

Utilisation des notebooks Jupyter pour la diffraction de poudre pour le « BAG matériaux historiques »

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Strahlenlinien (*beamline*), Kandinsky



SOME ARTEFACTS ANALYZED AT THE ESRF



Egyptian cosmetics
Louvre museum,
(18th dynasty, 1570-1292 BC)
Ph. Walter,
Paris



Inks in Egyptian papyri
Carlsberg Collection
(1st-3rd C.),
T. Christiansen,
Copenhagen



Ming porcelains
Beijing Archaeological
Institute (15th-16th C.),
Ph. Sciau,
Toulouse



Rembrandt's impasto
Rijksmuseum
(1634),
V. Gonzalez,
Delft



Van Gogh's *Sunflowers*
van Gogh Museum,
(1888-1889),
L. Monico,
Perugia, Antwerp



Munch's *Scream*,
Munch Museum
(1910),
L. Monico,
Perugia

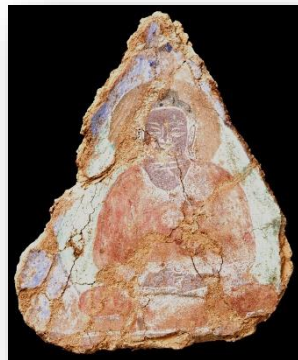


Rodin's sculptures
Rodin museum
(1908-1913),
J. Langlois,
Paris

Antiquity → **Today**



Opaque Egyptian glasses
Louvre museum and
British museum,
(18th dynasty, 1570-1292 BC)
I. Biron,
Paris



Bamiyan Buddhist paintings
(6th-9th C.)
Y. Taniguchi,
Tokyo



Leonardo da Vinci's whites
Louvre Museum
(1452-1519)
V. Gonzalez,
Paris



Ultramarine pigment
in *Girl with a Pearl Earring*,
Mauritshuis
(1665),
A. Gambardella,
Amsterdam

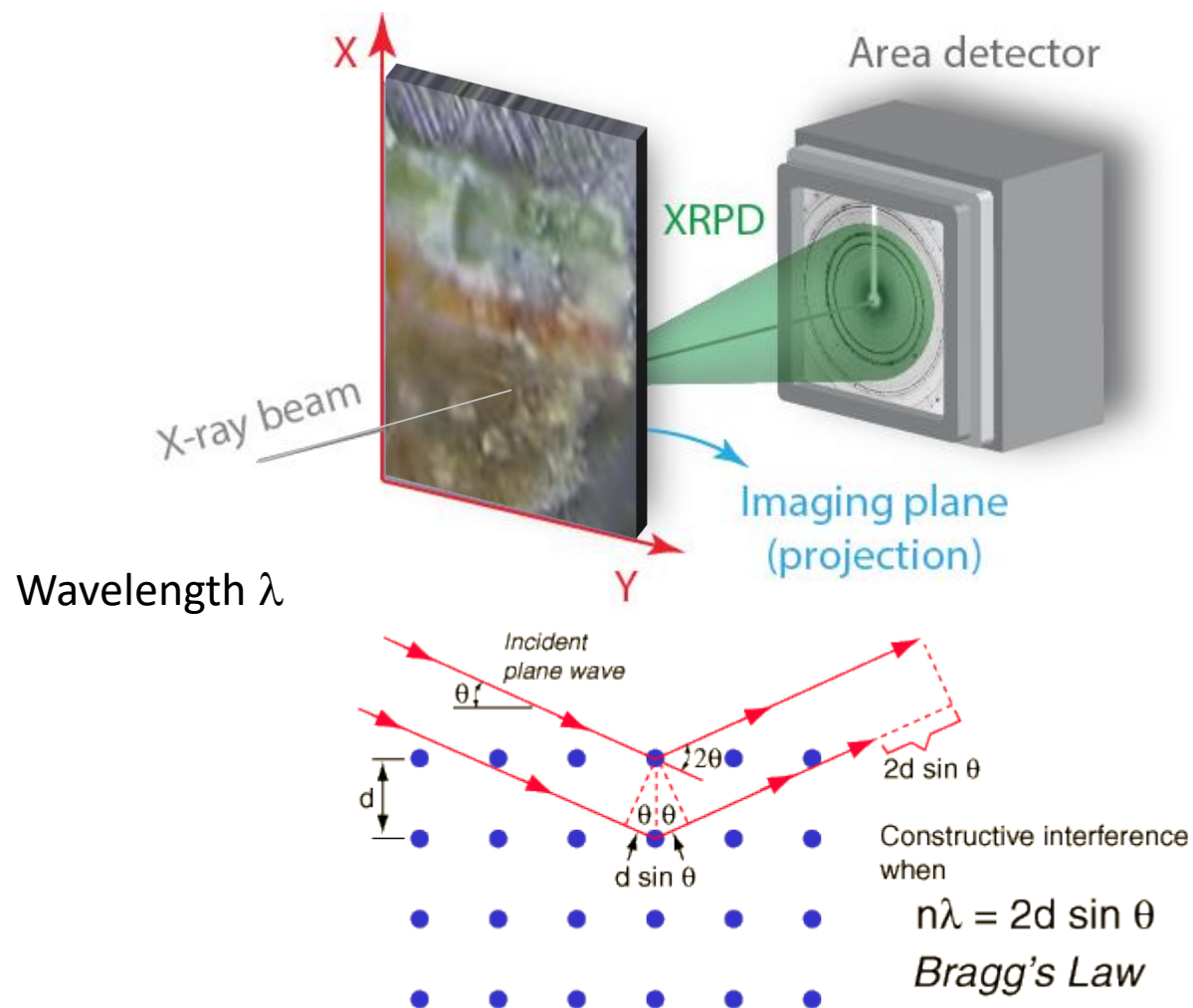


Matisse's *Joy of Life*
Barnes Foundation,
(1905-1906),
E. Pouyet,
Grenoble



Italian design
objects in plastics
private collection,
1960's, L. Toniolo,
Milano

X-RAY DIFFRACTION: IDENTIFICATION OF PHASES AND STRUCTURAL INFORMATION



Heritage Science

X-ray Diffraction Mapping for Cultural Heritage Science: a Review of Experimental Configurations and Applications

Victor Gonzalez^{+, * [a]}, Marine Cotte^{+, [b, c]}, Frederik Vanmeert^{+, [d]}, Wout de Nolf^[b] and Koen Janssens^[a]



V. Gonzalez, M. Cotte, F. Vanmeert, W. de Nolf and K. Janssens, "X-ray Diffraction Mapping for Cultural Heritage Science: a Review of Experimental Configurations and Applications", *Chemistry – A European Journal*, 26, 1703–1719 (2020).

REMBRANDT'S *IMPASTO* TECHNIQUE

WORKS LED BY

Victor Gonzalez, TU Delft and Rijksmuseum, Amsterdam

SAMPLES

Tiny fragments from *Portrait of Marten Soolmans*, 1634, Rijksmuseum, *Susanna*, 1636, Mauritshuis and *Bathsheba*, 1654, Louvre, from the *impasto* and the paint layers.

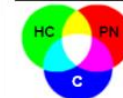
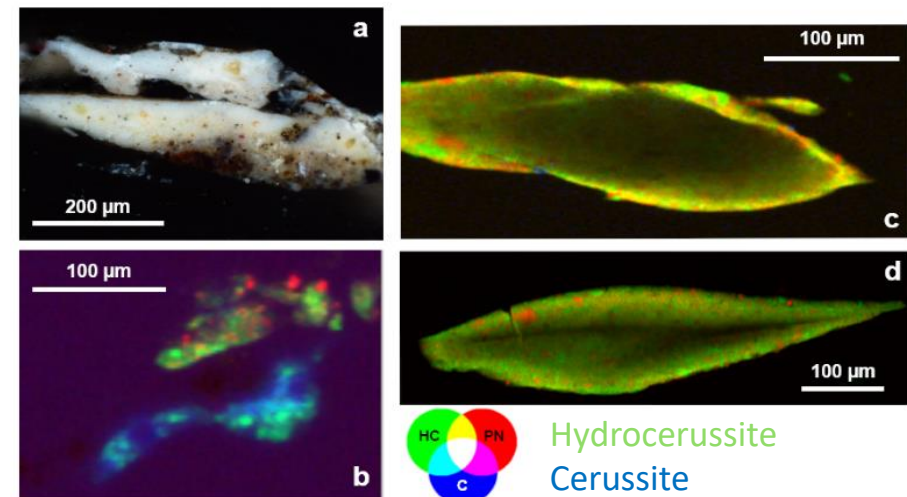
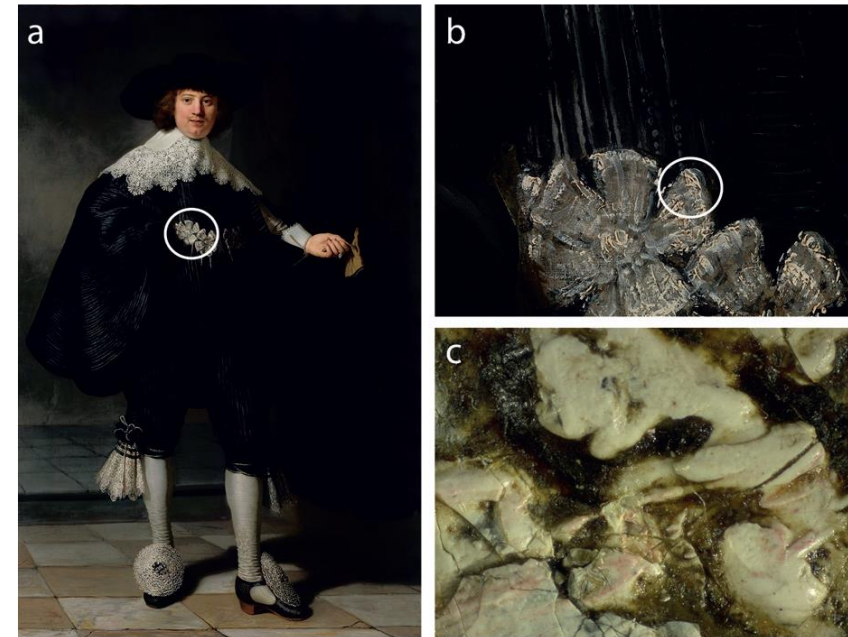
QUESTIONS

How did Rembrandt obtain his unique *impasto* effect?
Is there a chemical difference between *impasto* and paint layers giving a clue about his technique?

SOME RESULTS

Presence of a very rare lead phase (plumbonacrite), indicative of the treatment of oil with an alkaline lead.
In agreement with contemporaneous recipes to produce thick oils (made of lead soaps!).

V. Gonzalez, M. Cotte, G. Wallez, A. van Loon, W. de Nolf, M. Eveno, K. Keune, P. Noble and J. Dik, "Unraveling the Composition of Rembrandt's Impasto through the Identification of Unusual Plumbonacrite by Multimodal X-ray Diffraction Analysis", *Angewandte Chemie International Edition*, 58 (2019).

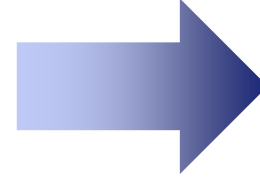


Hydrocerussite
Cerussite
Plumbonacrite

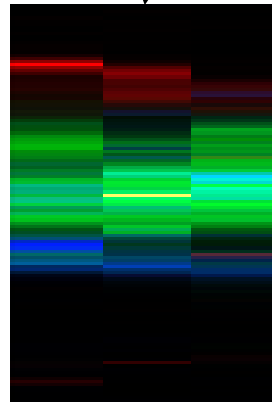
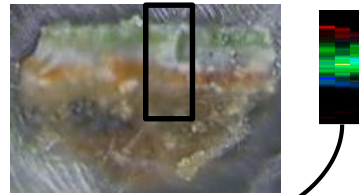
ESRF-EXTREMELY BRIGHT SOURCE (EBS) IN PRACTICE : A SMALLER AND BRIGHTER BEAM



Dec 2006
map size: $150 \times 60 \mu\text{m}^2$
pixel size: $1 \times 20 \mu\text{m}^2$
15s / pixel
1h52 for 450 pixels

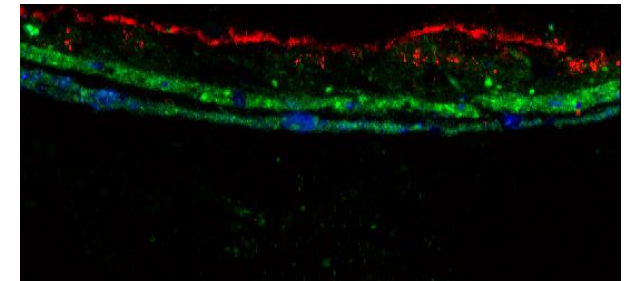
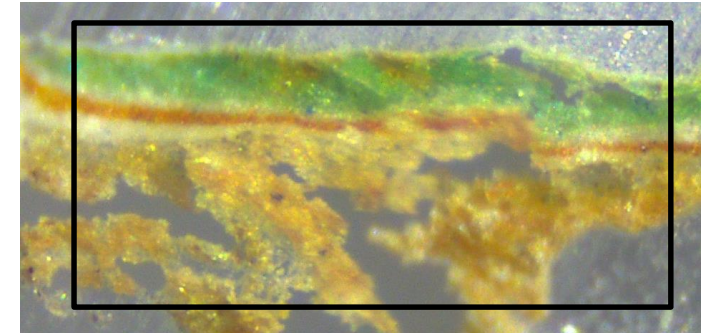


Nov 2021
map size: $800 \times 370 \mu\text{m}^2$
pixel size: $1 \times 1 \mu\text{m}^2$
0.016s / pixel
1h18 for 296 000 pixels



100μm

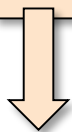
palmierite hydrocerussite
cerussite



- More samples
- Larger fields of view
- Higher resolution
- Better statistics

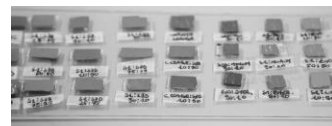
“STREAMLINE”: BEYOND DATA COLLECTION

- New access models
- New communities
- User outreach



Users

- ↗ More users
- ↗ New users
- ↗ More diverse users



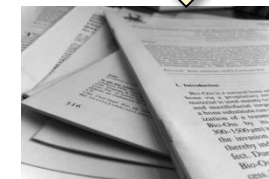
Samples

- New source (**EBS**)
- New/ refurbished beamlines
- New techniques



Data

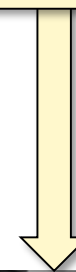
- ↗ Quantity
- ↗ Quality
- ↗ Complexity



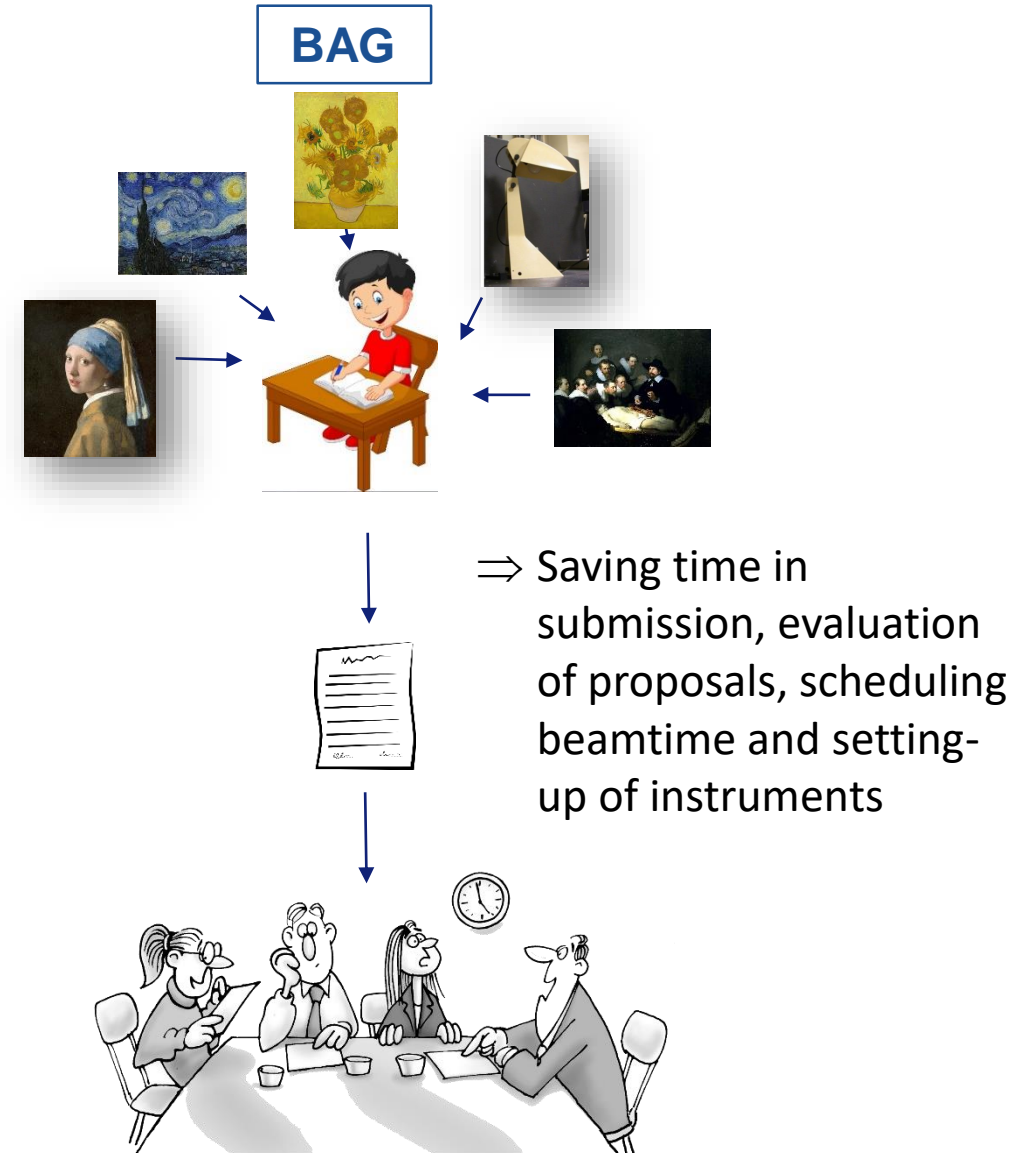
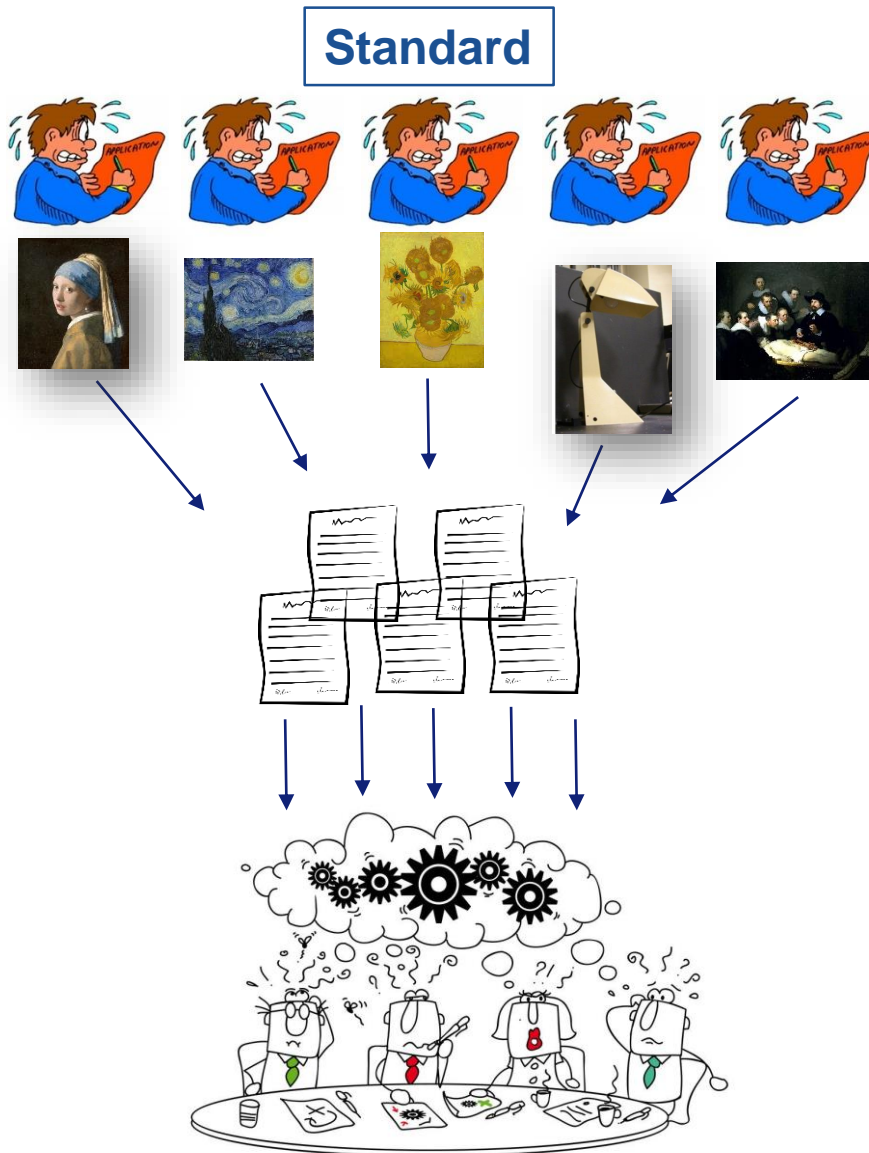
Results

- ↗ Quantity
- ↗ Quality
- ↗ FAIR

- New tools for data collection, on-line analysis,
- Open access



FROM STANDARD ACCESS MODELS TO BLOCK ALLOCATION GROUP (BAG) ACCESS



THE “HISTORICAL MATERIALS” BLOCK ALLOCATION GROUP: A NEW SHARED ACCESS



RIJKS MUSEUM



11 European teams

- ENS Paris-Saclay: V. Gonzalez
- CNR-SCITEC: L. Monico
- Courtauld Institute of Art: A. Nevin, A. Burnstock
- Politecnico di Milano: D. Comelli
- Rijksmuseum: K. Keune
- IRCP/C2RMF: I. Reiche
- Universitat Politècnica de Catalunya: N. Jiménez
- ESRF: M. Cotte
- IRCP: G. Wallez
- University of Antwerp: K. Janssens
- TU Delft: M. Alfeld

Access to 2 beamlines (ID13 and ID22), every 6 months for 2 years
⇒ Collaborative training of new users and development of tools for data acquisition, for data processing

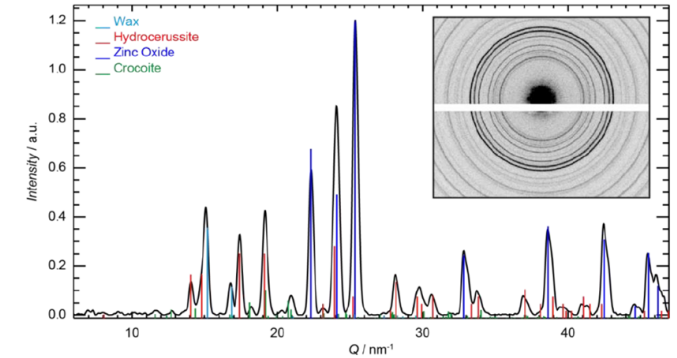
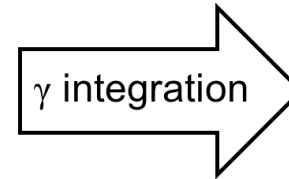
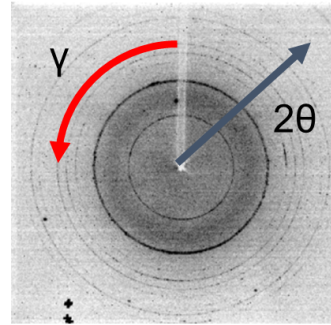
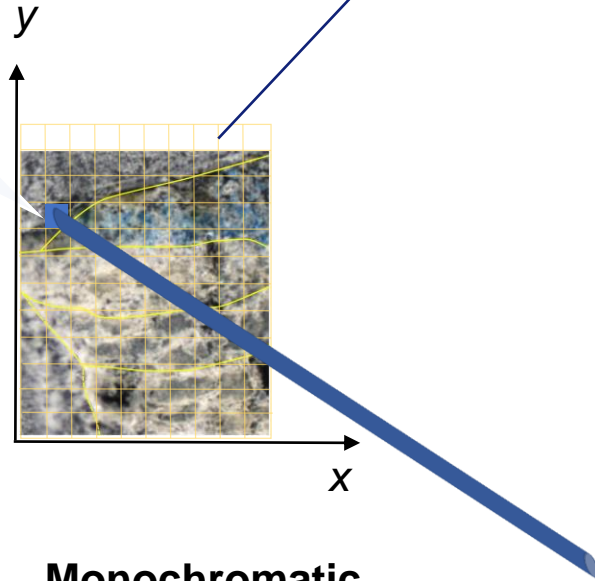
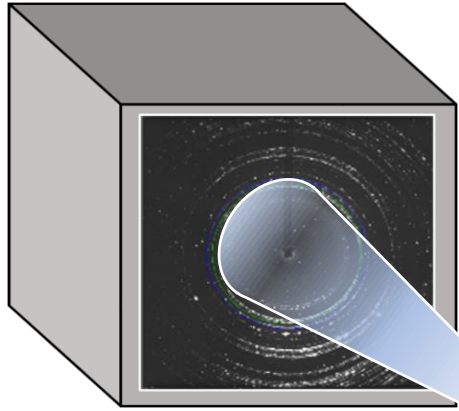


<https://www.esrf.fr/BAG/HG172>



THE DATA ACQUISITION AND PROCESSING WORKFLOW FOR ID13 MICRO-XRD MAPS

**XRD Detector :
EIGER 6M**

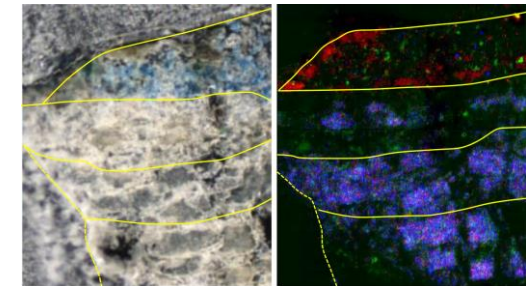


Identification of crystalline phases

Linear
combination
of reference
patterns

Integration on
regions of
interest

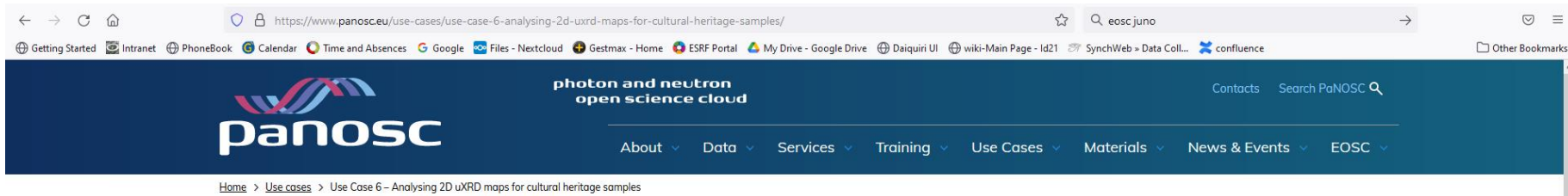
Quantitative
Rietveld fitting



Distribution Images

Nov 2021:
4 days
186 samples + 2 references
15 end-users

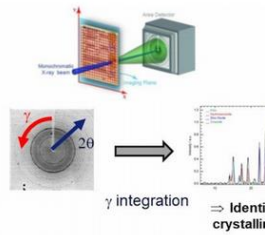
“JUNO”: JUPYTER NOTEBOOK



Home > Use cases > Use Case 6 – Analysing 2D uXRD maps for cultural heritage samples

Use cases

Use Case 6 – Analysing 2D uXRD maps for cultural heritage samples



Credits: M.Cotte (ESRF)

Improving the efficiency of 2D uXRD possible regular beamtime, remote

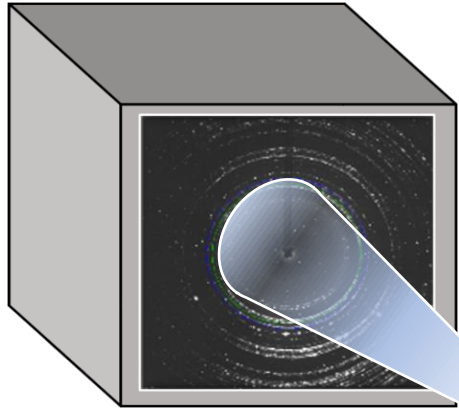


The screenshot shows the GitLab repository page for "juno" by Loic Huder. The repository has 175 commits, 4 branches, 20 tags, 645 KB files, 11.9 MB storage, and 16 releases. The description is "Jupyter notebooks for azimuthal integration". The page shows the "main" branch selected, with a commit hash of "4ef00aaf" and a message "Loic Huder authored 2 months ago". Below the commit information are links for "README", "MIT License", "CONTRIBUTING", and "CI/CD configuration". A table lists the repository's files and their last commit and update dates.

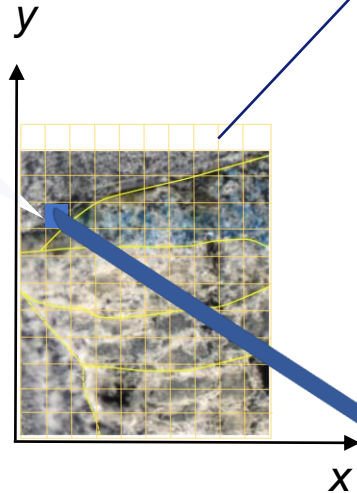
| Name | Last commit | Last update |
|------------------|---------------------|--------------|
| juno | 0.8.5 | 2 months ago |
| .bumpversion.cfg | 0.8.5 | 2 months ago |
| .gitignore | Edf instead of tiff | 1 year ago |

THE DATA ACQUISITION AND PROCESSING WORKFLOW FOR ID13 MICRO-XRD MAPS

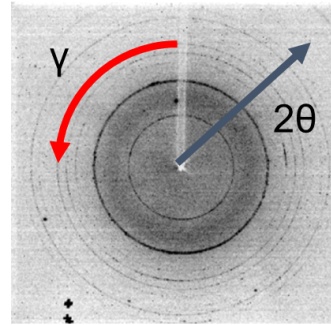
XRD Detector :
EIGER 6M



Steps 0 and 1:
set-up calibration

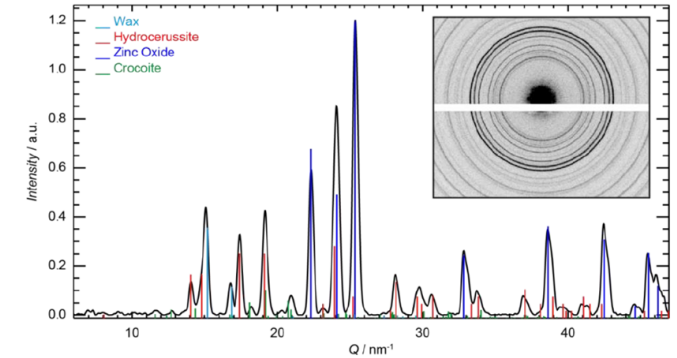


Monochromatic
X-ray beam



Step 2

γ integration



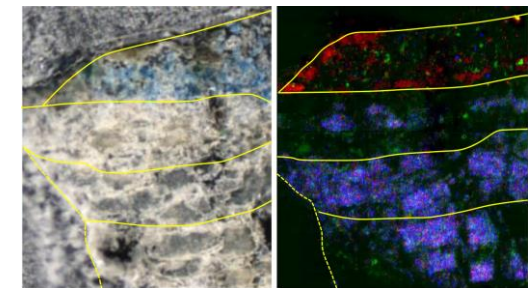
Identification of crystalline phases

Linear
combination
of reference
patterns

Step 3

Integration on
regions of
interest

Quantitative
Rietveld fitting



Distribution Images

Keeping a stable (but flexible) procedure for:

- **All BAG users**, with different teams working in parallel (avoid parallel scripts development)
- Including **non-expert users** (who just want results with basic procedure)
- But also **expert users** (requiring additional options for high quality analysis)
- **Without computing skills** (no complicated software installation, limited list of command lines)
- Coming **every 6 months**: (avoid re-develop tools every 6 months)
- Being **on-site or participating remotely** (web interface)
- **Future “data re-users”** in a couple of years (post embargo): very important taking into account the preciousness of samples (therefore of data)
- Using a stable experimental set-up (data acquisition, data format, data type)

The advantages of the Notebook

- Having texts explaining each step
- Having the possibility to change some parameters easily
- Having the possibility to display some results and easily check the acquisition
/ data processing quality

SOME RECENT OUTCOMES



Article

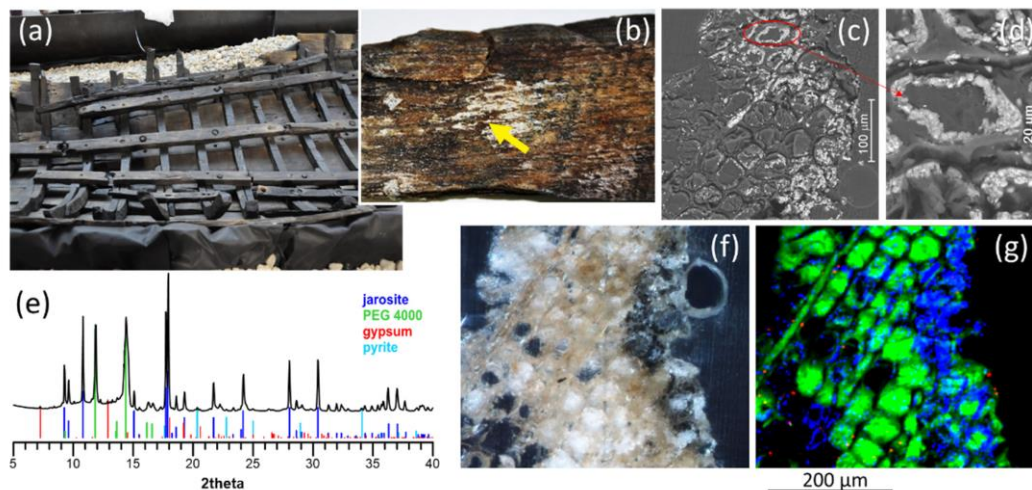
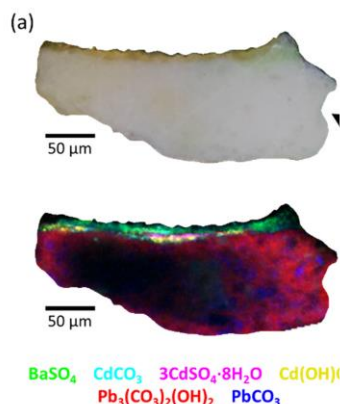
The “Historical Materials BAG”: A New Facilitated Access to Synchrotron X-ray Diffraction Analyses for Cultural Heritage Materials at the European Synchrotron Radiation Facility

Marine Cotte ^{1,2,*}, Victor Gonzalez ^{3,*}, Frederik Vanmeert ^{4,5,*}, Letizia Monaco ^{4,6,7,*}, Catherine Dejoie ¹, Manfred Burghammer ¹, Loïc Huder ¹, Wout de Nolf ¹, Stuart Fisher ¹, Ida Fazlic ^{1,8}, Christelle Chauffeton ^{9,10,11}, Gilles Wallez ^{9,11,12}, Núria Jiménez ¹³, Francesc Albert-Tortosa ¹³, Nati Salvadó ¹³, Elena Possenti ¹⁴, Chiara Colombo ¹⁴, Marta Ghirardello ¹⁵, Daniela Comelli ¹⁵, Ermanno Avranovich Clerici ^{4,16}, Riccardo Vivani ¹⁷, Aldo Romani ^{6,7}, Claudio Costantino ^{6,7}, Koen Janssens ^{4,8}, Yoko Taniguchi ¹⁸, Joanne McCarthy ¹, Harald Reichert ¹ and Jean Susini ^{1,†}

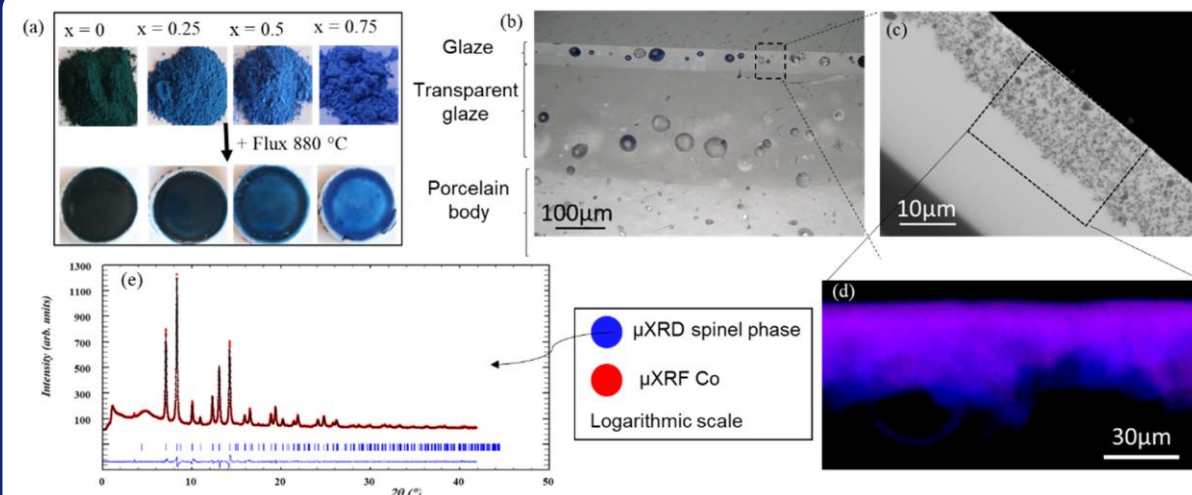


Femmes (1907), Picasso (Fondation Beyeler, Riehen/Basel)

Understanding cadmium yellow degradation in Picasso's *Femmes*
Marta Ghirardello, Daniela Comelli
 Politecnico di Milano



Study of the degradation of a waterlogged medieval timber
Núria Jiménez, Francesc Albert-Tortosa, Nati Salvadó,
 Departament d'Enginyeria Química EPSEVG, Universitat Politècnica de Catalunya



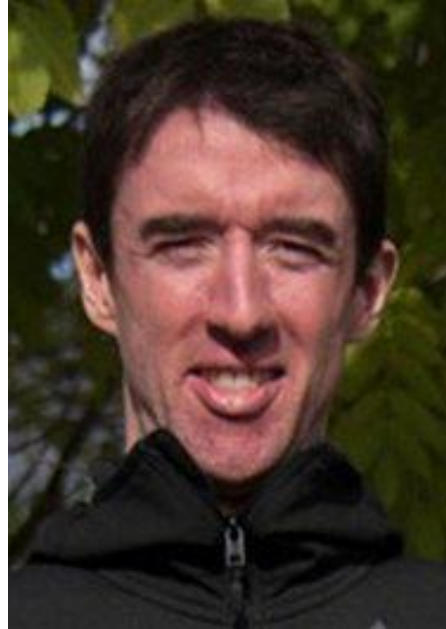
Understanding the composition of cobalt pigments in Sèvres porcelains
Christelle Chauffeton, Gilles Wallez Chimie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris

- Shared account on Jupyter/ slurm (to use the same file for all users of the same group)
- More tools for data analysis:
 - Just started: filtering the single crystals signal from the powder signal
 - Access to a reference database for phase identification and linear combination of reference patterns
 - Machine learning analysis (long term future; Jupyterlab?)

SPECIAL THANKS TO



Loïc Huder, ESRF



Wout de Nolf, ESRF



Frederik Vanmeert,
AXIS, University of Antwerp,
KIK-IRPA, Brussels



PIONEERING SYNCHROTRON SCIENCE



STREAMLINE



THANK YOU FOR YOUR INVITATION AND YOUR ATTENTION
Thanks to all users and colleagues involved in this research!



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