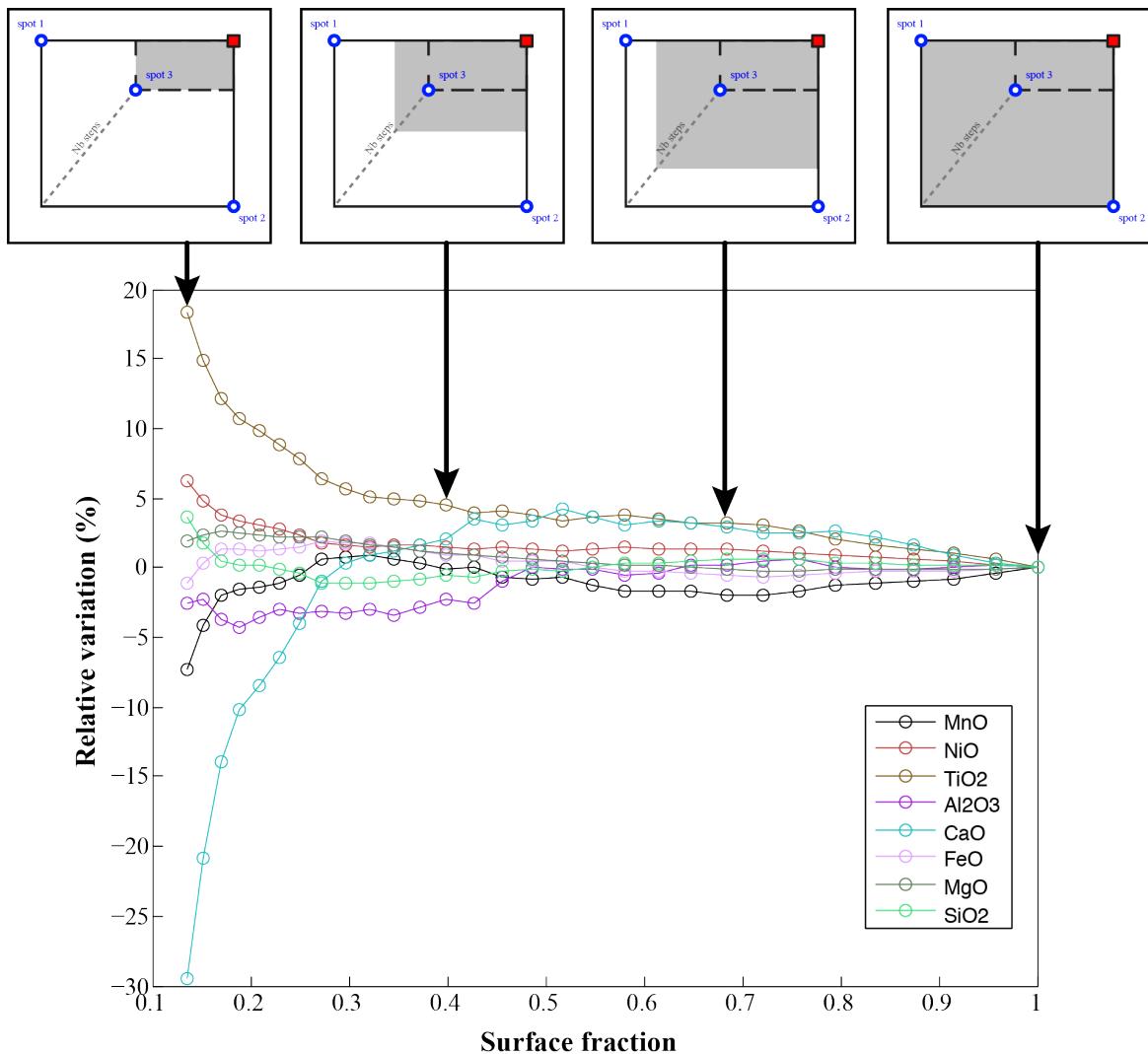


Figure 3.31 – Result exporting compositions with a variable-size rectangle

- Define the smallest rectangle from the selected corner (see Fig. 3.30-d).
- Define the number of steps, i.e. the number of samples along the dashed line in figure 3.30-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. 3.31). 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.

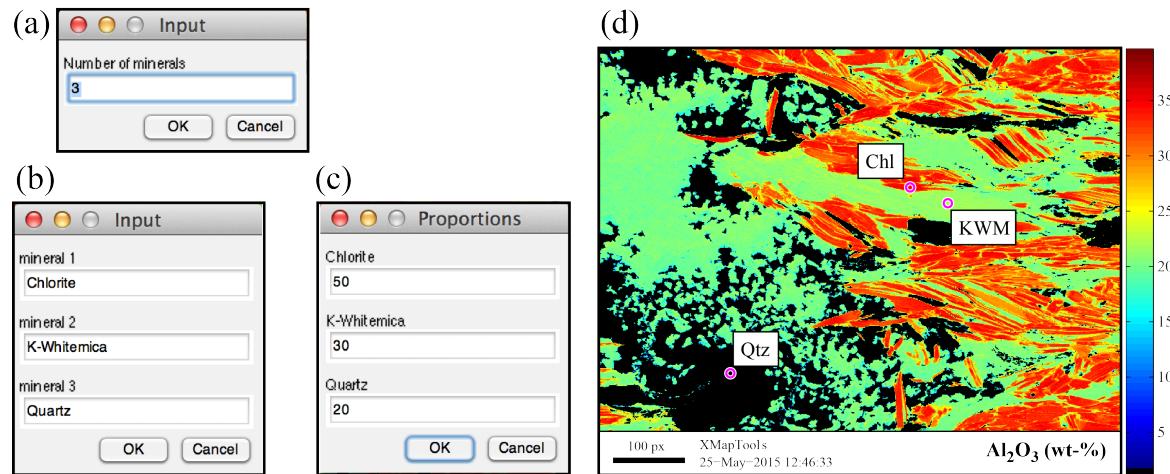


Figure 3.32 – Procedure to export composition build from proportions. (a) number of phases and their (b) names, (c) modal proportion, and (d) compositions.

**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]** The button `export composition build from proportions` enables exporting a local bulk composition computed using mineral compositions and mineral proportions set by user. 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. 3.32). The following steps are required:

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

The generated file (see code 3.14) 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 <sub>2</sub> O <sub>3</sub>	21.6714	34.5545	0.0000
FeO	31.0584	1.454	0.0000
K <sub>2</sub> O	0.0094	9.0293	0.0000
MgO	12.2202	1.2115	0.0000
Na <sub>2</sub> O	0.018231	1.4428	0.0000
SiO <sub>2</sub>	25.3511	46.49	99.612
TiO <sub>2</sub>	0.029867	0.36857	0.0000

**(3) Local Composition:**

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

Code 3.16 – Example of exported file in /Exported-LocalCompos

## 3.6 RESULTS

### 3.6.1 Results from external functions (Results)

**[M3101]** The menu *results phase* enables to select the *result* (corresponding to the output of an *external function*) that is displayed in the main figure window. All the *results* computed 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]** The menu *elements & variables* allows the variable of the *result* to be selected. This menu is updated for each *result* selected in [M3101].

**[B3101]** The button *rename result* enables editing the name of the *result* selected in [M3101]. This name was automatically defined during the computation of the external function (format: [*FunctionName*]).

**[B3102]** The button *delete result* allows the *result* selected in [M3101] to be deleted. This button is available only if two or more *results* have been computed.

**[B3103]** The button *export compositions (results)* enables exporting variables from the *result* selected in [M3101]. One file is generated for each selected variable. The generated files are matrixes with the same size as the original map. This file is exported in the directory *Exported-Results*. If this directory does not exist the program makes it in the working directory.

```
Export ... (RESULTS in ascii format) ...
Export ... (mineral: K-WhiteMica) ...
Export ... (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 3.17 – 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].

**[B3105]** The button *delete a variable* enables deleting the variable selected in [M3102] of the *result* selected in [M3101].

### 3.6.2 Other functions for trace element maps

**[B3301]** The button *spider* opens the *Spider module*. A complete description of this module is given in the following section (see §3.7.5).

**[B3302]** The button *compute a relative map*  allows a relative map to be computed. A reference pixel shall be defined by clicking on the image (Fig. 3.33a). 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. 3.33b). This map has no unit. For a map  $A$  (matrix) and a reference pixel with a composition  $R$ ,  $Diff\_rel$  is simply obtained by:

$$Diff_{rel} = \frac{A}{R} \quad (3.20)$$

- **Diff\_per** shows the relative difference in composition for each pixel to the reference pixel expressed in percentage (e.g. Fig. 3.33c).

$$Diff_{per} = \frac{(A - R)}{R} \times 100 \quad (3.21)$$

**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. 3.33c). Only the pixel with positive values are considered by the *auto-contrast* function.

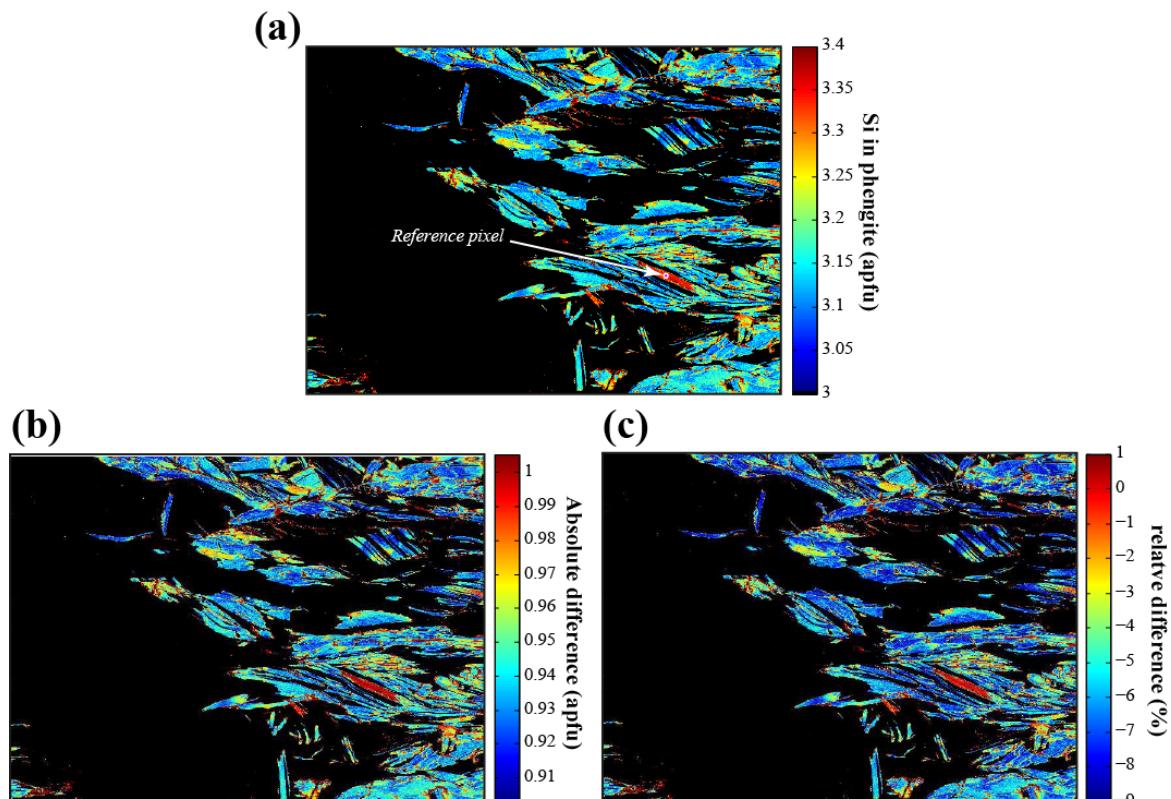


Figure 3.33 – Relative maps. (a) Silicon map of phengite in atom per formula unit (apfu). The reference pixel used to compute (b) and (c) was selected in the Si-rich phengite (3.37 apfu) and is plotted in magenta. (b) Map of Si in phengite showing the relative composition of each pixel to the reference pixel (see Eq. 3.20). (c) Map of relative differences expressed as percentage (see Eq. 3.21).

### 3.7 CHEMICAL MODULES

Any map displayed in the main window (e.g. *X-ray maps*, *concentration map*, *merged map*, *result*) can be treated in binary diagrams (Fig. 3.35a), in ternary diagrams (Fig. 3.35b) or displayed as composite RGB image (Fig. 3.40). It is also possible to generate new maps (variables) from existing maps (variables). The chemical modules BINARY, TRIPLOT3D, RGB and GENERATOR are called using the buttons [B5301], [B5302], [B5303] and [B5304], only if the number of selected variables is greater than two or three for ternary diagrams. A complete 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 having compatible names (see §2.6.2).

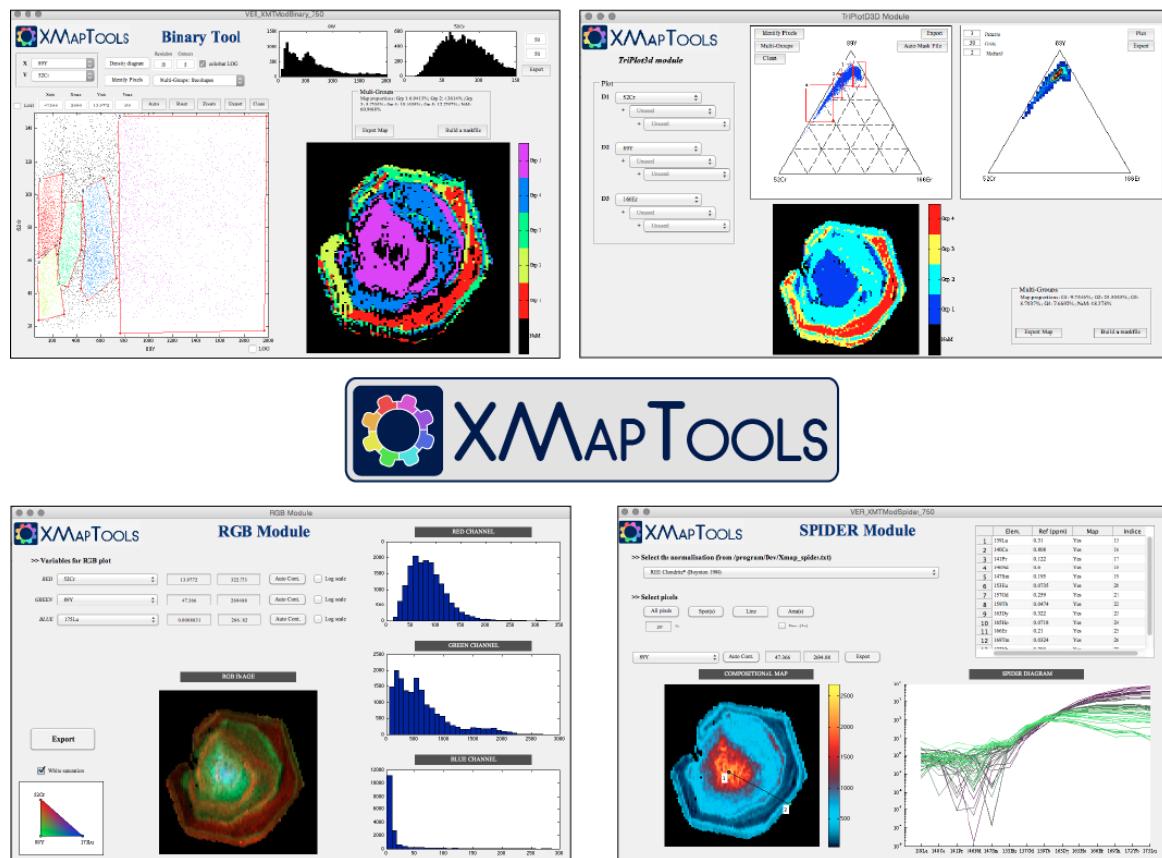
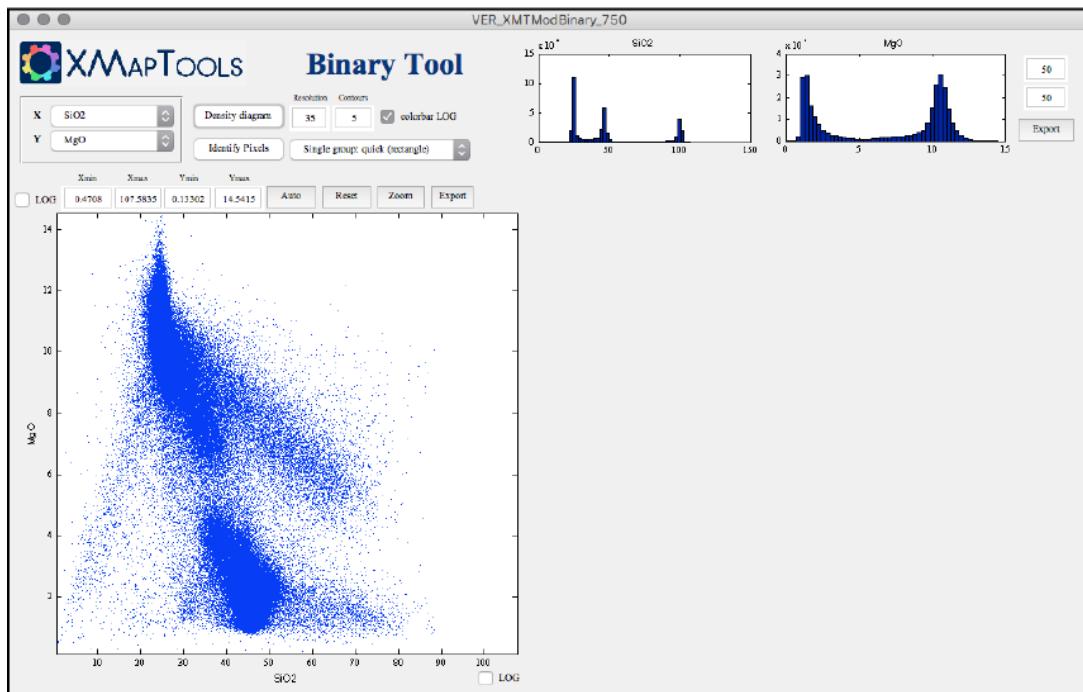


Figure 3.34 – Chemical modules available in XMapTools

(a)



(b)

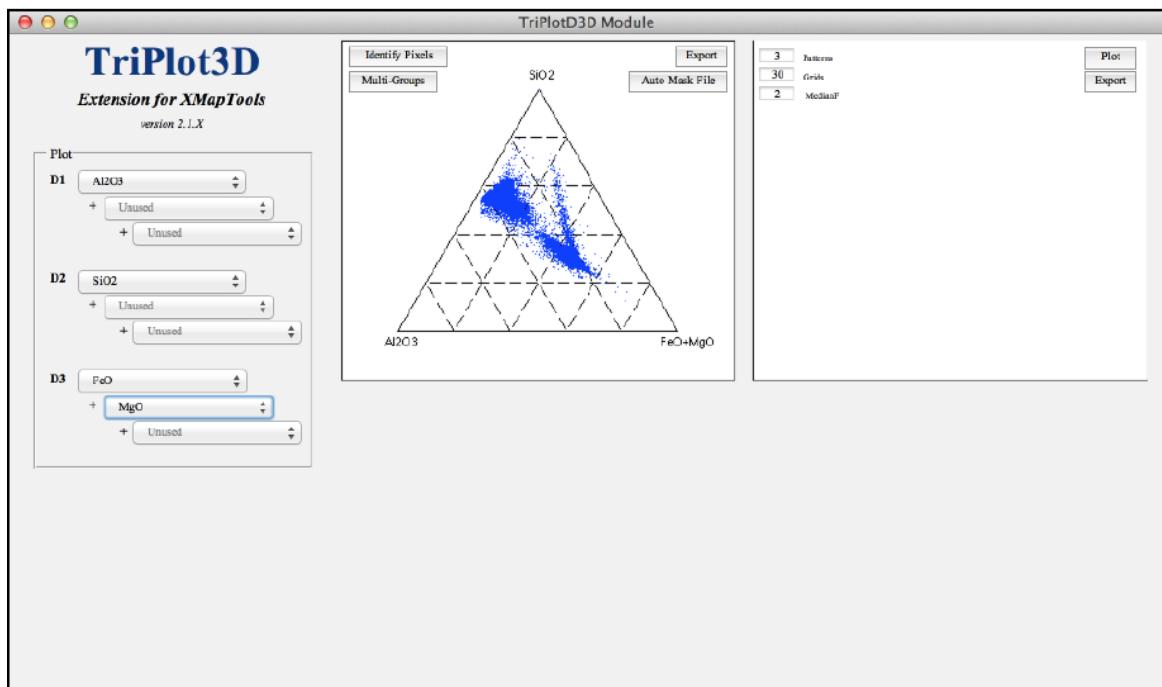


Figure 3.35 – Chemical modules (a) Binary and (b) TriPlot3D

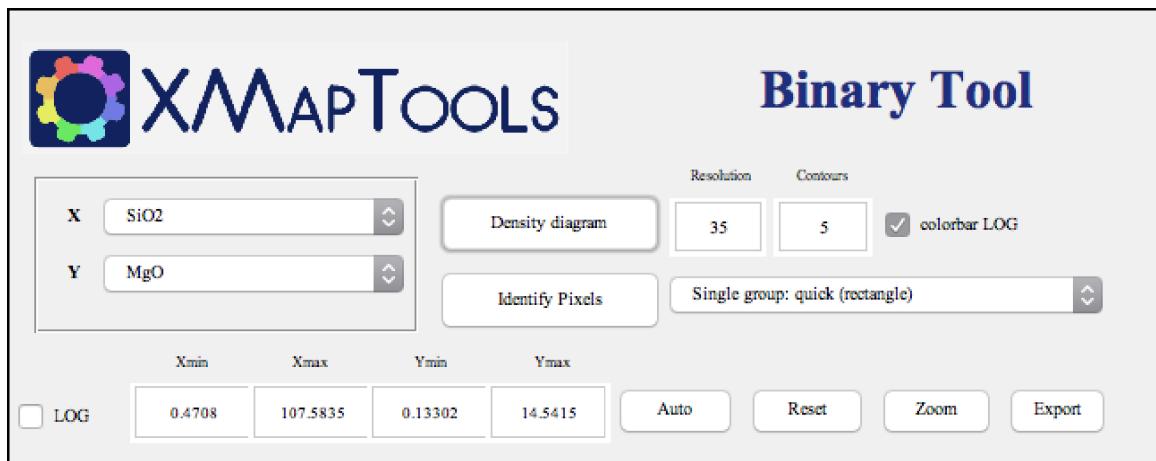


Figure 3.36 – Buttons and options of the Binary module

### 3.7.1 Binary Module

BINARY is a module (see 3.3.4) with an additional graphic user interface that is included in the XMAPTOOLS’ package. This module can be used in the three workspaces *X-ray*, *Quanti* and *Results*. Once in use, this module remains independent of 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 metapelitic from the western Alps investigated by Aude Verly.

The main buttons and options are available in the *Binary* module (see Fig. 3.36) 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. 3.36). The maps listed in these menus depend on the workspace from which *Binary* is called.

**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.

**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.

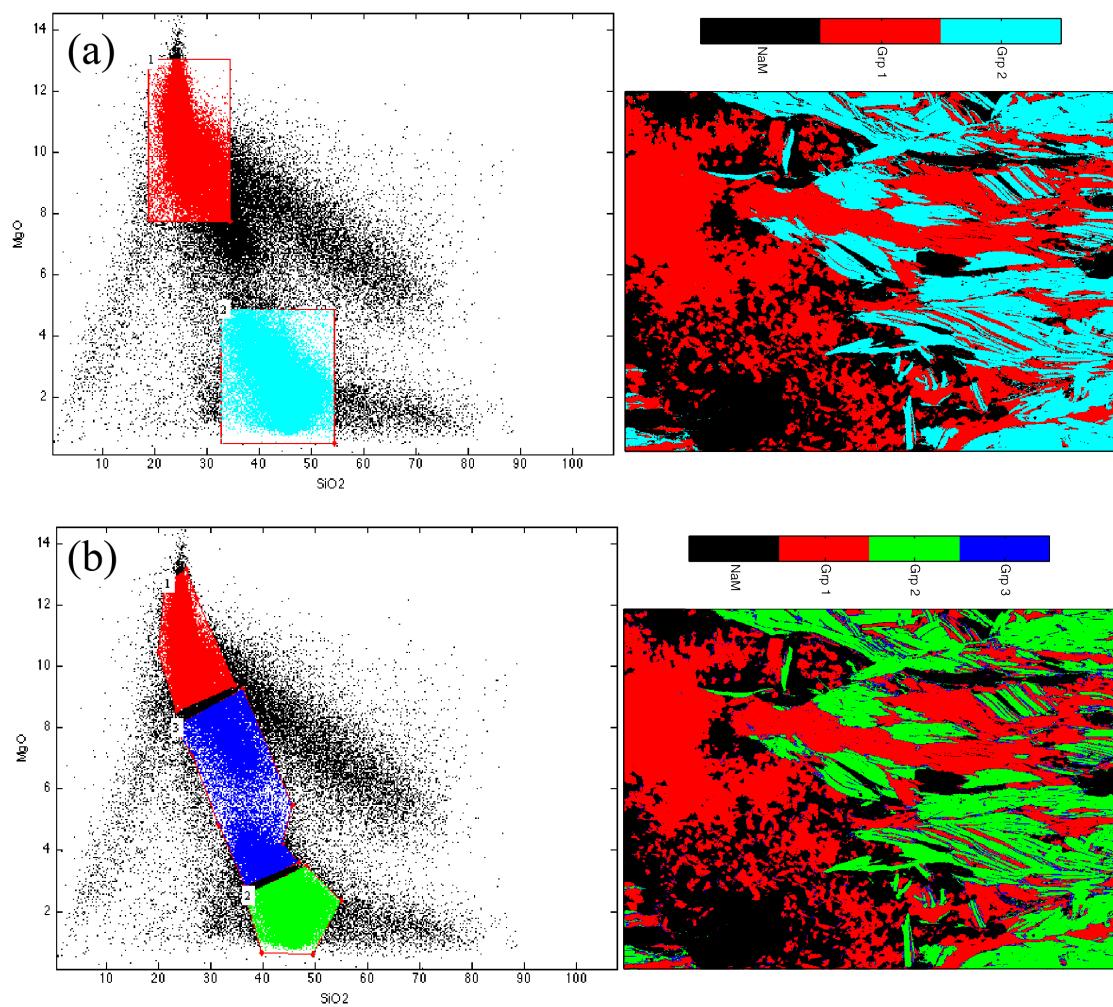


Figure 3.37 – Multi-Groups functions in the Binary module. (a) Quick (rectangle) using 2 groups: chlorite (red) and phengite (blue). (b) Free shape using 3 groups: chlorite (red), phengite (green) and the mixing pixels between them (blue)

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

### 3.7.1.1 Density diagrams in the Binary module

**Density diagram (button)** generate a density diagram from the points plotted in the binary diagram. The resolution and the number of patterns (default values 35 and 5) can be edited before to call the function. The resolution is the number of vertical and horizontal pixels in the density image. A high resolution increases significantly the duration of the calculation. Note that the density map is plotted using a color bar with a logarithmic scale if the option *colorbar LOG* is selected.

### 3.7.1.2 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. 3.36):

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

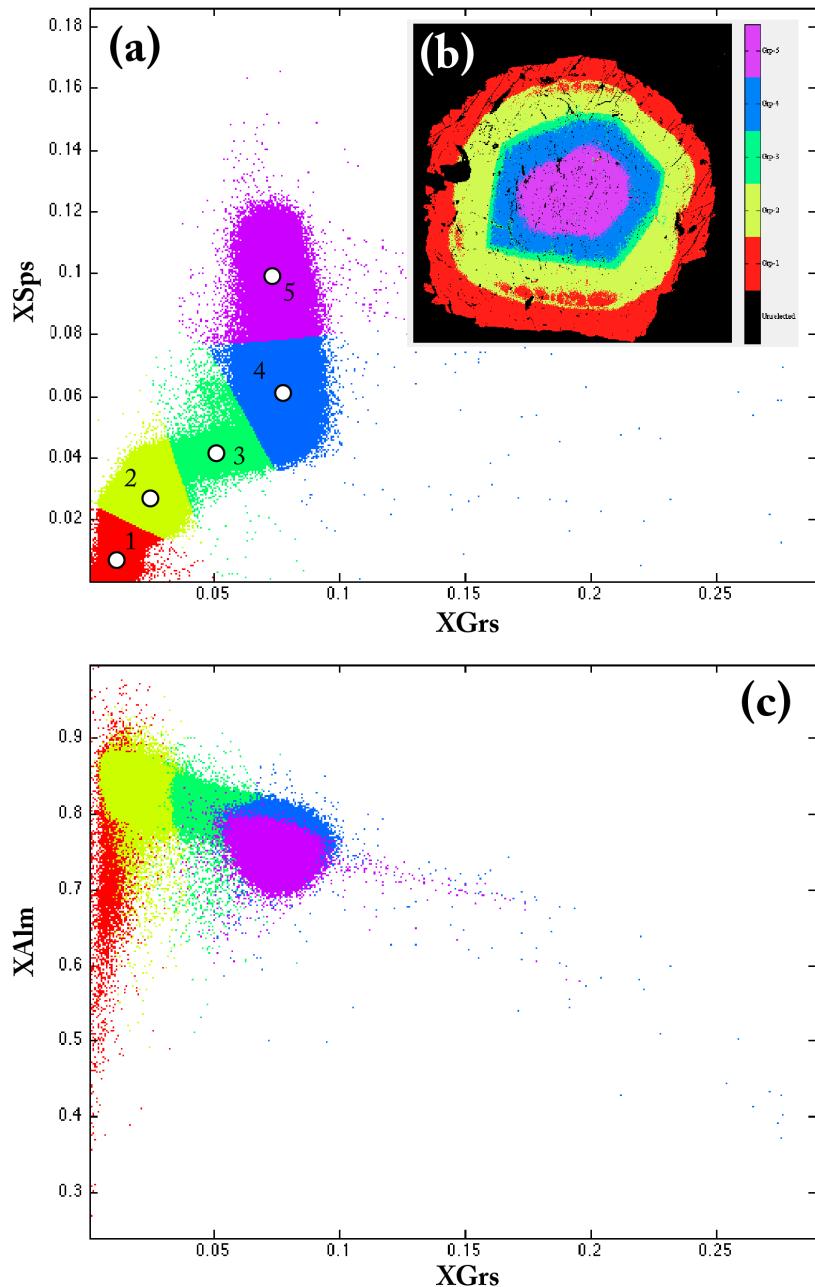


Figure 3.38 – *k*-means clustering in the Binary module. (a) clustering in the system  $[X_{Grs}, X_{Sps}]$  using 5 clusters (see the spots for the initial centroids) and the method *sqEuclidian*. (b) map showing the spatial distribution of each final cluster. (c) The clusters are plotted in a binary 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 ( $X_{Grs}$ )

- *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 3.37.

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

### 3.7.1.3 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.

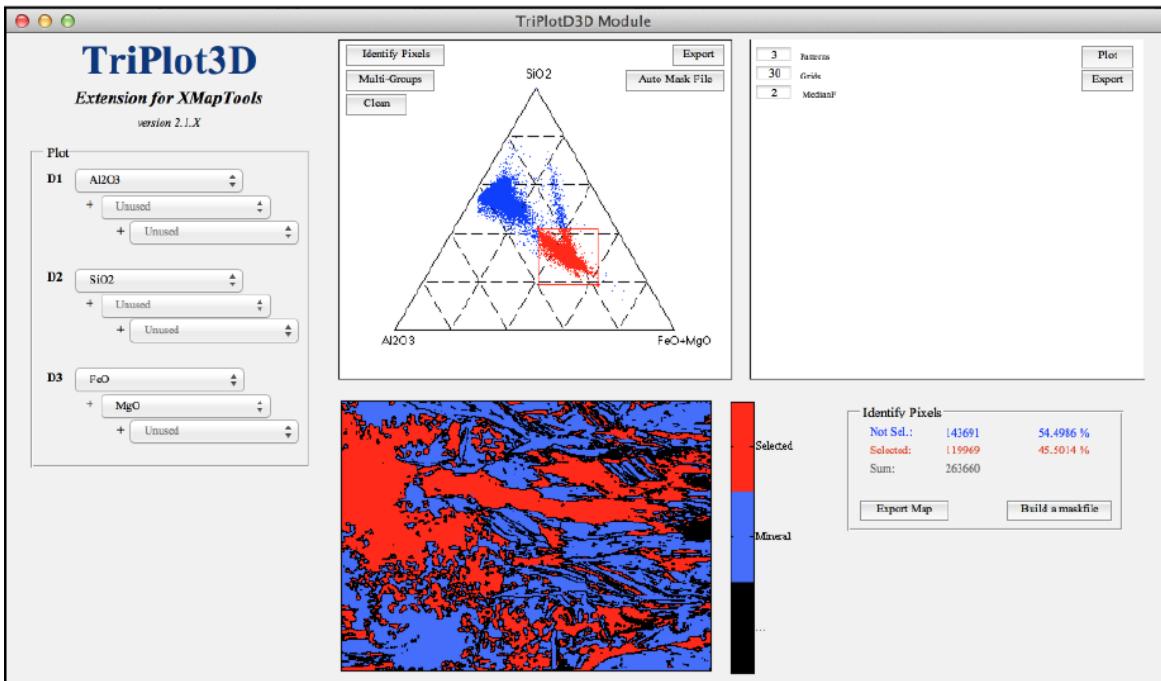
**Plot (button)** this button allows the original binary diagram in which the clusters of the selected mask file were generated to be plotted. This button is only available when a mask file is selected.

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

## 3.7.2 TriPlot3D Module

TRIPILOT3D is a module (see 3.3.4) with an additional graphic user interface that is included in the XMAPTOOLS' package. The functions available in TRIPILOT3D (Fig. 3.39) are similar to those described above for BINARY. This section of the user-guide and this module will be improved in a future update.

(a)



(b)

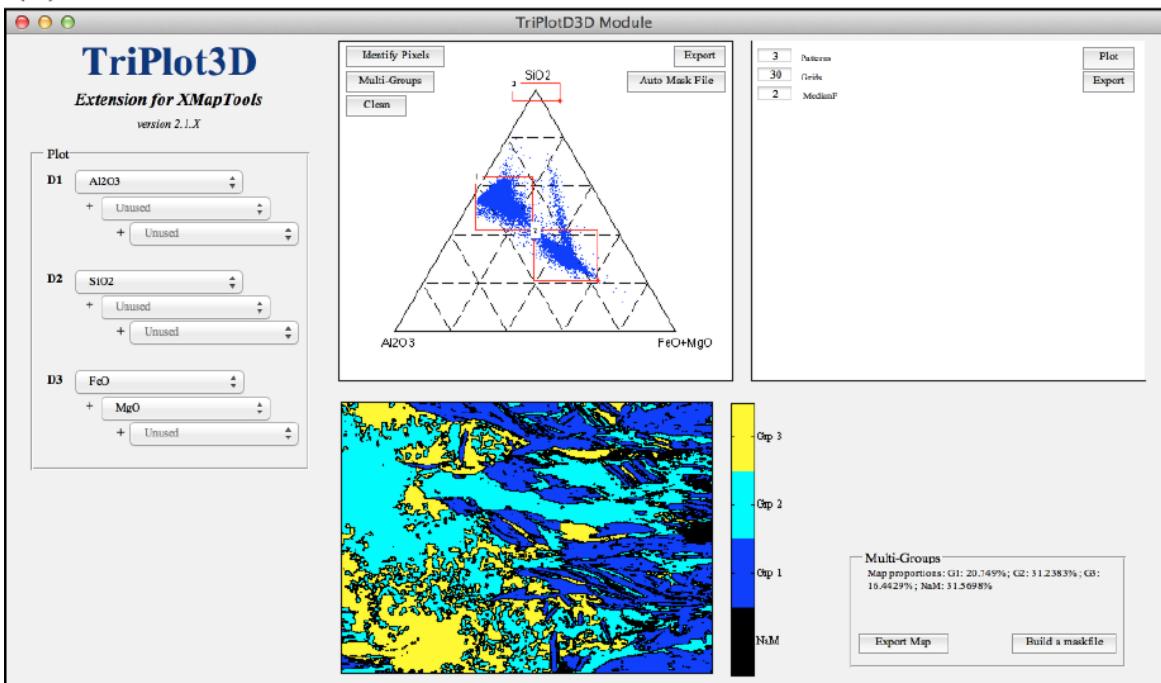


Figure 3.39 – Chemical modules TriPlot3D (a) identify pixels, (b) multi-group

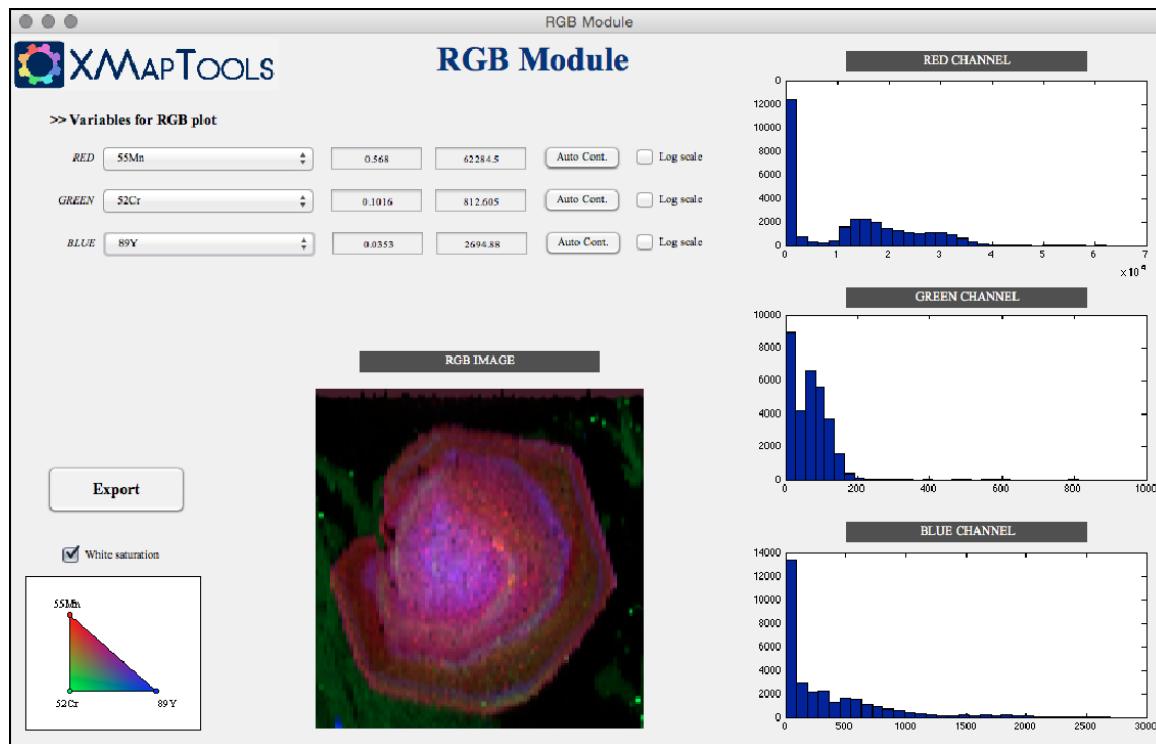


Figure 3.40 – Chemical modules RGB (see text for details)

### 3.7.3 RGB Module

RGB is an XMAPTOOLS’ module (see 3.3.4) that generates three channels composite images (RGB for red, green and blue) from compositional maps. In figure 3.40 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*.

The *variables for RGB* spot window (Fig. 3.40) enables selecting three maps that will be used to generate the RGB map. The *auto-contrat* buttons works in the same way as those available 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<sup>©</sup> 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 an option available below the *export* button.

### 3.7.4 Generator Module

GENERATOR is an XMAPTOOLS’ module (see 3.3.4) that can be used to generate new maps (i.e. variables) from existing maps in any workspace (*X-ray*, *Quanti* or *Results*). Once the new maps are generated they can be send back to the main XMAPTOOLS window. Note that the main XMAPTOOLS window is frozen when the GENERATOR module is in use. Close the GENERATOR window to unfreeze XMAPTOOLS.

### 3.7.4.1 Code format

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

$$[Output] = [Operation] \quad (3.22)$$

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 3.18 – Array arithmetic commands in MATLAB<sup>©</sup> using the period character "."

Additional information regarding the MATLAB<sup>©</sup> operators can be found at [https://www.mathworks.com/help/matlab/matlab\\_prog/matlab-operators-and-special-characters.html](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:

$$Fe/Mg = Fe./Mg; \quad (3.23)$$

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:

$$Mg\# = (Mg./ (Mg + Fe)) * 100 \quad (3.24)$$

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:

$$HREE\_slope = (x175Lu/0.0381)./(x147Sm/0.231) \quad (3.25)$$

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](https://www.mathworks.com/help/matlab/matlab_prog/variable-names.html)

### 3.7.4.2 Graphical User Interface of the Generator module

The interface of the GENERATOR module is shown in Figure 3.41. The description is divided into two parts:

Before to generate new maps:

**[1] Plot options** (Fig. 3.41a) 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<sup>®</sup> windows (see [B5102] for details).

**[2] List of maps** (Fig. 3.41a) 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. 3.41a) 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. 3.41a) Input for the code that will be evaluated to generate new variables (maps).

**[5] Generate** (Fig. 3.41a) Button to generate the map using the code given in (4).

**[6] Classical operations** (Fig. 3.41a) 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. 3.41a) 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.

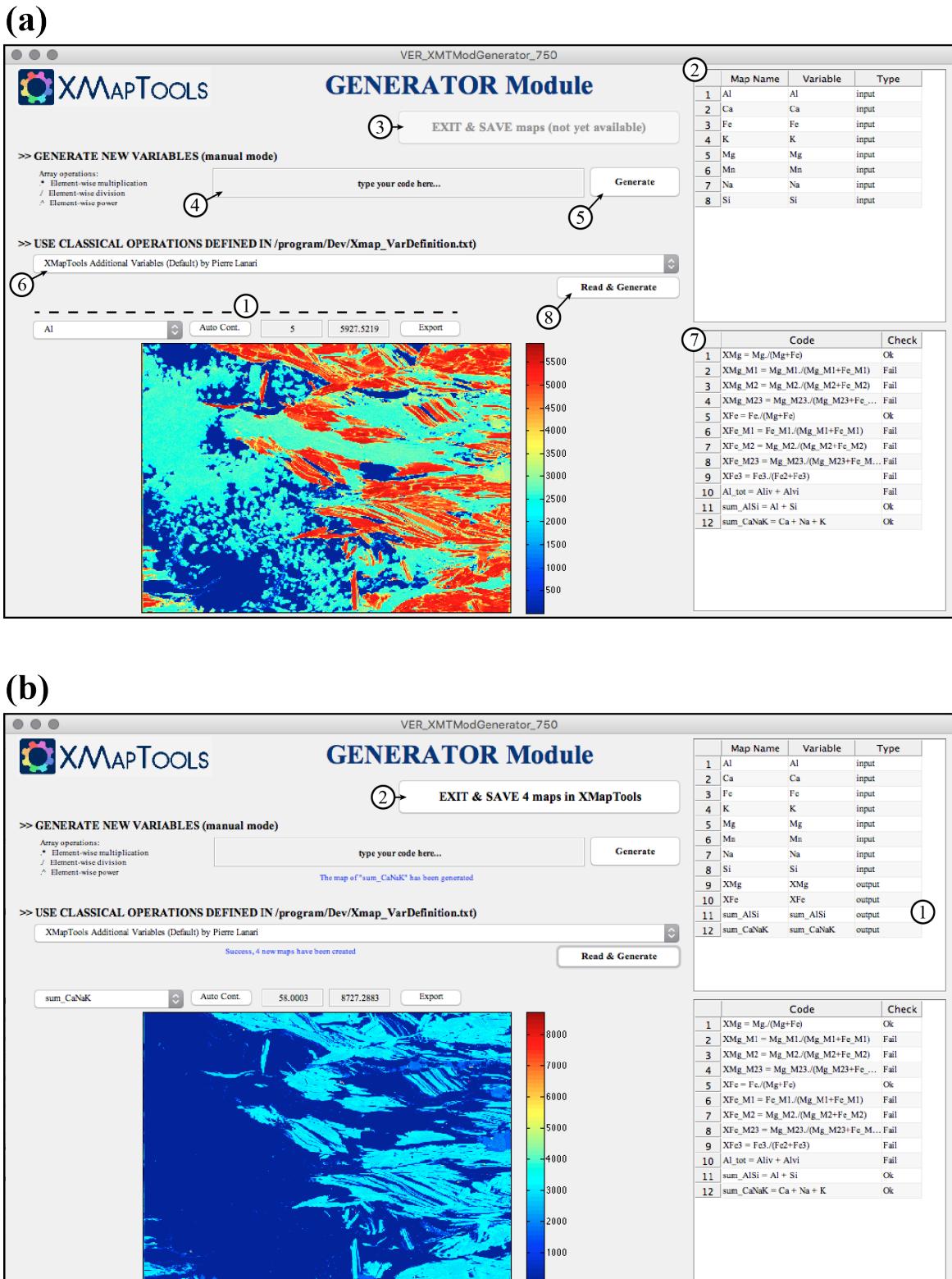


Figure 3.41 – GENERATOR module graphical user interface (a) before to generate a new map; (b) after generating new maps

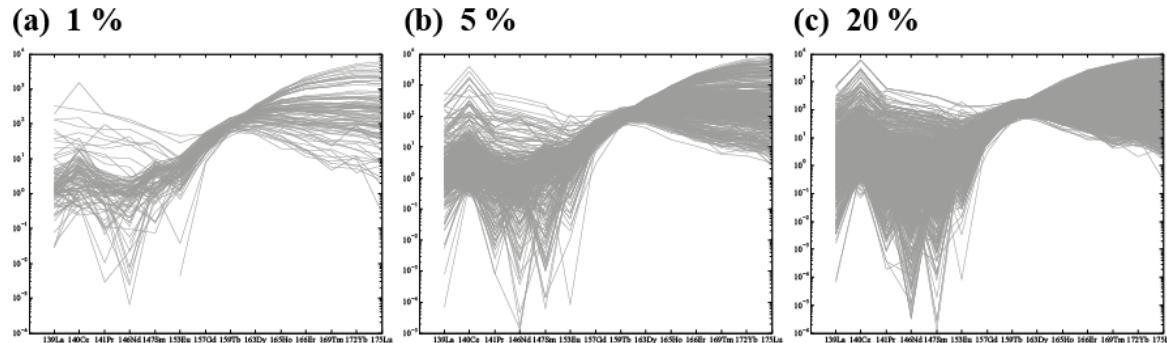


Figure 3.42 – *Spider diagram of REE in garnet using (a) 1%, (b) 5% and (c) 20% of the pixels of the map. See Fig. 3.43 for x labels.*

**[8] Read and Generate** (Fig. 3.41a) 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. 3.41b) 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. 3.41a) 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.

### 3.7.5 Spider Module

The SPIDER module (Fig. 3.34) generates spider diagrams of trace element maps. The SPIDER module is available in the workspace *Results*, provided that trace element maps of isotopes are available (see §2.6.2). The list of the isotopes and the reference compositions used in the selected normalization are shown in the table (see 1 in Fig. 3.44)

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

- Select a normalization in the normalization menu (2 in Fig. 3.44)
- Select a color scheme in the color menu (3 in Fig. 3.44)
- Select pixels of the map using the sampling functions: (1) All; (2) Spot(s); (3) Line; (4) Areas (see below)

#### 3.7.5.1 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 exemple of pixel fractions of 1%, 5% and 20% are reported in figure 3.42. Note that in this example, there is no significant difference between 20% and 100% because of the large number of pixels used.

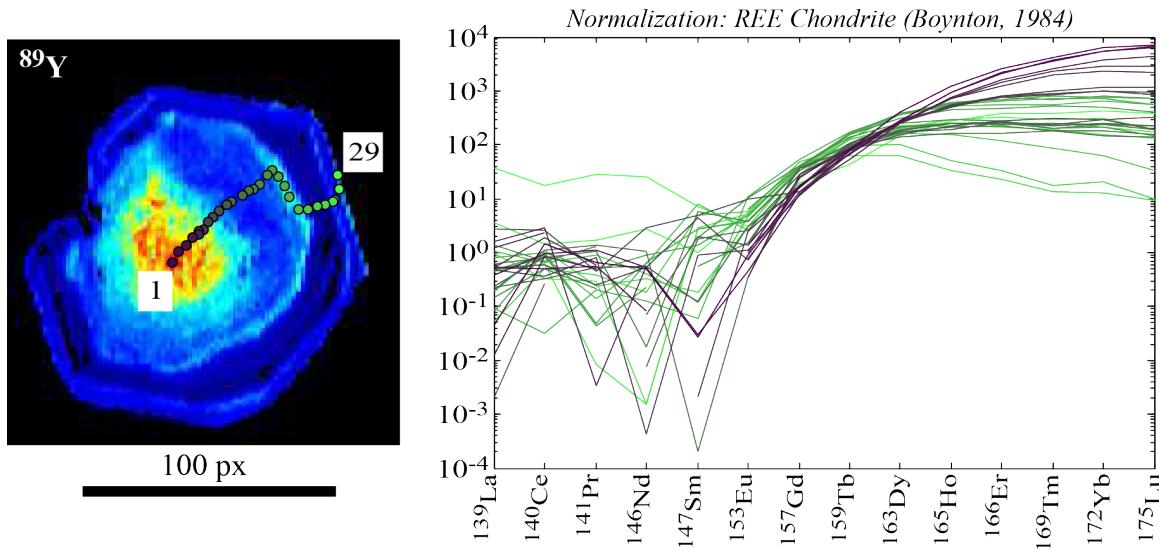


Figure 3.43 – Spider diagram of REE in garnet using the sampling method: spot analyses. Map:  $^{89}\text{Y}$  (red high concentration, blue low concentration, in ppm, see Fig. 3.44 for color scheme)

**[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 3.43. 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 3.44. 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 3.45. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram. In this case the standard deviation ( $1\sigma$ ) 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  $(\text{mean} - \text{std}) < 0$  or  $(\text{mean} - \text{std}) = 0$ .

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. 3.44) can be selected in order to add a new set of curves onto an existing spider diagram.

### 3.7.5.2 Figure and colors

The map can be managed using the following functions (see 5 in Fig. 3.34):

- *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*)

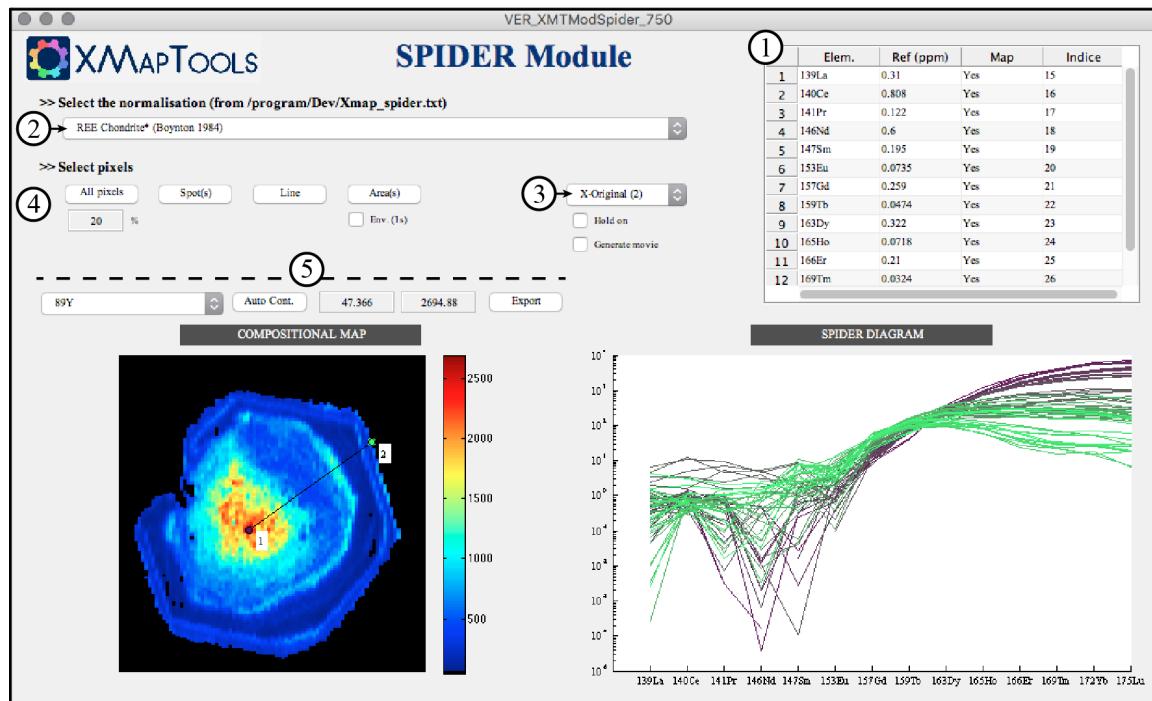


Figure 3.44 – Spider diagram module; sampling mode: line.

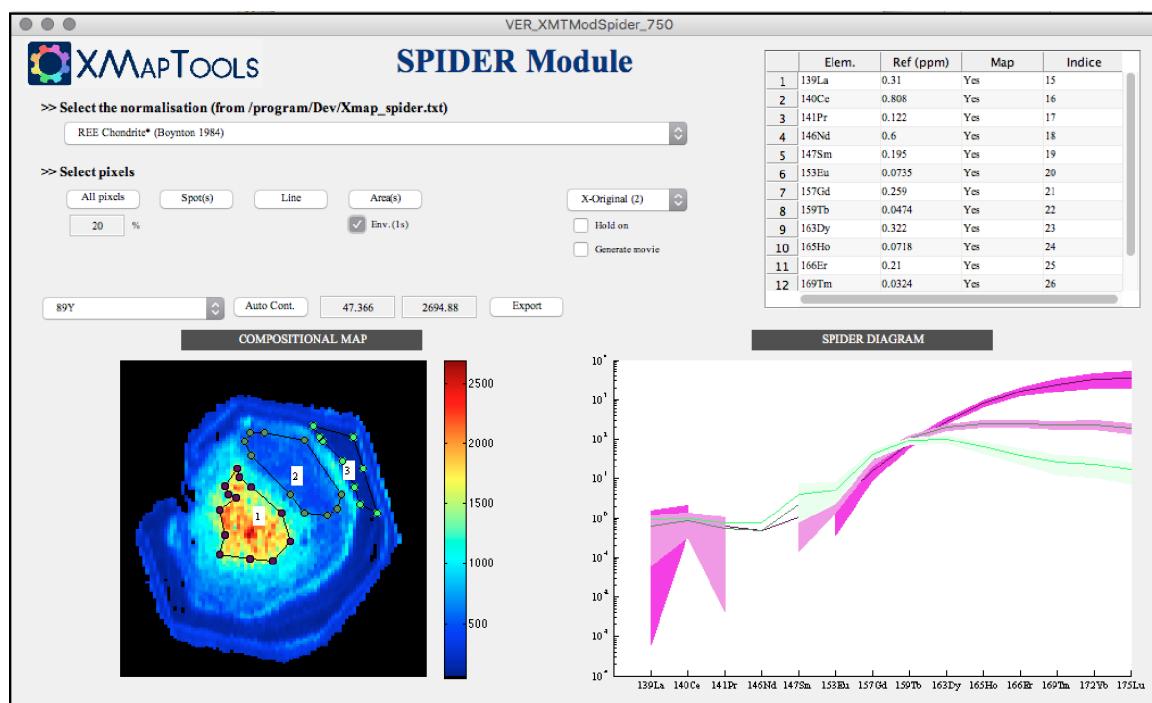


Figure 3.45 – Spider diagram module; sampling mode: area(s)

- *Export* this function allows the map and spider diagrams to be exported in new MATLAB<sup>©</sup> 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. 3.46a)
- *Bred* blue to red (Fig. 3.46b)
- *Greyl* green to yellow (Fig. 3.46c)
- *Pinor* pink to orange (Fig. 3.46d)
- *Shicy* braun to green to blue (Fig. 3.46e)
- *Jet (4)* blue to green to orange to red (Fig. 3.46f)

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

### 3.7.5.3 Create a movie with 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. 3.47a).
- Unactivate the option *hold on*
- Activate the option *Generate movie*: two new fields appear (see Fig. 3.47a)
- 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. 3.47b)
- 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.

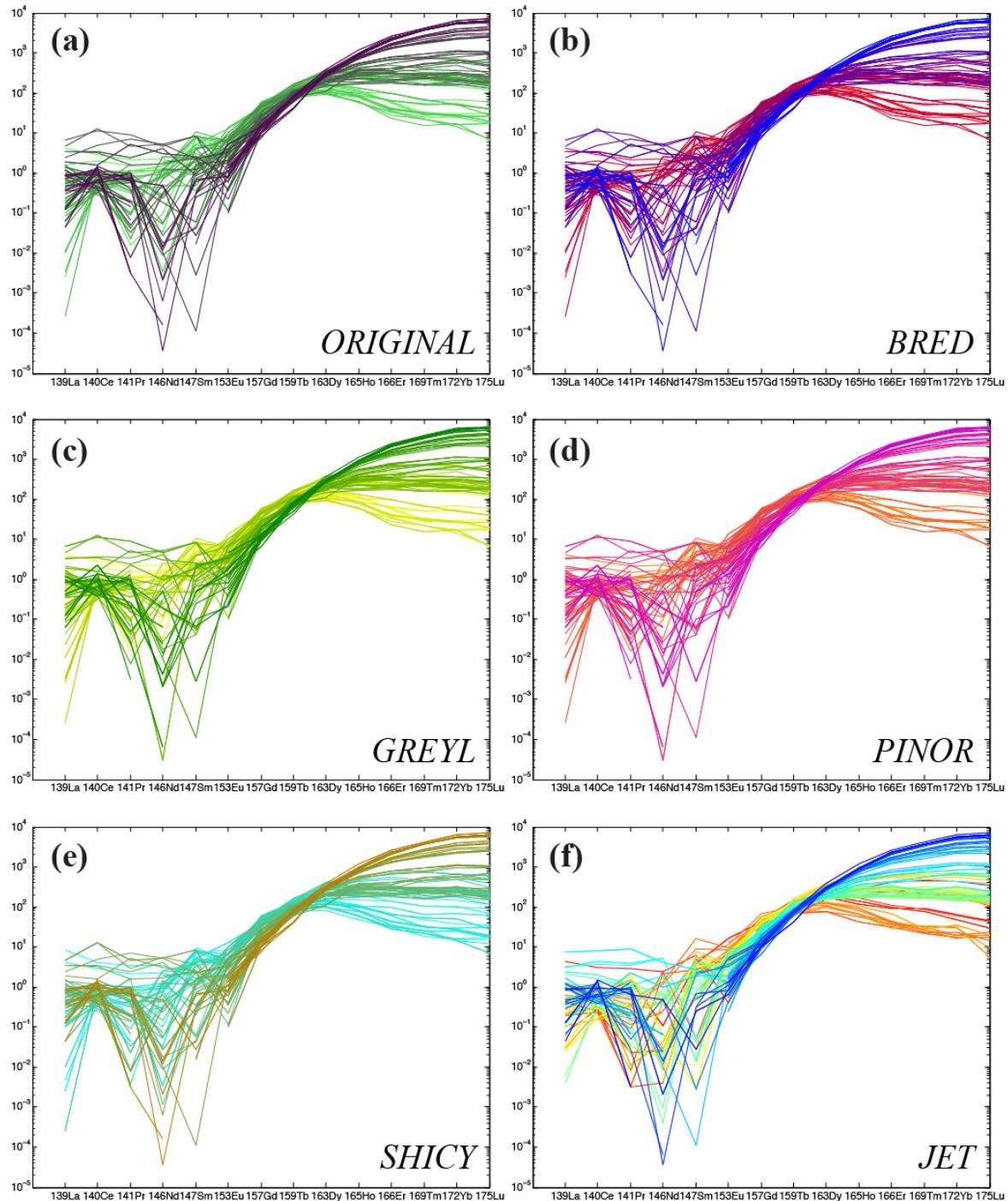


Figure 3.46 – Color schemes available in the SPIDER module

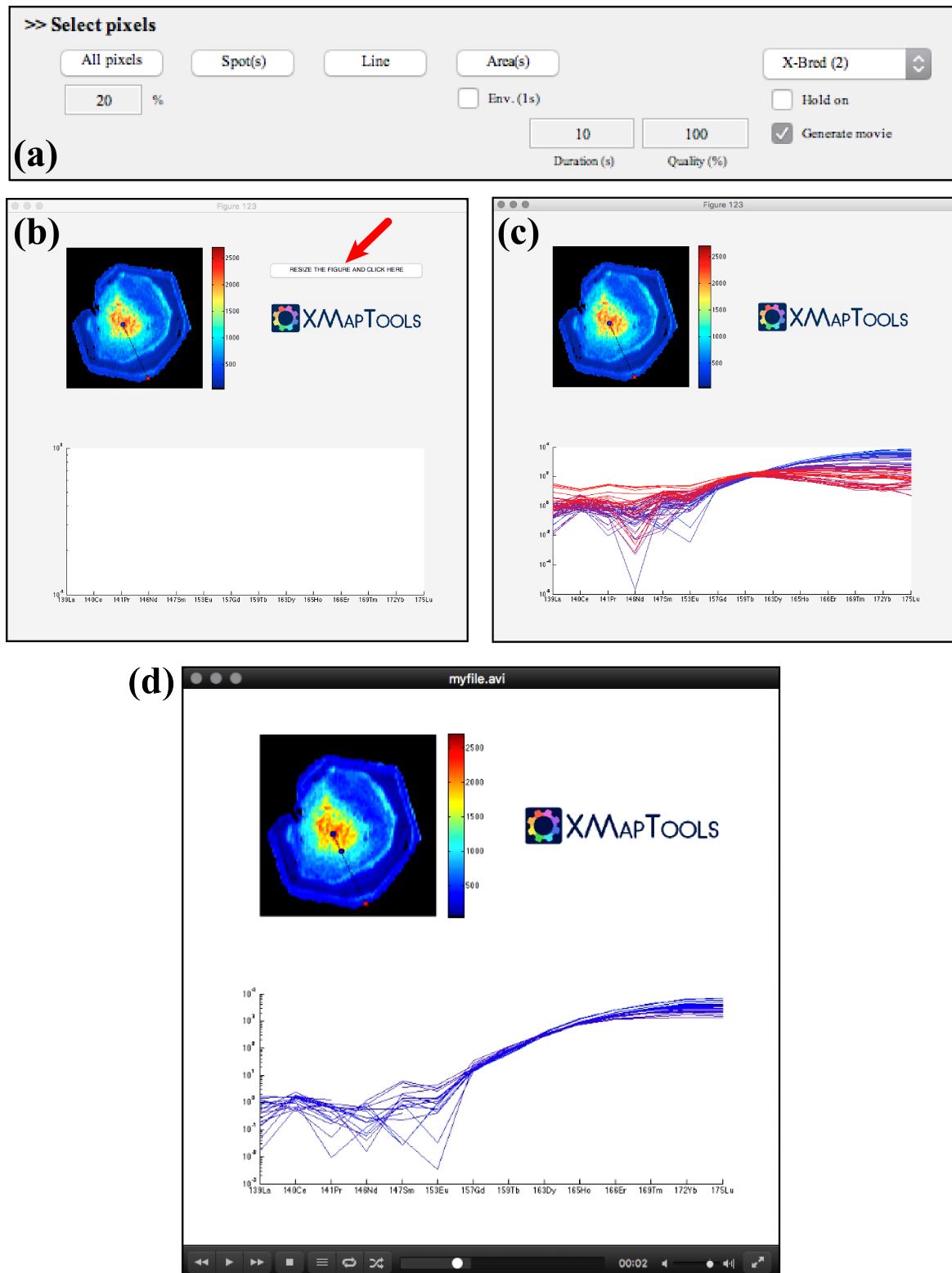


Figure 3.47 – Video mode of the SPIDER module. (a) The option Generate movie is active and it is possible to edit the duration of the video in second and the quality (between 10 and 100 %). (b) Figure used to generate the movie; this figure can be resized before to start recording the movie. (c) live 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 colorbar 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.

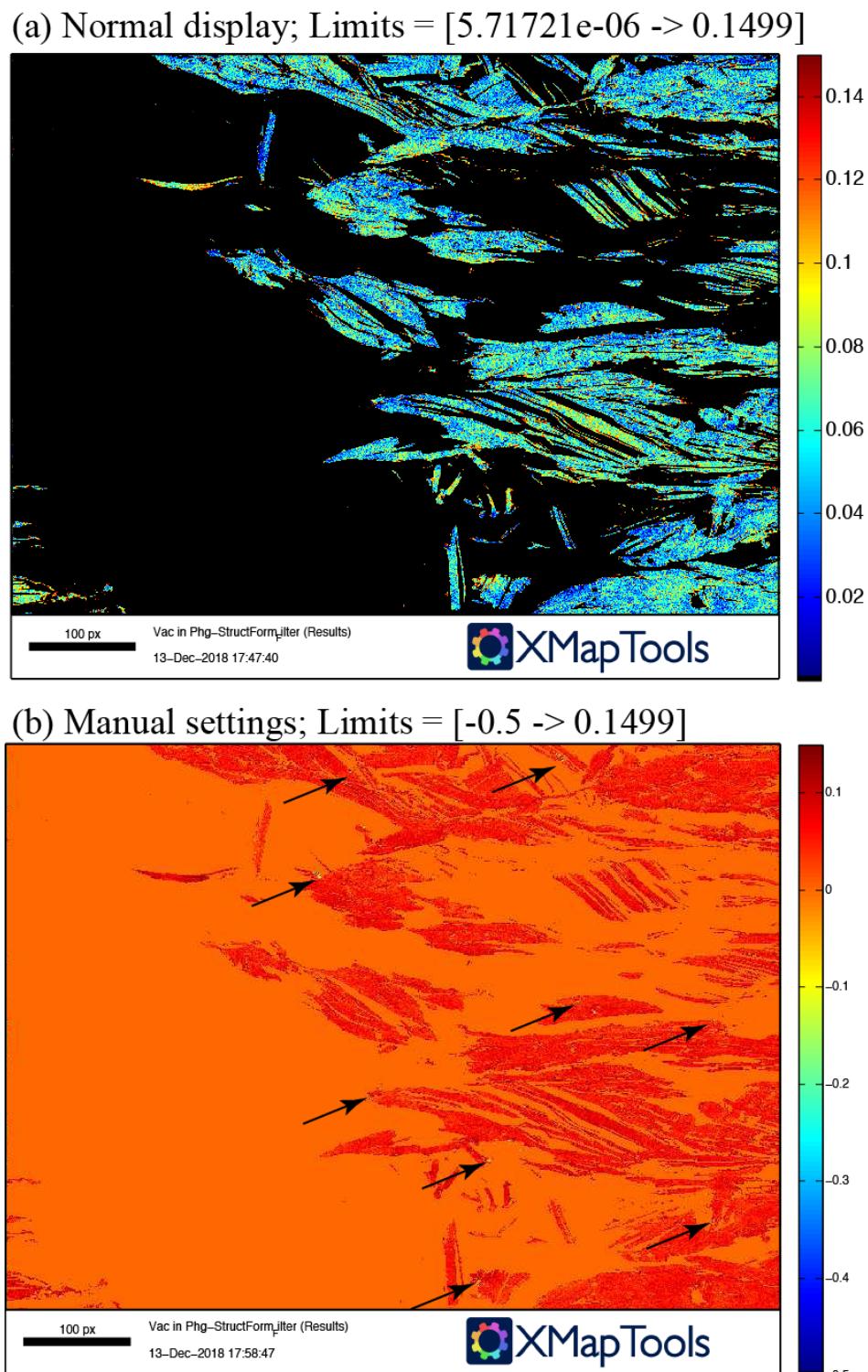


Figure 4.1 – Example of image with negative values that are (1) ignored by the automatic display; (2) visible if the lower limit of the displayed values is set manually

## 4.2 EXPORT MASK IMAGES WITH PERSONALIZED COLORS

It is possible to use the figure tools of MATLAB<sup>©</sup> 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<sup>©</sup> 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...*

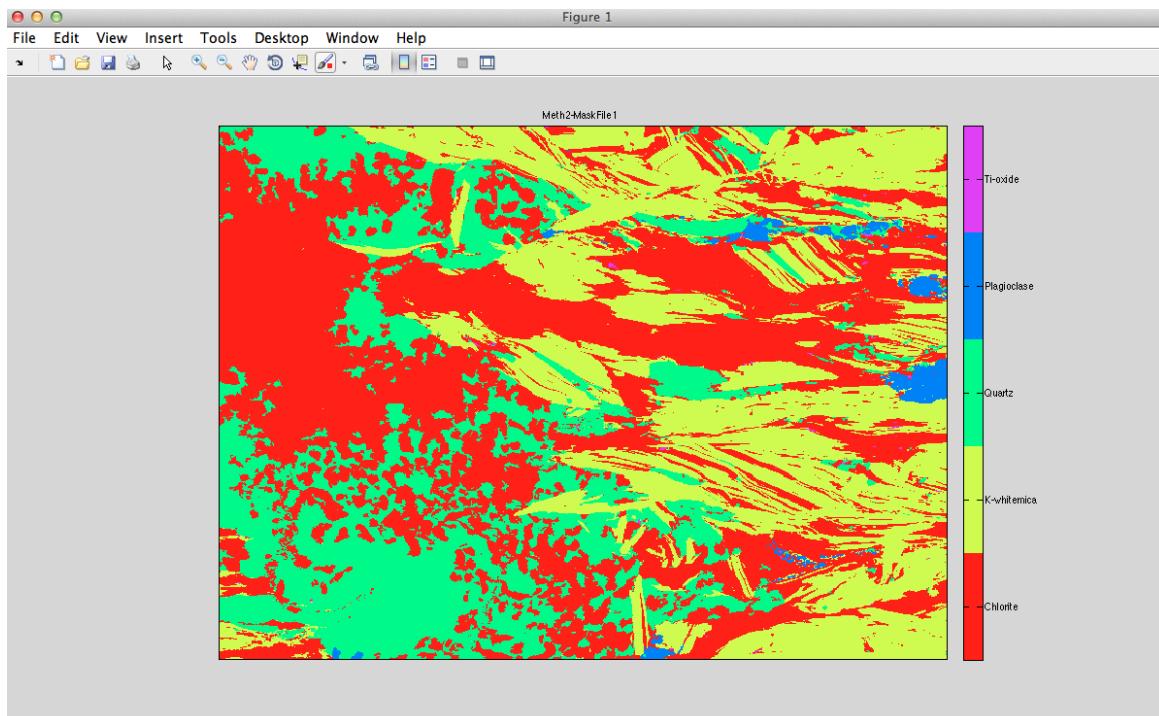


Figure 4.2 – Mask image exported using the function *export mask image* (see text)

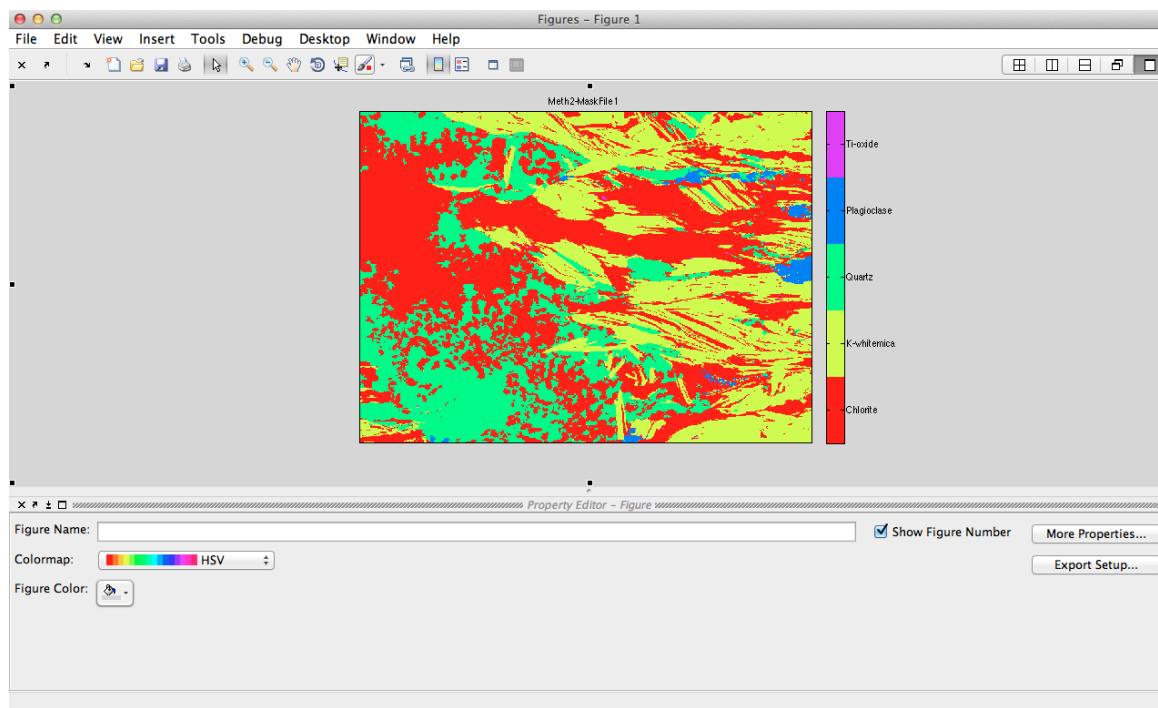


Figure 4.3 – Mask-image with the Figure editor

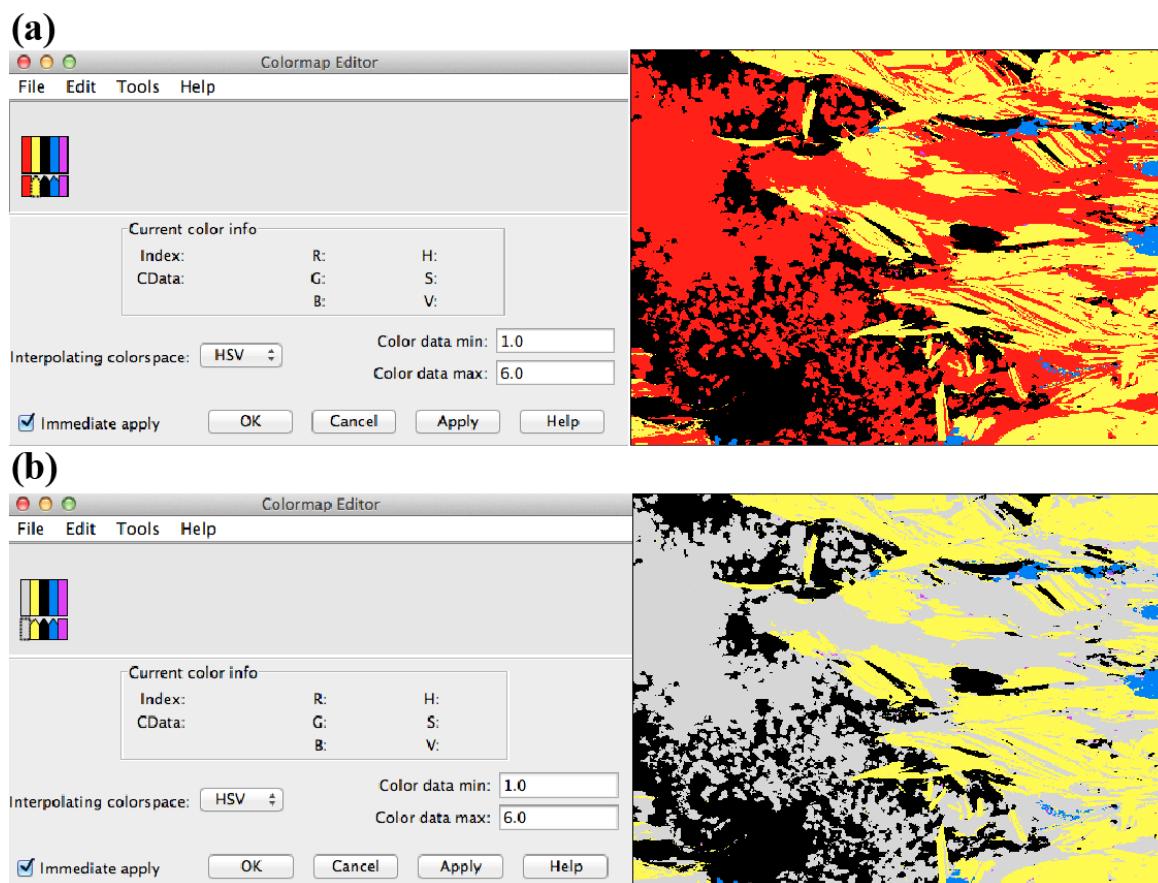


Figure 4.4 – Colormap Editor with the new colors

## 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.
- **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<sup>©</sup> 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: Na<sub>2</sub>O, MgO, Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, P<sub>2</sub>O<sub>5</sub>, SO<sub>2</sub>, Cl<sub>2</sub>O, K<sub>2</sub>O, CaO, TiO<sub>2</sub>, V<sub>2</sub>O<sub>5</sub>, Cr<sub>2</sub>O<sub>3</sub>, MnO, FeO, CoO, NiO, CuO, ZnO, ZrO<sub>2</sub>, AgO, CdO, SnO<sub>2</sub>, Ce<sub>2</sub>O<sub>3</sub>, As<sub>2</sub>O<sub>5</sub>, Sb<sub>2</sub>O<sub>3</sub>, Cs<sub>2</sub>O, La<sub>2</sub>O<sub>3</sub>, Nd<sub>2</sub>O<sub>3</sub>, PbO, SrO, ThO<sub>2</sub>, UO<sub>2</sub>, Y<sub>2</sub>O<sub>3</sub>, Sm<sub>2</sub>O<sub>3</sub>, Gd<sub>2</sub>O<sub>3</sub>, Dy<sub>2</sub>O<sub>3</sub>, Pr<sub>2</sub>O<sub>3</sub>. 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.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

Not yet available...

### 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>SiO<sub>2</sub> TiO<sub>2</sub> Al<sub>2</sub>O<sub>3</sub> FeO MnO MgO CaO Na<sub>2</sub>O K<sub>2</sub>O>

- **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 et al 1999*
- **Function name** is *NThermoCCVidal1999.m*
- **Output variables** are: T and lnKd
- **Input variables** are SiO<sub>2</sub>, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, FeO, MnO, MgO, CaO, Na<sub>2</sub>O, K<sub>2</sub>O
- **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: [SiO<sub>2</sub>, TiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, FeO, MnO, MgO, CaO, Na<sub>2</sub>O, K<sub>2</sub>O].

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<sup>©</sup> *Current Folder* tool. Use the following code into the *Command Window* to test the function:

Code 4.1 – *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 4.2 – *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<sup>©</sup> 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 4.3 – *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]

## 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 2.3.2.1.

## 5.3 INTERFACE ERRORS

The up to date list of identified bug is available at [https://www.xmaptools.com/?page\\_id=84](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.

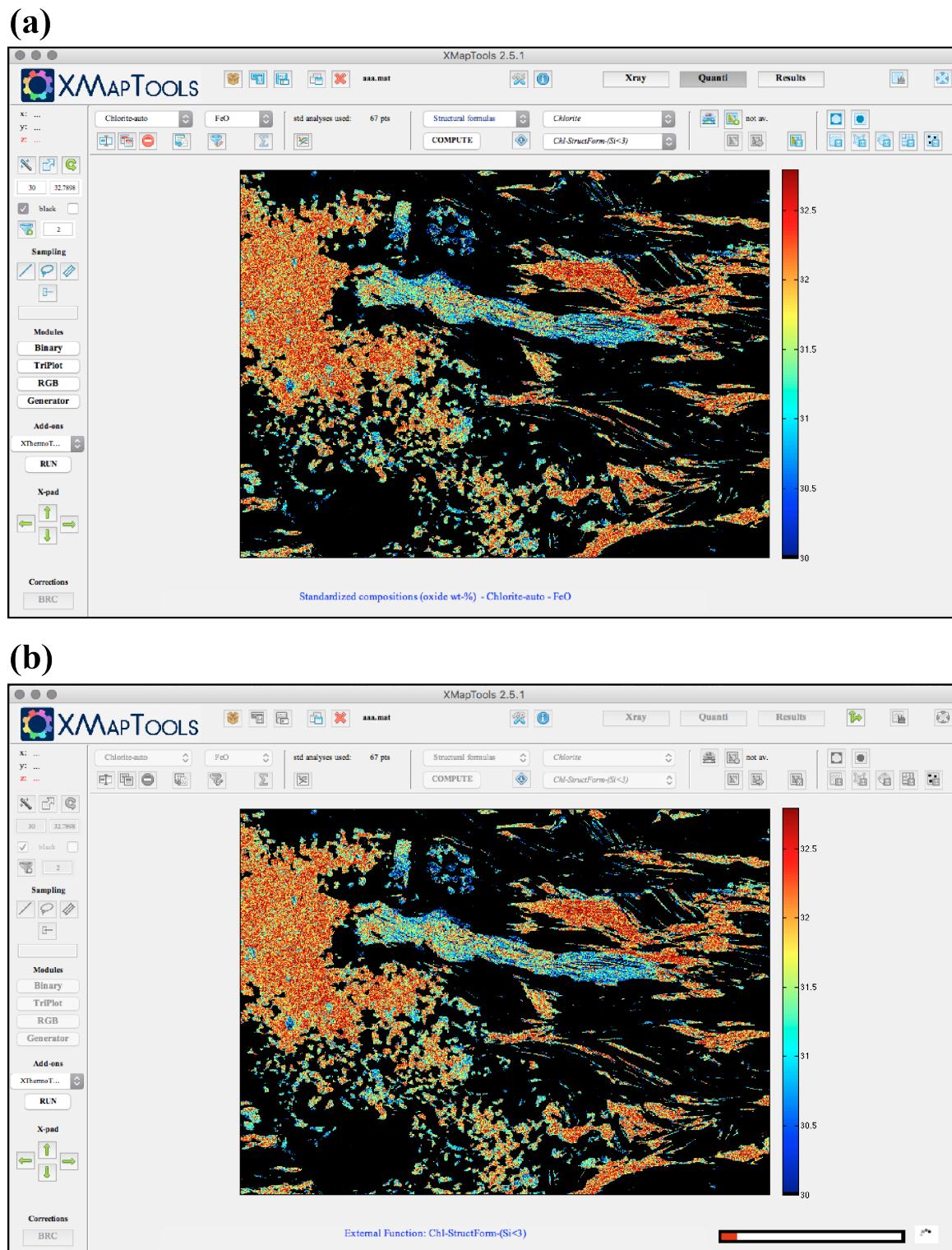


Figure 5.1 – XMAPTOOLS main interface: (a) normal (b) busy

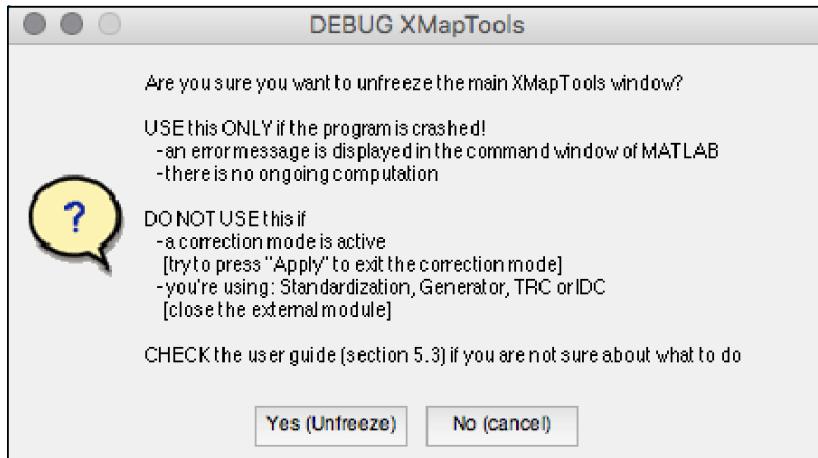


Figure 5.2 – Warning message appearing when the button unfreeze the interface has been pressed

- 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<sup>©</sup> *Command Window* and hit *Ctrl + C* to kill the job first; then, and only then press the button *unfreeze the interface* .

# TUTORIAL 1: ELECTRON MICROPROBE X-RAY MAPS PROCESSING

6

## 6.1 INTRODUCTION

A set of X-ray maps is provided as an example with XMAPTOOLS 2.1.1. In this chapter we described 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 to start using the 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 \(2012\)](#).

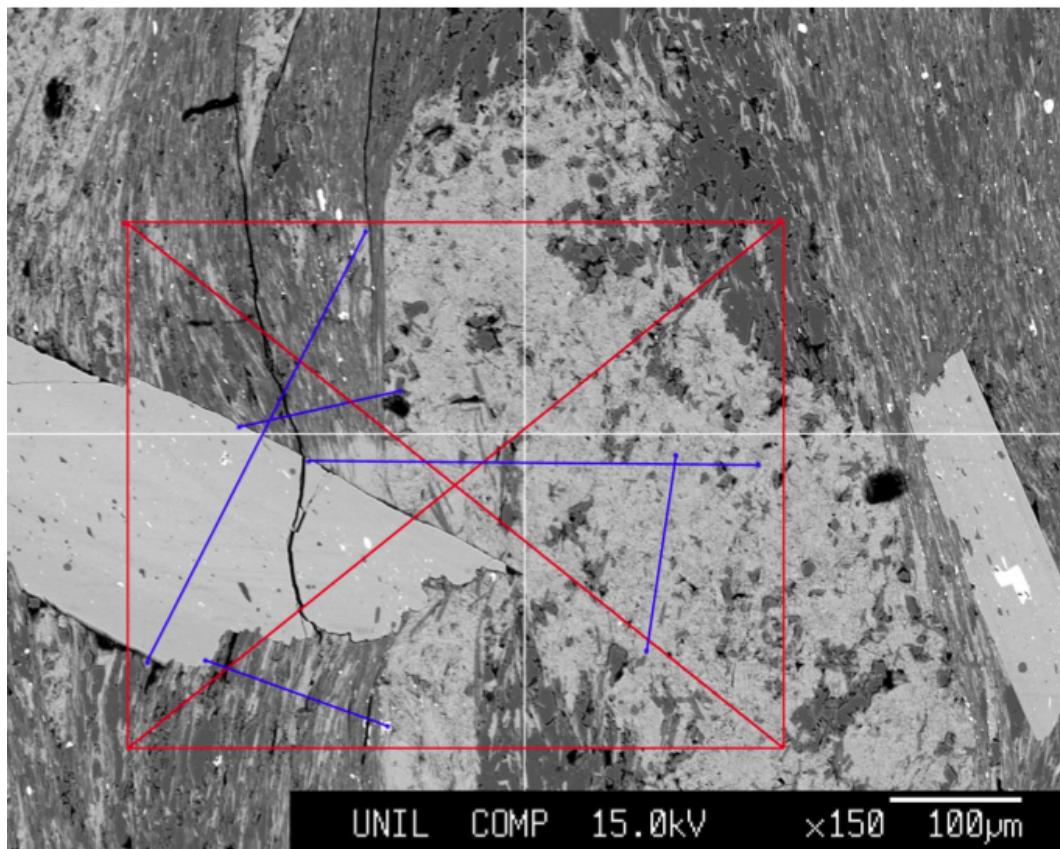


Figure 6.1 – BSE image of the studied area (red rectangle) with transect of spot analyses (blue lines) from [Bernier \(2011\)](#).

### 6.1.1 How to get started

XMAPTOOLS is a software that can only be executed from the MATLAB<sup>©</sup> environment. The following steps explain how to run XMAPTOOLS in your computer.

- (1) Run MATLAB<sup>©</sup>
- (2) Go to the data example repertory using the *Current Folder* window in the MATLAB<sup>©</sup> 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 6.2a.
- (3) Run XMAPTOOLS using the command: » **XMapTools** (case sensitive, example in Fig. 6.2a)
- (4) Information such as software release and attached files are reported in the MATLAB<sup>©</sup> command window (Fig. 6.3b) XMAPTOOLS main window appears after few seconds (Fig. 6.3)

As discussed in Introduction, XMAPTOOLS is divided into three workspaces: X-ray, Quanti and Results. The next sections described the corresponding operations of data processing.

## 6.2 X-RAY WORKSPACE

### 6.2.1 Add new data

- (1) Press the button *add*  to import X-ray files (arrow in Fig. 6.4).
- (2) A dialog box opens in which files can be selected (6.4a). 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) Select the automated method (see step 4 below). If you do not want to use the automated method, for each map the program asks for a corresponding element. Each map/element couple are automatically detected with the file name and should be validated. You must check if the automatically selected element fit with the selected map and press *OK*. Repeat this operation until all the files have been checked and imported.
- (4) The program scans the maps and finds the corresponding element. Then it opens the *Import Tool* (Fig. 6.4b).
- (5) 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. 6.4b). Then press *Apply Corrections* to correct for dead time and import the maps in the main window.

**Warning:** Do not apply any transformation such as rotation to EPMA maps, otherwise the map coordinates in Standard.txt will not work anymore. The rotation correction should only be used with standardized maps such as LA-ICP-MS maps.

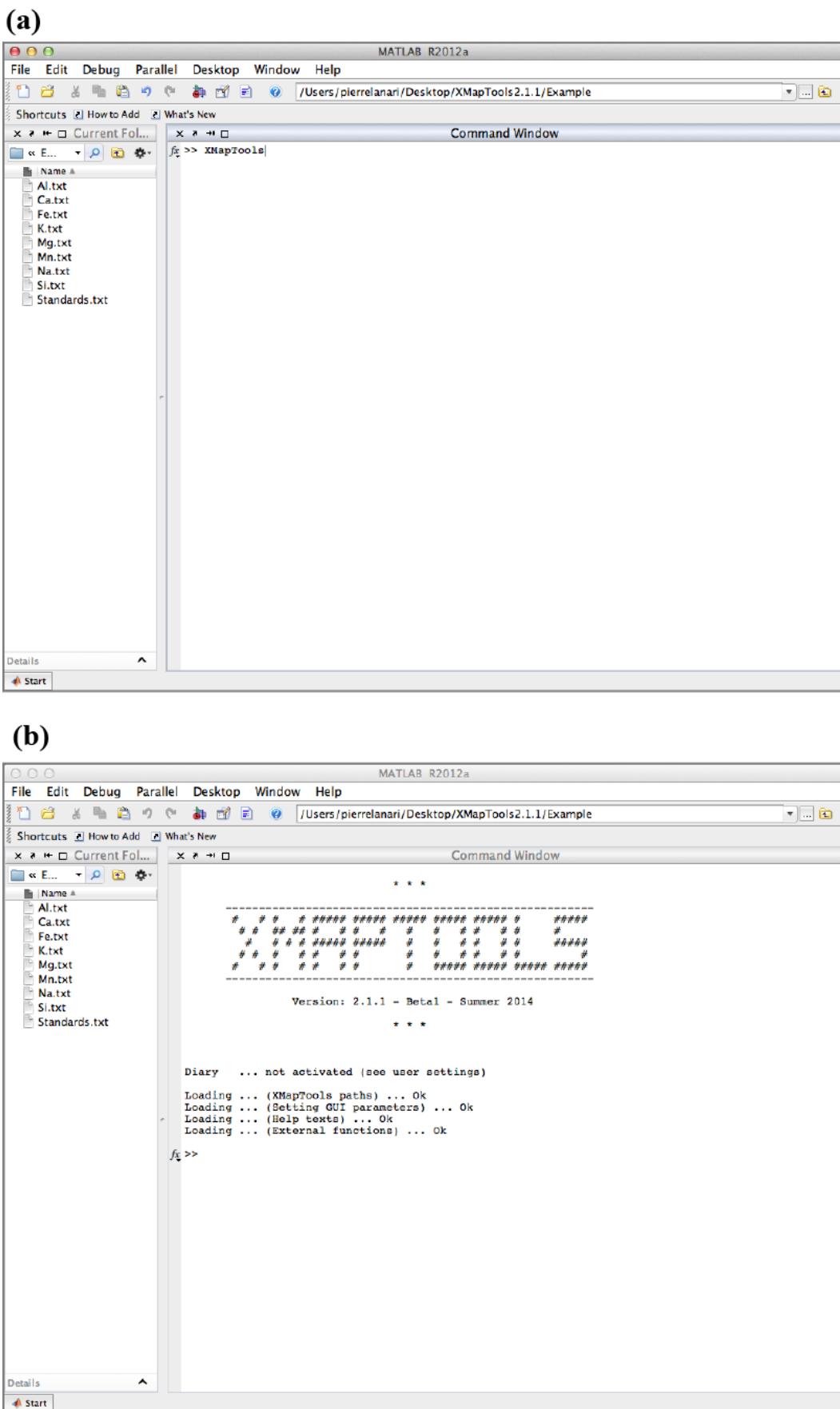
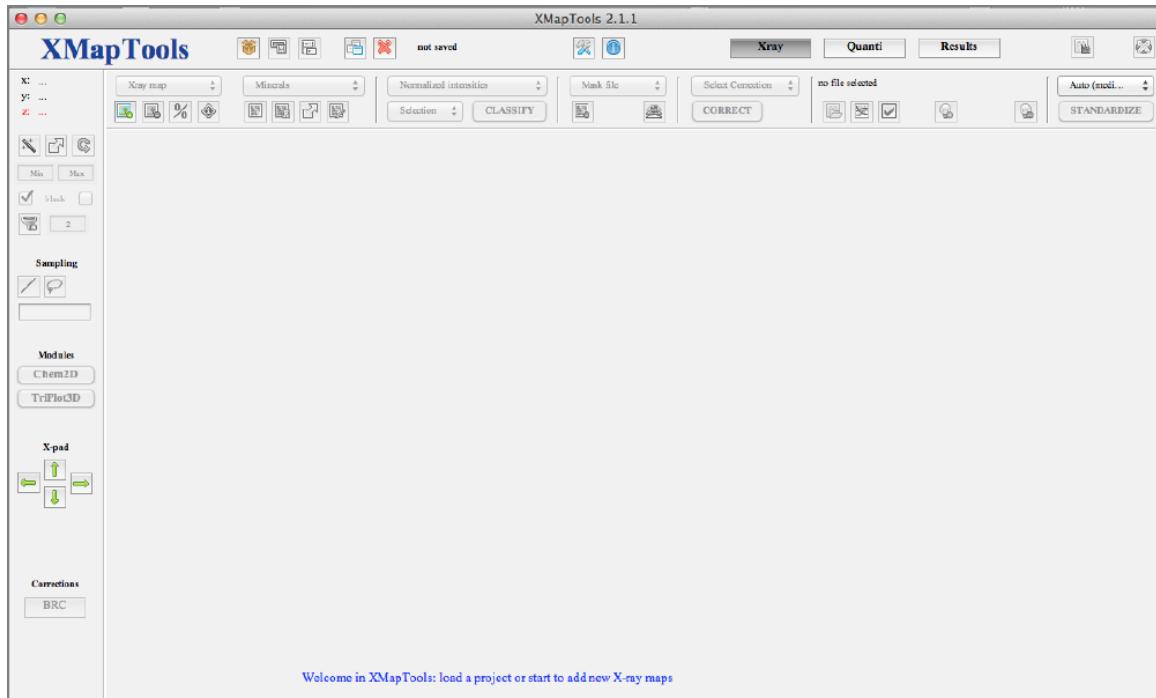


Figure 6.2 – Procedure to run XmapTools from the MATLAB<sup>©</sup> command window

Figure 6.3 – *XMapTools* main window

(6) When all the corrected files have been imported, XMAPTOOLS displays the first map in the main figure area (Fig. 6.5). The details about the maps and the corrections are displayed in the MATLAB<sup>©</sup> *Command Window* (see insert 6.1).

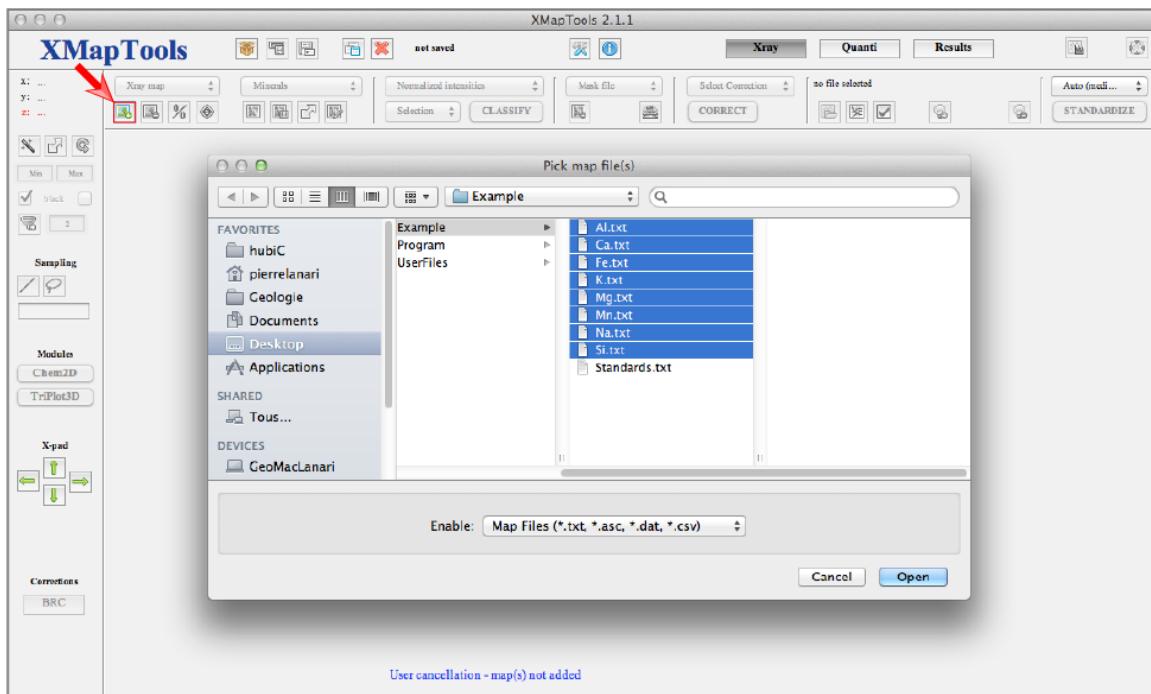
```
Import Tool ... (apply corrections) ...
- Map: Al      [type: 1]
  * Dead time correction applied: DwellT(200); DeadT(300)
- Map: Ca      [type: 1]
  * Dead time correction applied: DwellT(200); DeadT(300)
- Map: Fe      [type: 1]
  * Dead time correction applied: DwellT(200); DeadT(300)
- Map: K       [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 6.1 – *Import Tool*

### 6.2.2 Display X-ray images

X-ray images can be displayed using the X-ray menu (red arrow in Fig. 6.5). Use this menu and select a new map. The figure is automatically updated and the new map displayed.

(a)



(b)

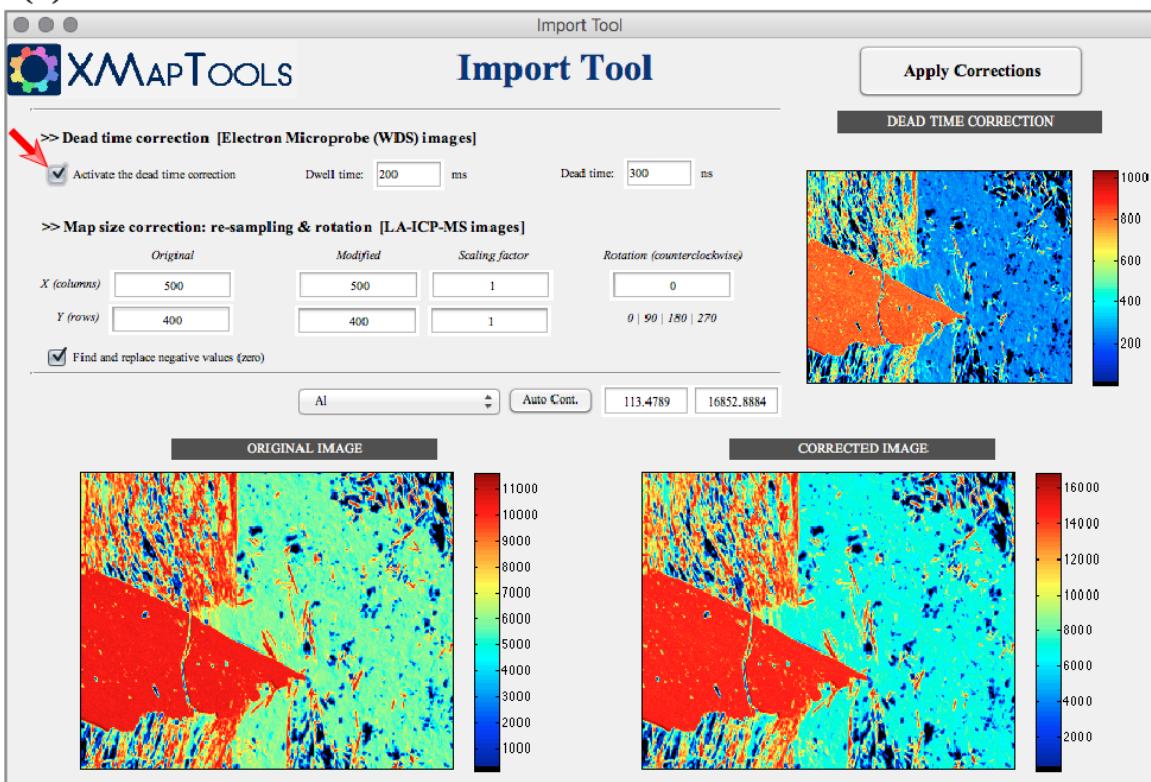


Figure 6.4 – Add new X-ray map(s) and Import Tool

**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 intensities for raw X-ray data). In order to change this values, figure options must be used (see below).

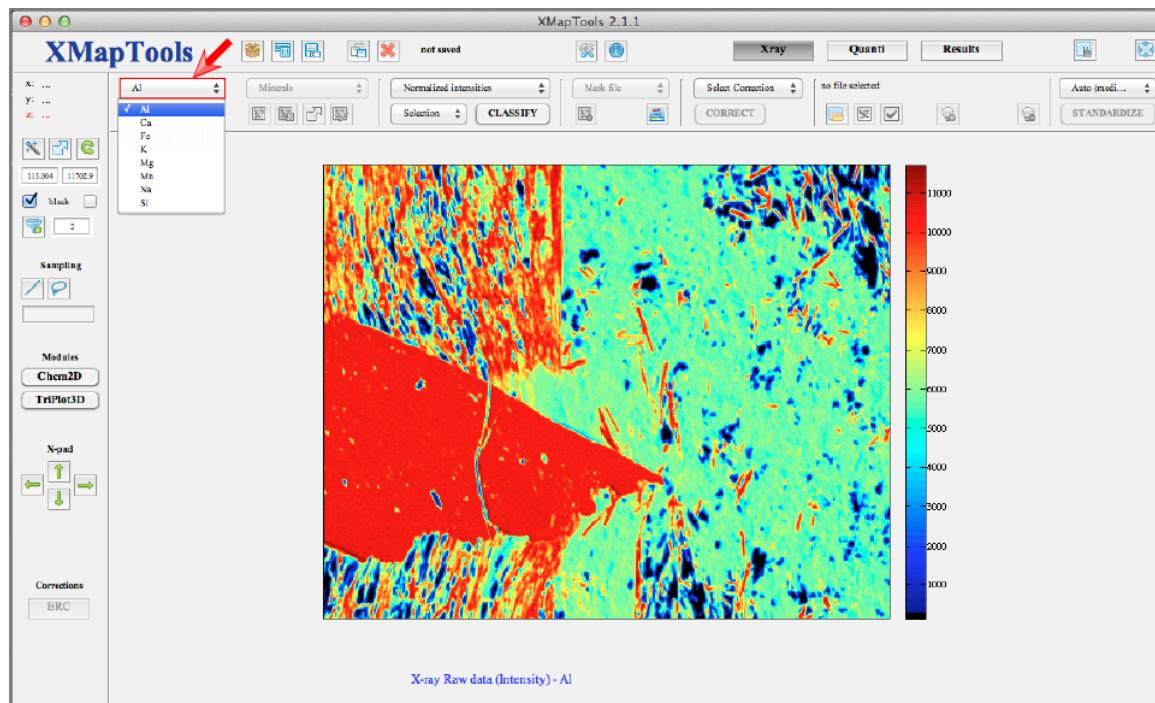


Figure 6.5 – X-ray menu is available to display X-ray images

### 6.2.3 Figure options

The window allowing to manage Figure options is available on the left part of the main XMAPTOOLS GUI (Fig. 6.6a).

#### 6.2.3.1 Live coordinates

- (1) Display the map *Al* using the X-ray menu (red arrow in Fig. 6.5, 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.

#### 6.2.3.2 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. 6.6b).

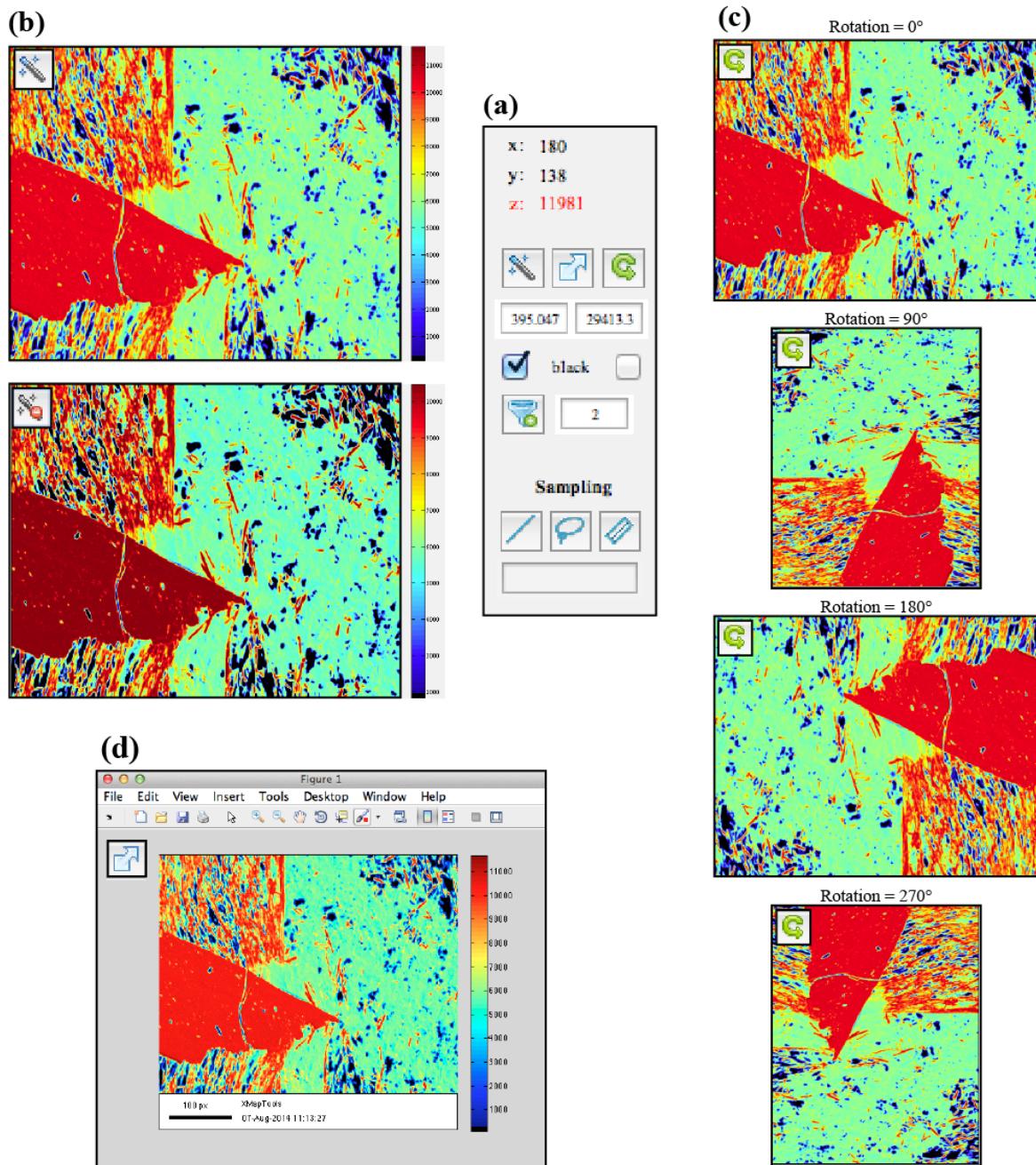


Figure 6.6 – Display options. (a) Display option menu; (b) auto-contrast mode activated (down), unactivated (up); (c) rotation mode for different rotation angles.

(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* .

**NB:** In this example, the displayed image does not change significantly (6.6b). 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. 6.5, 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

#### 6.2.3.3 Image rotation

(9) Image orientation can be changed using the button *rotate* . Press this button to rotate the image of  $90^\circ$  (counterclockwise). Four positions corresponding to  $0^\circ$ ,  $90^\circ$ ,  $180^\circ$  and  $270^\circ$  are available (Fig. 6.6c).

**NB:** The image coordinates displayed in the live coordinate screen are coordinates in the original system that correspond to  $0^\circ$  rotation, i.e. the coordinates of an object are exactly the same in all the rotation modes.

#### 6.2.3.4 Export and save image

(10) The Image displayed in the figure area can be exported by using the button *export* . A new window opens with the same figure (Fig. 6.6d). 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<sup>©</sup>

#### 6.2.3.5 Black layers in color bar

(1) Display the map *Ca* using the X-ray menu (red arrow in Fig. 6.5, second map)

(2) Manually adjust the color bar limits to: lower = 5000 and upper = 7000 (Fig. 6.7)

(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. 6.7) is automatically activated.

(4) Enable the upper black color by selecting the second checkbox (right in Fig. 6.7). 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. 6.7). All the pixels with intensities higher than 7000 are displayed in the last red color of the color bar (normal mode).

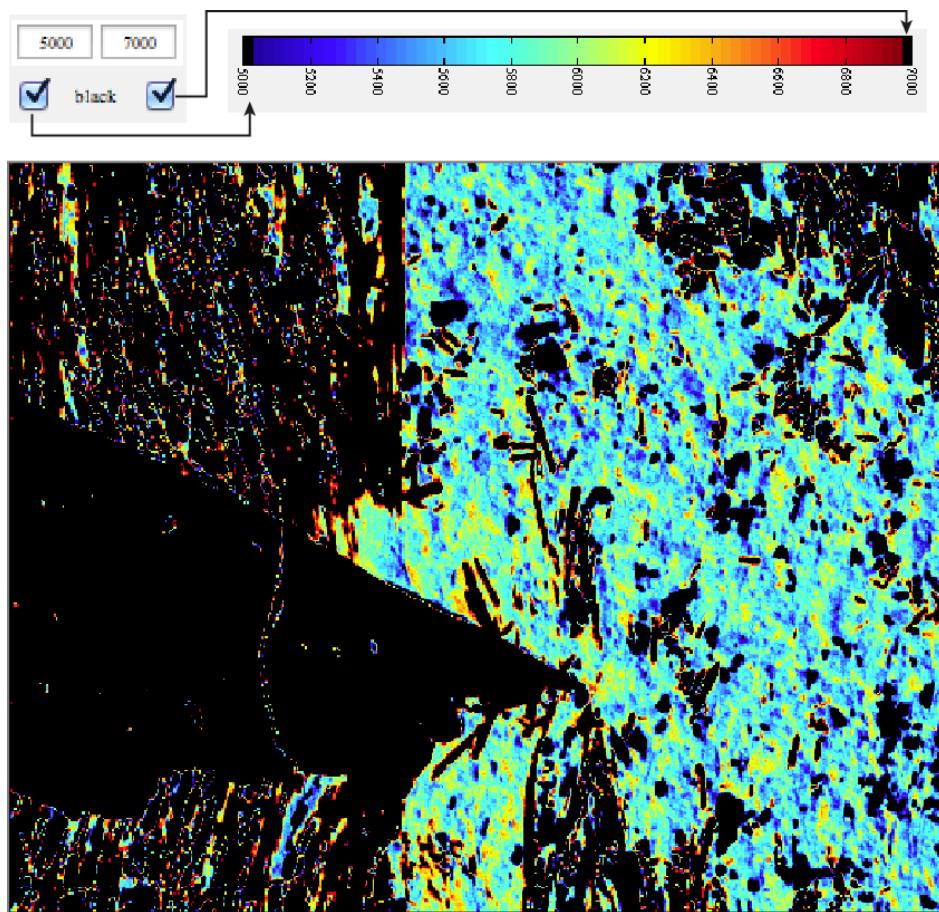


Figure 6.7 – *Display options*. (a) *Display option menu*; (b) *auto-contrast mode enabled (down), disabled (up)*; (c) *rotation mode for different rotation angles*.

#### 6.2.3.6 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. 6.8a).
- (3) Press the button *median filter* A rectangular median filter is applied to the displayed map (Fig. 6.8b).
- (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. 6.8c).
- (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.

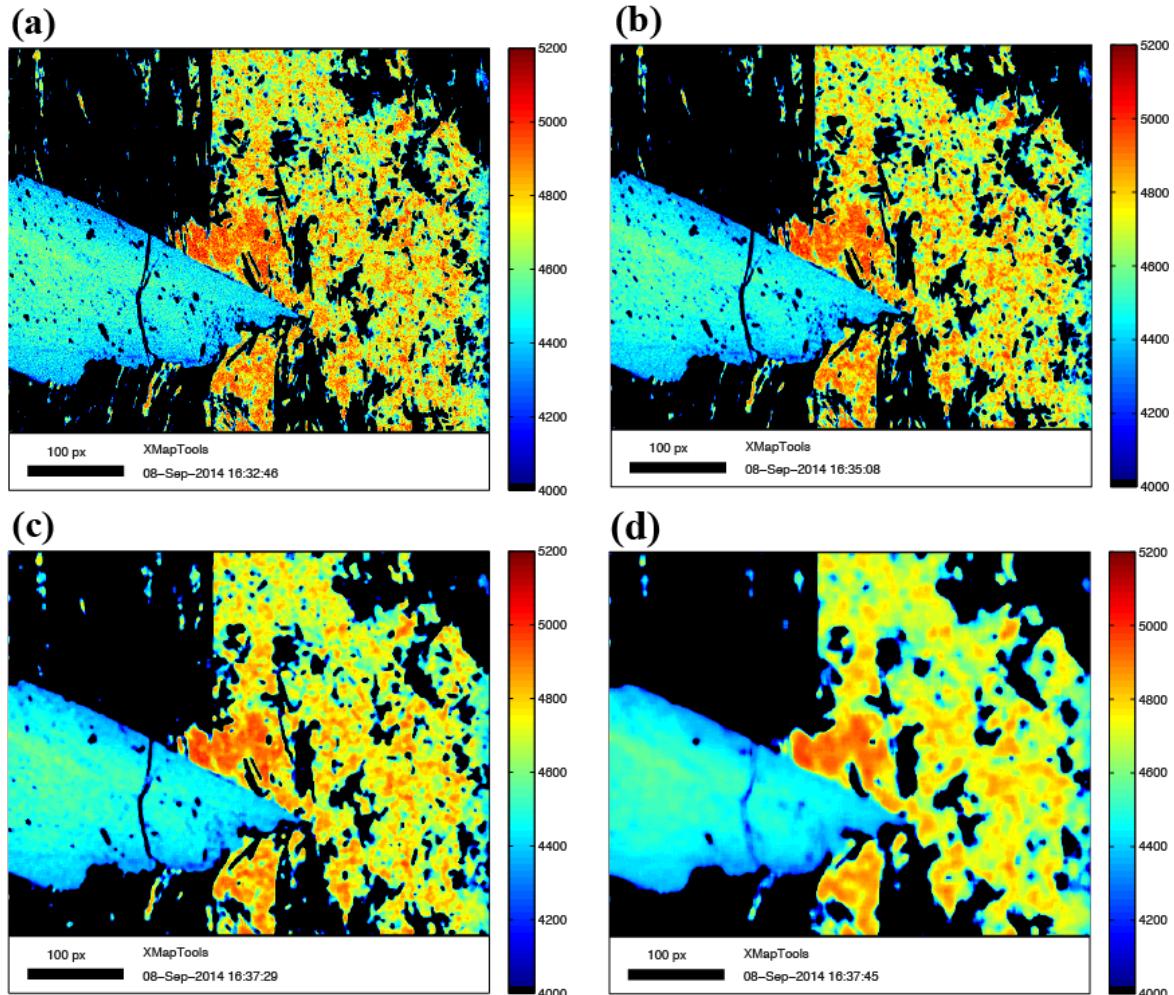


Figure 6.8 – Median Filter. (a) not used; (b) size = 2; (c) size = 5; (d) size = 10;

### 6.2.3.7 Sampling

(1) Display the map  $Mg$  using the X-ray menu (fifth map) and apply the auto contrast using the button *auto-contrast*

(2) Press the button *sampling* (line) , select the mode *single map* and define two points of a transect going across the porphyroblast (see points 1 and 2 in Fig. 6.9a). The program open a new figure window with the diagram *pixel position* against *chemical composition*. The program asks you if you want to save the corresponding map with the transect line into a FIG file that can be opened with MATLAB<sup>®</sup> and converted to PDF. In this example the diagram is pixels (from 1 to 168) 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* .

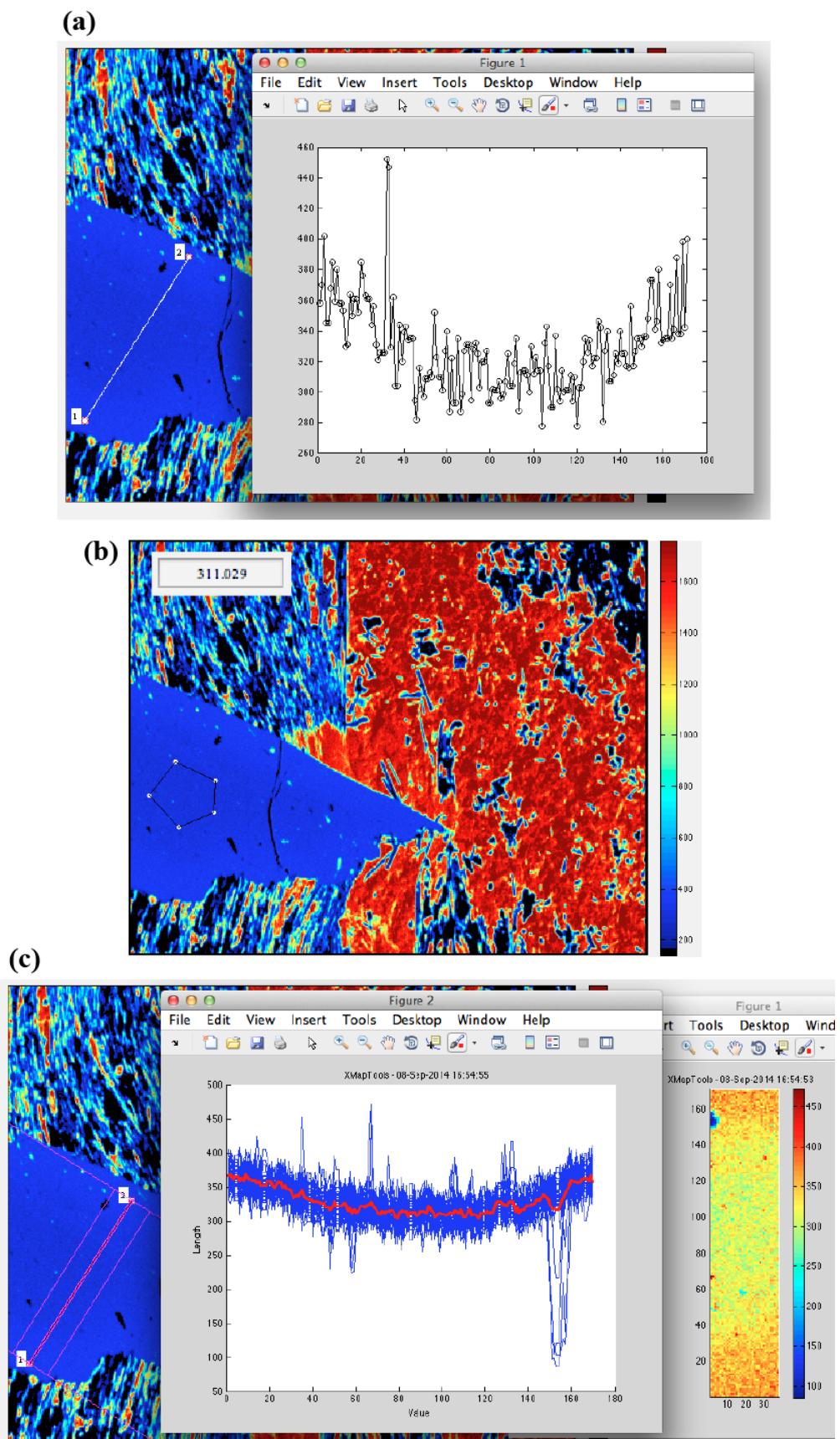


Figure 6.9 – Sampling functions. (a) mode: line; (b) mode: area (c) mode: integrated lines.

(4) Press the button *sampling* (area)  and select an area in the same porphyroblast (Fig. 6.9b). The program display the mean composition of this area in the box within the figure option window. In this example the mean intensity of Fe is  $311 \pm 18$  counts ( $1\sigma$ ).

(5) Press the button *sampling* (integrated lines)  and select two points across the porphyroblast and an 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. 6.9c). The program open a new figure with the map of the integrated area (labeled *Fig. 1* in 6.9c). Then a new figure window is opened with the diagram *pixel position* 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 proposes to save the results of the profile in ASCII files with a dialogue windows. The figures displayed are not saved and must be exported by user using the button *export*  and the option *save as* available in the menu (see §6.2.3.4).

## 6.2.4 X-ray images options

### 6.2.4.1 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. 6.10a) to generate a precision image (in  $2\sigma$ ) that opens in a new window (Fig. 6.10b). 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 1.4.1.2.

(3) Set the precision image as the current active figure by selecting the window.

(4) In the MATLAB<sup>©</sup> command window, set the color axis range of the figure to 1-11% using the following command. The result is displayed in figure 6.10c.

```
caxis ([1 11])
```

Code 6.2 – *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 6.10d. 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 ...*

### 6.2.4.2 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* .

(2) Display the *X-ray info window* using button *X-ray info* 

(3) The resulting info window is displayed in Fig. 6.11 and the text reported in the box 6.3

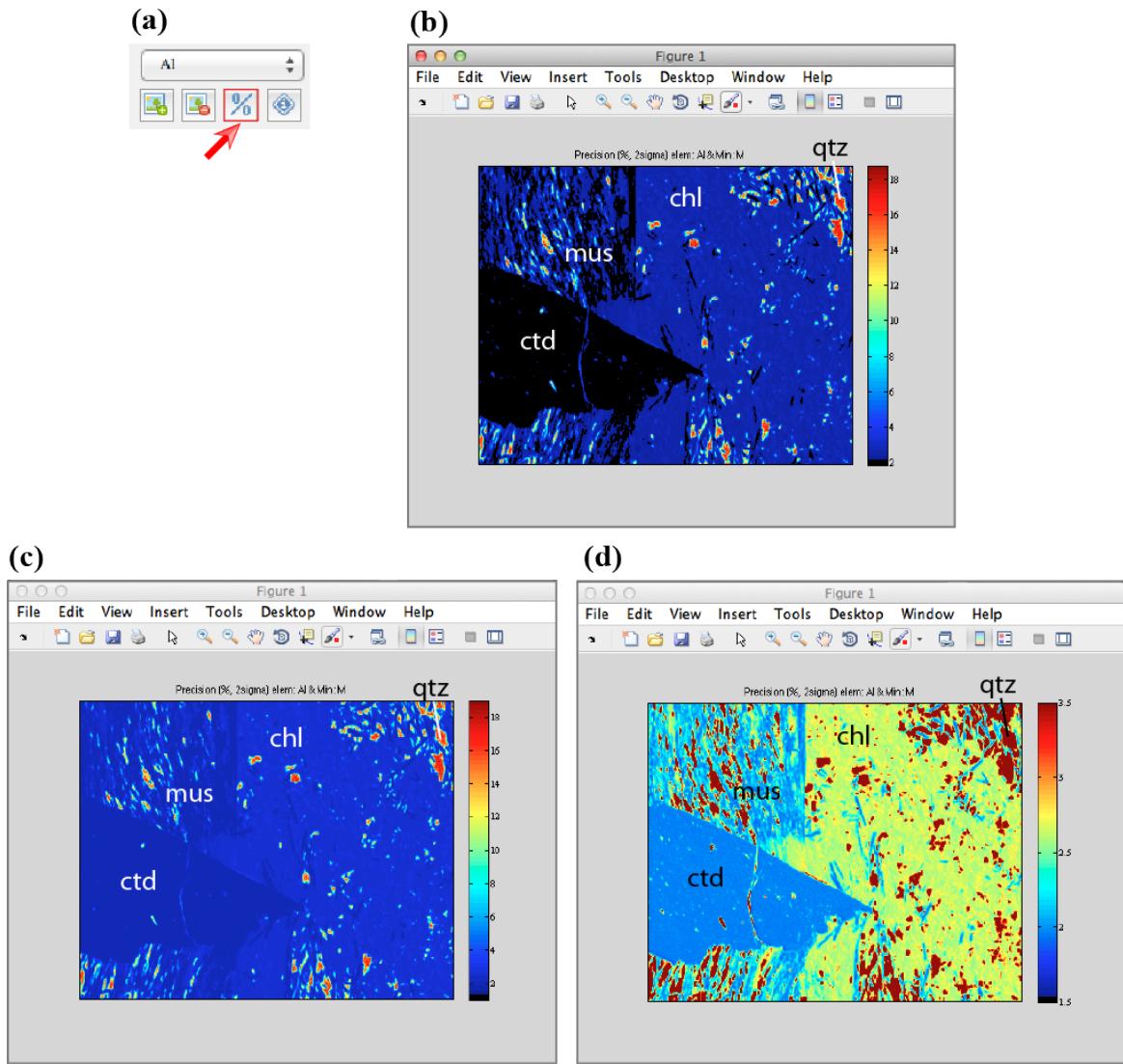


Figure 6.10 – Precision image in % calculated from the X-ray map of Al. (b), (c) and (d) are the same data (precision image for Al in %) plotted with different color bar axis values (see text)

```

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 6.3 – Text printed in the info window

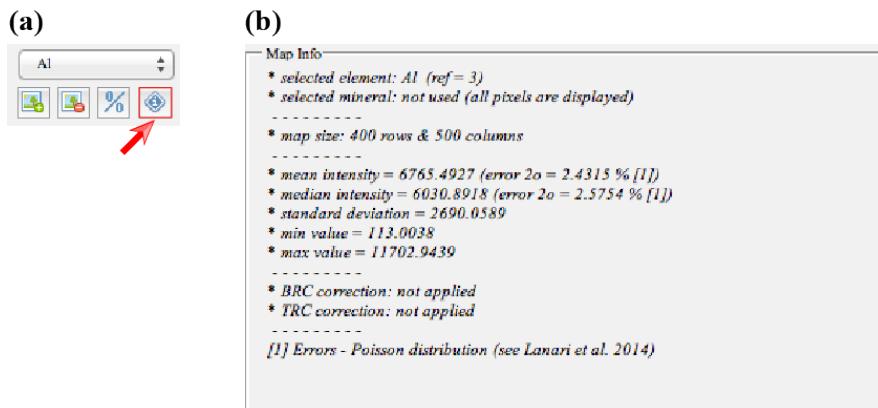


Figure 6.11 – Info button (a) and window (b) available into the workspace X-ray

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.

### 6.2.5 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 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 ([6.2.5.1](#)).

A manual classification is available in XMAPTOOLS 2 and will be discussed later (see section [6.2.5.3](#)).

#### 6.2.5.1 Automatic classification (normalized and classical modes)

(1) Display the map *Al* using the X-ray menu (first map) and in the classification window, select *Normalized intensities* and the mode *selection* (see Fig. [6.12](#)). 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. [6.12](#))

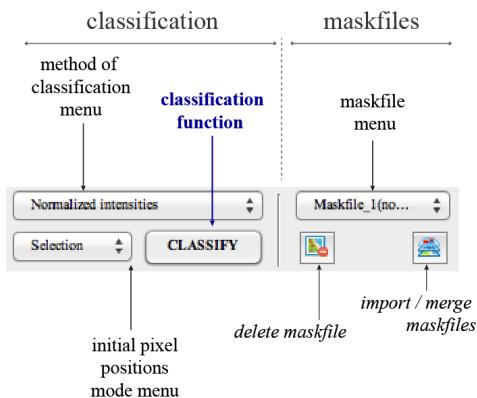


Figure 6.12 – Classification and mask file menus and buttons

- (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. 6.13a) 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-clic 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. 6.13b). 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 correspond to a distinct phase that have been classified, indicating that a new phase must be defined for quartz. Information regarding the classification are printed out in the Command Window (Code 6.4).

```
Mask creating ... (Maskfile_1(norm)) ...
Mask creating ... (Selected maps: Al Ca Fe K Mg Mn Na Si)
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 6.4 – Text printed in the command window during the classification

- (7) The name of the phases may be edited using the function *rename phases*. Press the button (Fig. 6.12) 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).

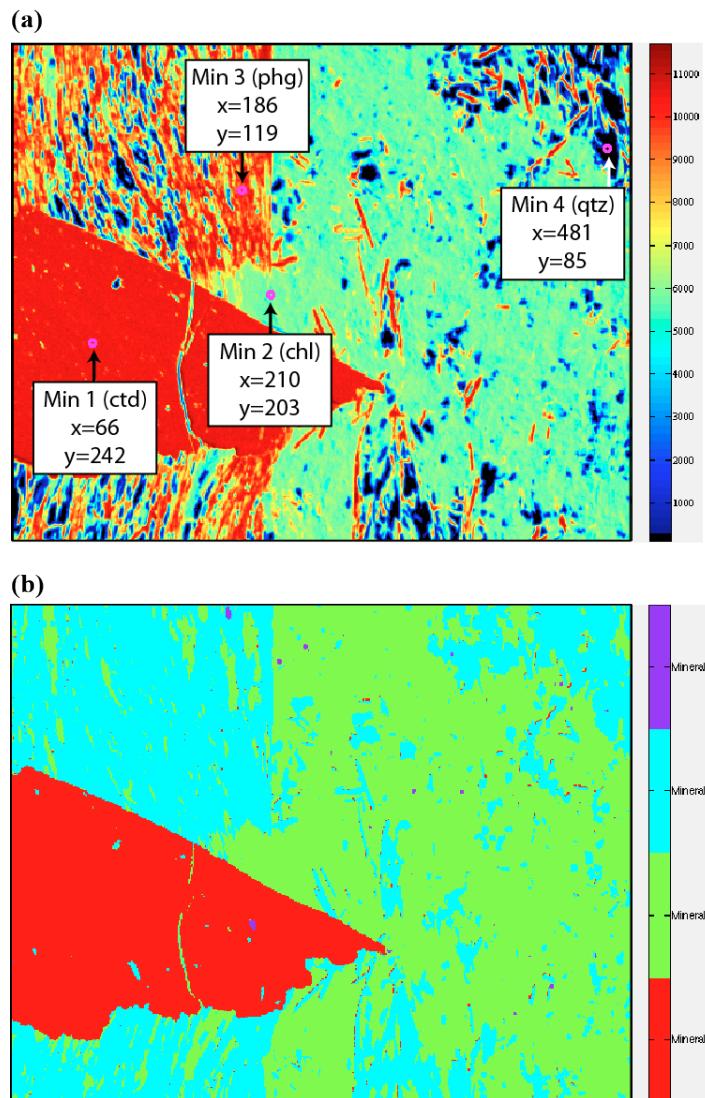


Figure 6.13 – Classification: (a) Coordinates and position of the input pixels selected by the user in order to define the compositions of the minerals (map: Al in number of counts). (b) Mask image generated using the mode Normalized intensities and the mode Selection (see [6])

(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 6.14. 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. 6.12) to delete it.

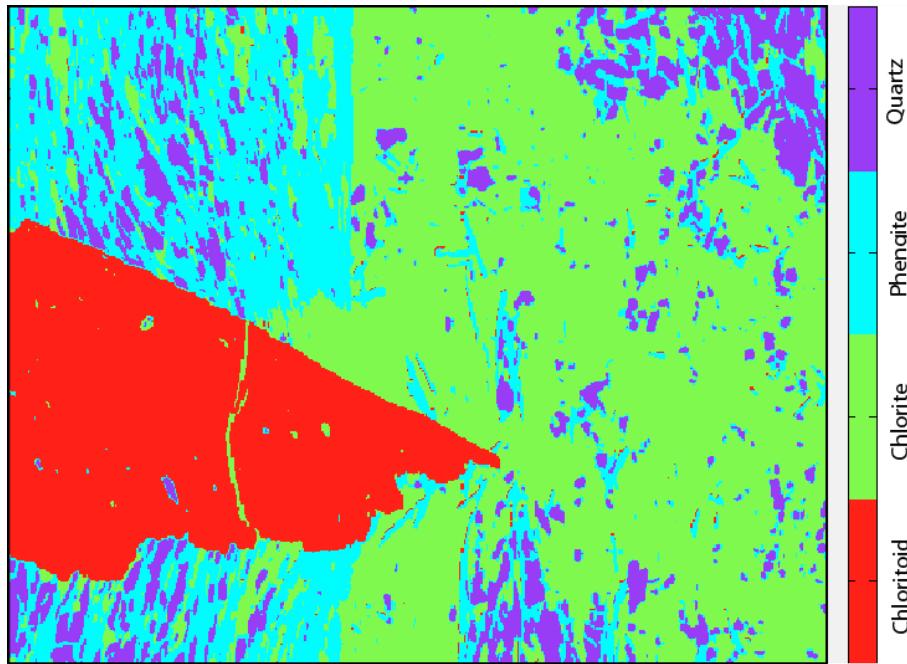


Figure 6.14 – *Classification: Mask image generated using the mode Classical computation and the mode File (see [8])*

#### 6.2.5.2 Display X-ray images of a specific phase

Once the classification is achieved a mask file is active. The menu *phase (masks)* (Fig. 6.15b) 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 6.15a. All the pixels are displayed.
- (2) Select the phase *chloritoid* in the mask menu. Adjust the contrast by pressing the button *auto-contrast* . The result is reported in figure 6.15b. In this case, only the pixels that belong to the mask *chloritoid* are displayed.

#### 6.2.5.3 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 6.2.5.1). 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*.

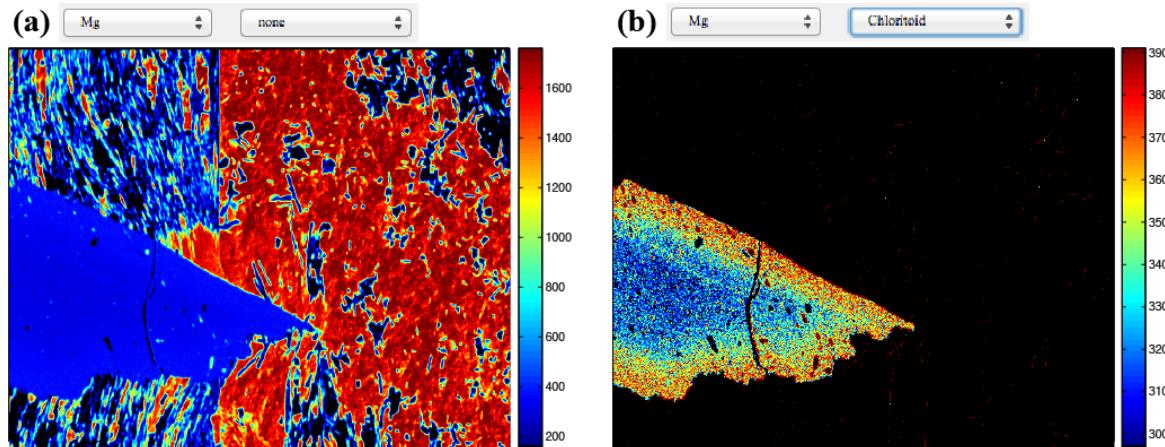


Figure 6.15 – Display X-ray image Mg (a) with none selected in the mask menu and (b) with chloritoid selected in the mask menu. The auto-contrast function has been used before to generate the images.

(3) Plot  $Fe$  vs  $Mg$  using the menus  $X$  and  $Y$  (see Fig. 6.16).

In the diagram displayed in figure 6.16, 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. 6.17). 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. 6.17).

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.

(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. 6.18a).

(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. 6.18b).

(7) In a diagram  $K$  vs  $Al$  select the points belonging to the group phengite and generate a mask file named *Phengite.txt* (Fig. 6.18c).

(8) In a diagram  $Si$  vs  $Al$  select the points belonging to the group quartz and generate a mask file named *Quartz.txt* (Fig. 6.18d).

Individual or merged Mask files can be imported in XMAPTOOLS.

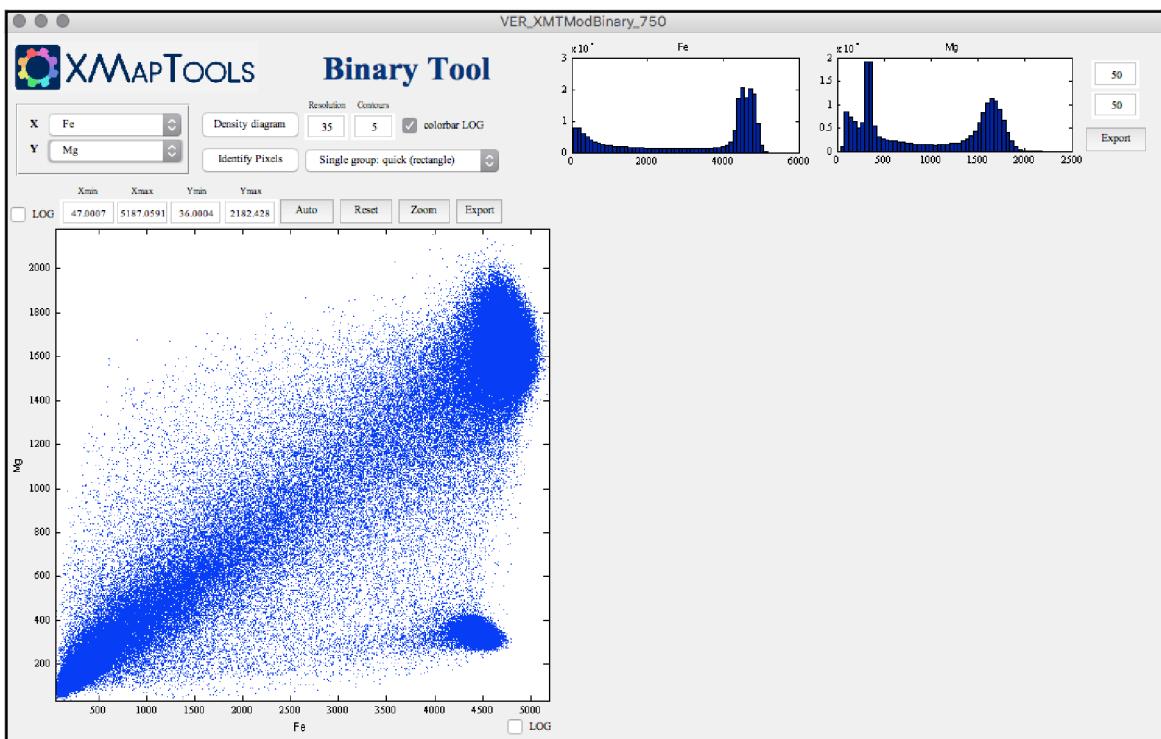


Figure 6.16 – Binary module (diagram Fe vs Mg)

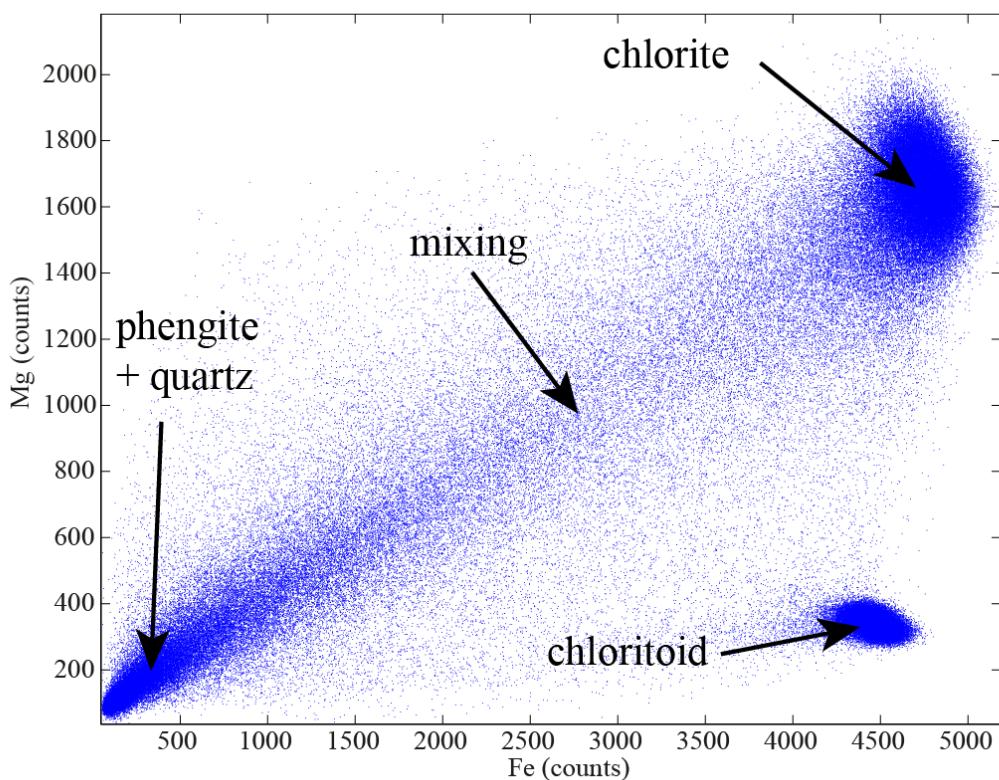


Figure 6.17 – Chemical diagram Fe vs Mg exported from the Binary diagram

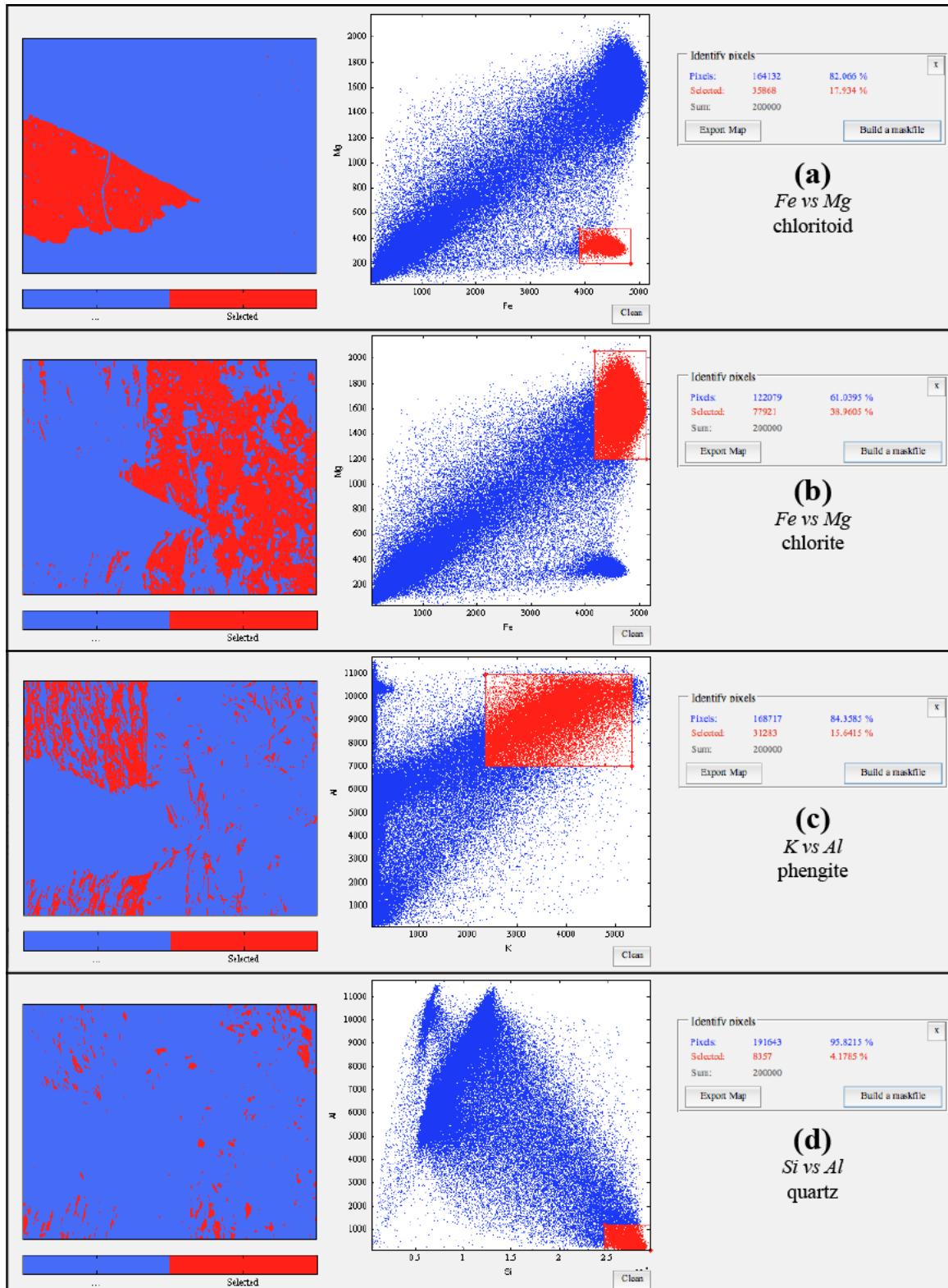


Figure 6.18 – Function identify pixels in the Binary diagram

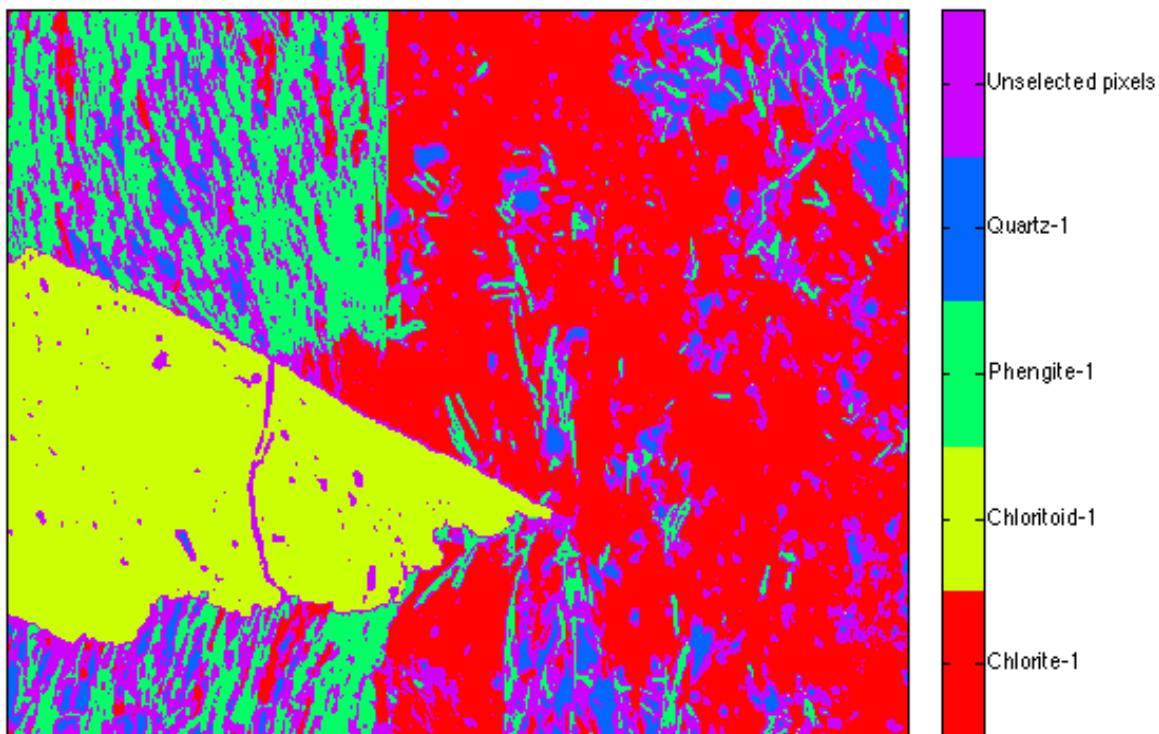


Figure 6.19 – Mask image of the mask file: *Merged-Maskfile*

(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 6.19.

(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.

#### 6.2.5.4 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) .

#### 6.2.6 Corrections

The full description of all corrections available in XMAPTOOLS is provided in the section 3.4.4.

*Work in progress.*

### 6.2.7 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. \(2018\)](#).

#### 6.2.7.1 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 [2.6.6](#) 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. [6.20a](#)).
- (3) As a file *Standards.txt* exists in the working directory, XMAPTOOLS suggests to open that file (Fig. [6.20b](#)). 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. [6.20d](#)). The group of buttons for internal standards has also been updated (Fig. [6.20c](#)).
- (5) Hide the spots analyses using the function *hide standards*  and display them again using the function *display standards* 

#### 6.2.7.2 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 *SiO<sub>2</sub>* (wt-%). The result is reported in figure [6.23](#) (case: original position). The correlation coefficient between the two spectra is 0.78 (see Code [6.5](#)).

```
Standards testing ... (Element: Si) ...
Standards testing ... (Correlation: 0.77956)
Standards testing ... (Element: Si) .... Ok
```

Code 6.5 – Text printed in the command window by the function *display intensity vs composition chart*

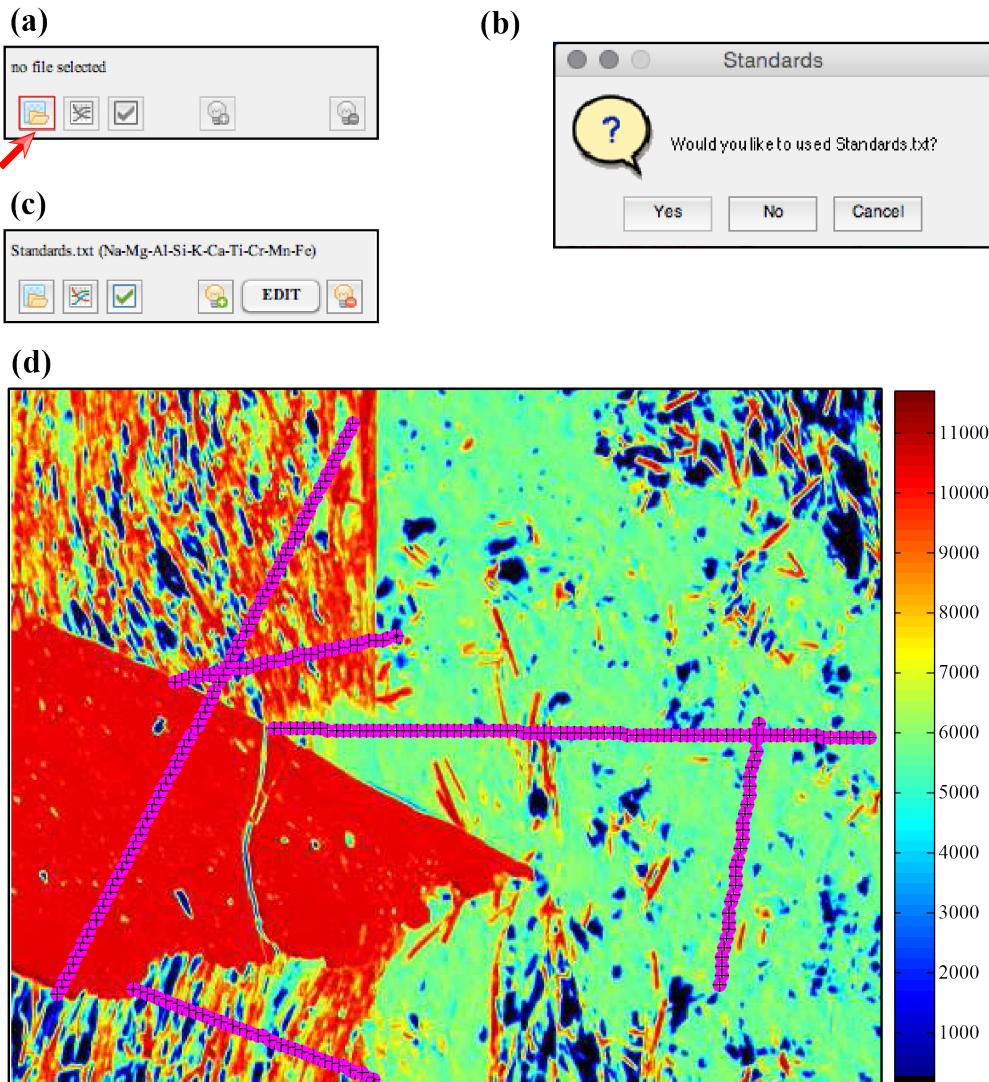


Figure 6.20 – Procedure to load standards. (a) Group of buttons for internal standards (no standard file) (b) If a file Standards.txt exists in the working directory, the program proposes to open that file. (c) Group of buttons for internal standards (standard file loaded). (d) Map of Al with the spot 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. 6.21).

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  $20 \times 20$  pixels for which the center pixel (0,0) is the original position of the spot analyses (marked by a black star in Fig. 6.22).

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

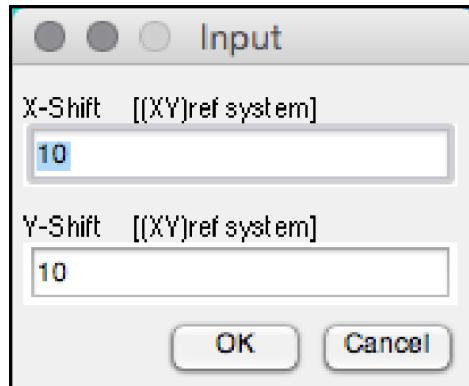


Figure 6.21 – Window to define X and Y shifts

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<sup>©</sup> Command Window (see Code 6.6).

```
SPC ... [ Standard Position Correction ]
SPC ... X correction of 1 pixels applied ... OK
SPC ... Y correction of 2 pixels applied ... OK
SPC ... Done
```

Code 6.6 – 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. 6.21). The results are reported in figure 6.23 (case: corrected positions).

The new correlation coefficient between Si and SiO<sub>2</sub> 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.

#### 6.2.7.3 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*

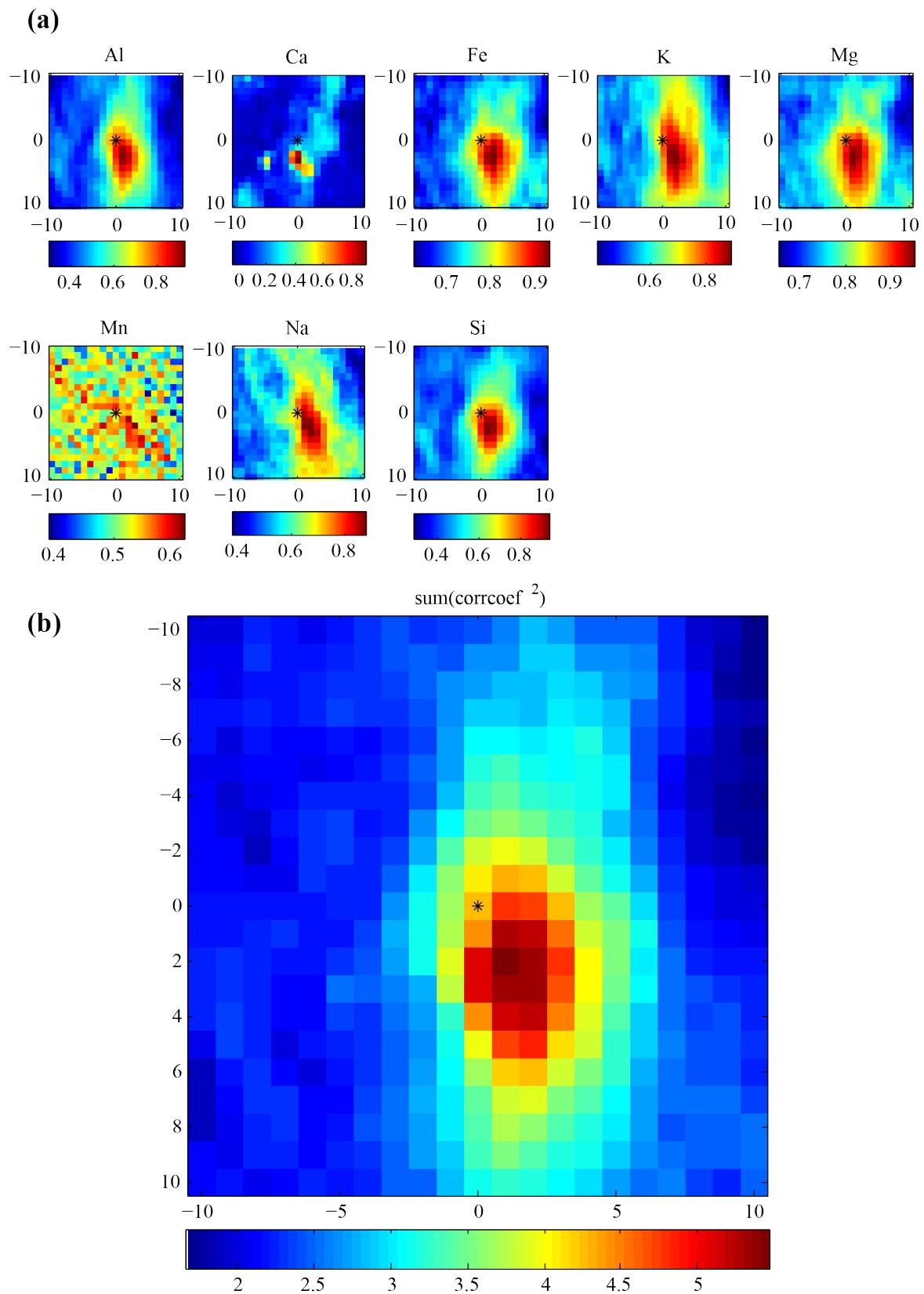


Figure 6.22 – Results of the check quality of std/maps positions

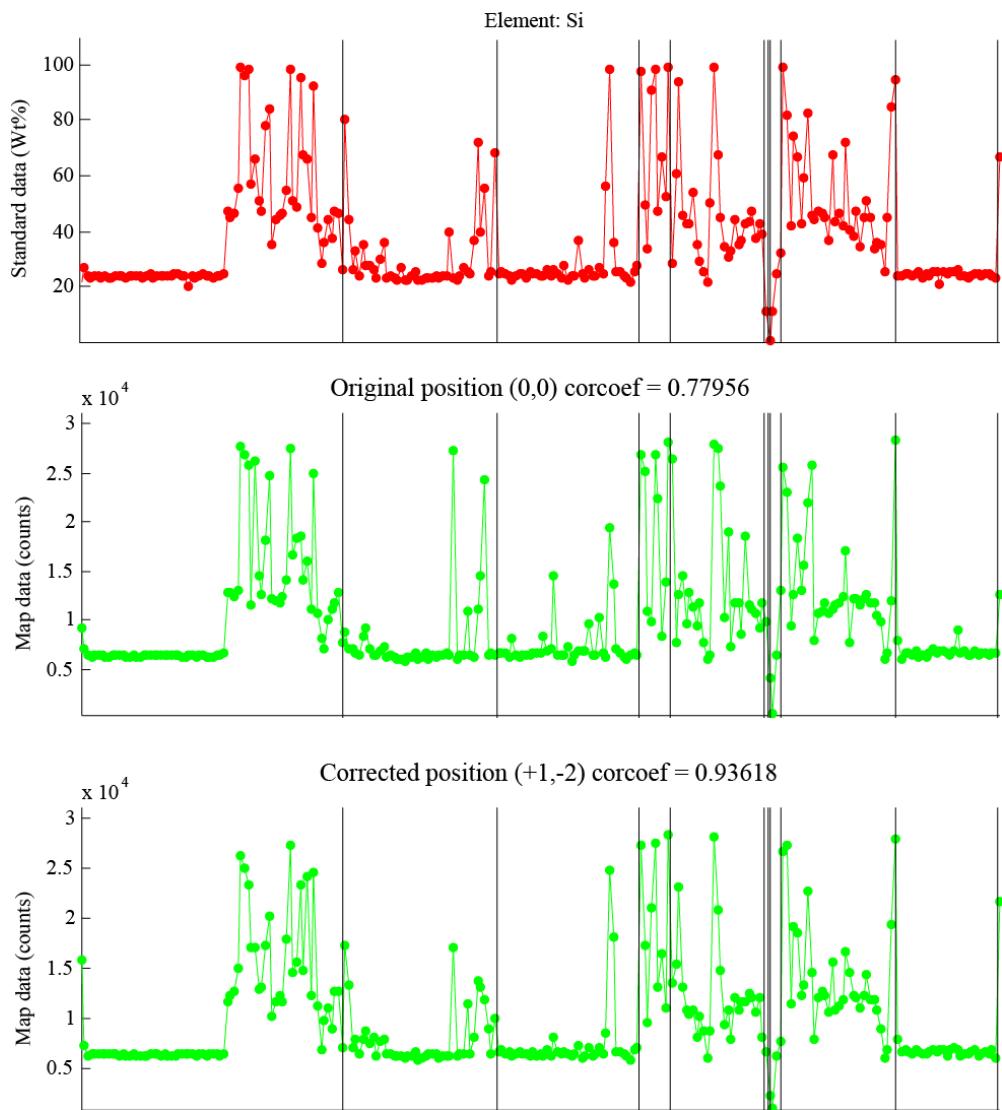


Figure 6.23 – Results of display intensity vs composition chart for the original and corrected positions

- (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. 6.24).
- (9) Display the spot analyses using the function *display standards*
- (10) Save the project.

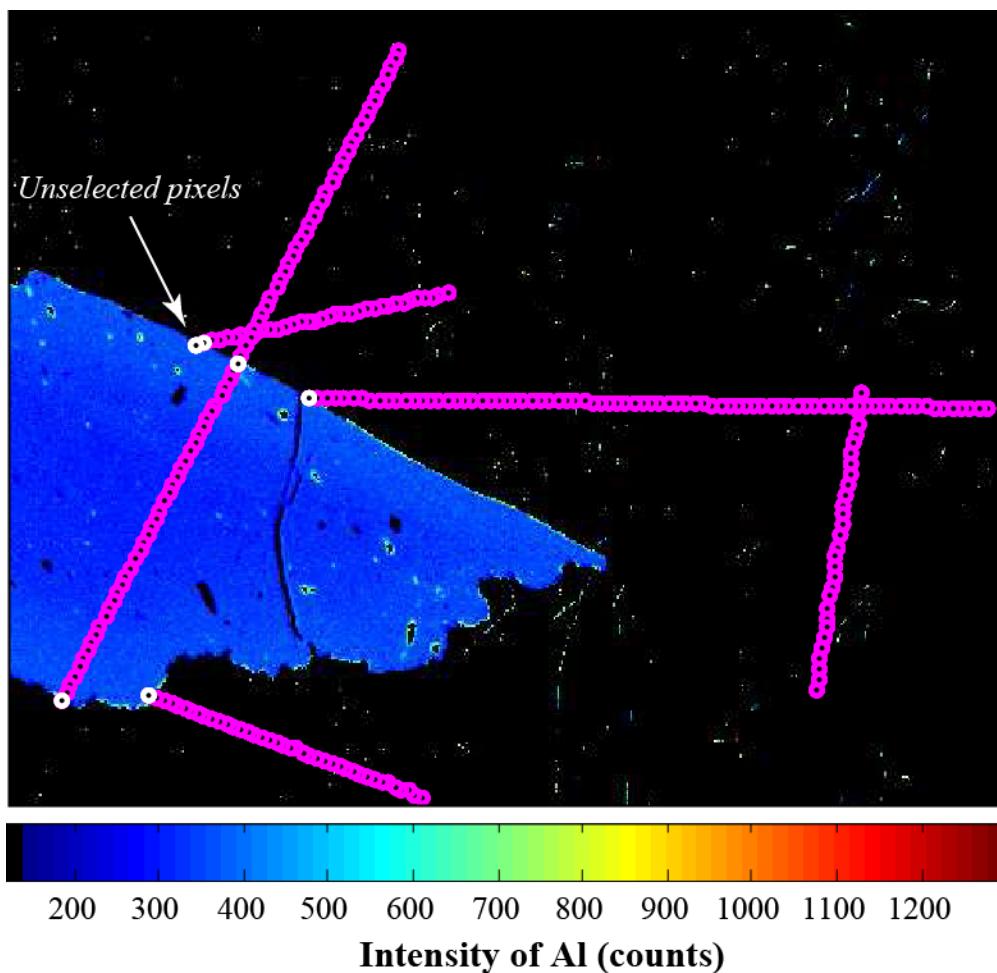


Figure 6.24 – Internal standards for chloritoid. Note that the spot analyses near the grain boundaries are unselected (white circles)

#### 6.2.7.4 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. 6.25).

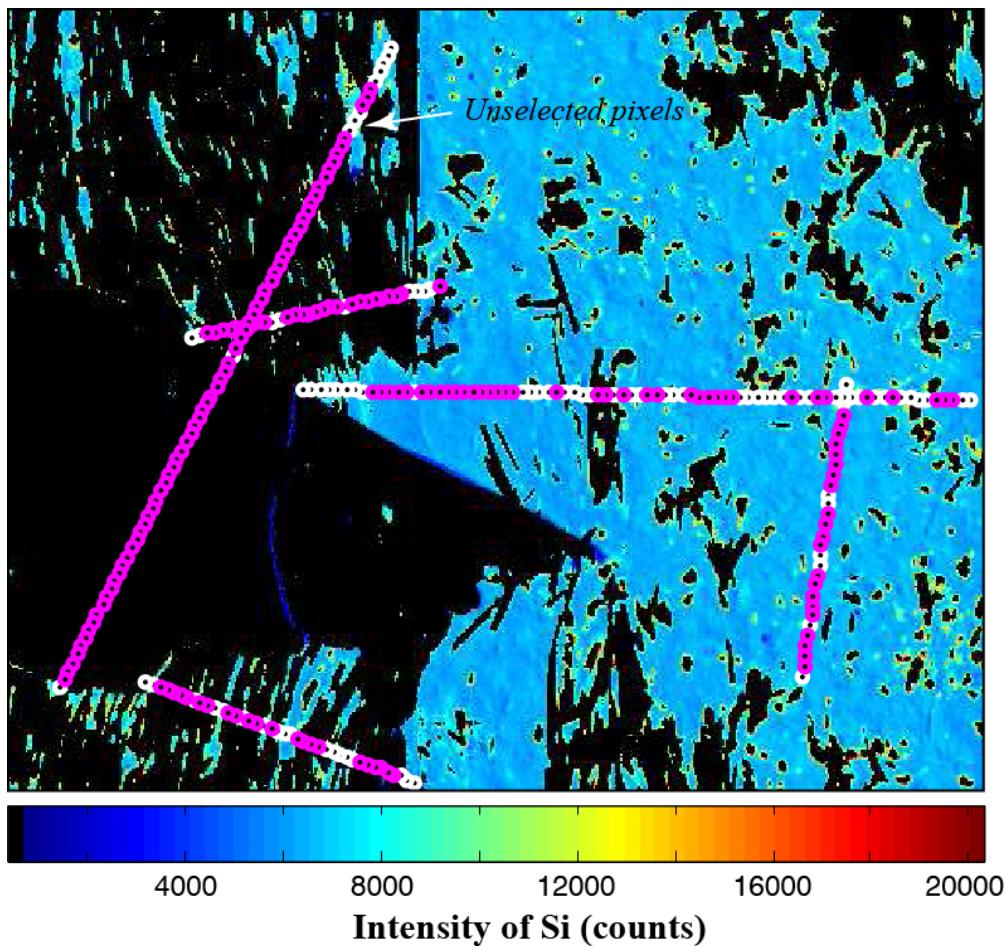


Figure 6.25 – Internal standards for chlorite. Note that the spot analyses near the grain boundaries are unselected (white circles)

- (7) Display the spot analyses using the function *display standards* 
- (8) Save the project.

#### 6.2.7.5 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 §6.2.7.3 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. 6.26). 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

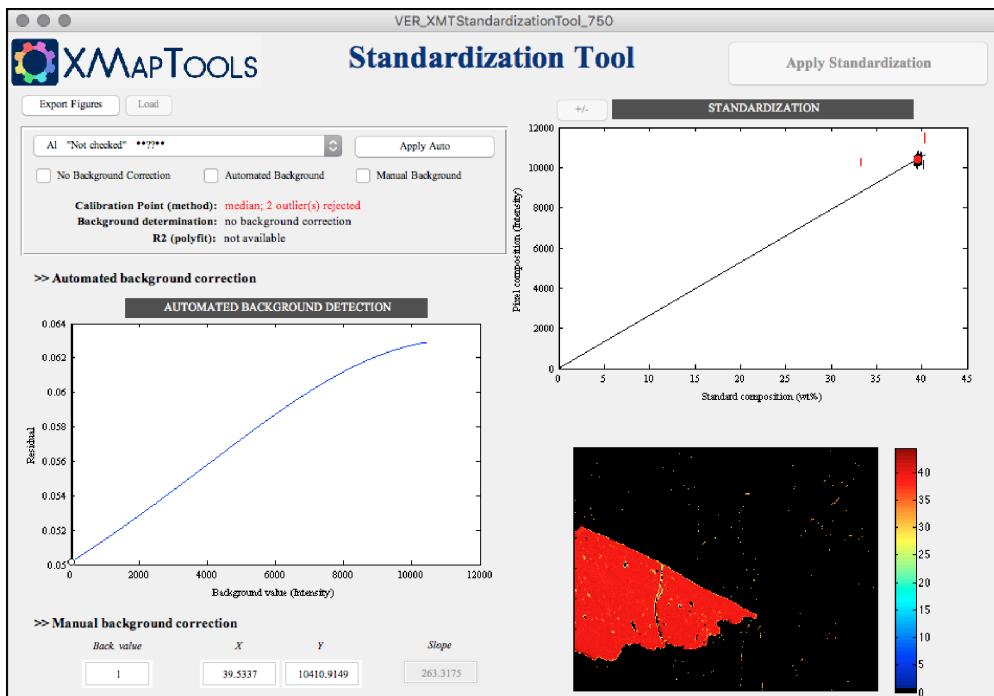


Figure 6.26 – Advanced standardization tool

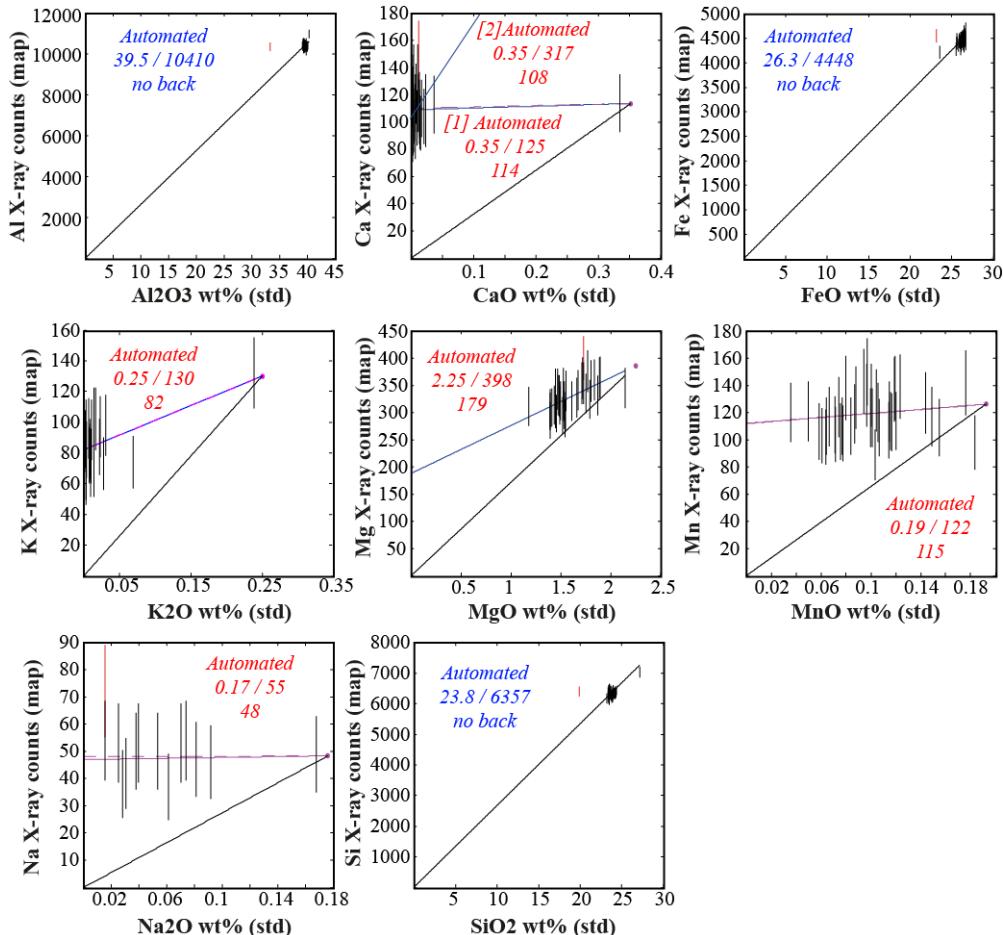


Figure 6.27 – Standardization diagrams for chloritoid

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  $X = 39.53 \text{ wt\%}$ ;  $Y = 10410$  counts (Figs. 6.26 & 6.27). 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  $X = 0.35 \text{ wt\%}$ ;  $Y = 125$  counts; a background value of 114 counts is estimated ([1] in Fig 6.27). A warning message is displayed as there are 3 pixels with concentration of  $\text{CaO}$  above 110 %. This is unrealistic for this example and it suggests that the spot analysis with a concentration of  $\text{CaO} = 0.32 \text{ wt\%}$  is an outlier. Press the button  $+$ / $-$  and click onto this point. The new calibration curve is defined by the point  $X = 0.35 \text{ wt\%}$ ;  $Y = 317$  counts; a background value of 108 counts is estimated ([2] in Fig 6.27). This is more realistic and the highest concentration of  $\text{CaO}$  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  $X = 26.3 \text{ wt\%}$ ;  $Y = 4448$  counts; no background correction needed (Fig. 6.27).

(6) Select the next element K and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point  $X = 0.25 \text{ wt\%}$ ;  $Y = 130$  counts; a background value of 82 counts is estimated (Fig 6.27). The  $\text{K}_2\text{O}$  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 6.27.

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. 2018). 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. 6.27). 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. 6.26).

(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.

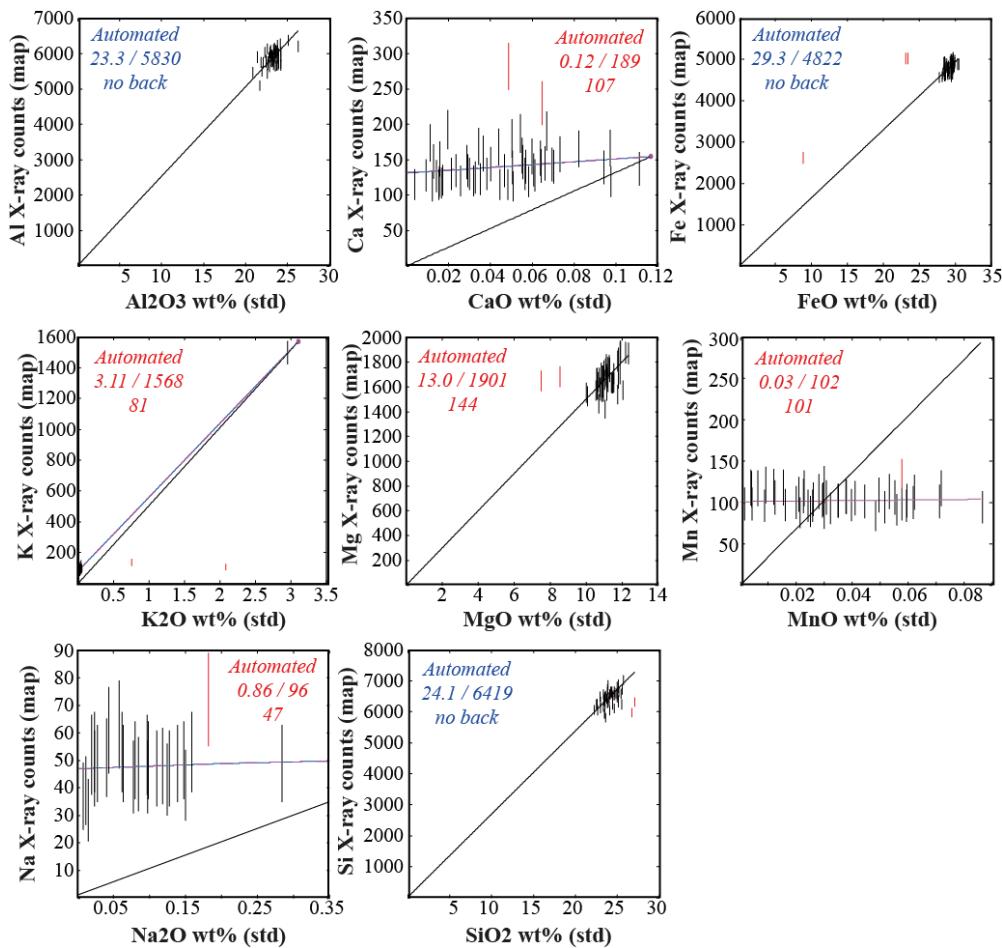


Figure 6.28 – Standardization diagrams for chlorite

(12) Check the quality of standardization using the function *Generate the oxide wt% sum map*  $\Sigma$

#### 6.2.7.6 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 6.28.
- (3) Once all the calibration curves haven been defined, press the button *Apply Standardization* (Fig. 6.26) and save the standardization parameters.
- (4) Check the quality of standardization using the function *Generate the oxide wt% sum map*  $\Sigma$
- (5) Save the project.

### 6.2.7.7 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<sub>2</sub>* 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<sub>2</sub> 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<sub>2</sub>* and press *OK*.

(6) In the workspace *Quanti*, check the concentration of *SiO<sub>2</sub>* in quartz.

(7) Save the project.

### 6.2.7.8 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 μm). In the file *Standards.txt*, the values of K<sub>2</sub>O 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 μm) 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 §6.2.7.3) to obtain a cluster in the standardization tool. This is not possible.

For the following sections of the tutorial, the phengite pixels are ignored.

## 6.3 QUANTI WORKSPACE

### 6.3.1 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 et Engi \(2017\)](#).

#### 6.3.1.1 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. 6.29a). 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.

#### 6.3.1.2 Quanti files of specific areas

- (1) Duplicate the *Quanti* file *Merged\_Map* using the button *Duplicate Quanti file*  [B2106] (Fig. 6.30a). A new *Quanti* file labeled *Merged\_Map\_copy* is created (Fig. 6.30b).
- (2) Use the function *select and area and delete the pixels inside*  [B2410] (Fig. 6.30c) 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. 6.30d). 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. 3.19).

#### 6.3.1.3 Density map and density correction

As discussed in [Lanari et 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 6.8 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.

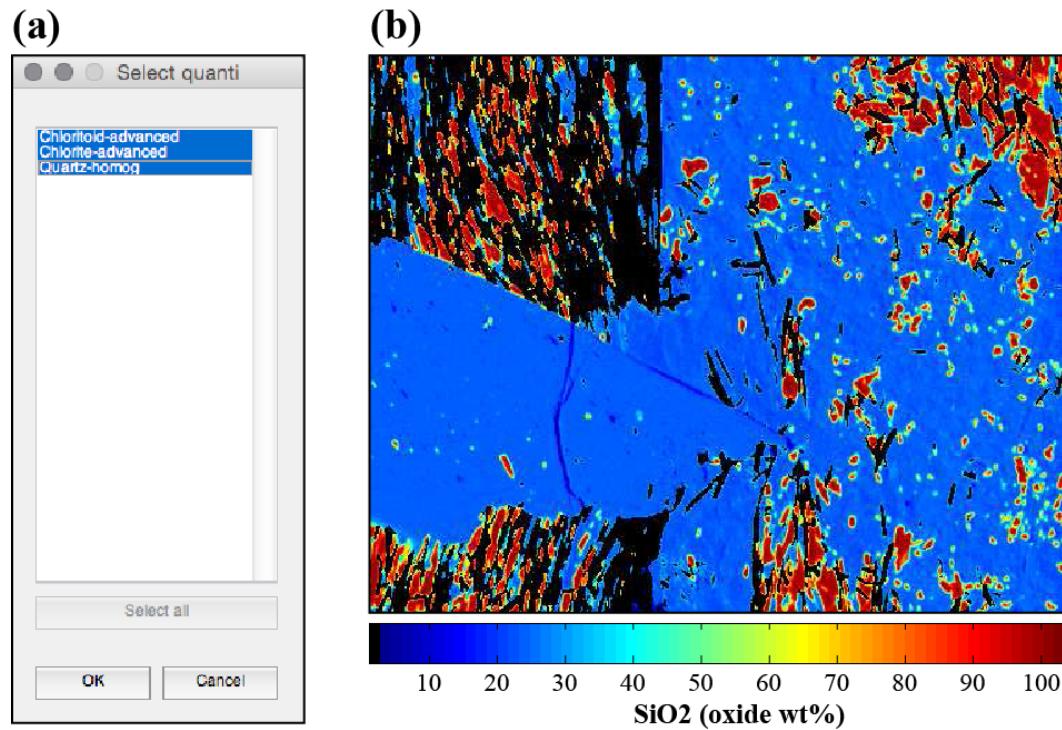


Figure 6.29 – Merge 'Quanti' files. (a) Select the maps. (b) map of silica

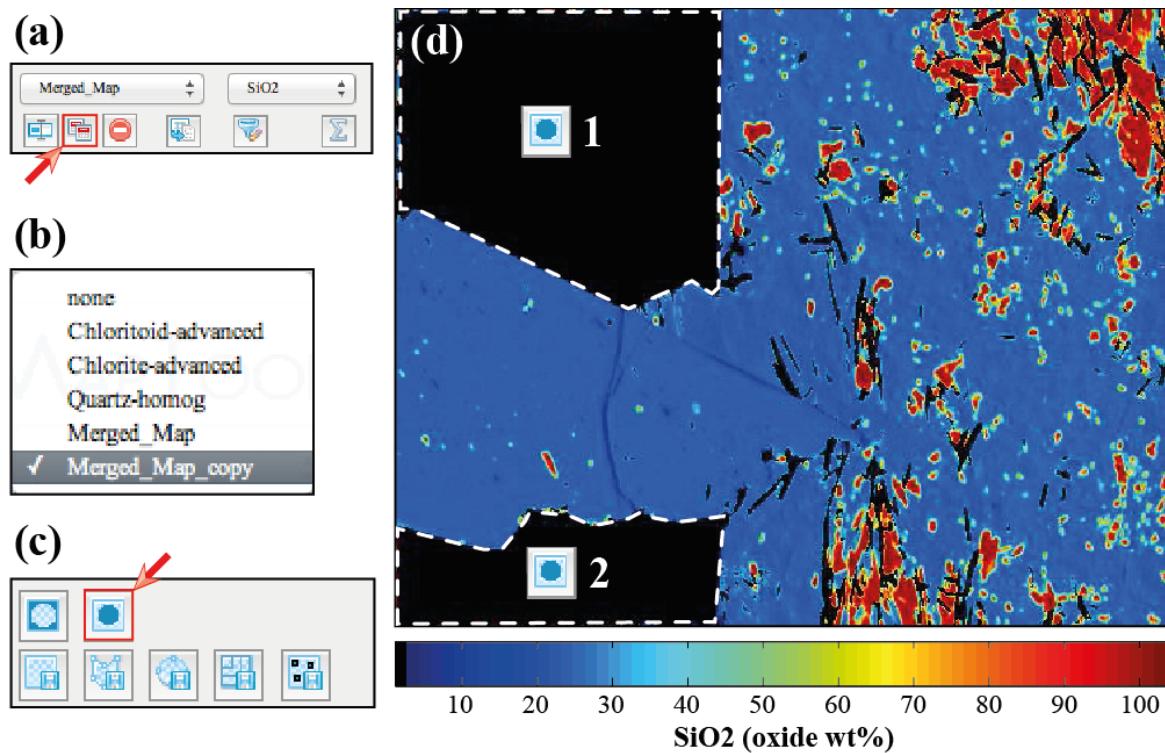


Figure 6.30 – (a) Duplicate the Quanti file 'Merged map'. (b) The 'Quanti' file 'Merged\_Map' has been duplicated. (c) Function used to delete the selected pixels of an area. (d) The pixels of two domains (labeled 1 and 2) have been deleted, i.e. they will not be used to extract the local bulk composition.

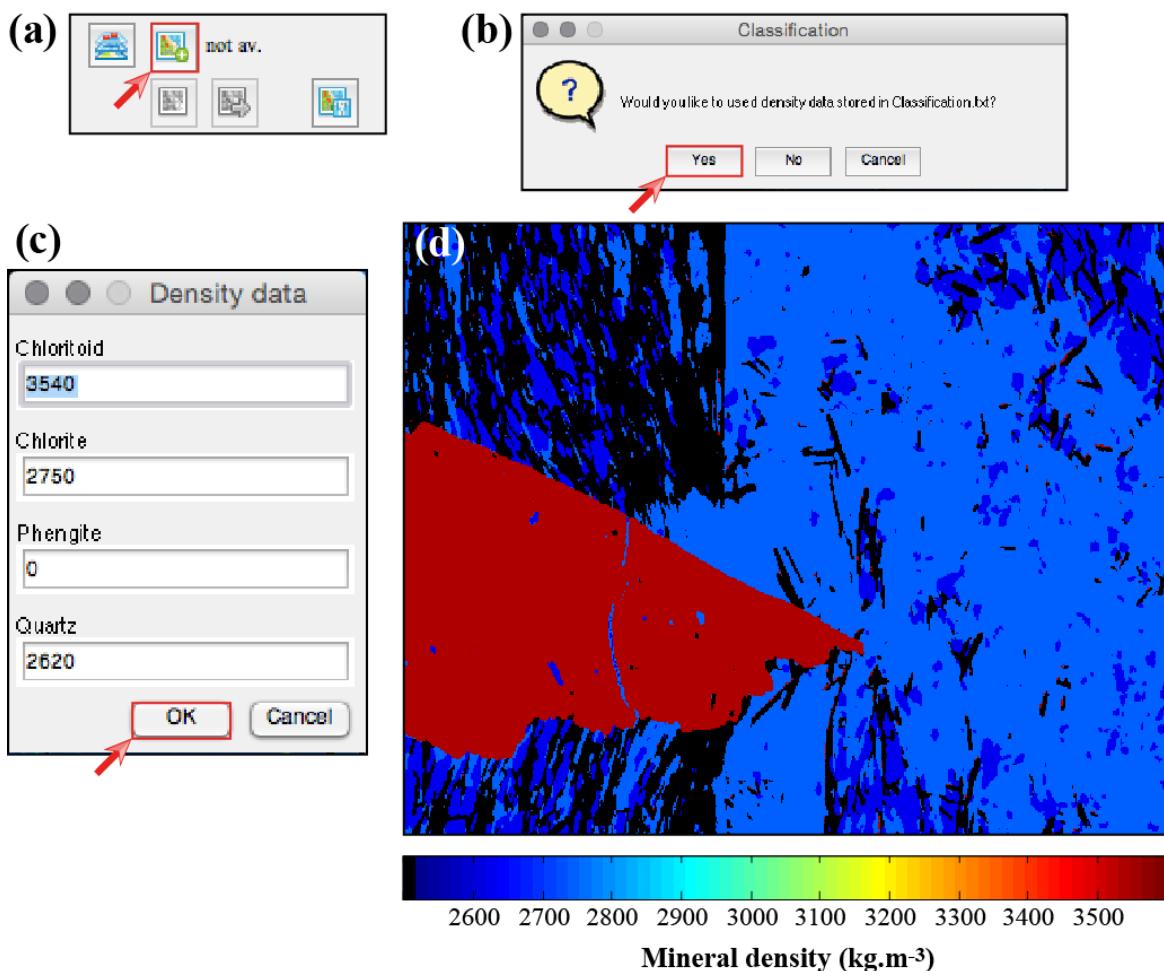


Figure 6.31 – (a) Define a new density map (b) Read the density data stored in the file Classification.txt. (c) Density values for each phase. (d) Density map used to apply the density corrections.

```
>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 6.7 – 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. 6.31a). The program reads the density data stored in *Classification.txt*, provided that this option is activated (Fig. 6.31b). The density values can be edited in the input dialog-box shown in Figure 6.31c.

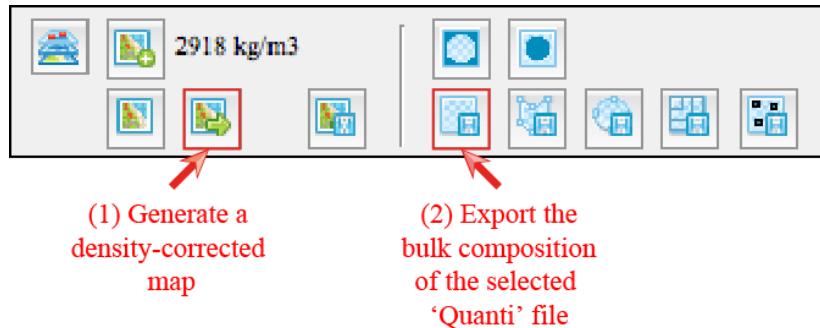


Figure 6.32 – Buttons to apply the density correction and export local bulk compositions

- (3) You can display the density map any time (Fig. 6.31d) by pressing the button *display the density map* [B2407].

#### 6.3.1.4 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. 6.32).

#### 6.3.1.5 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 6.8. If no density correction is applied for this example, the Al contained in the chloritoid is significantly underestimated.

Elem.	DCM	noDCM
Al <sub>2</sub> O <sub>3</sub>	25.7	22.8
CaO	0.36	0.32
FeO	24.3	22.4
K <sub>2</sub> O	0.29	0.28
MgO	6.73	6.57
MnO	0.07	0.07
Na <sub>2</sub> O	0.52	0.48
SiO <sub>2</sub>	30.8	29.4

Code 6.8 – Comparisons between local bulk composition determined for *\*DCM\_Merged\_Map\_Copy* (*DCM*) and *Merged\_Map\_Copy* (*noDCM*).

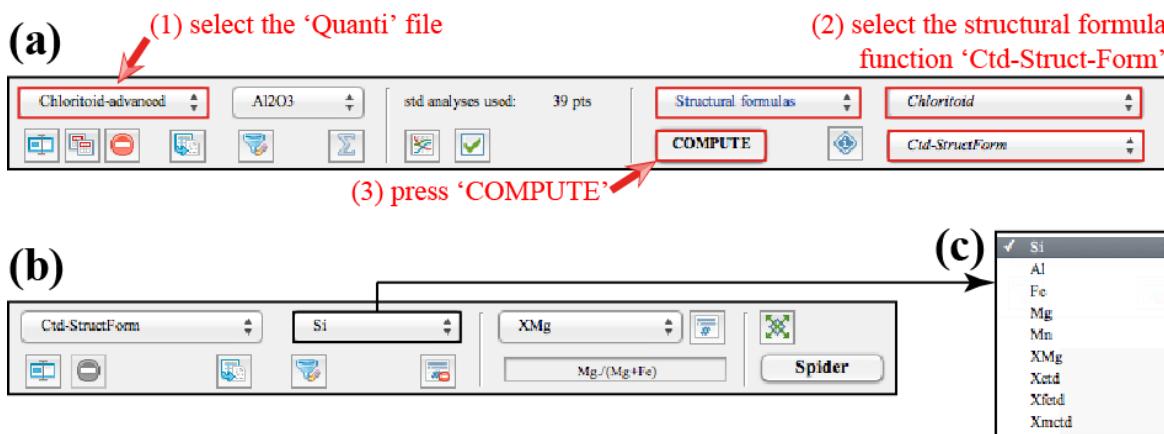


Figure 6.33 – Computation of structural formula maps: chloritoid. (a) select the ‘Quanti’ file and the external function Ctd-Struct-Form. (b, c) Buttons and menu of in the workspace Results.

### 6.3.2 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.

#### 6.3.2.1 Structural formula of chloritoid

(1) Select the *Quanti* file *Chloritoid-advanced* in the workspace *Quanti* (Fig. 6.33a).

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. 6.33a).

(3) Press the button *COMPUTE* (Fig. 6.33a).

(4) XMAPTOOLS opens the workspace *Results* and display the first element of the structural formula, here Si (in apfu, see Fig. 6.33b,c).

(5) Display the variable *XMg* (corresponding to  $\frac{Mg^{2+}}{Mg^{2+} + Fe^{2+}}$ ) using the menu shown in Figure 6.33c.

Additional variables can be generated in the workspace *Quanti* (see section 6.4.1 below).

## 6.4 RESULTS WORKSPACE

### 6.4.1 How to generate additional variables?

Use the GENERATOR module to generate new variables (see [3.7.4](#)).



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