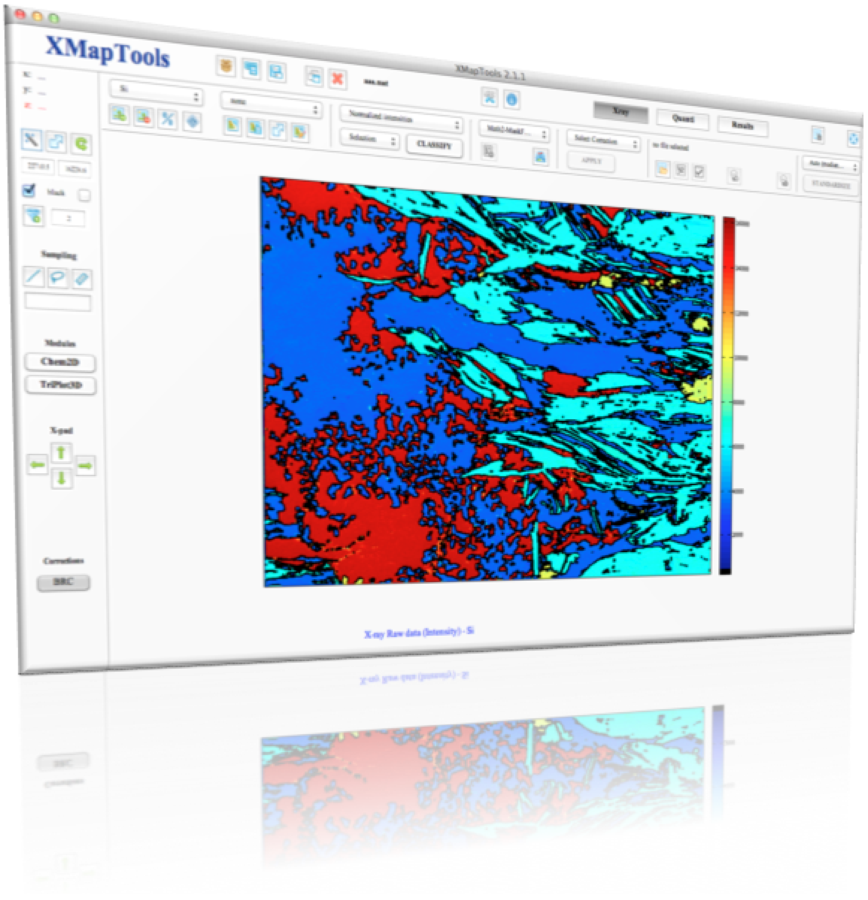
Dr. Pierre Lanari

An Introduction to
XMapTools 2.4

numerical tools for quantitative petrology



University of Bern

Bern, Monday 28th August, 2017

Dear XMapTools' users,

It is a great pleasure to introduce XMapTools, a software for the processing of compositional images from EPMA, SEM or LA-ICP-MS. This project has been initiated in 2009 when I was PhD student in Grenoble. Since the first release in 2012, the program has continuously been improved with numerous updates. This user guide aims to assist the users to ensure the better experience possible with textscXMapTools. However, before to go further into details and see how it works, it is important to acknowledge the students, 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) has been 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 (University of Bergen); M. Engi, J. Hermann, D. Rubatto, A. Vho, T. Bovay, M. Burn, A. Berger, M. Tedeschi, E. Kempf and F. Guintoli (University of Bern); C. Loury, Y. Rolland (GeoAzur Nice); T. Raimondo (University of South Australia); E. Duesterhoeft and R. Bousquet (Kiel University); C. Martin (University of Charlotte); E. Grosch (University of Bergen); G. Plissart (Universidad Austral de Chile); 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 (Univeristy of Milano); D. Waters (University of Oxford); G. Ortolano (Catania University) for help, suggestions, comments, data and/or collaborations in order to develop and test XMapTools.

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INTRODUCTION

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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 past year 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) to standardize semi-quantitative X-ray map data from electron microprobe analyses into maps of mineral oxide composition. This goal is achieved using high precision spot analyses as internal standards. Chemical groups corresponding to the mineral phases and other entities are separated using a K-means statistical approach (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 composition, structural formulae and phase equilibrium conditions, such as pressure and temperature, at each pixel. This allows for integrated textural interpretation of recorded physico-chemical conditions on a micro-scale. This goal is achieved using various geothermometers or geobarometers (about 50 functions available). In addition, binary and ternary chemical diagrams can be plotted using the modules CHEM2D and TRIPLOT3D. These modules may be used to identify the 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 CITATIONS GUIDELINES

Please use appropriate references for calculations done with XMAPTOOLS. The XMAPTOOLS release number must be specified just after the name. For instance: *Data were proceeded using* XMAPTOOLS *2.1.3 (Lanari et al. 2014)*

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

LA-ICPMS 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

Mapping technique: 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.

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)

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.

On the other hand, we would like to reassure also the Commercial World. Indeed, the Scientific Software Open Source Academic For Free License IS NOT like other, commonly spread Open Source Free licenses, GNU-GPL or other. In the sense that the present License well keeps into account all the needs and the way of functioning of the Commercial and Profit Institutions World. Into this world, XMapTools is going to be distributed under other Licenses, to be negotiated from case to case. In this case it is a paying code, and exclusiveness for a certain merceological sector, or even full exclusiveness can be agreed with commercial institutions. This protects commercial institutions investments on applied research lines using the XMapTools code against concurrential actions, a posteriori possible to concurrent commercial institutions for codes licensed under commonly spread Open Source Free licenses. We agree with the Commercial World that these licenses revealed not compatible with the ordinary way of functioning in the Commercial World. This is the reason why we choose a different license policy for XMapTools: to make Commercial Institutions profit of the Basic Research ByProducts. And at the same time, to make the Basic Research benefit of the funding coming from the Commercial World, to finance the Basic Research itself.

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

1.4 ANALYTICAL PROCEDURE (ELECTRON MICROPROBE)

To acquire high-quality X-ray maps to be standardized, it is strongly recommended to follow the procedures proposed by De Andrade et al. (2006) and described in details in Lanari et al. (2014b). Basically, the analytical session is divided into two parts: (1) in-situ spot analyses measurements of phase compositions to be used as internal standard during analytical standardization and (2) X-ray compositional mapping in wavelength dispersive mode, i.e using WDS spectrometers.

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 moderne 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 increase 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-intenisty 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 80×120 μm^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 grains 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 $1 \mu m$. 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 $1\mu m$) 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.

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:

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

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 8×16 μm^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 36×35 μm^2. Pixel sizes of 1, 2, 3 and 4 μm will generates images of 36×35, 18×17, 12×11 and 9×8 pixels respectively. For a given surface to be analyzed, the size of the image (in pixels) strongly affects the measurement time. In this example, estimated measurement times are 756 s, 184 s, 79 s and 43 s for 1, 2, 3 and 4 μm spot size respectively with dwell time of 300 ms and two passes.

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

An other characteristic feature of X-ray images is that at the contact between two phases, mixing compositions are analyzed. It is important to remember that the compositions of the pixels at the

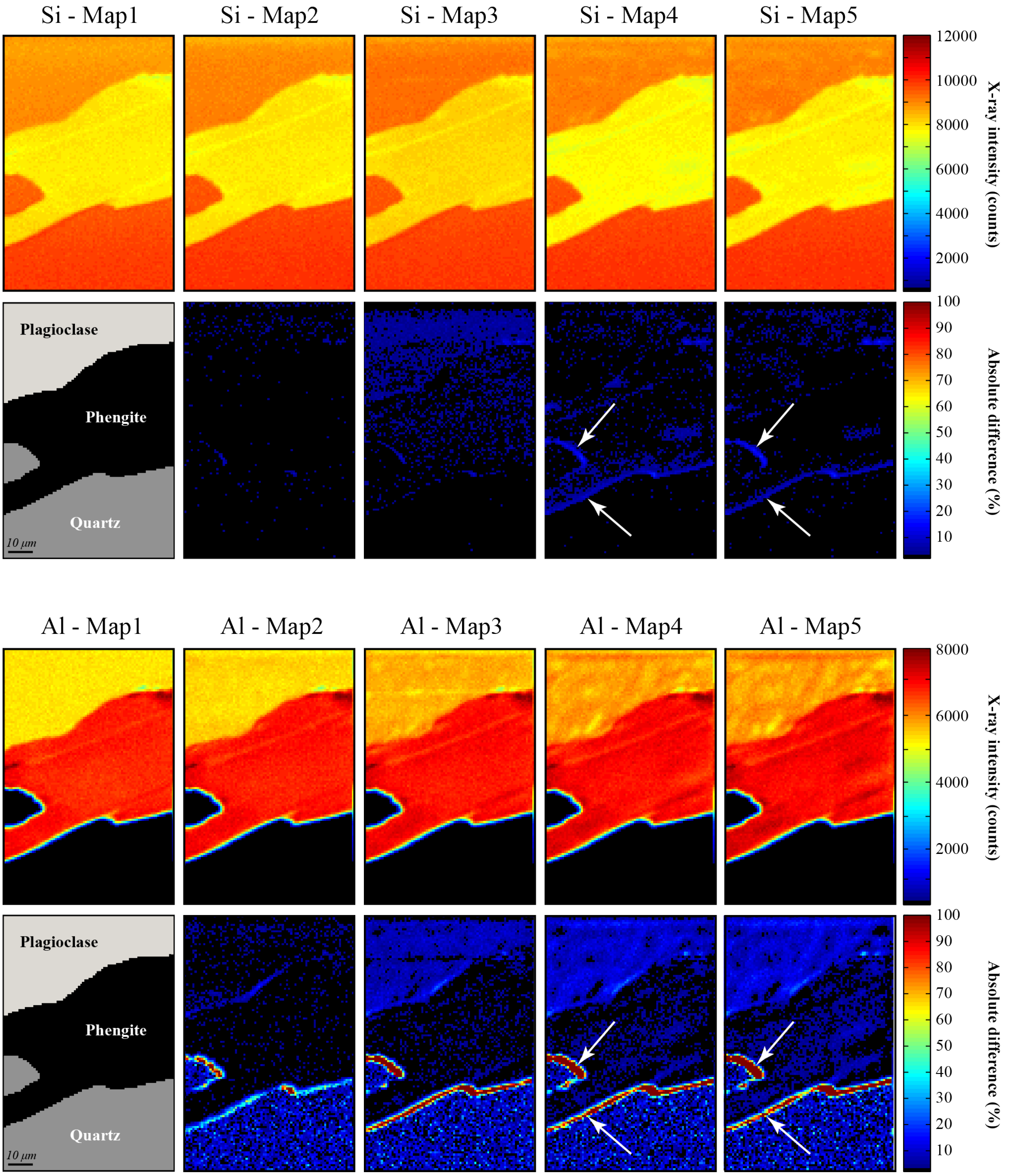


Figure 1.1 – *X-ray maps Si (top) and Al (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating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

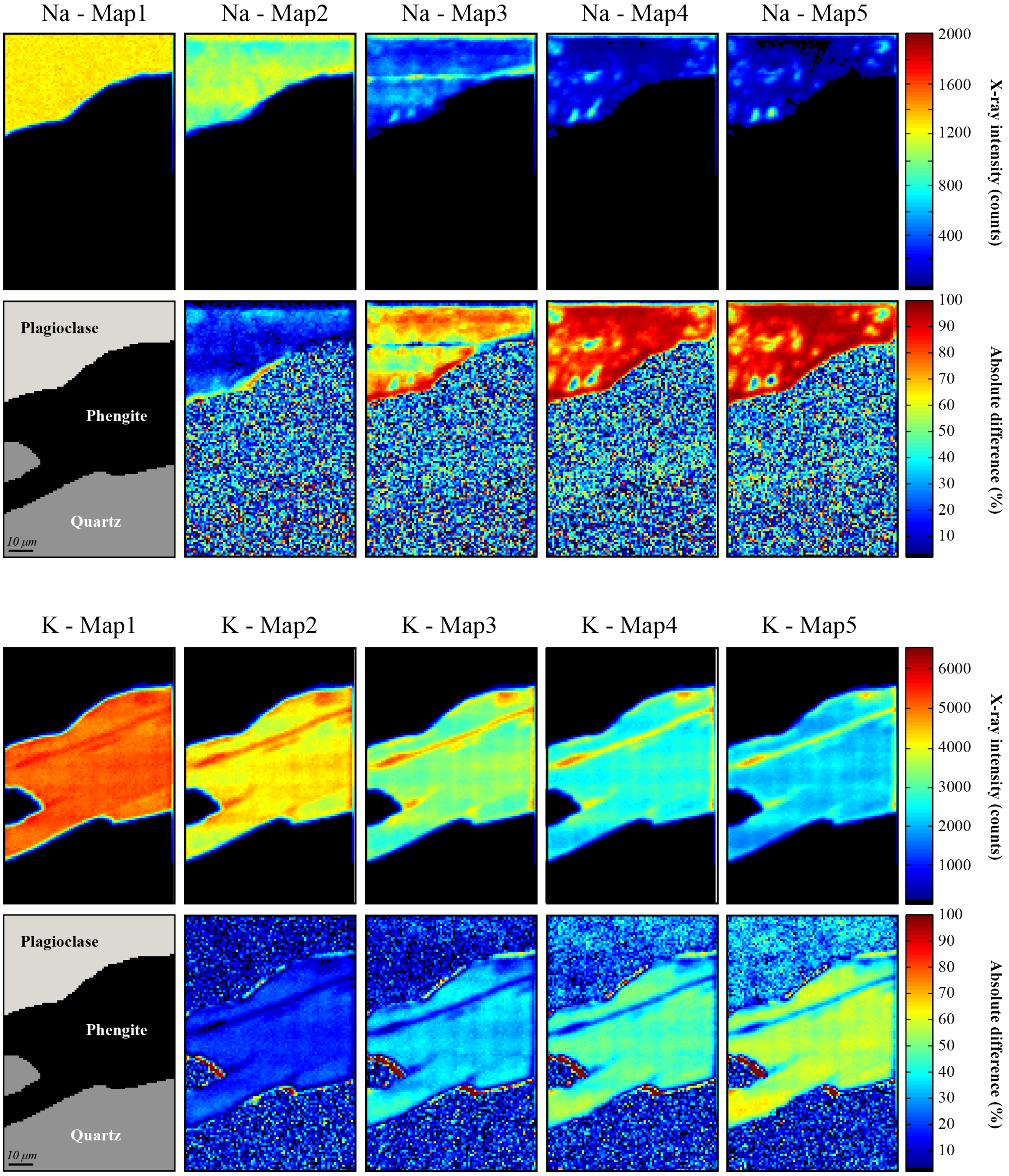


Figure 1.2 – *X-ray maps Na (top) and K (bottom) and absolute differences in % compared to the first map. Data were measured on a JEOL 8200 microprobe at the University of Bern, by acquiring five consecutive maps of the same area (corresponding to 10 passes: Na, Si, Ca, Al, Fe & Ti, K, Mg, Mn). Accelerating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

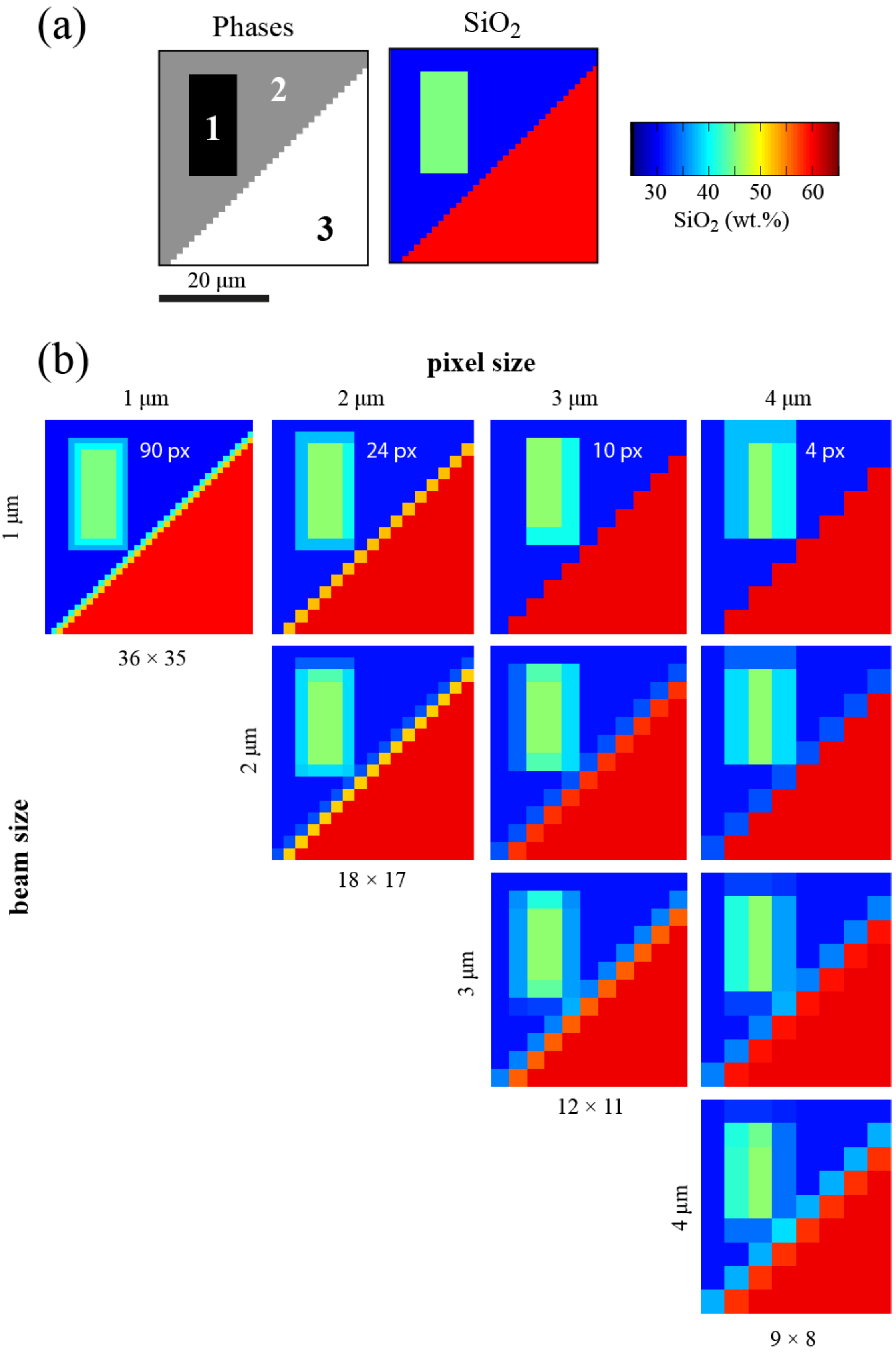


Figure 1.3 – *Spatial resolution dependency to pixel size and beam size. (a) Images of the different phases (left) and compositions of* SiO_2 *(right). The phase compositions are assumed to be perfectly homogeneous with* SiO_2 *composition of 45 wt.%, 30 wt.% and 60 wt.% for phases 1, 2 and 3 respectively.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

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

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):

$$P = \frac{2}{\sqrt{n}} \tag{1.2}$$

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

Example: A map of chlorite was acquire at the Institute of Geological Sciences (University of Bern) on a metasediment from the Western Alps, using an electron beam focussed at $1\mu m$, 15 KeV accelerating voltage, 100 nA specimen current, 200 ms dwell time and $3\mu m$ step size. The chlorite composition is $SiO_2 = 25.0$ $wt-\%$; $Al_2O_3 = 20.1$ $wt-\%$; $FeO = 32.1$ $wt-\%$; $MgO = 10.6$ $wt-\%$. 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 $SiO_2 = 0.82$ $wt-\%$; $Al_2O_3 = 0.78$ $wt-\%$; $FeO = 1.12$ $wt-\%$; $MgO = 0.534$ 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).

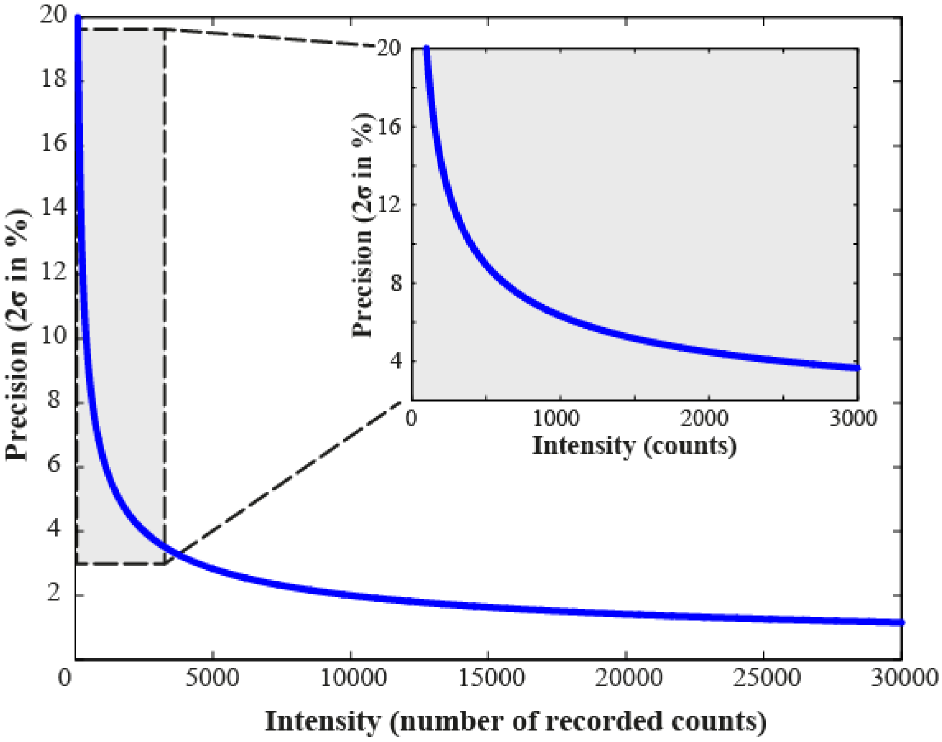


Figure 1.4 – *Relation between the number of recorder counts and the analytical precision of an analysis*

1.5 THEORETICAL CONSIDERATIONS

The following sections outline some fundament aspects of quantitative mapping through theoretical descriptions. This section is expected to growth 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:

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

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:

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

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

$$v_i = s_i \tag{1.5}$$

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

$$\rho_{mixture} = \sum_{i=1}^{i=n} v_i \rho_i \tag{1.6}$$

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

$$\rho_i = \frac{M_i}{V_i} \tag{1.7}$$

and consequently the mass of phase i is

$$M_i = \rho_i v_i \sum j = 1 j = n V_j \tag{1.8}$$

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 ($M_{mixture}$)

$$w_i = \frac{M_i}{M_{mixture}} \tag{1.9}$$

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

$$w_i = \frac{\rho_i}{\rho_{mixture}} v_i \tag{1.10}$$

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

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

If a significant density difference exists between the considered phase the local bulk composition i 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. 3.16).

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

XMapTools may be run with MATLAB© version 7.5 release R2007b or more recent releases. It has been developed on a MacBook Pro using MATLAB© R2012a and it has been intensively tested on MATLAB© R2014b and on Windows 7 with MATLAB© R2013b.

XMapTools 2.1.7 seems to be fully compatible with MATLAB© R2014b on OSX with some display issues that will be fixed in a future release. The program check which MATLAB© version is used and run the recommended GUI: *VER_XMapTools_750* from MATLAB© 2009b to MATLAB© 2014a and *VER_XMapTools_804* from MATLAB© 2014b to MATLAB© 2015b. This compatibility check ensures a better compatibility of XMapTools with the recent versions of MATLAB© in which a new graphical engine has been deployed.

XMapTools does not require any additional MATLAB© 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.

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 the new XMapTools.

(1) Run MATLAB©

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

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

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

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

(6) Follow the installation procedure described below (section 2.3).

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

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

2.3 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 proceed to the setup on your computer.

The XMAPTOOLS package is available at: www.xmaptools.com in the section XMAPTOOLS 2.1.X 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.*

(1) Login to XMAPTOOLS website using you user name and password

(2) Go to the download page [XMAPTOOLS 2.1.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.*

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 */UserHome/Documents/MATLAB/* (Fig. 2.1). It is strongly recommended to use this directory to install XMAPTOOLS. Here, MATLAB© always has the permissions to write in files. It is recommended to not 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 edited by user. *UserFiles* contains user's functions and codes. The use of this functionality is explained in details in section 4.2 and is reserved to

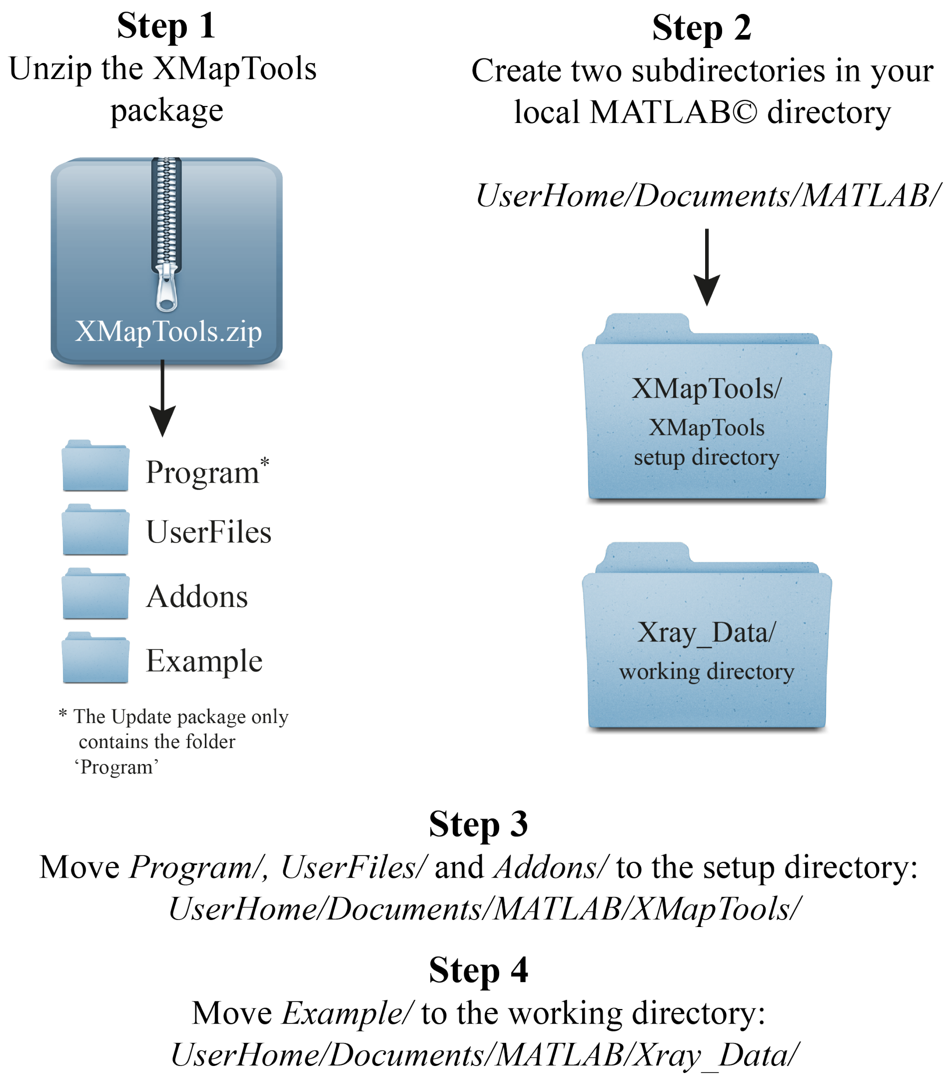


Figure 2.1 – XMAPTOOLS *files, folders, repertories and the starting procedure. The* XMAPTOOLS *setup package contains four folders:* Program, UserFiles, Addons *and* Example.

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 4.3. *Example* contains a set of microprobe X-ray maps that are used in the tutorial (see chapter 6).

(2) Create two subdirectories in your local MATLAB© directory: *../UserHome/Documents/MATLAB/XMapTools/* for the prorgam 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.

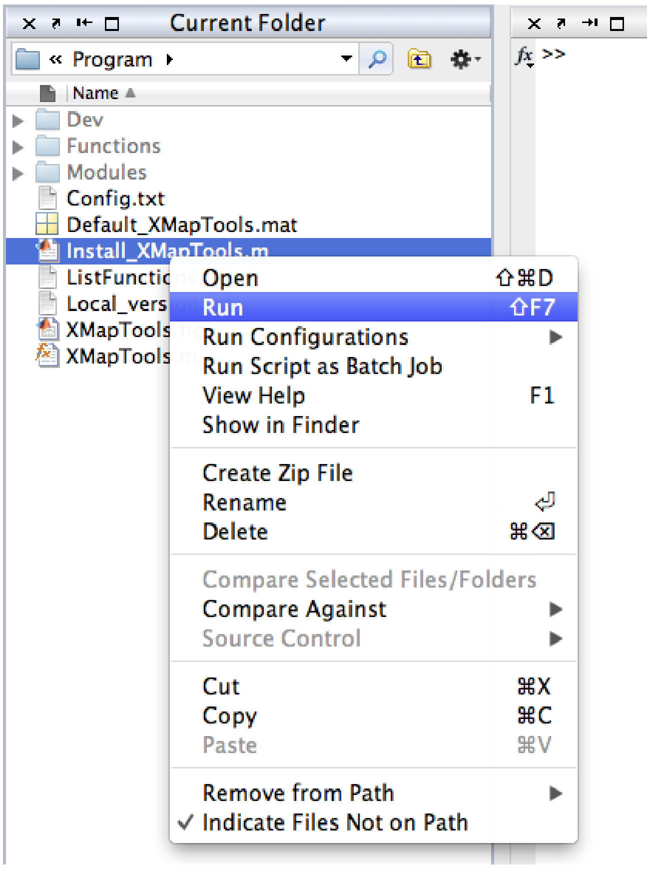


Figure 2.2 – XMapTools *setup. Make a right-click on Install_XMapTools.p and press run to install XMapTools on your computer.*

2.3.2.2 Run Install_XMapTools.p

(1) Run MATLAB$^{©}$

(2) Go to the XMapTools directory (*/Program*) using the *Current Folder* window in MATLAB$^{©}$

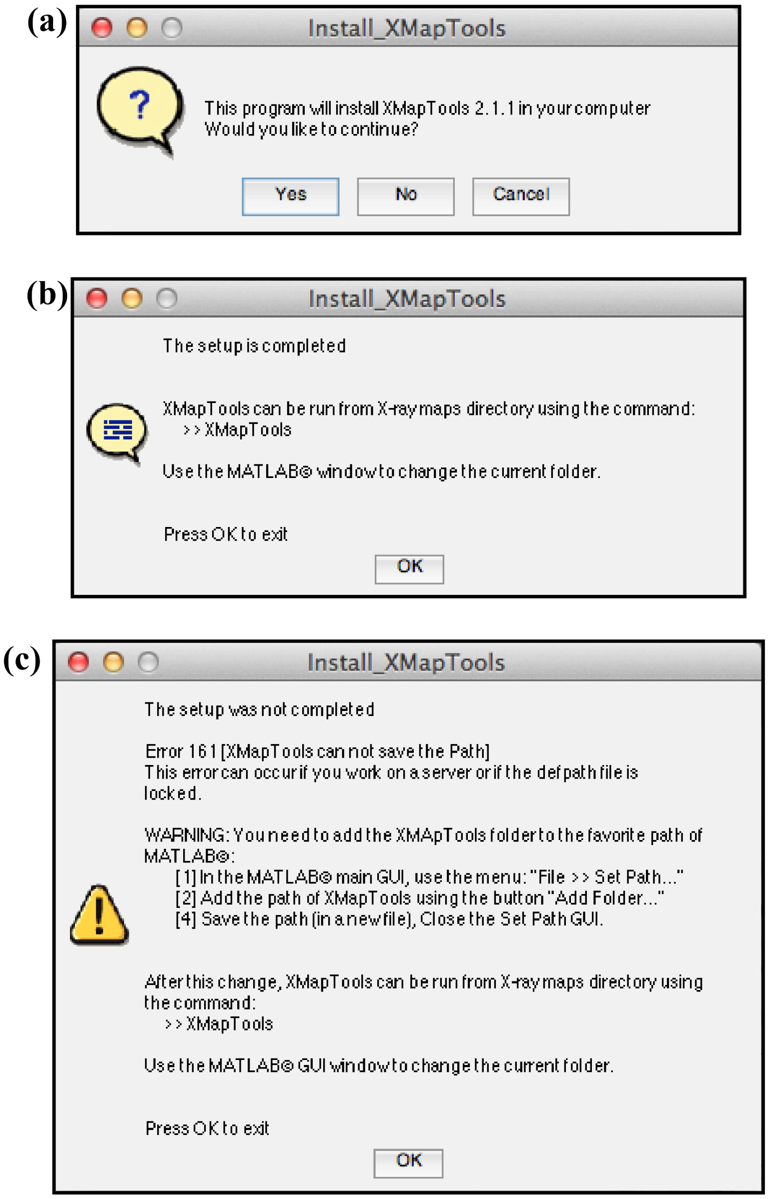
(3) Run the program *Install_XMapTools.p* (see Fig. 2.2, or using in the *MATLAB*$^{©}$ *command window* the case-sensitive command: *» Install_XMapTools*)

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

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

Case 1: **Setup is completed** (see message in Fig. 2.3b). This message is displayed if XMapTools was correctly installed in you 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 you computer. Two solutions may be used to solve the problem (7a and 7b):



This program will install XMapTools 2.1.1 in your computer
Would you like to continue?

The setup is completed

XMapTools can be run from X-ray maps directory using the command:
>> XMapTools

Use the MATLAB© window to change the current folder.

Press OK to exit

The setup was not completed

Error 161 [XMapTools can not save the Path]
This error can occur if you work on a server or if the defpath file is locked.

WARNING: You need to add the XMApTools folder to the favorite path of MATLAB©:
[1] In the MATLAB© main GUI, use the menu: "File >> Set Path..."
[2] Add the path of XMapTools using the button "Add Folder..."
[4] Save the path (in a new file), Close the Set Path GUI.

After this change, XMapTools can be run from X-ray maps directory using the command:
>> XMapTools

Use the MATLAB© GUI window to change the current folder.

Press OK to exit

Figure 2.3 – XMAPTOOLS *setup dialogue boxes*

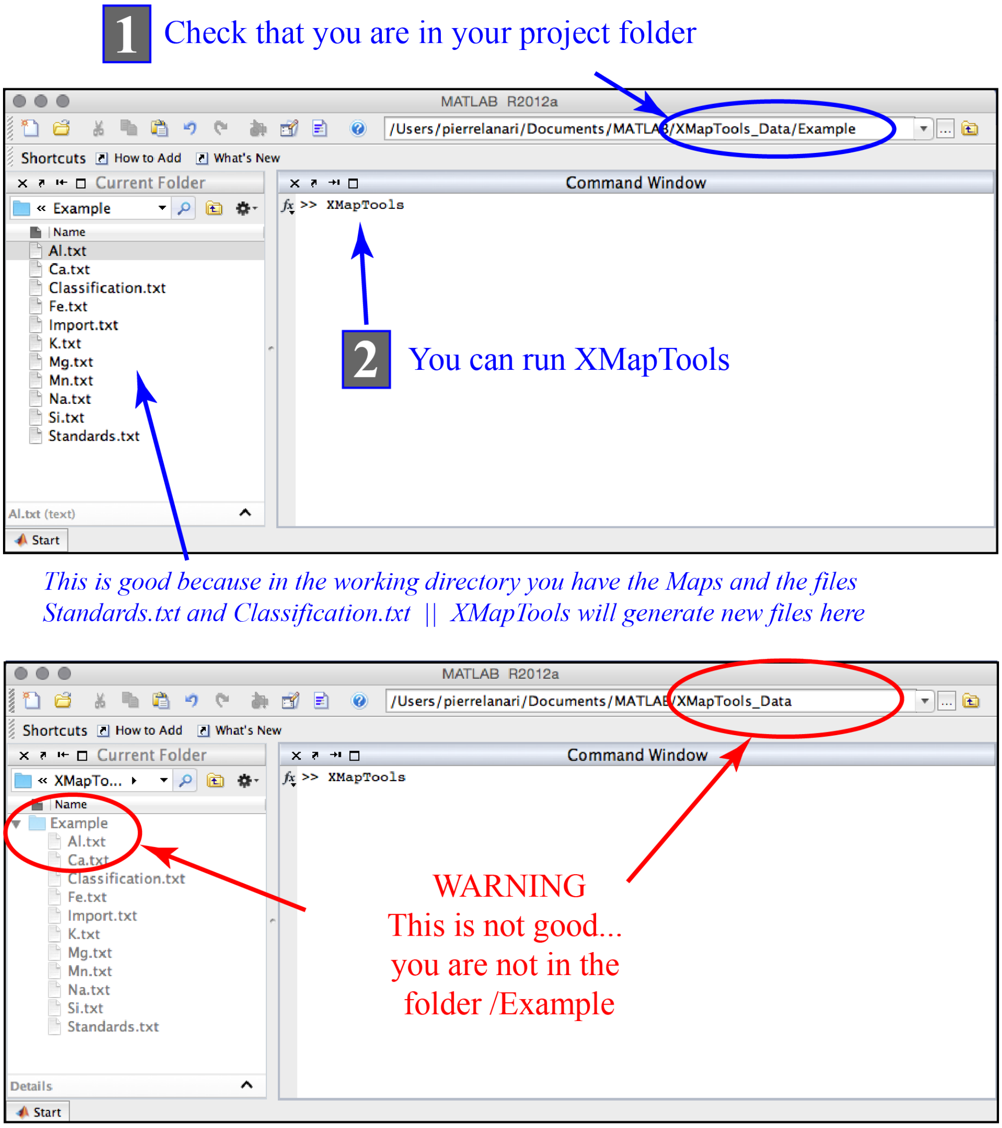
(6a) In the main MATLAB© window, select the menu *File* and *Set Path...* Use the button *Add folder* to add your XMAPTOOLS folder in your favourite paths. Use the button *Save* to save the favourite path file that will be loaded when MATLAB© is launched.

(6b) Try to look at *pathdef.m* file 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© environment. The following steps explain how to run the program in you computer from the MATLAB© command window.

Warning: after setup or update, close MATLAB© and run it again. On some computers, XMAP-


1 Check that you are in your project folder

/Users/pierrelanari/Documents/MATLAB/XMapTools_Data/Example

```
>> XMapTools
```

2 You can run XMapTools

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

/Users/pierrelanari/Documents/MATLAB/XMapTools_Data

```
>> XMapTools
```

WARNING
This is not good...
you are not in the
folder /Example

Figure 2.4 – *Directory check before to run XMapTools*

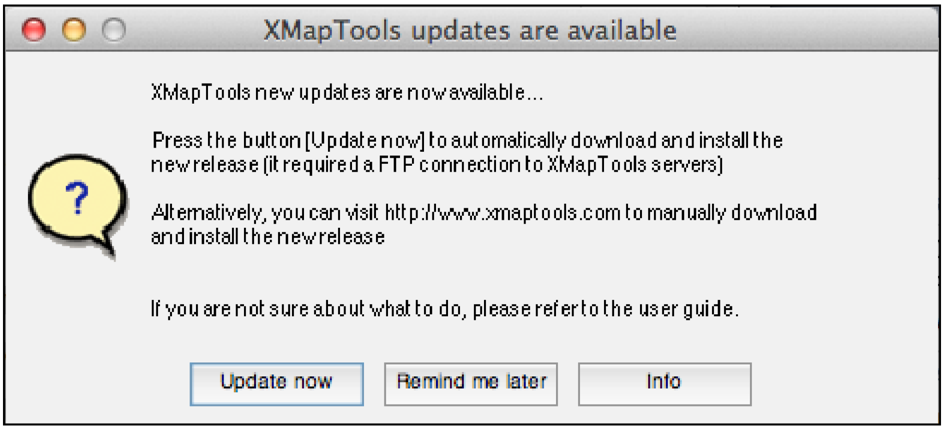
TOOLS graphic user interface seems to not always launched after the setup. this problem is easily solved by restarting MATLAB©.

(1) Run MATLAB©

(2) Set the MATLAB© directory to your XMapTools working directory were are stored the X-ray maps: *.../UserHome/Documents/MATLAB/Xray_Data/ProjectX/*. It is vitally important to set the MATLAB© path to the working directory containing the maps and then to 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© main window.

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

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



XMapTools updates are available

XMapTools new updates are now available...

Press the button [Update now] to automatically download and install the new release (it required a FTP connection to XMapTools servers)

Alternatively, you can visit http://www.xmaptools.com to manually download and install the new release

If you are not sure about what to do, please refer to the user guide.

Figure 2.5 – XMapTools *automatic update dialogue box*

2.4 Update XMapTools

A system that automatically check for updates is included in XMapTools (release 2.1.X and later). 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 the FTP connection used to download the new package. This problem has been fixed in XMapTools 2.1 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 release from the website (see details in section 2.4.1). The folder *Program* stored in the XMapTools setup directory is updated in contrast to the folders: *Examples* and *UserFiles* that are kept unchanged. The user files stored in *UserFiles* are not removed by the automatic update (if *UserFiles* is not stored in *Program*).

In you do not want do 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. A new release must be available on the website.

(1) Run MATLAB©

(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 first removes 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 (not yet implemented)

(1) Login to XMAPTOOLS website using you user name and password and download the new update (not the XMapTools package for first setup, but only the update part that contains the new files in the folder *Program*)

(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© and run the program *Install_XMapTools.p* (follow 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	X-ray maps (WDS, type 1) with compatible names (see below)	Yes
_P.txt - _S.txt - _Zr.txt - _Ni.txt	X-ray maps (EDS, type 2) with compatible names and the EDS code (_)	Optional
TOPO.txt - SEI.txt	Topo and SEI images used for the corrections	Optional
Standards.txt	This file includes maps coordinates and spot analyses for the analytical standardization	Yes
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 SiO2, TiO2, Al2O3, FeO, MnO, MgO, CaO, Na2O, K2O.

The metalloids available are Fe_m, Cu_m.

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

2.6.4 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*

2.6.5 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 the functions in XMAPTOOLS to proceed through the successive steps of the process (e.g. classification, analytical standardization, thermobarometry).

This program description chapter 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 description

General:

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

Display and corrections:

menus: *Add-ons* [M5601]

buttons: *figure/display tools* [B5101] [B5102] [B5103] [B5104] [B5105] [B5106] - *sampling tools* [B5201] [B5202] [B5203] [B5204] - *chemical modules* [B5301] [B5302] [B5303] - *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]

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] [B2411] [B2412]

Results:

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

buttons: *results from external functions* [B3101] [B3102] [B3103] [B3104] - *filtering* [B3201]

3.1.2 XMapTools strategy

The strategy behind XMapTools is intensively described in Lanari et al. (2014b). 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 part enables to (1) add and display 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(%) composition.

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.

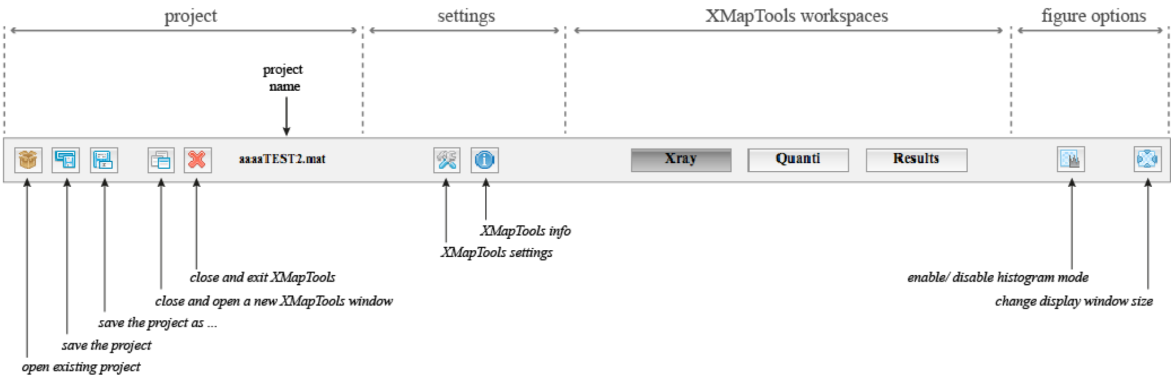
Results workspace allows the calculated results (mineral structural formulas, P-T maps) to be displayed, the results to be exported and enables to compute new variables from the maps.

General functions are provided in all the workspaces such as: (1) plot options, (2) filters, (3) sampling functions and (4) external modules (chemical diagrams): Chem2D,Triplot3D and RGB.

LA-ICP-MS data can be proceeded with 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.

XMapTools projects can be saved as **.mat* files and all the variables becomes easily accessible from the MATLAB© command window.

(a) General



(b) Display and corrections

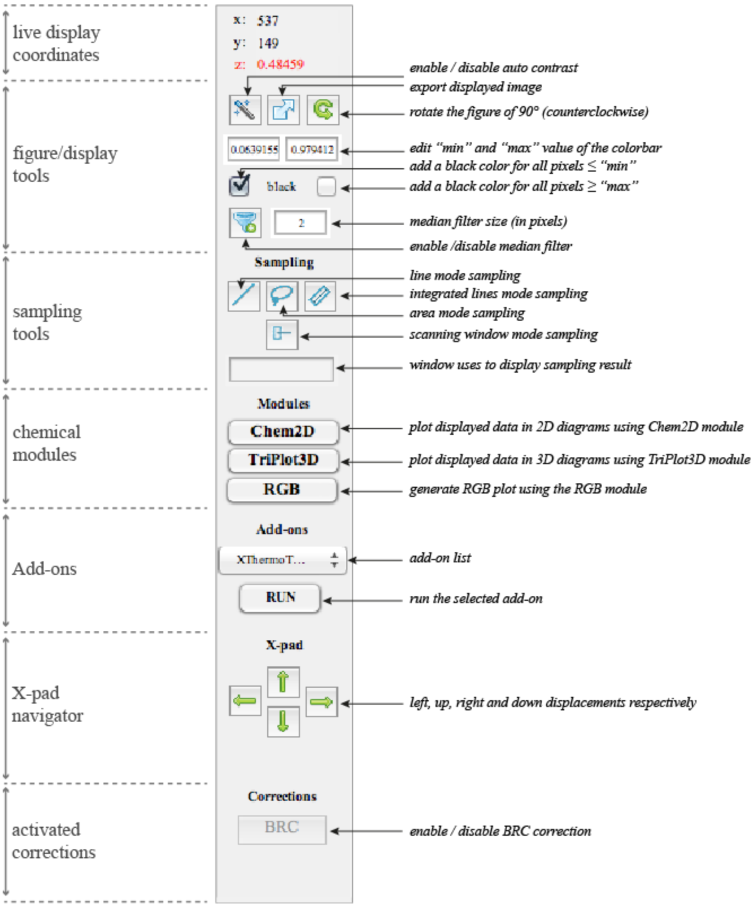
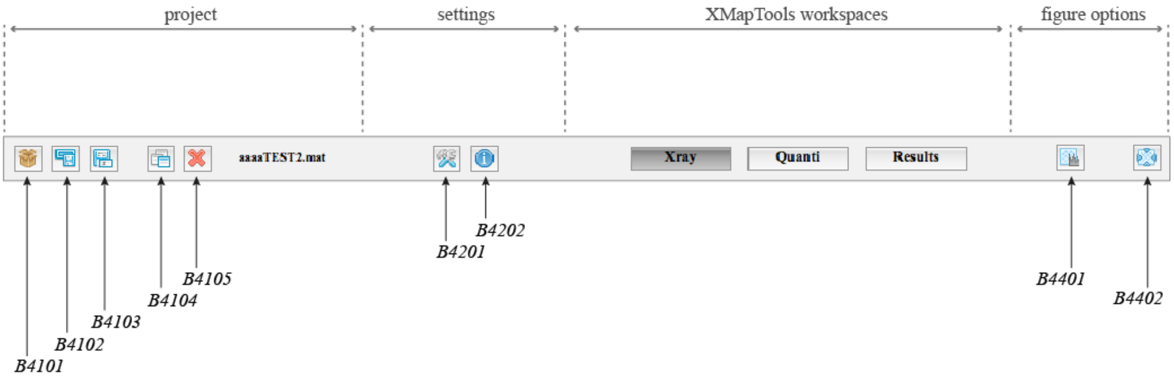


Figure 3.1 – *XMapTools objects and corresponding functions for (a) "general" and (b) "display" windows.*

(a) General



(b) Display and corrections

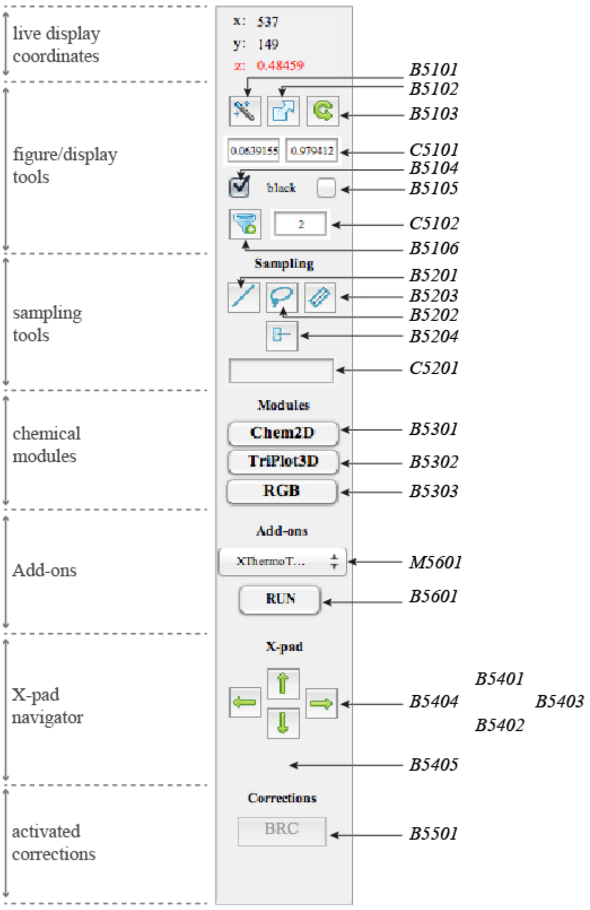


Figure 3.2 – *XMapTools objects and corresponding functions for (a) "general" and (b) "display" windows.*

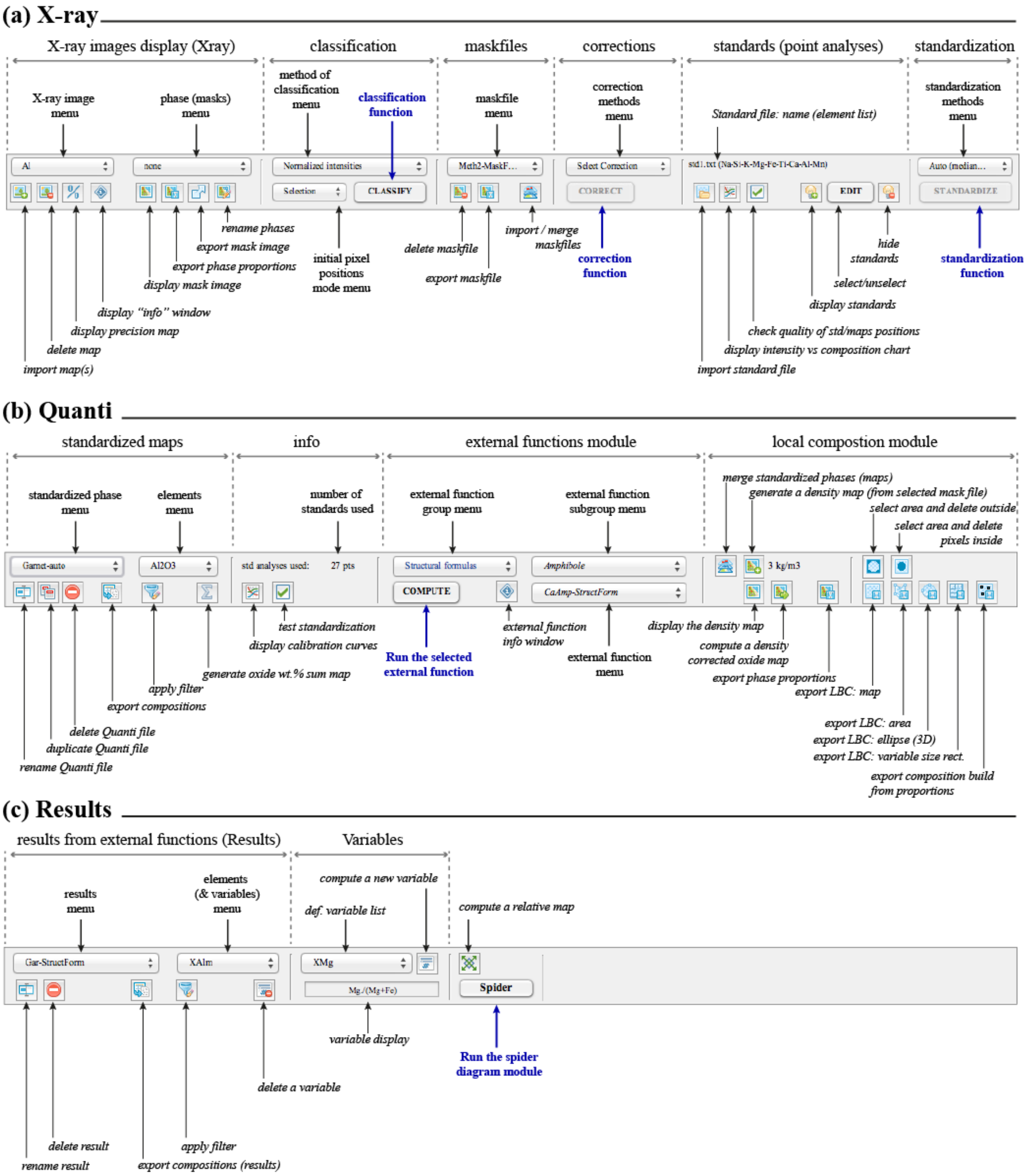


Figure 3.3 – *XMapTools objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.*

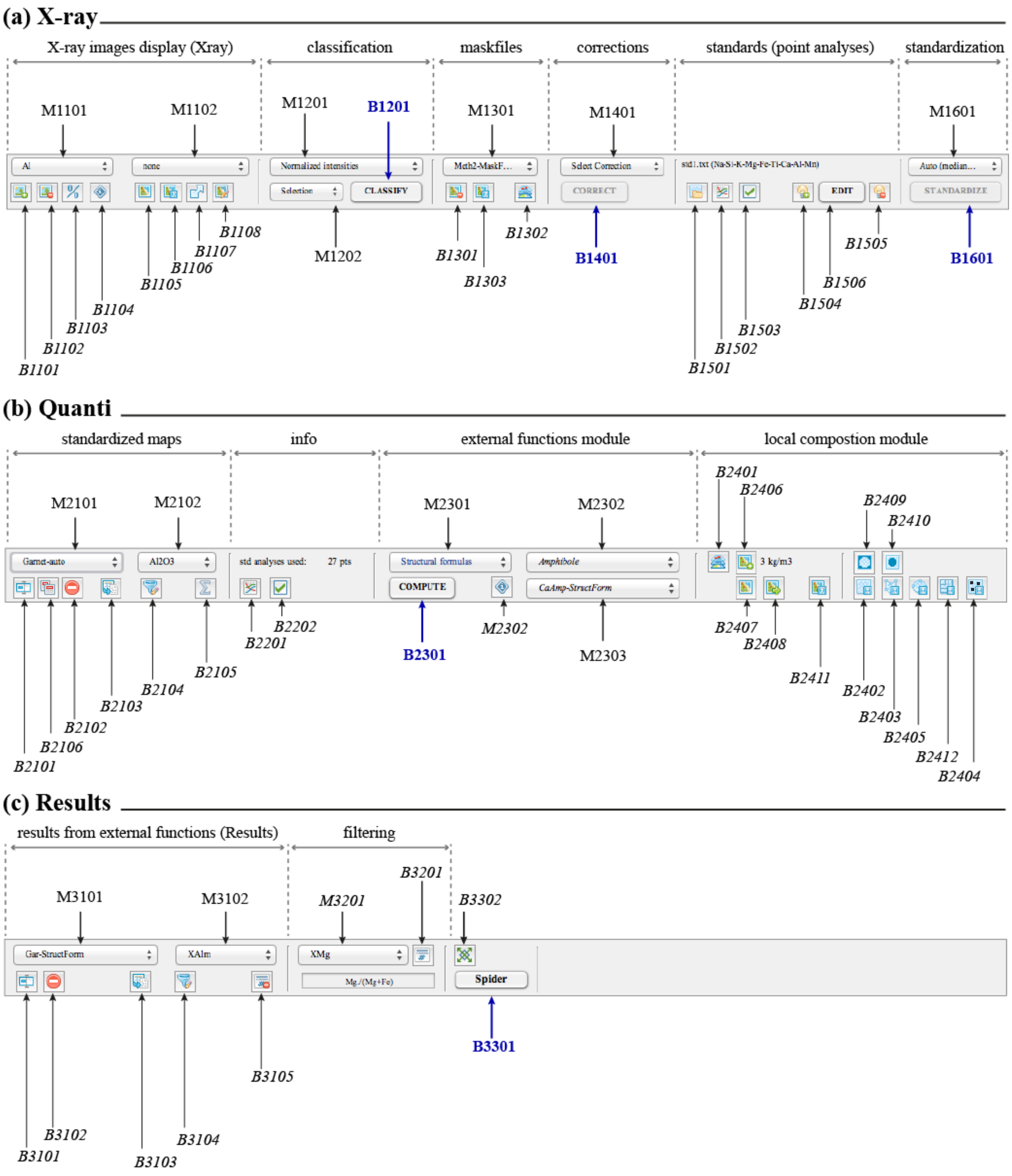


Figure 3.4 – *XMapTools objects and corresponding processing functions for (a) "X-ray", (b) "Quanti" and (c) "Results" workspaces.*

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© formatted binary file (MAT-file, extension: _*.mat_). The following variables (structures): *Corrections, Data, Directory, ListMap, MaskFile, Profils, 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 close the current XMapTools session, clear all the variables of the workspace and run a new XMapTools session. This function must be used before to load a new project, because it allows to clear all the variables from the previous work.

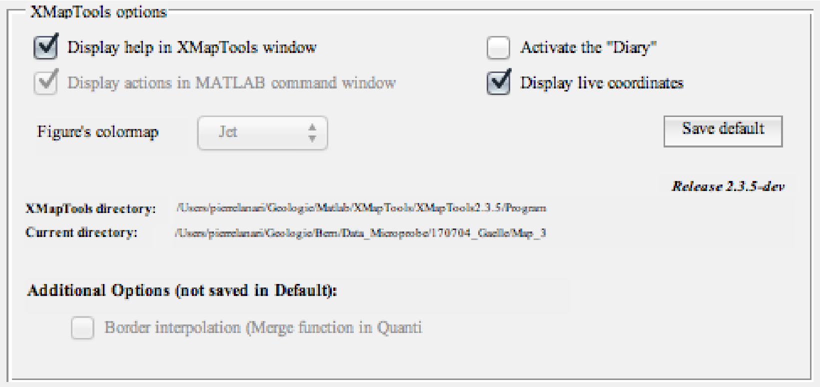
[B4105] The button *close and exit* may be used to end the current XMapTools session and to close the program.

3.2.2 General settings

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

XMapTools settings options are:

- **Display help in XMapTools window [default: enabled]** allowing the user help texts to be displayed into the main window (blue text at the bottom).
- **Activate the diary [default: disabled]** enables to save all the info displayed in the MATLAB© command window in a diary file.
- **Display live coordinates [default: enabled]** allowing the live coordinate to be displayed in the main window (top left, see description in section 3.3). This option may on some old computer cause notable slowing down during the use of the software; it can be disabled here.
- **Figure's colormap [default: JET]** allows the figure's colormap to be set. Available sets are: Jet (Default); ColdWarm; WYRK; Hot; Gray; HSV; Cool; Spring; Summer; Autumn; Winter; Bone; Copper; Pink.
- **Border interpolation (merge function in Quanti) [default: unselected]** activates the border interpolation option in the function merge [B2401].



XMapTools options

☑ Display help in XMapTools window

☑ Display actions in MATLAB command window

☐ Activate the "Diary"

☑ Display live coordinates

Figure's colormap: Jet

Release 2.3.5-dev

XMapTools directory: /Users/pierrelanari/Geologie/Matlab/XMapTools/XMapTools2.3.5/Program

Current directory: /Users/pierrelanari/Geologie/Bern/Data_Microprobe/170704_Gaelle/Map_3

Additional Options (not saved in Default):

☐ Border interpolation (Merge function in Quanti

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

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 alos 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).

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 axe 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

[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* allows the image currently displayed in the figure window to be exported in a new window. This function opens exactly the same figure (including images and user's selections, points, lines...) in a new MATLAB© figure window.

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: $*.fig$, $*.ai$, $*.eps$, $*.jpg$, $*.pcx$, $*.pbm$, $*.pdf$, $*.pgm$, $*.png$, $*.ppm$, $*.pkm$ and $*.tif$ (list depending on the MATLAB© version used). Pdf files are convenient as they can be easily edited using a program such as Adobe Illustrator©.

[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

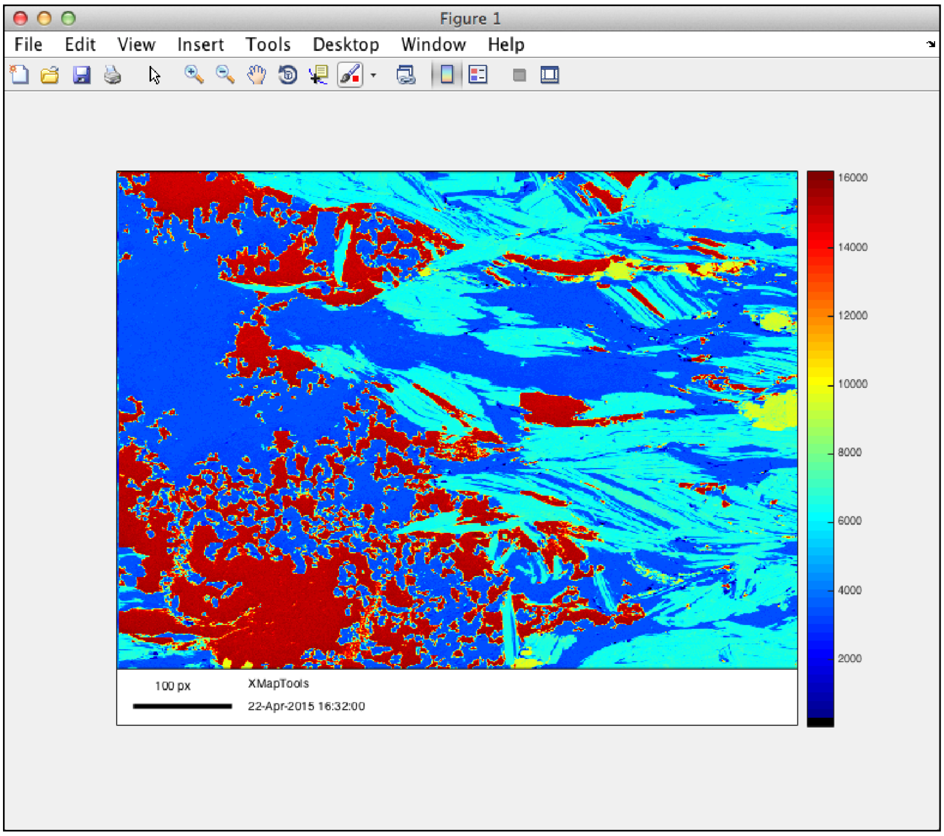


Figure 3.6 – *MATLAB© Window with the exported figure (see button [B5102])*

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

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

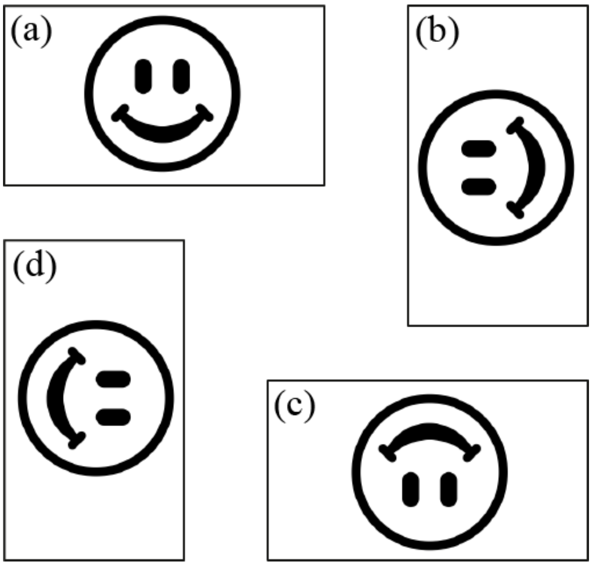


Figure 3.7 – *Orientation positions available for the main figure display (see rotate function [B5103])*

3.3.3 Sampling tools

[B5201] The button *line mode sampling* enables to generate a diagram showing the variation of the pixel compositions along a given transect (line). The sampling line is defined by two spots 1 and 2; the direction is from spot 1 to spot 2 (1 and 2, see Fig. 3.9).

This sampling function can be applied to (1) the displayed map [single map mode] or (2) to a list of maps selected by the user [multi maps mode]. A menu enables to select the sampling mode (Fig. 3.8). If the multi maps mode is selected, it is possible to select the list of element maps from the selected X-ray, quanti or result.

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

```
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)*

```
Sampling from XMapTools
08–Aug–2017
Method: Area

Ref      Value    StdDev   N       StdErr
1.0000   167.55   15.48    2140    0.3347
```

Code 3.2 – *Example of exported file (sampling mode area)*

[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. 3.9b). Selection mode is disabled using right-clicking (spot 11, in Fig. 3.9b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.9b. The result is displayed in the cell [C5201]. The results including the average, the standard deviation (1σ), the number of

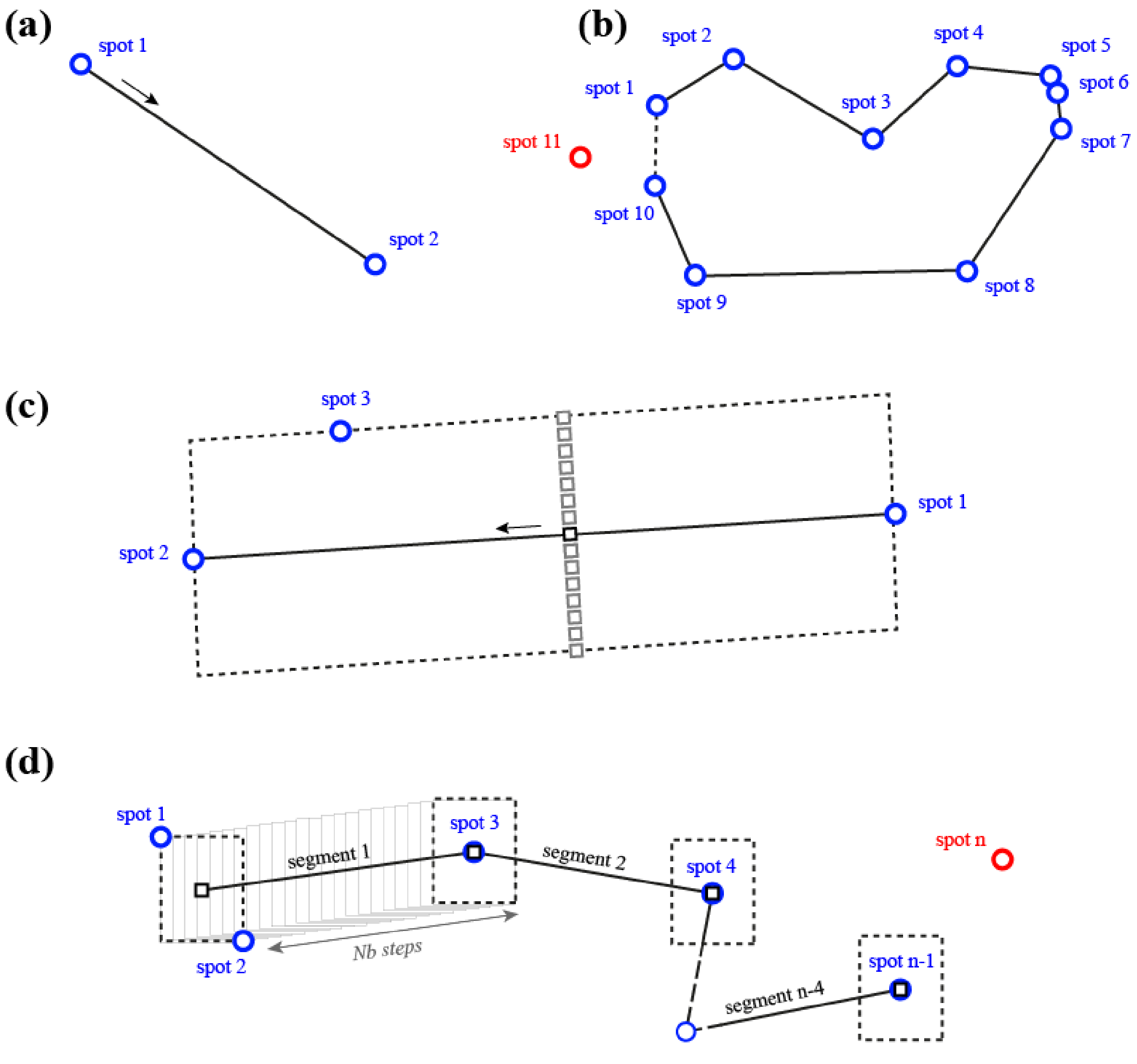


Figure 3.9 – *Sampling functions: (a) line mode [C5201], (b) area mode [C5202], (c) integrated lines mode [C5203] and (d) scanning window [C5204]*

pixels and the standard error (1σ) 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*.

[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. 3.9c). 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. 3.9c).

Seven display options are available:

- [1] Mean + All
- [2] Mean only
- [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. 3.10.

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 and 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. 3.11). In the given example, the rectangle is displaced from the starting point (left on Fig. 3.11-a) to the end of the path (right on Fig. 3.11-a) along 3 segments with 3 × 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. 3.11-b).

Click two points to define the reference rectangle and successively select the location where you want to move next the center (see Fig. 3.9) 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 3.11 the distances have been converted from pixels to μm.

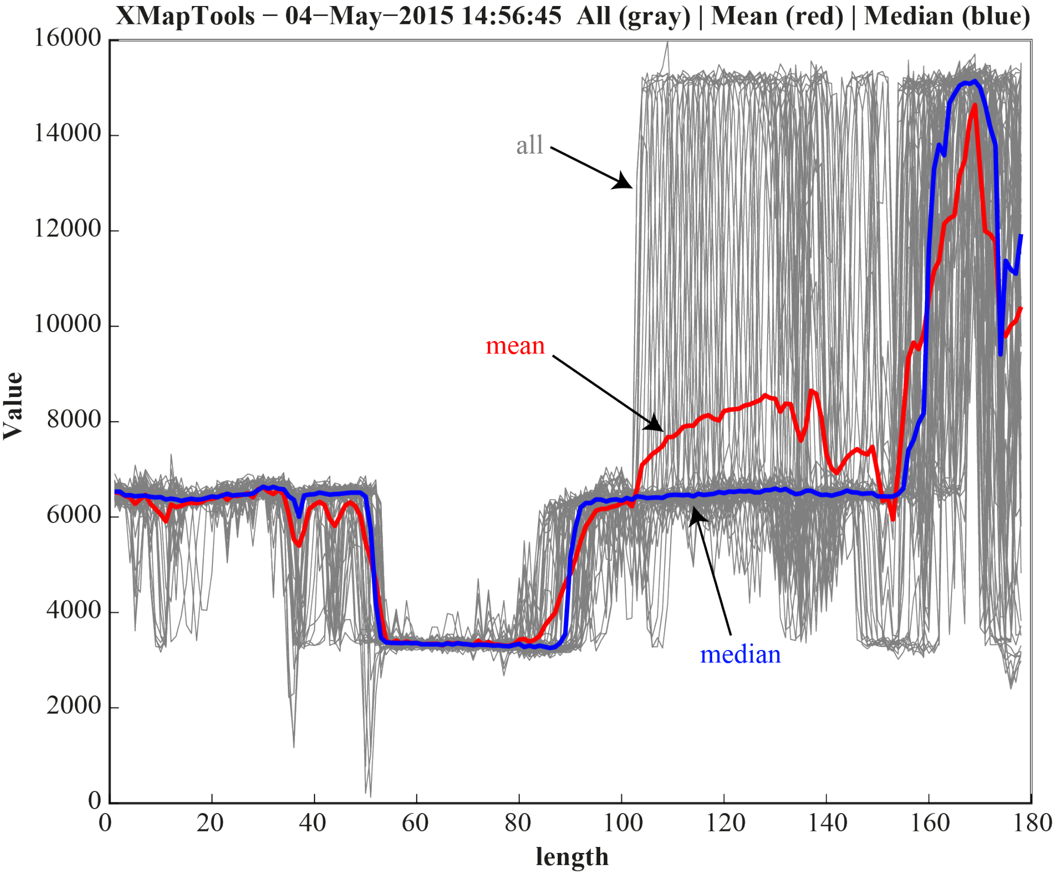


Figure 3.10 – *Example of sampling integrated lines mode.*

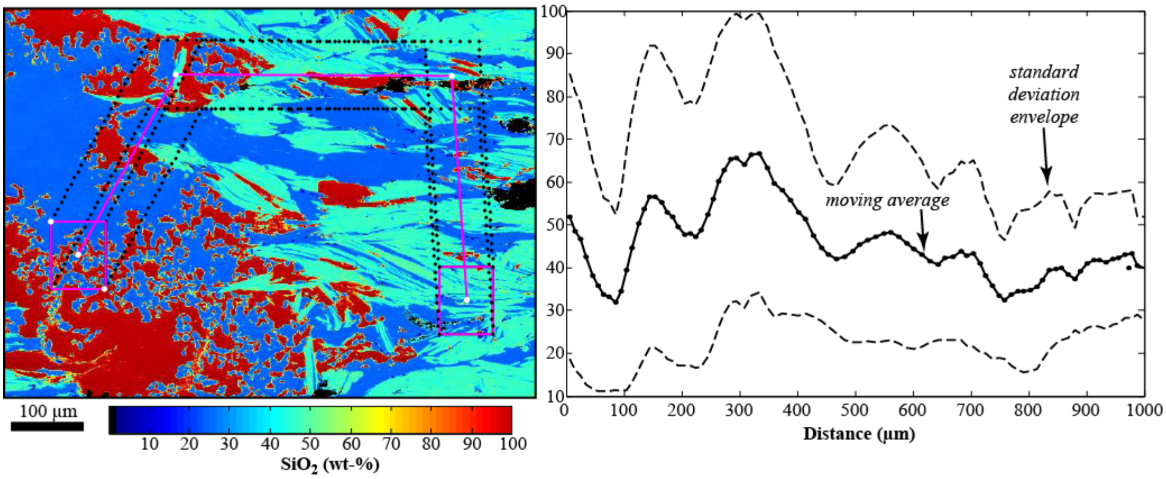


Figure 3.11 – *Example of sampling using (a) a scanning window and the exported (b) the moving average and standard deviation.*

3.3.4 Chemical modules

The buttons [B5301] *Chem2D*, [B5302] *TriPlot2D* and [B5303] *RGB* 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.

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].

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. 3.12) contains some correction fonctions 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:

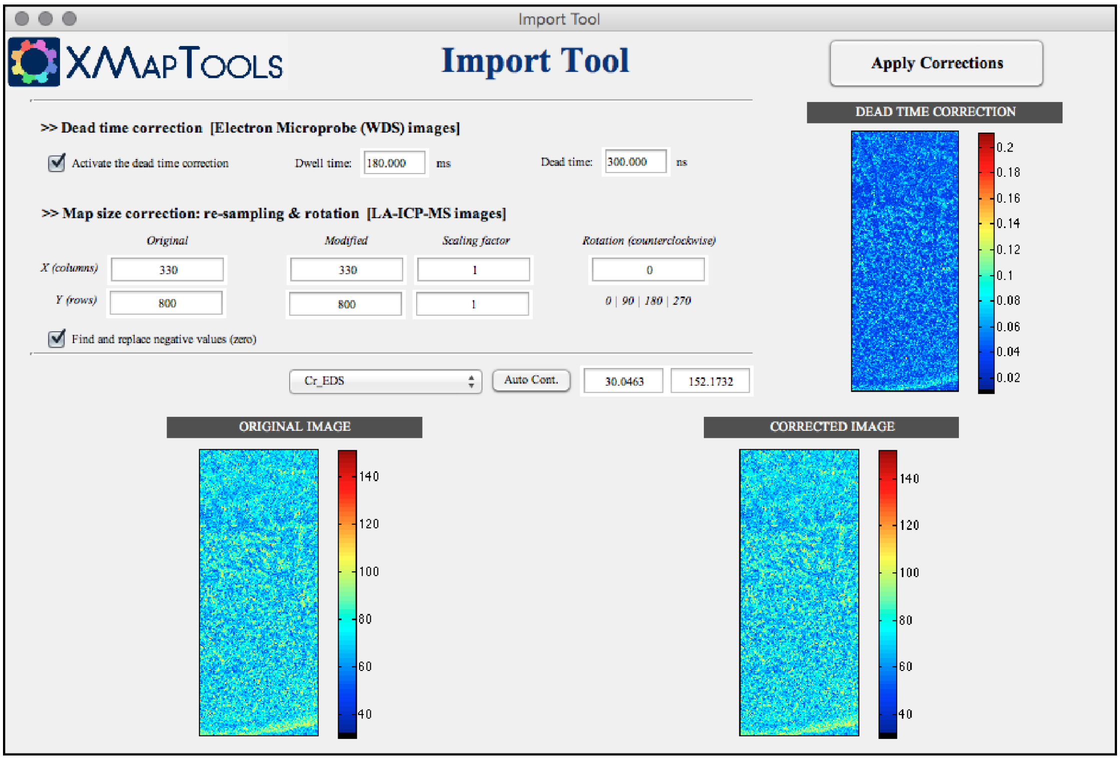
  $$I_{corr} = \frac{I_{measured}}{1 - DT \times 10^{-9} \times I_{measured}} \tag{3.1}$$

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

- *LA-ICP-MS*: Map-size correction: re-sampling and rotation. Scaling factors (integers) can be use to modify the size of the map. Positive scaling factors shrink the image using re-sampling, whereas negative scaling factors expend the image by duplicating the pixels. An example of re-sampling is provided in figure 3.13.

- *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© command window (see examples for EPMA insert 3.4 and LA-ICP-MS insert 3.5 below)



>> Dead time correction [Electron Microprobe (WDS) images]

☑ Activate the dead time correction Dwell time: 180.000 ms Dead time: 300.000 ns

>> Map size correction: re-sampling & rotation [LA-ICP-MS images]

	Original	*Modified*	*Scaling factor*	*Rotation (counterclockwise)*
X (columns)	330	330	1	0
Y (rows)	800	800	1	*0 | 90 | 180 | 270*

☑ Find and replace negative values (zero)

Cr_EDS Auto Cont. 30.0463 152.1732

Figure 3.12 – *Import module of XMapTools*

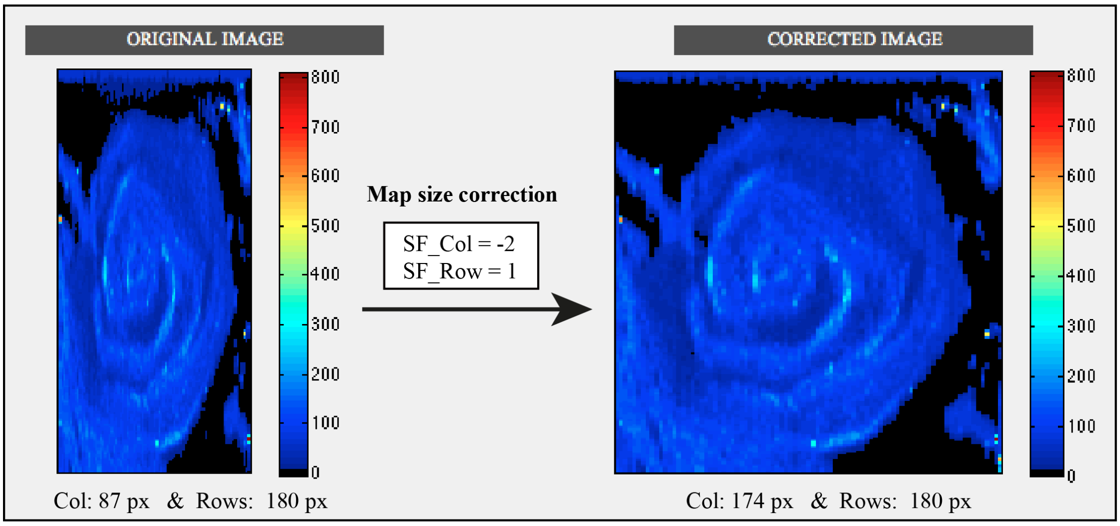


Figure 3.13 – *Example of map size correction for LA-ICP-MS images*

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 2σ (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 2σ; (5) median intensity of displayed pixels and the corresponding uncertainty at 2σ; (6) standard deviation; (7) lower and (8) upper intensity values; (9) BRC, (10) TRC and (11) MPC correction info (see section 3.4.4).

[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 2.6.4. 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 used this file to specify the initial pixel set during the classification. Press yes to continue and no to open an other 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 *Chem2D* 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© (see example below).

Example: Four mask files (Chlorite.txt; Phengite.txt; Plagioclase.txt; and Quartz.txt) generated from *Chem2D* 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
BRC	Border-removing correction	APPLY	No	existing mask file
TRC	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

Table 3.1 – *Corrections available in XMapTools, modes and requirements*

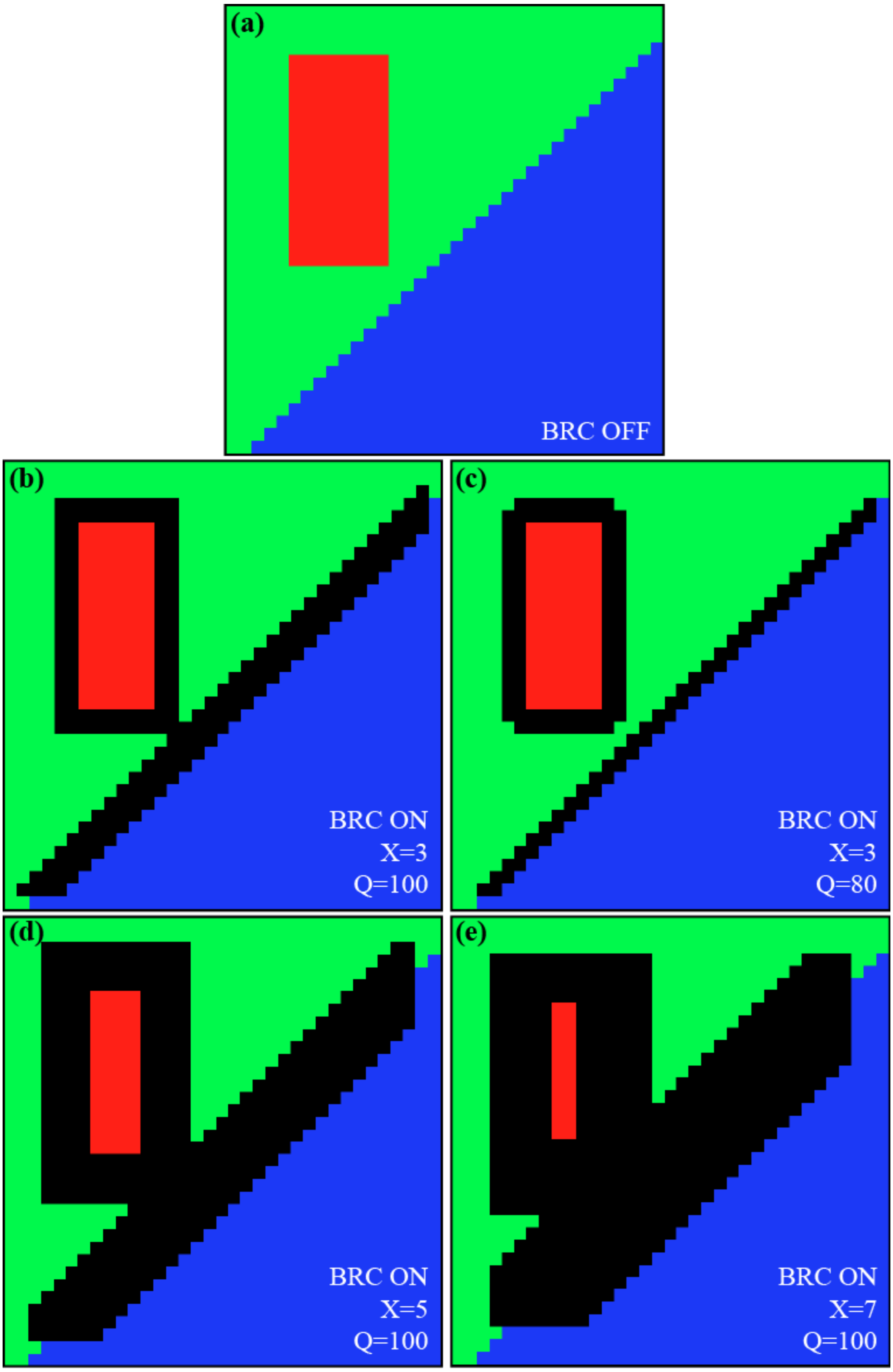


Figure 3.14 – *Examples of BRC correction with various X and Q parameters. This small map* (35×35 *pixels*^{2}*) exhibits three phases (Phase 1 in red; Phase 2 in green; Phase 3 in blue). Pixels removed by BRC are plotted in black. A complete description of this map can be found in Fig. 1.3.*

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 3.14. 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:

$$px(i,j) \tag{3.2}$$

with

$$((X-1)/2) < i < i_{max} - ((X-1)/2) \tag{3.3}$$

and

$$((X-1)/2) < j < j_{max} - ((X-1)/2) \tag{3.4}$$

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

$$\sum_{1}^{X^2} (px(i-(X-1)/2 : i+(X-1)/2, j-(X-1)/2 : j+(X-1)/2))) < X^2 \frac{Q}{100} \tag{3.5}$$

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

The equation (3.5) 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.

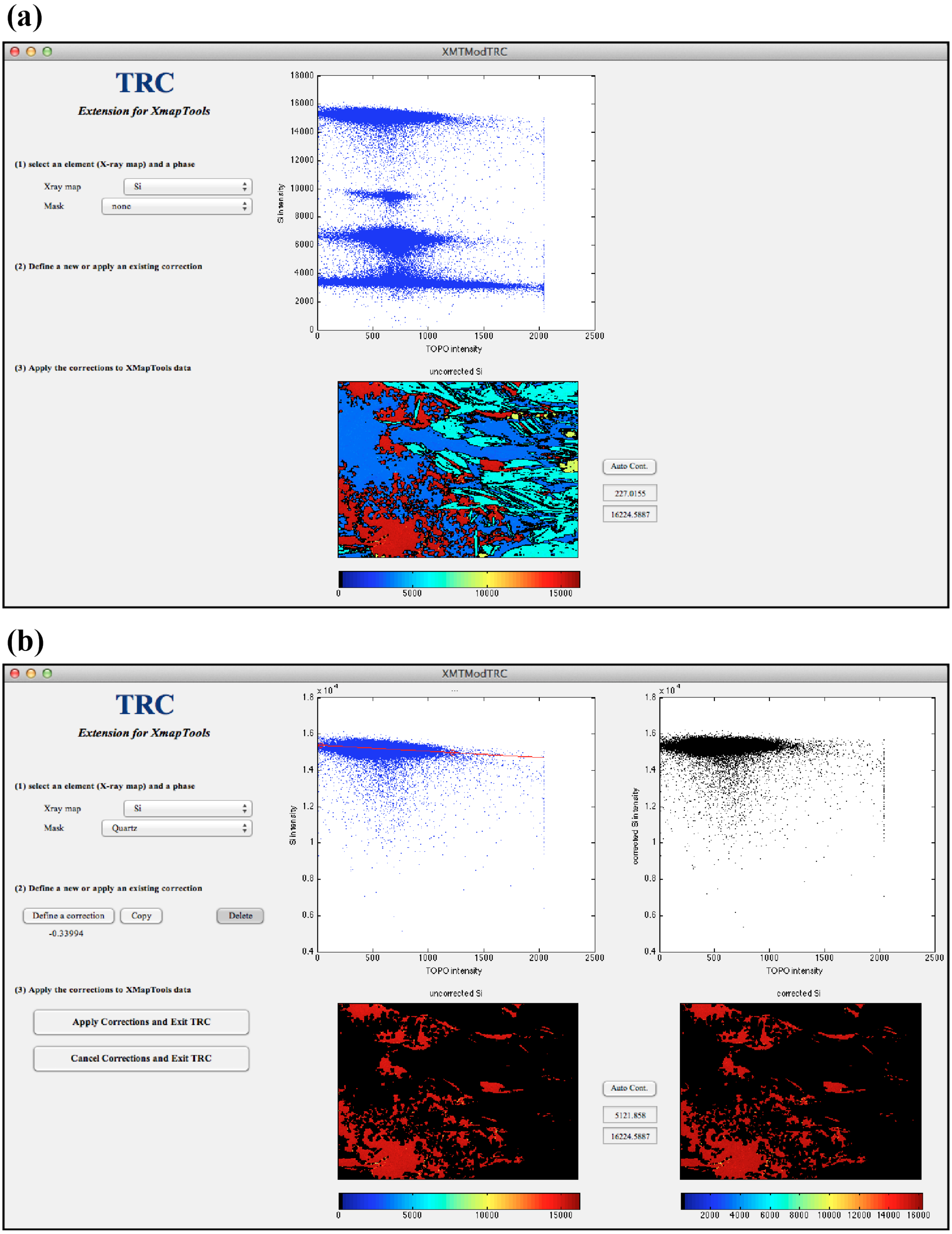
Examples of *BRC* correction are given in fig. 3.14. Corrections are applied to a small map exhibiting three phases plotted with three colors (red, green and blue in Fig. 3.14a). Several combinations of X and Q parameters have been tested and results are reported in figs. 3.14b, c, d and e. For a fixed 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. 3.15) 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.



(a)

(1) select an element (X-ray map) and a phase

Xray map: Si

Mask: none

(2) Define a new or apply an existing correction

(3) Apply the corrections to XMapTools data

227.0155

16224.5887

(b)

(1) select an element (X-ray map) and a phase

Xray map: Si

Mask: Quartz

(2) Define a new or apply an existing correction

-0.33994

(3) Apply the corrections to XMapTools data

5121.858

16224.5887

Figure 3.15 – *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 3.15. One element (e.g. Si) can be selected using the menu *X-ray maps* (Fig. 3.15a). 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 3.15b the phase quartz is selected to correct for Si. A linear relationship (red line in Fig. 3.15b) 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. 3.15b).

The correction straight line defined above may be written as:

$$\Delta I = a \times I_{topo} \tag{3.6}$$

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

$$I_{corr} = I_{meas} - \Delta I \tag{3.7}$$

Together with Eq. 3.6 this gives:

$$I_{corr} = I_{meas} - a \times I_{topo} \tag{3.8}$$

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

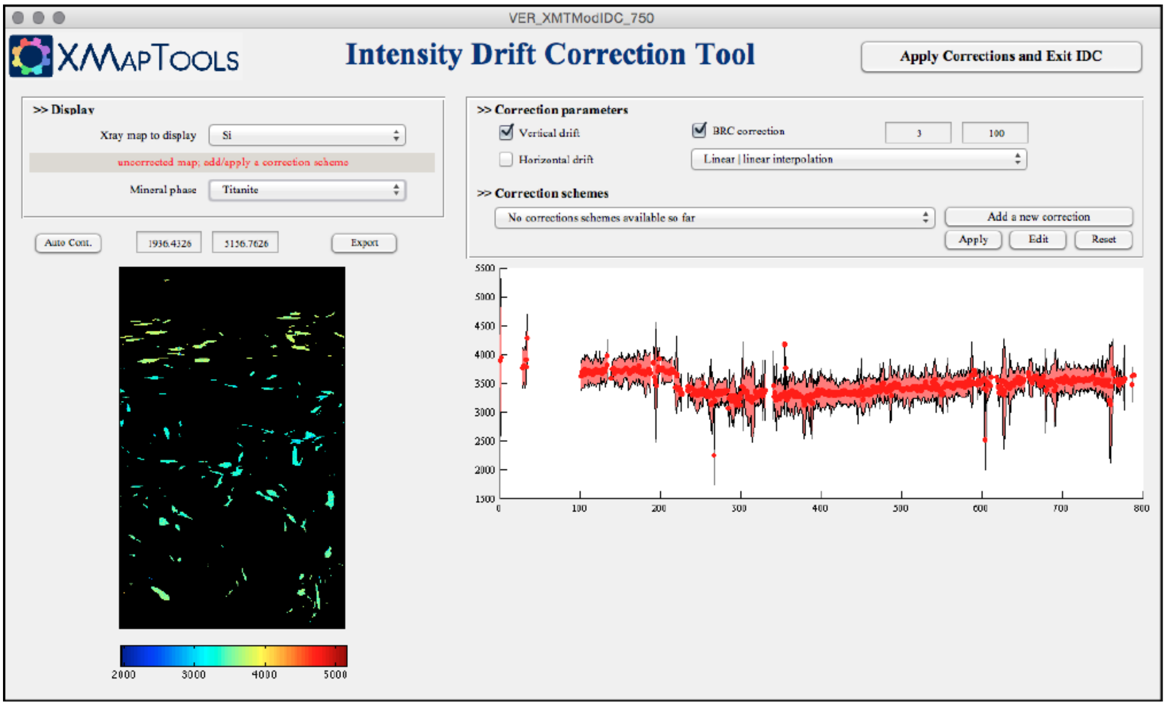
Intensity drift correction (*IDC*) is a correction function that aims to correct any time-dependent intensity drift that can have occurred during the acquisition. Relatively slight drifts (few %) are systematically reported on some EPMA instruments mainly caused by variations of the beam current at the 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 accros 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. 3.16) 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 3.16. The measured map of Si in titanite (Fig. 3.16a) exhibit vertical variations of the number of counts for Si. this variation is caused by a 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. 3.16) it is possible to specify the direction of acquisition, i.e. *horizontal* or *vertical* (vertical in the example shown in Fig. 3.16). 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)


VER_XMTModIDC_750

Intensity Drift Correction Tool

>> Display

Xray map to display: Si

uncorrected map; add/apply a correction scheme

Mineral phase: Titanite

1936.4326 5156.7626

>> Correction parameters

☑ Vertical drift

☐ Horizontal drift

☑ BRC correction 3 100

Linear | linear interpolation

>> Correction schemes

No corrections schemes available so far

Figure 3.16 – *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* (neareast 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. 3.16). The red dot show the average intensity of each line or column with the relative error and standard deviation uncertainty envelopppe (at 2σ).

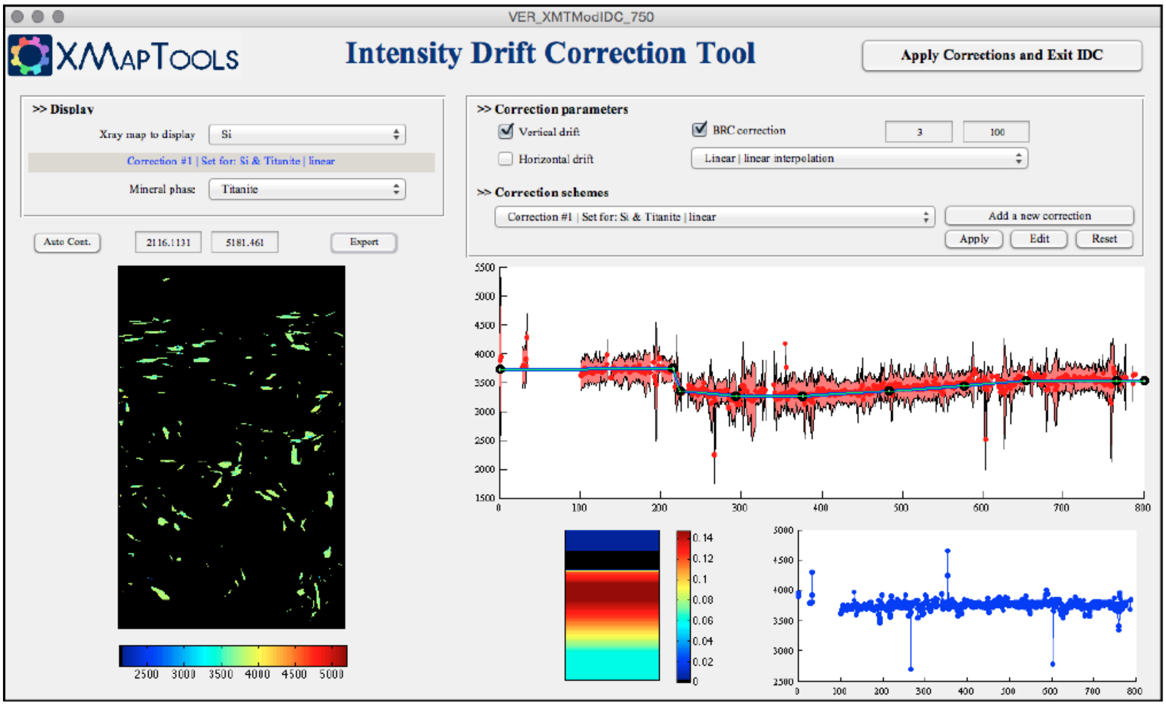
A correction scheme can be defined by pressing the button *Add a new correction*. The interpolation points used to define the correction function are selected by clicking onto the figure (see black points in Fig. 3.17). This selection is always done from left to right; a new point is registered only 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. 3.17). The interpolation method can be changed after the selection of the points.

The correction map (see map in Fig. 3.17 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. 3.16 and Fig. 3.17).

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



VER_XMTModIDC_750

Intensity Drift Correction Tool

>> Display

Xray map to display: Si

Correction #1 | Set for: Si & Titanite | linear

Mineral phase: Titanite

2116.1131

5181.461

>> Correction parameters

☑ Vertical drift

☐ Horizontal drift

☑ BRC correction 3 100

Linear | linear interpolation

>> Correction schemes

Correction #1 | Set for: Si & Titanite | linear

Figure 3.17 – *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 BC1 - Background correction (map)

This function is not yet available for public use. Work in progress.

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 2.6.5). 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  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 3.18a) and in the X-ray map Al (Fig 3.18b). 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*

[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 ΔX and ΔY two variables expressed in pixels. For a given spot analysis with the initial coordinate X_j and Y_j, the map of the correlation coefficient (τ) for the element El_i is calculated from the position:

$$(X_j - \Delta X, Y_j - \Delta Y) \tag{3.9}$$

to the position

$$(X_j + \Delta X, Y_j + \Delta Y) \tag{3.10}$$

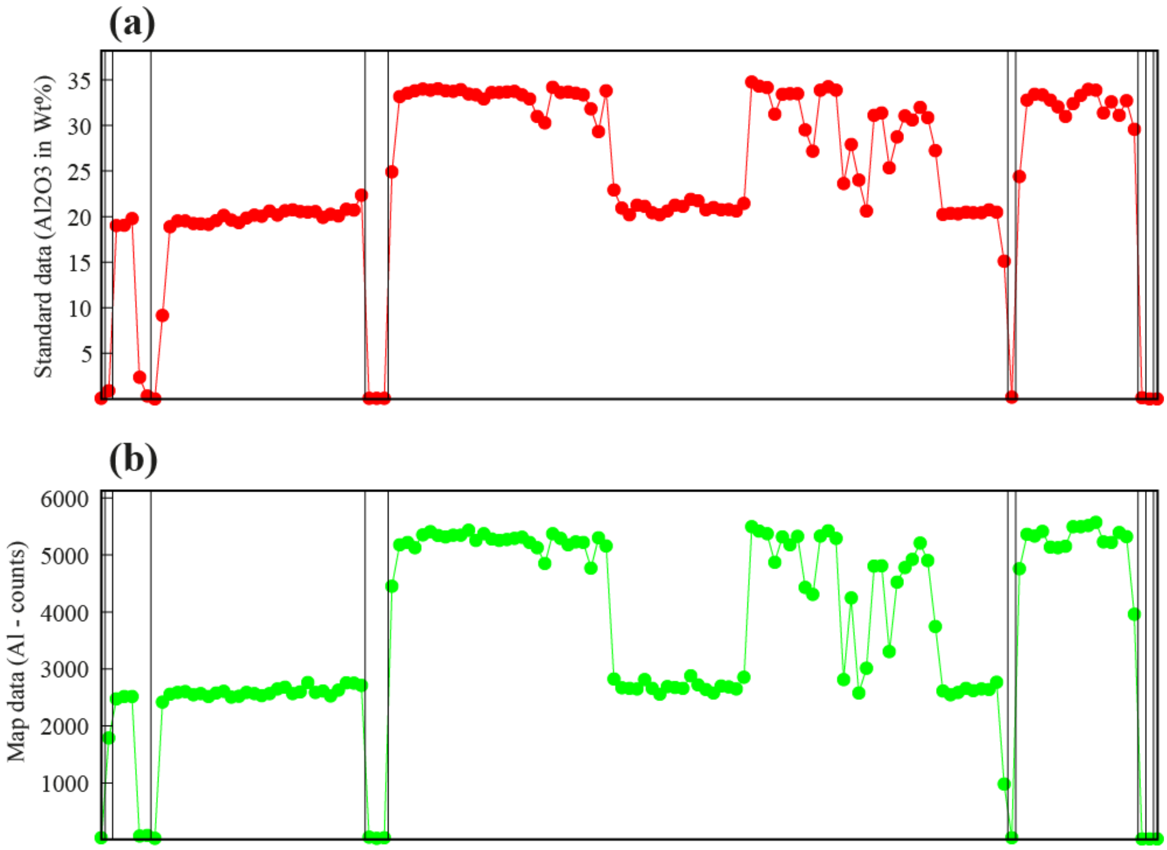


Figure 3.18 – *Function display intensity vs composition chart*

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

Two figures are generated by the function *check quality of std/maps positions*. The first figure contains the maps of the correlation coefficients $\tau(El_i)$ (Fig. 3.19). 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 3.19 and 3.20). The axis values are given in pixels from $-\Delta X$ to ΔX and from $-\Delta Y$ to ΔY. In this example the default values $\Delta X = 10px$ and $\Delta Y = 10px$ are used.

The second figure 3.20 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):

$$M = \sum El = 1n(\tau_i)^2 \tag{3.11}$$

This method works provided that the individual maps from figure 3.19 show contrasted τ values ranging from $0.2 - 0.4$ to $0.9 - 1$. If no good correlation exists, the higher value of the second figure could not be the optimal position. In this case a problem should have occurred with the transformation of the map coordinates or the best position can be out of range. Greater values of ΔX and ΔY might be used.

[B1504] 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.

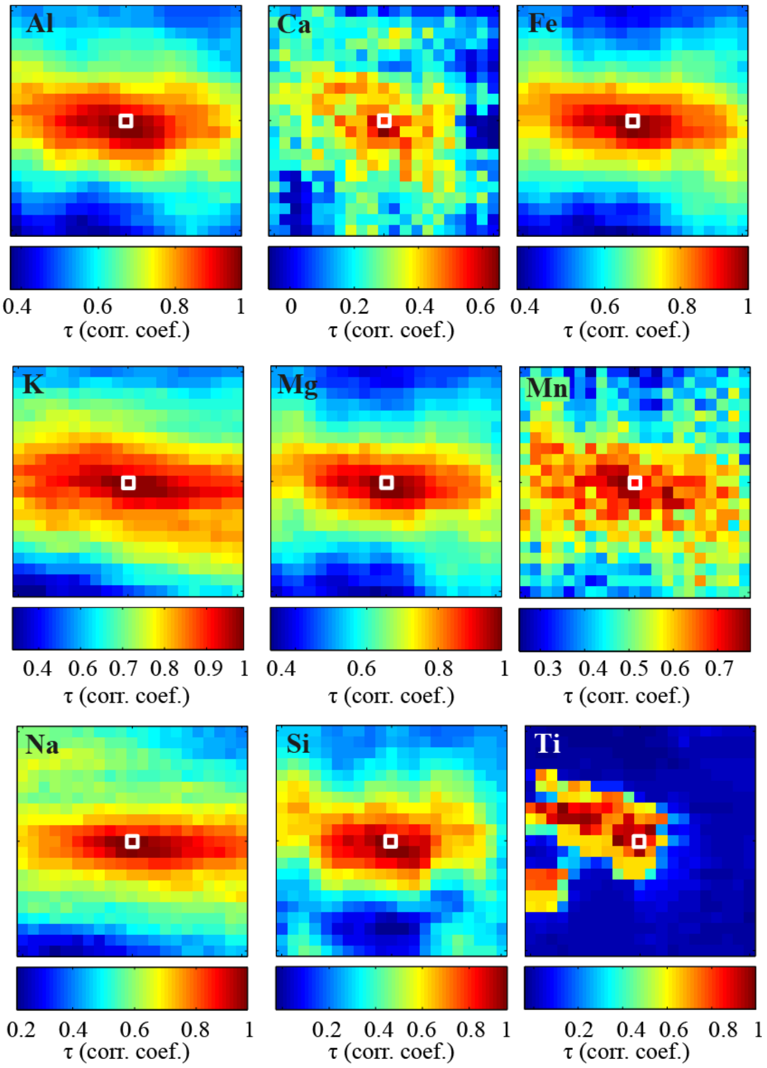


Figure 3.19 – *Function: check quality of std/maps positions. Correlation coefficients (τ) maps for each element (El_i) (see text for details)*

[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.

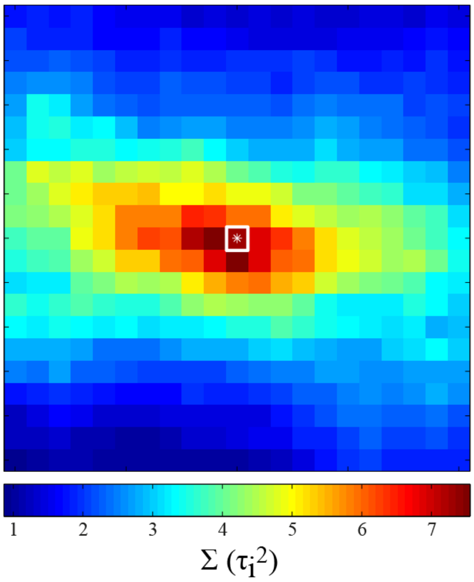


Figure 3.20 – *Function: check quality of std/maps positions.* $\sum(\tau_i)^2$ *(see text for details)*

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 the XMapTools paper Lanari et al. (2014b) and references therein.

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

Four standardization methods are available in XMapTools:

- *Advanced standardization* is a semi-automatic method of standardization that includes a background correction (Lanari et al. submitted). The advanced standardization is applied using the module *XMTStandardizationTool* (see §3.4.6.3). This method is the default method.
- *Auto (median approach)* is an automatic method of standardization in which the calibration curves were defined automatically using a median approach.
- *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 for the standardization of homogeneous phases with known composition such as quartz (100% of SiO_2). The calibration curve is defined using the median values of the intensities and the composition provided by the user.
- *Transfert to Quanti* allows 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 standardized.

NB: When the standardization is achieved (end of the standardization function) the program generate a *standardized phase* containing the standardized data and switches automatically to the second 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).

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:

$$Y = \frac{Y_C}{X_C} X \tag{3.12}$$

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

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

$$X_i^p = \frac{X_C}{YX_C} Y_i^p \tag{3.13}$$

Any calibration curve defined with the equation 3.12 intersects the X- and Y-axis origin $(0, 0)$. This assumption generates systematic deviations for the low-concentrated elements and result in an imprecise standardization.

Example: An example of the advanced standardization of garnet is shown in Figure 3.21. The advanced standardization is compared with the automated approach for element showing low concentrations such as MnO and MgO. A complete description is provided in Lanari et al. (submitted).

3.4.6.2 Background correction in XMapTools

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

$$Y = \frac{Y_C - Y_B}{X_C} X + Y_B \tag{3.14}$$

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

$$X_i^p = (Y_i^p - Y_B) \frac{X_C}{Y_C - Y_B} \tag{3.15}$$

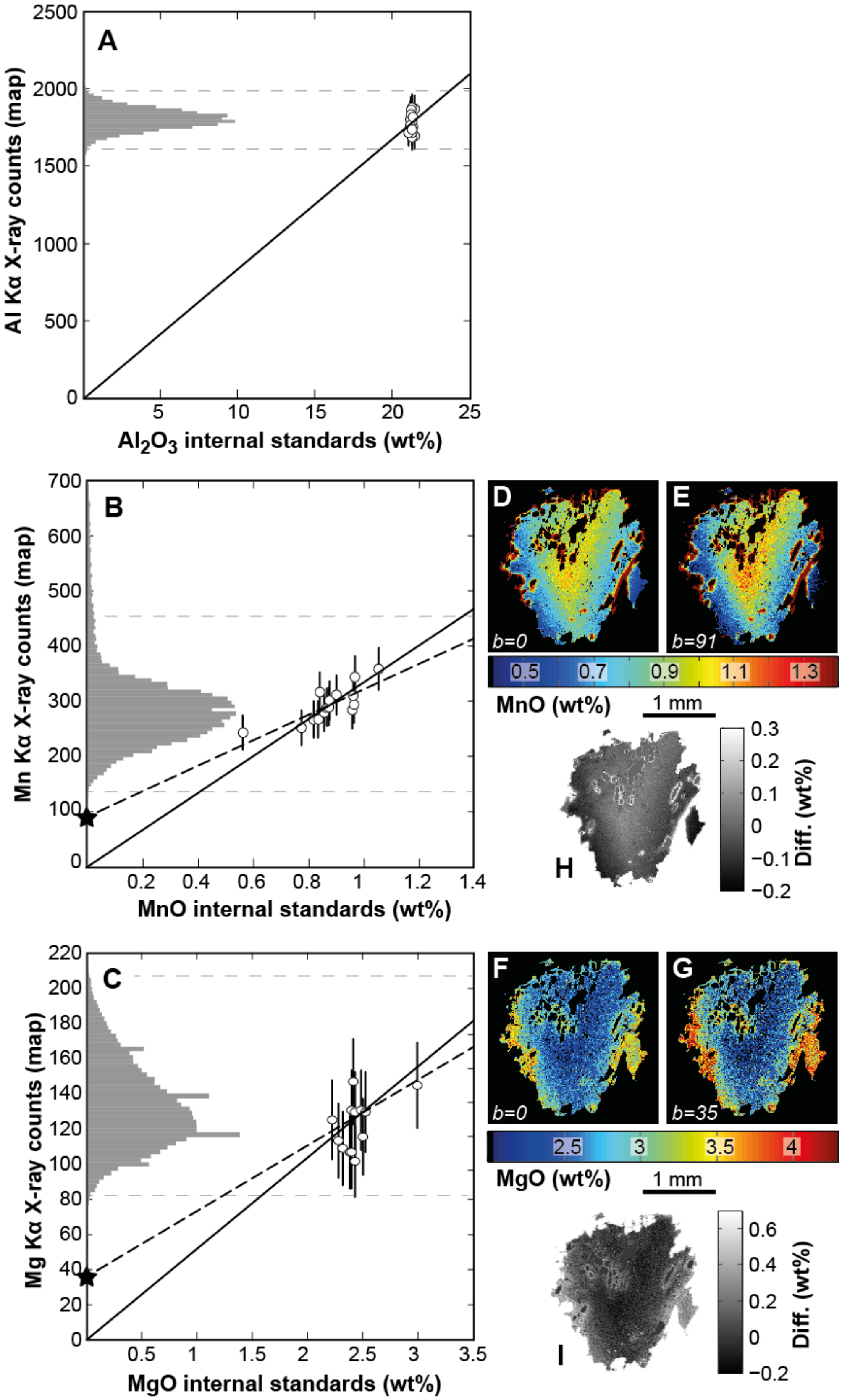
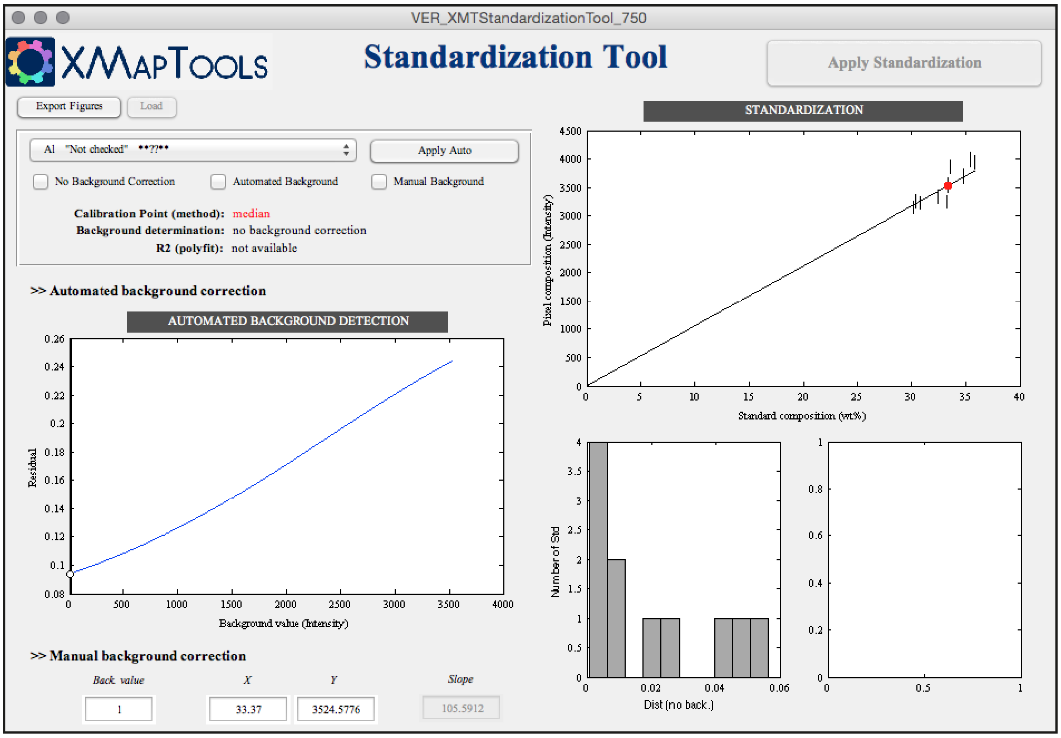


Figure 3.21 – *Example of standardization for a garnet of the Central Alps after Lanari et al. (submitted).*

(a)



Al "Not checked" **??**

☐ No Background Correction ☐ Automated Background ☐ Manual Background

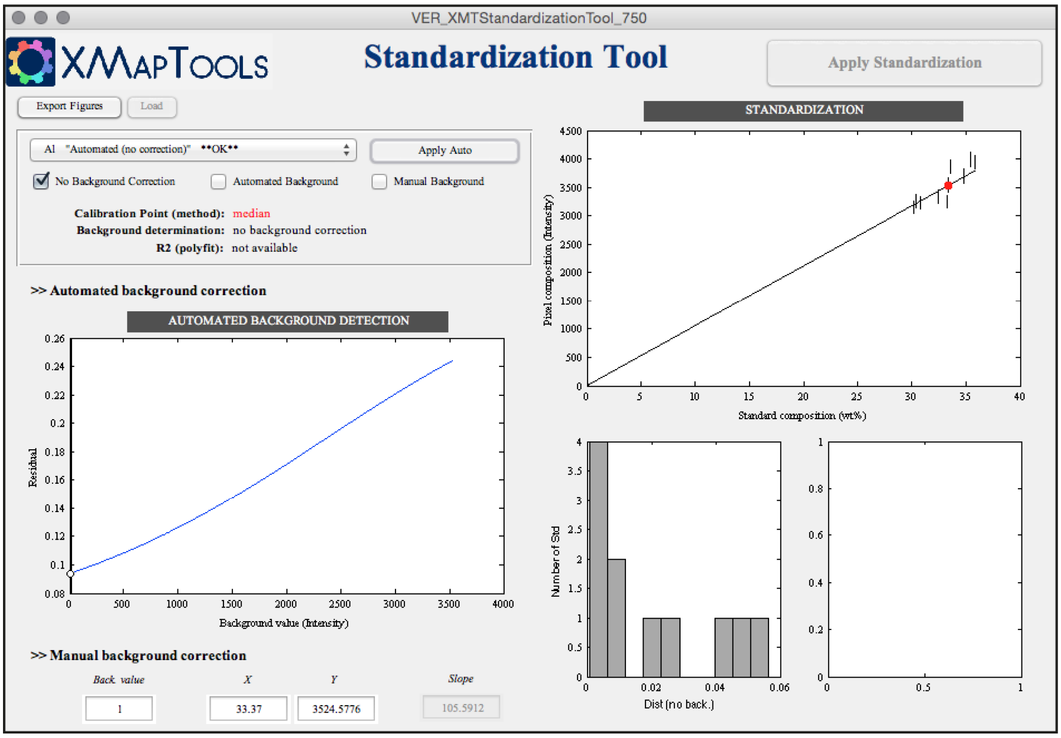
Calibration Point (method): median
Background determination: no background correction
R2 (polyfit): not available

>> Automated background correction

>> Manual background correction

Back value	X	Y	Slope
1	33.37	3524.5776	105.5912

(b)



Al "Automated (no correction)" **OK**

☑ No Background Correction ☐ Automated Background ☐ Manual Background

Calibration Point (method): median
Background determination: no background correction
R2 (polyfit): not available

>> Automated background correction

>> Manual background correction

Back value	X	Y	Slope
1	33.37	3524.5776	105.5912

Figure 3.22 – *Advanced standardization; case: automated - no background correction (here Al in garnet). (a) no calibration, (b) automated calibration (no background correction).*

3.4.6.3 Module XMTStandardizationTool

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. 3.22). Each item string contains the element name and the method used to define the calibration curve. For a given element, in this example aluminium, the string can be:

- **Al "Not checked" **??**** - No calibration curve has been defined for this element
- **Al "Automated (no correction)" **OK**** - A calibration curve has been defined using the automated method without any background correction. In this case the X-ray intensity of the element is high and no background correction is required (Lanari et al. submitted).
- **Al "Automated (with background correction)" **OK**** - A calibration curve has been defined using the automated method including a background correction that is based on an approximation of the background value.
- **Al "Manual" **OK**** - A calibration curve has been defined using the manual mode. In this case it is not specified if a background correction has been applied or not.

The button *Apply Auto* allows the automated mode to be activated. 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.

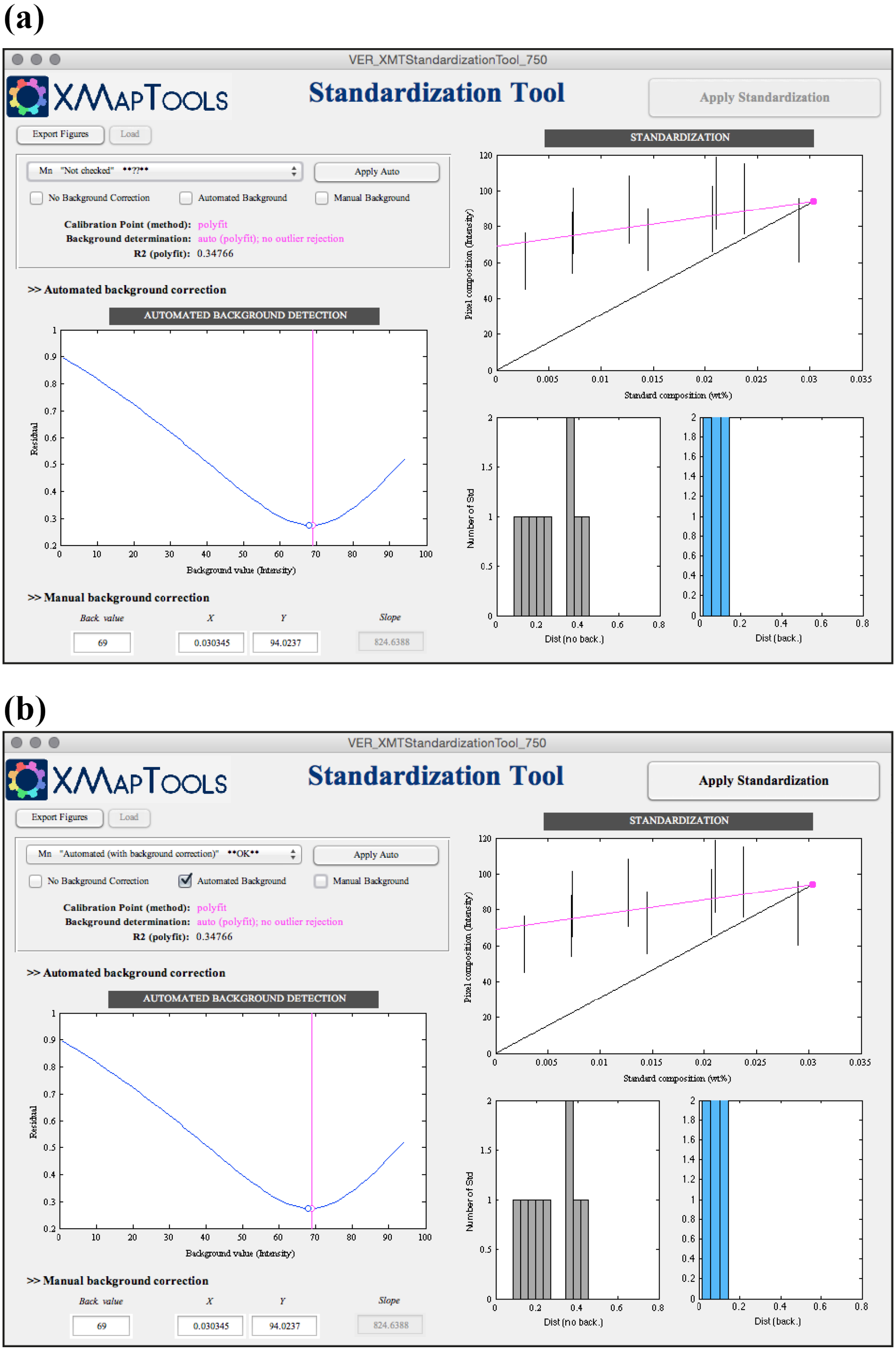
The check buttons *No background correction*, *Automated background* and *Manual background* indicate the mode being used for the selected element.

Additional informations are also displayed:

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

The calibration curve without background correction is displayed in black. The calibration point determined using the median values in red and the one determined using the polyfit approach in magenta. The calibration curves based on the polyfit approach are shown in magenta (dashed line, not used, continuous line, used). The calibration curve based on the least-square residual approach is shown in blue.

The figure *Automated background correction* show the evolution of the residuals with the background value (e.g. Fig. 3.23). The residuals are computed as the sum of the distances between the calibration curve and the internal standards.



(a)

Mn "Not checked" **??**

☐ No Background Correction ☐ Automated Background ☐ Manual Background

Calibration Point (method): polyfit
Background determination: auto (polyfit); no outlier rejection
R2 (polyfit): 0.34766

>> Automated background correction

>> Manual background correction

Back. value: 69
X: 0.030345
Y: 94.0237
Slope: 824.6388

(b)

Mn "Automated (with background correction)" **OK**

☐ No Background Correction ☑ Automated Background ☐ Manual Background

Calibration Point (method): polyfit
Background determination: auto (polyfit); no outlier rejection
R2 (polyfit): 0.34766

>> Automated background correction

>> Manual background correction

Back. value: 69
X: 0.030345
Y: 94.0237
Slope: 824.6388

Figure 3.23 – *Advanced standardization; case: automated - background correction (here Mn in garnet). (a) no calibration, (b) automated calibration (background correction).*

The background value as well as the X and Y coordinates of the calibration point are reported in the window *Manual background correction* (Fig. 3.23). These values can be edited in manual mode.

The window *Standardization* displays the calibration curve(s) and the internal standards. The two histogram diagrams show the distribution of the distances between the calibration curve and the internal standards (left, no background correction; right with background correction).

Three examples are given in the Figures 3.22, 3.23 and 3.24. In this case the calibration curve is plotted in black.

(1) Automated calibration curve without any background correction (Fig. 3.22).

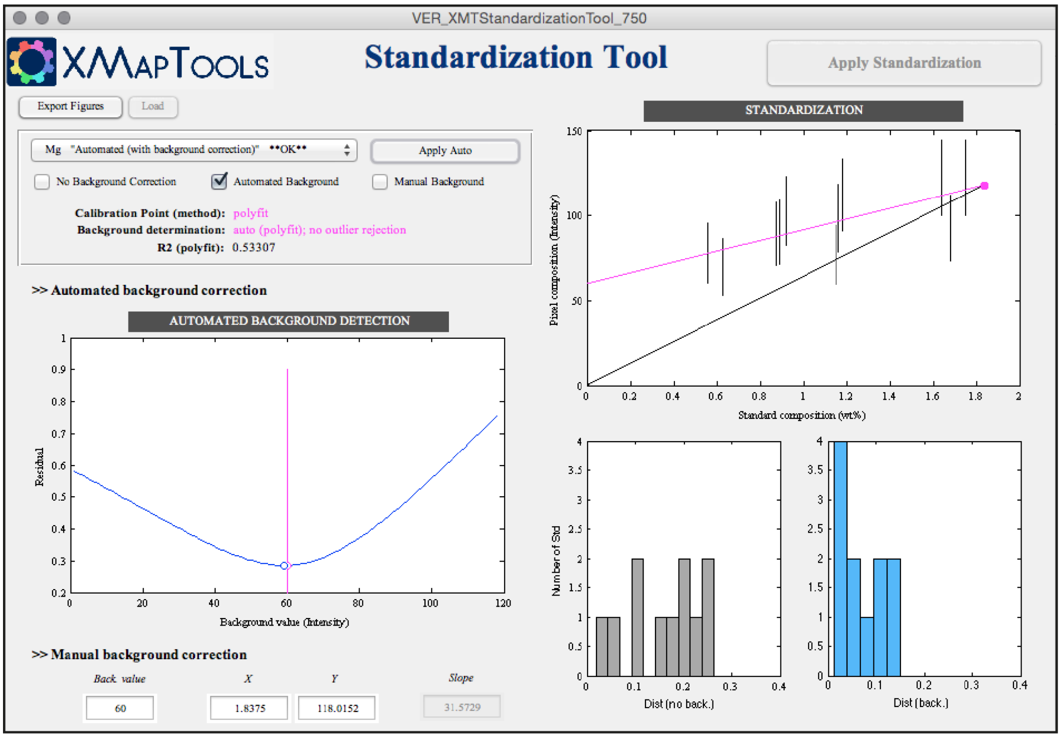
(2) Automated calibration curve with background correction (Fig. 3.23). In this case the calibration curve is plotted in magenta.

(3) Manual calibration curve with background correction (Fig. 3.24). In this case the calibration curve is plotted in green. The dashed curve show the result of the polyfit function (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 is necessary to switch to the *manual mode*. The goal is to obtained a reasonable calibration curve.
- 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, it might be necessary to standardize again each phase to be able to use all the new functionalities.

(a)



Mg "Automated (with background correction)" **OK**

☐ No Background Correction ☑ Automated Background ☐ Manual Background

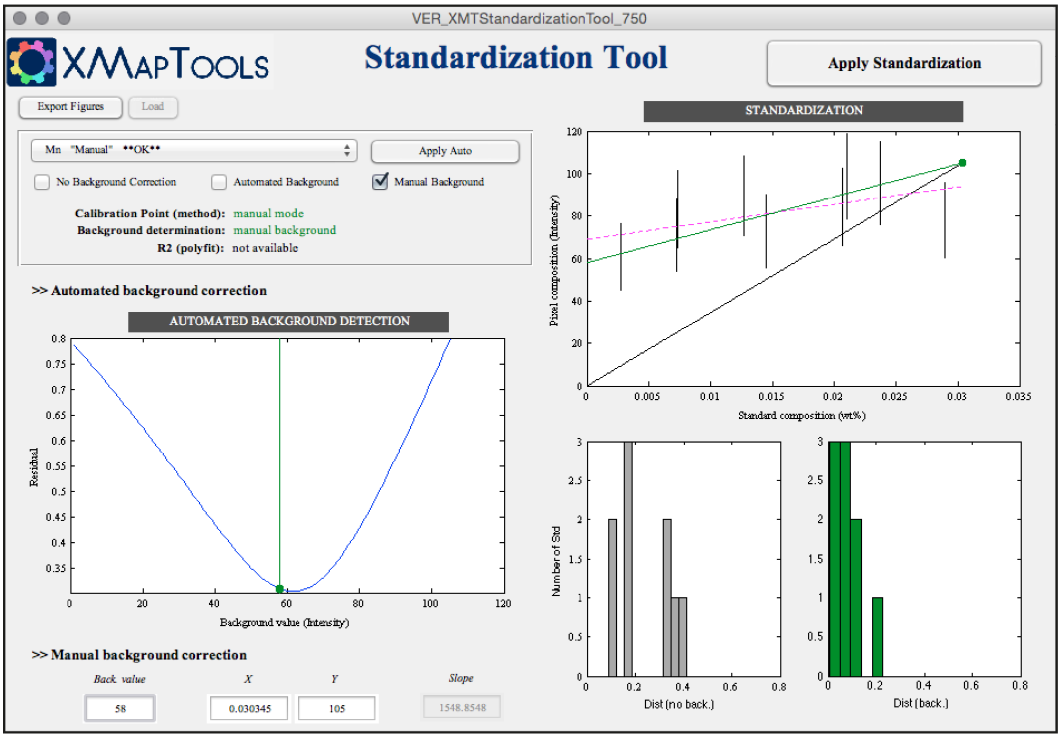
Calibration Point (method): polyfit
Background determination: auto (polyfit); no outlier rejection
R2 (polyfit): 0.53307

>> Automated background correction

>> Manual background correction

Back. value	*X*	*Y*	*Slope*
60	1.8375	118.0152	31.5729

(b)



Mn "Manual" **OK**

☐ No Background Correction ☐ Automated Background ☑ Manual Background

Calibration Point (method): manual mode
Background determination: manual background
R2 (polyfit): not available

>> Automated background correction

>> Manual background correction

Back. value	*X*	*Y*	*Slope*
58	0.030345	105	1548.8548

Figure 3.24 – *Advanced standardization; case: manual - background correction (here Mg in garnet). (a) no calibration, (b) manual calibration (background correction).*

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. 3.25)

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 Fe2O3 and XFe3+. 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 Chem2D 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.

[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.

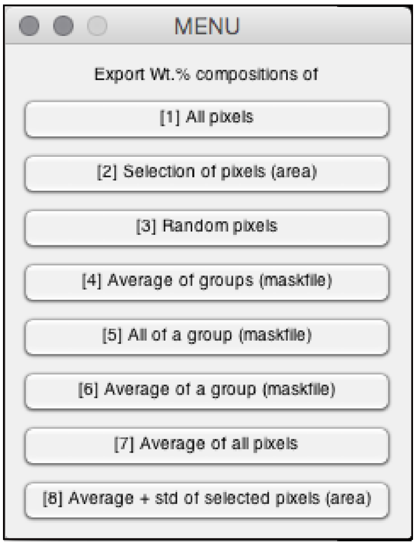


Figure 3.25 – *Menu listing the methods available to export oxide analyses from the selected Quanti file*

[B2105] The button *generate oxide wt-% sum map* Σ 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.

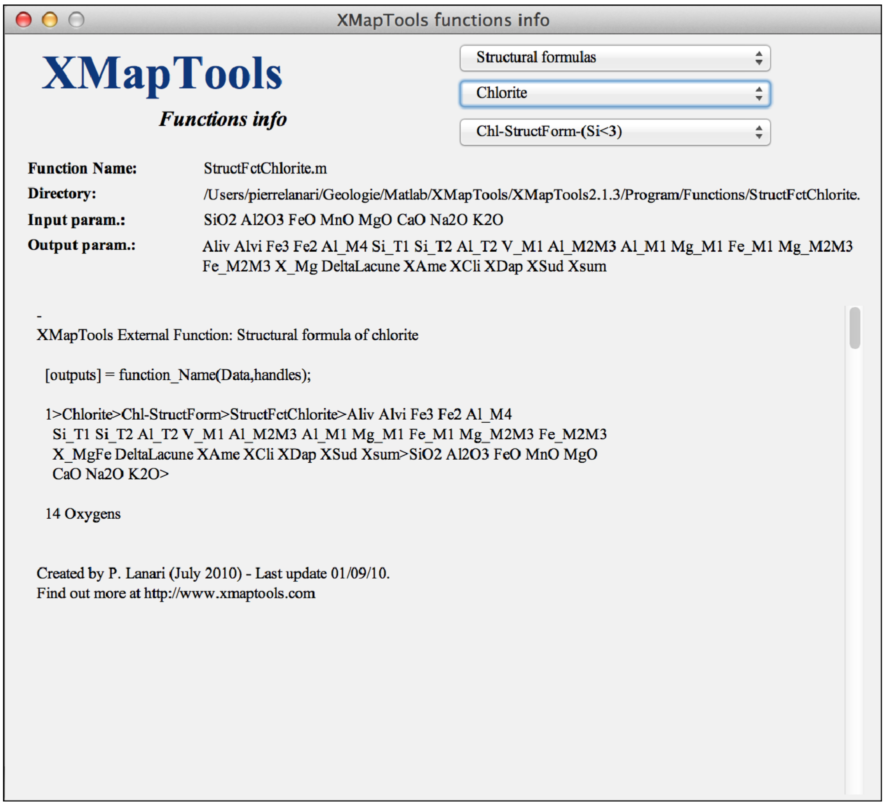
Warning: This functionality is not available in the version 2.4.1 (and the following updates) for standardizations that have been computed with 2.3.1 and previous versions. In this case, it is recommended to re-standardize your phases. Note that the following function is not affected and can still be 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 4.2.3 *How can I check the results of an external function?*)



Structural formulas
Chlorite
Chl-StructForm-(Si<3)

Function Name: StructFctChlorite.m
Directory: /Users/pierrelanari/Geologie/Matlab/XMapTools/XMapTools2.1.3/Program/Functions/StructFctChlorite.
Input param.: SiO2 Al2O3 FeO MnO MgO CaO Na2O K2O
Output param.: 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

```
-
XMapTools External Function: Structural formula of chlorite

 [outputs] = function_Name(Data,handles);

 1>Chlorite>Chl-StructForm>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_MgFe DeltaLacune XAme XCli XDap XSud Xsum>SiO2 Al2O3 FeO MnO MgO
  CaO Na2O K2O>

 14 Oxygens


Created by P. Lanari (July 2010) - Last update 01/09/10.
Find out more at http://www.xmaptools.com
```

Figure 3.26 – *XMapTools function info GUI*

[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. 3.26) 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

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 functions 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 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 additionally 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 an 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

$$DCM_i = \frac{\rho_i}{\rho_{mixture}} C_i^{wt} \tag{3.16}$$

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

Information regarding the density-correction are reported in the MATLAB© Command Window (see code 3.13). 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© Command Window)*

[B2409] The button *select an area and delete pixels outside* enables removing 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. 3.9b). Selection mode is disabled using right-clicking (spot 11, in Fig. 3.9b). The polygon is closed without taking into account the right clicking position, see dashed line in figure 3.9b. For the standardized phase selected in [M2101] all pixels outside the region-of-interest are deleted.

[B2410] The button *select an area and delete pixels inside* enables removing 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 deleted.

[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.

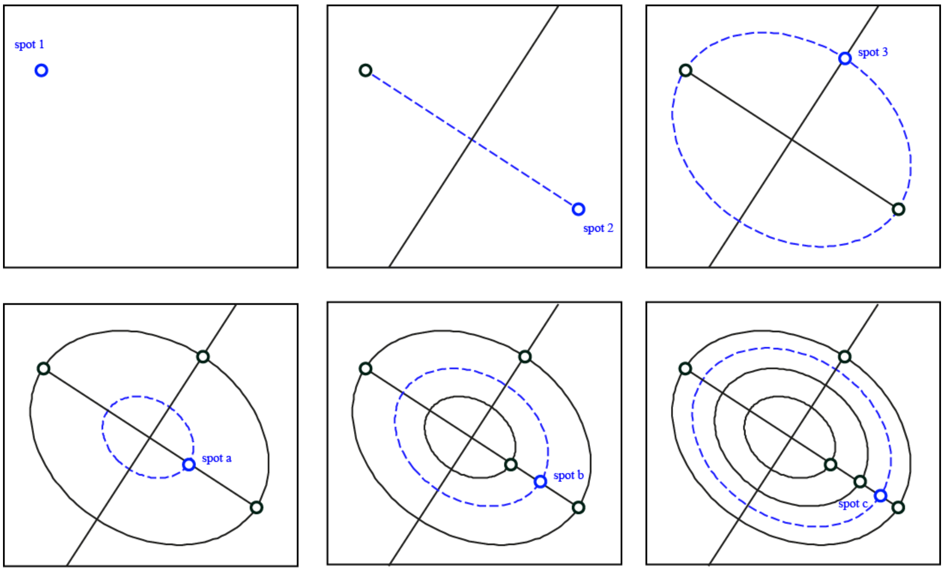


Figure 3.27 – *Procedure to define an ellipse and export composition extrapolated in 3D*

```
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. 3.27). Then integrations are defined from the conter to the rim of the primary ellipse (see points a, b and c on Fig. 3.27).

```
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^2)     1546191.93

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

Compositions integrations:
Al2O3    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
K2O      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
Na2O     7.985    9.470    11.300   11.425
TiO2     1.529    2.183    1.775    0.360
SiO2     54.799   56.254   59.698   62.701

Extrapolated (ellipsoid) local Compositions:
Al2O3    23.421
CaO      0.336
FeO      0.758
K2O      1.439
MgO      1.388
MnO      0.058
Na2O     10.754
TiO2     1.249
SiO2     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. 3.28 and 3.29).

The procedure consists of the following steps:

- Define the reference domain with a rectangle shape by clicking two pixels (see Fig. 3.28-a).
- Choose from which corner of this rectangle you want to define the smallest rectangle (see Fig. 3.28-b). The available options are: *top-left corner*, *top-right corner*, *bottom-left corner*, *bottom-top corner*. In the example shown in figure 3.28-c, the *top-right corner* is selected (red arrow in b).
- Define the smallest rectangle from the selected corner (see Fig. 3.28-d).
- Define the number of steps, i.e. the number of samples along the dahsed line in figure 3.28-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. 3.29). 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.

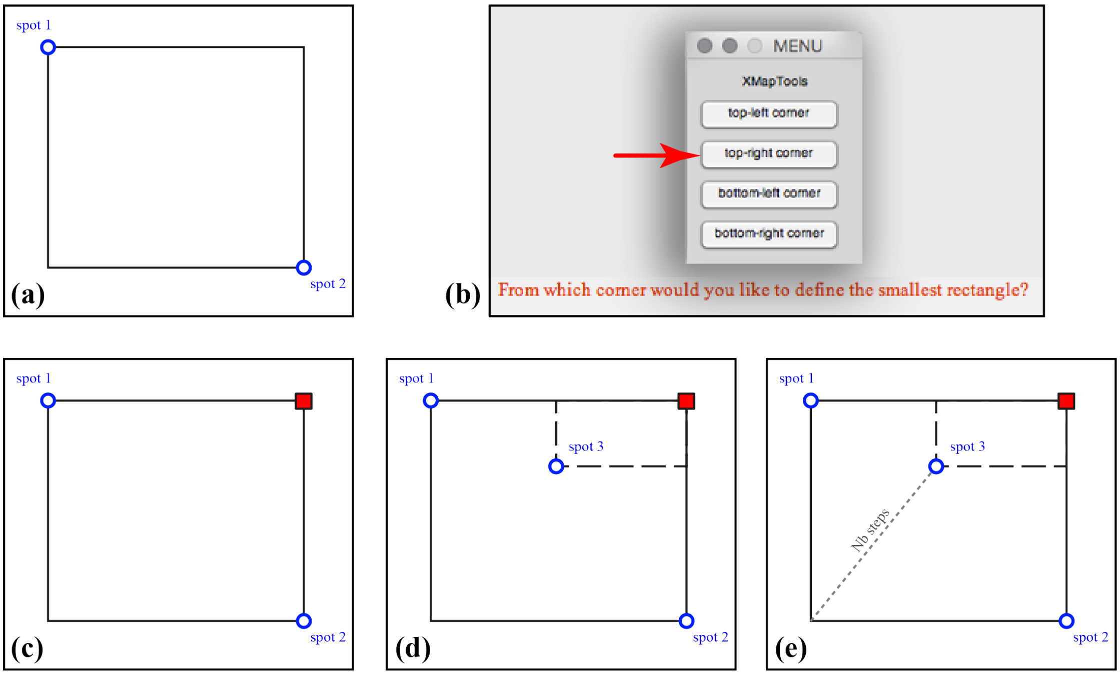
Note: This function does not save any file with the composition of the successive domains.

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. 3.30). 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.



From which corner would you like to define the smallest rectangle?

Figure 3.28 – *Procedure to export compositions with a variable-size rectangle*

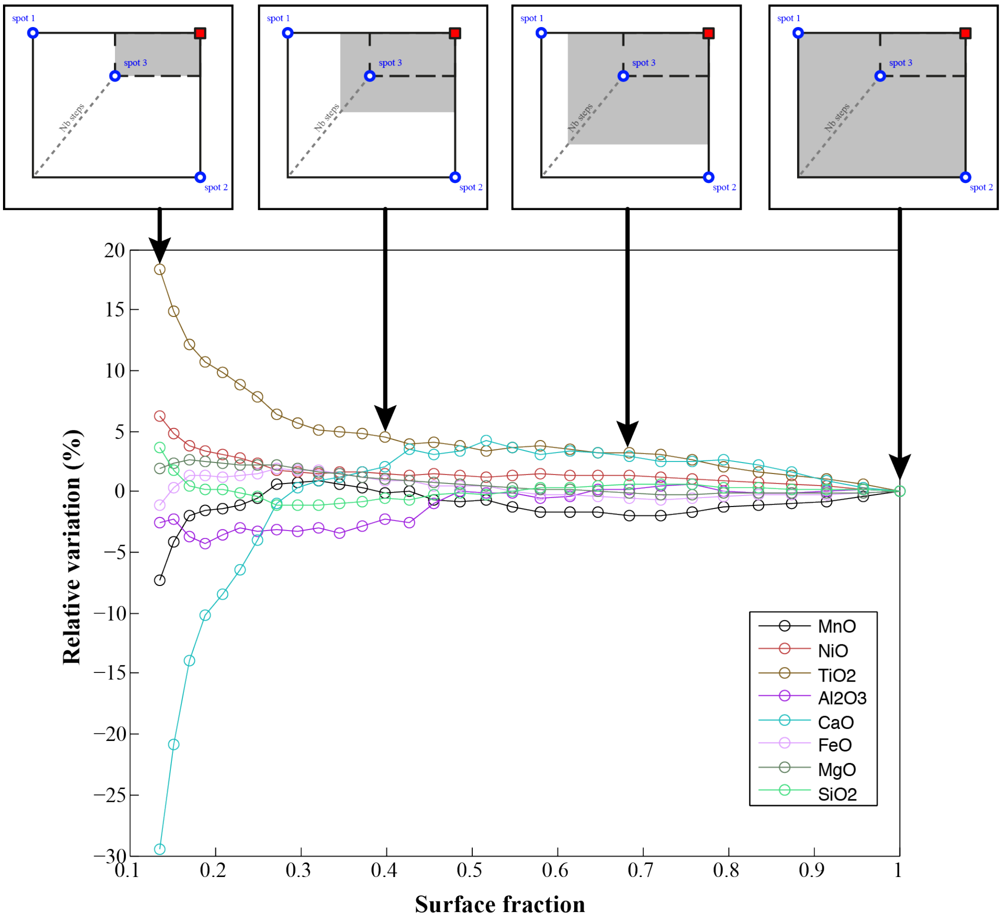
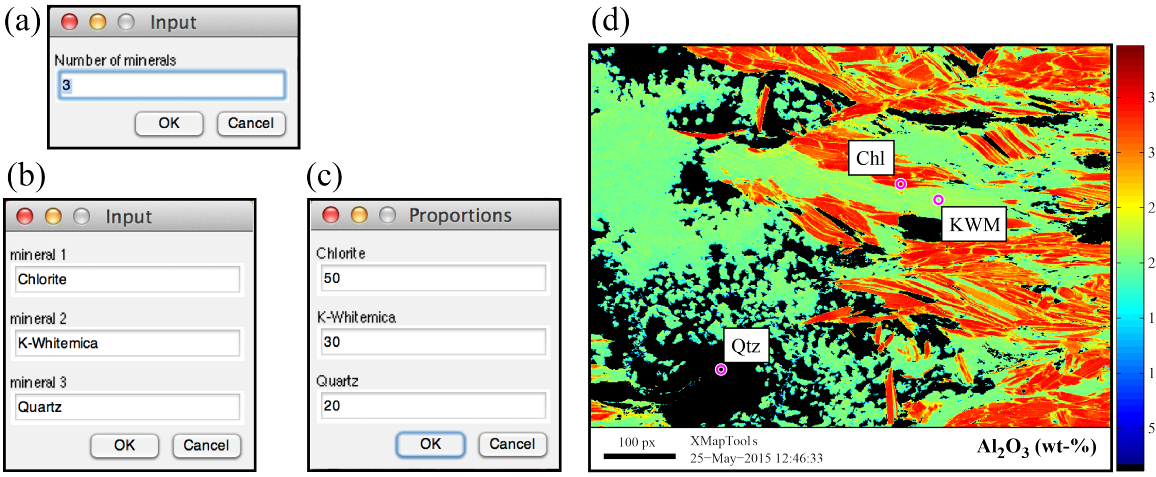


Figure 3.29 – *Result exporting compositions with a variable-size rectangle*

```
Local composition (Proportions) from XMapTools

(1) Mineral proportions:
Chlorite        50
K-Whitemica     30
Quartz          20

(2) Mineral compositions:
        Chlorite        K-Whitemica     Quartz
Al2O3   21.6714         34.5545         0.0000
CaO     0.02484         0.0033          0.0000
FeO     31.0584         1.454           0.0000
K2O     0.0094          9.0293          0.0000
MgO     12.2202         1.2115          0.0000
MnO     0.42126         0.0653          0.0000
Na2O    0.018231        1.4428          0.0000
SiO2    25.3511         46.49           99.612
TiO2    0.029867        0.36857         0.0000

(3) Local Composition:
Al2O3   21.202
CaO     0.01341
FeO     15.9654
K2O     2.7135
MgO     6.4736
MnO     0.23022
Na2O    0.44197
SiO2    46.5449
TiO2    0.1255
```

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



Number of minerals: 3

mineral 1: Chlorite
mineral 2: K-Whitemica
mineral 3: Quartz

Chlorite: 50
K-Whitemica: 30
Quartz: 20

Figure 3.30 – *Procedure to export composition build from proportions. (a) number of phases and their (b) names, (c) modal proportion, and (d) compositions.*

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

Code 3.17 – *Export results (info reported in the Command Window)*

[B3104] The button *compute a new variable* allows a new variable to be computed from the variables available in the *result* selected in [M3101]. The name and the code to compute the new variable are defined in a new window. The code must be written in MATLAB© and should use the existing variable names which are the names of the variables in the selected *result* (List available in [M3102]). Arithmetic combinations of maps must use the array arithmetic code as illustrated below (find out more at http://www.mathworks.fr/help/techdoc/ref/arithmeticoperators.html). Note that arithmetic operators should not be used in variable names.

For example, the *XFe* of chlorite may be computed from the Mg and Fe amounts in the M1 site (variables Mg_M1 and Fe_M1 see 3.17):

```
Enter the new variable name: XFe
Enter the MATLAB code (using ./, .* and .^): Fe_M1./(Mg_M1+Fe_M1)
```

Code 3.18 – *Example: How to compute a new variable*

the code ./ is used to generate an arithmetic division of two matrices. In case of error in the provided code, a warning window display the detected elements that were not found in the list.

```
A+B          % addition
A-B          % substraction
A.*B         % multiplication
A./B         % division
```

Code 3.19 – *Array arithmetic commands in MATLAB©:*

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

3.6.2 Filtering

[B3201] The button *APPLY FILTER* allows a new *result* to be created from the emphresult selected in [M3101], but containing only the pixels with the composition values ranging between the minimum and maximum values of the color bar set in [C5101].

3.7 CHEMICAL MODULES

Any displayed map (such as *X-ray maps*, *standardized phase*, *merged map*, *result*) can be treated in binary diagrams (Fig. 3.32a), in triangular diagrams (Fig. 3.32b) or displayed as composite RGB image (Fig. 3.35). The chemical modules CHEM2D, TRIPLOT3D and RGB are called using the buttons [B5301], [B5302] and [B5303], only if the number of selected variables is greater than two and three respectively. A description of the modules is available 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 with compatible names (see §2.6.2).

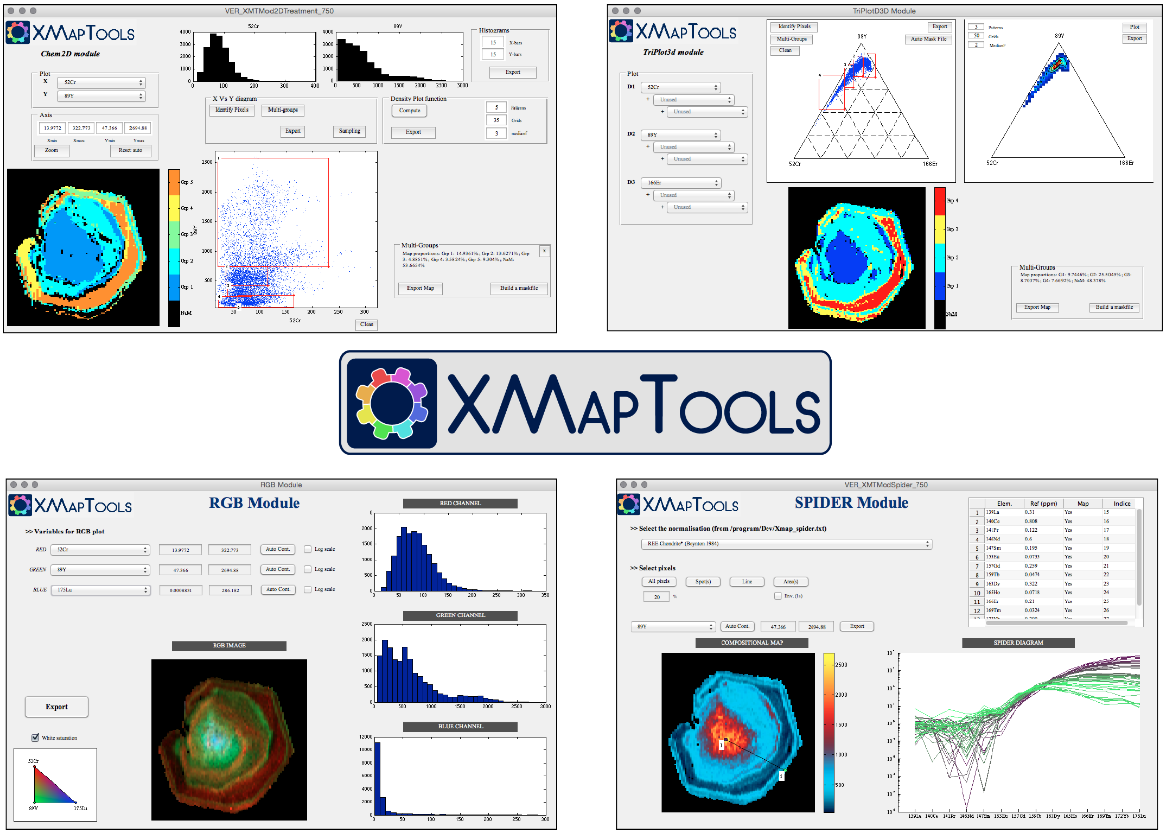


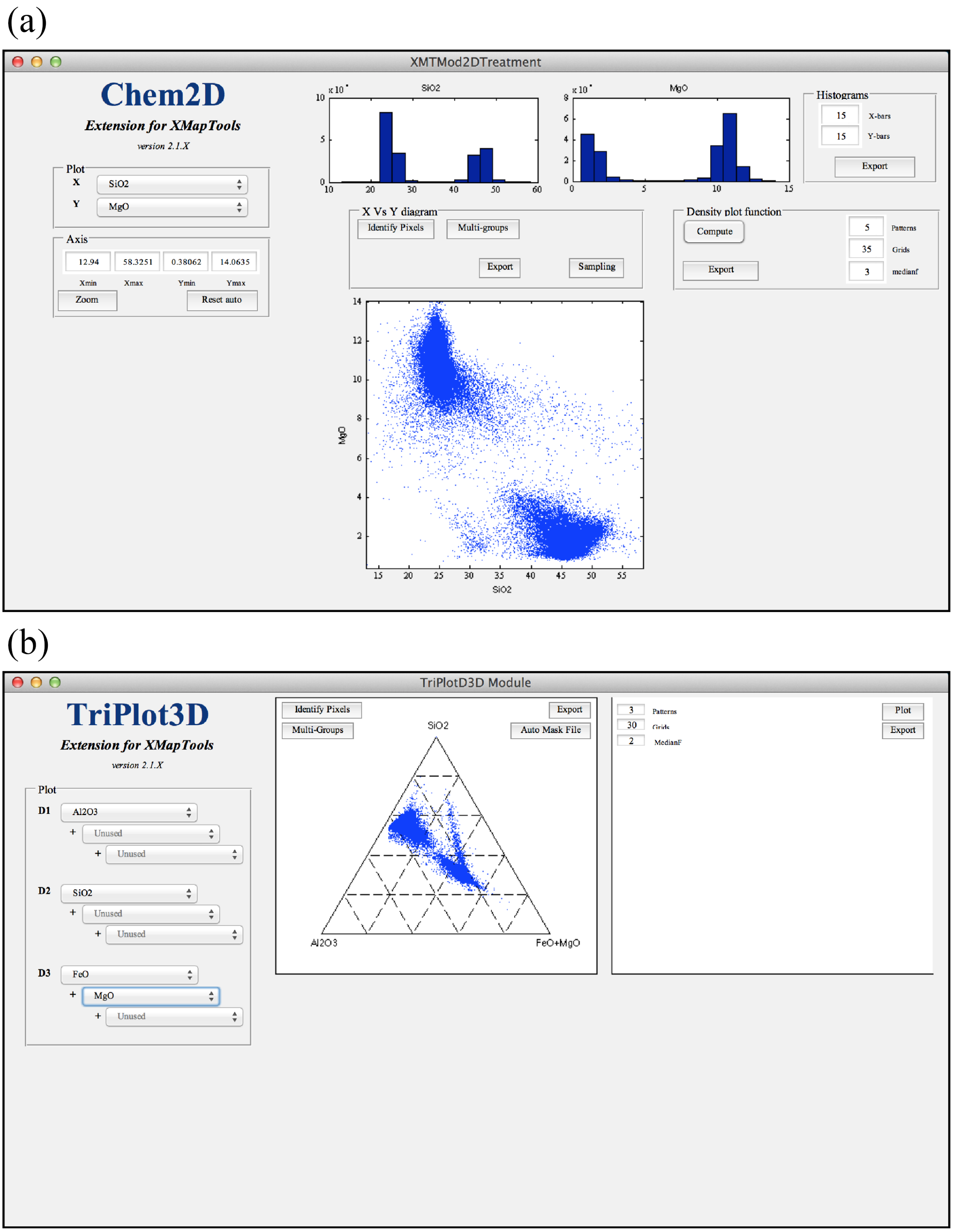
Figure 3.31 – *Chemical modules available in XMapTools*

3.7.1 Chem2D

CHEM2D is an additional graphic user interface called by XMAPTOOLS. 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. 3.33a). The sample used in the figure is a greenschist facies metapelite from the western Alps studied by Aude Verly.

The *plot* window (Fig. 3.33a) enables selecting the X and Y variables to be plotted in the binary diagram X against Y.

The *axis* window (Fig. 3.33a) enables defining both X and Y ranges (Xmin, Xmax, Ymin, Ymax)



X: SiO2
Y: MgO

Xmin: 12.94
Xmax: 58.3251
Ymin: 0.38062
Ymax: 14.0635

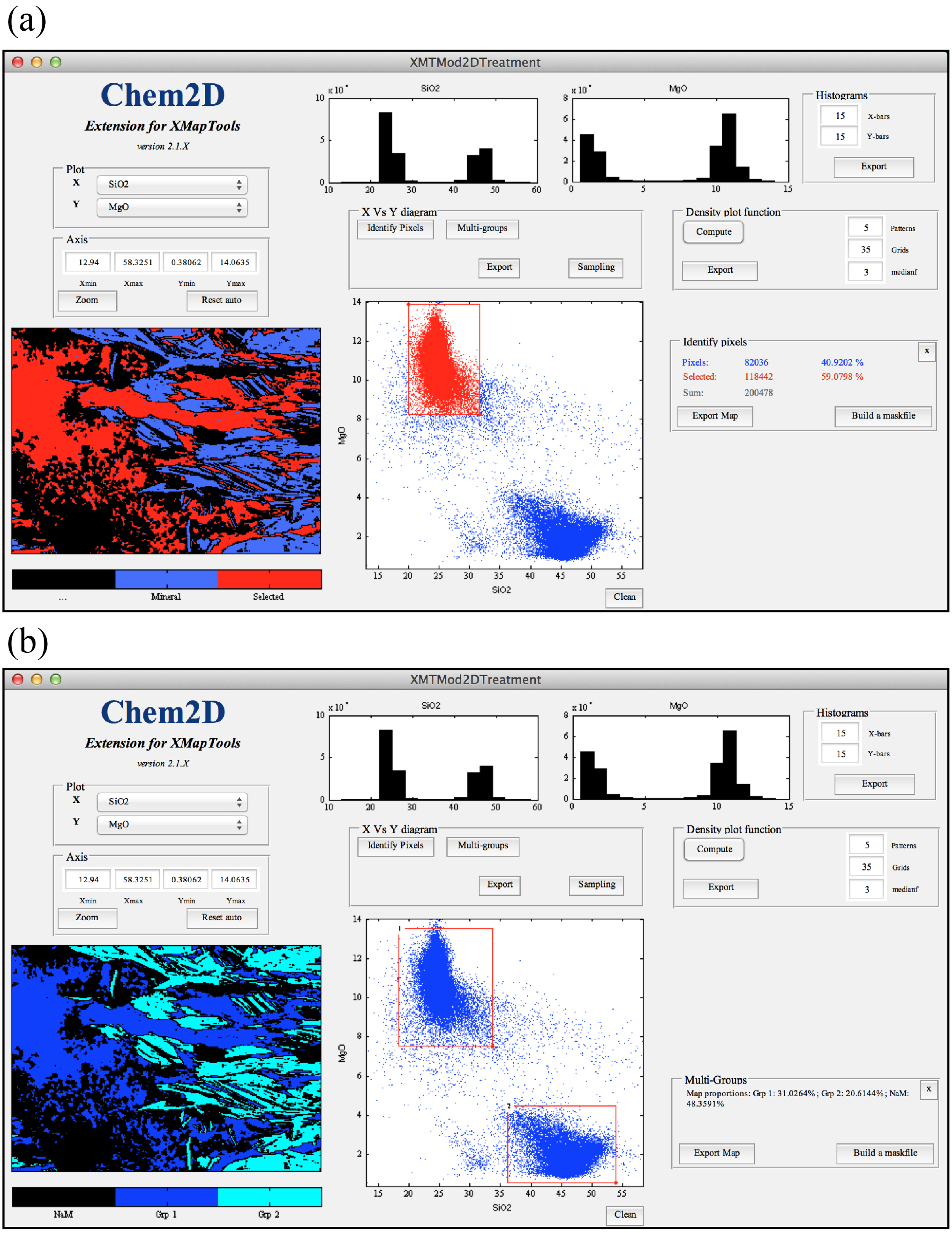
X-bars: 15
Y-bars: 15

Patterns: 5
Grids: 35
medianf: 3

D1: Al2O3 + Unused + Unused
D2: SiO2 + Unused + Unused
D3: FeO + MgO + Unused

Patterns: 3
Grids: 30
MedianF: 2

Figure 3.32 – *Chemical modules (a) Chem2D and (b) TriPlot3D*



(a)

Plot: X SiO2; Y MgO

Axis: Xmin 12.94; Xmax 58.3251; Ymin 0.38062; Ymax 14.0635

Histograms: 15 X-bars; 15 Y-bars

Density plot function: 5 Patterns; 35 Grids; 3 medianf

Identify pixels

Pixels: 82036 40.9202 %

Selected: 118442 59.0798 %

Sum: 200478

(b)

Plot: X SiO2; Y MgO

Axis: Xmin 12.94; Xmax 58.3251; Ymin 0.38062; Ymax 14.0635

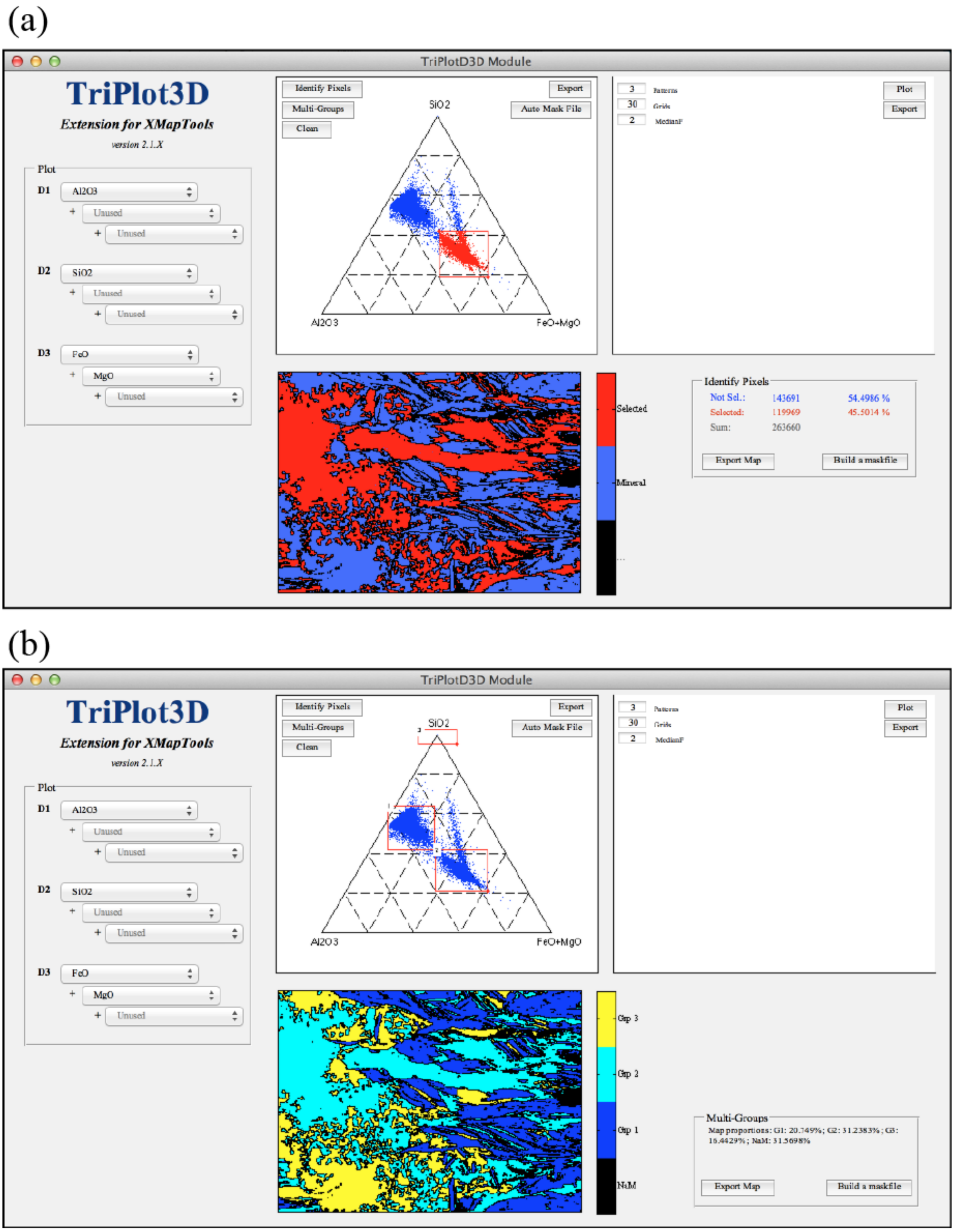
Histograms: 15 X-bars; 15 Y-bars

Density plot function: 5 Patterns; 35 Grids; 3 medianf

Multi-Groups

Map proportions: Grp 1: 31.0264% ; Grp 2: 20.6144% ; NaM: 48.3591%

Figure 3.33 – *Chemical modules Chem2D (a) identify pixels, (b) multi-group*



D1 Al2O3 + Unused + Unused
D2 SiO2 + Unused + Unused
D3 FeO + MgO + Unused

3 Patterns
30 Grids
2 MedianF

Identify Pixels

Not Sel.:	143691	54.4986 %
Selected:	119969	45.5014 %
Sum:	263660	

Multi-Groups

Map proportions: G1: 20.749%; G2: 31.2383% ; G3: 16.4429% ; NaM: 31.5698%

Figure 3.34 – *Chemical modules TriPlot3D (a) identify pixels, (b) multi-group*

of the main plot. The zoom function can be used to define these values directly in the figure by clicking with the cursor two points that define a rectangle. The button *reset auto* resets the range to the minimum and maximum values (default display values).

The *density plot function* is available to plot a point density diagram. The user must set the number of density curves (patterns), the grid size and the median filter to be used and press the button *compute*.

Two selection functions are available, the *Identify pixels* and *Multi-groups* functions. In both cases, the user can select a group of pixel compositions in the binary plot and display the corresponding pixels in a map. Statistics are displayed in a small window on the right hand side.

3.7.2 TriPlot3D

The functions available in TRIPLOT3D (Fig. 3.34) are similar to those described above for CHEM2D. This section of the user-guide will be improved later.

3.7.3 RGB

The RGB modules generates three channels composite images (RGB for red, green and blue) from compositional maps. In figure 3.35 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. 3.35) 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 buttton *export* allows opening the figure in a new MATLAB© figure window (check the description of [B5102] to see how to save the figures).

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

3.7.4 Spider

The SPIDER modules (Fig. 3.31) generates spider diagrams of trace element maps. The module can be called only from the workspace result with compatible data (see §2.6.2).

To display the spider diagram, it is necessary to:

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

[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 3.36. Note that in this example, there is no significant difference between 20% and 100% because of the large number of pixels used.

[2] Spot(s): The button *Spot(s)* enables selecting pixels to plot in the spider diagram. As usual in XMAPTOOLS, use right-clicking to leave the selection mode. An example of selection of 20 spots from garnet core to the rim is provided in figure 3.37. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram.

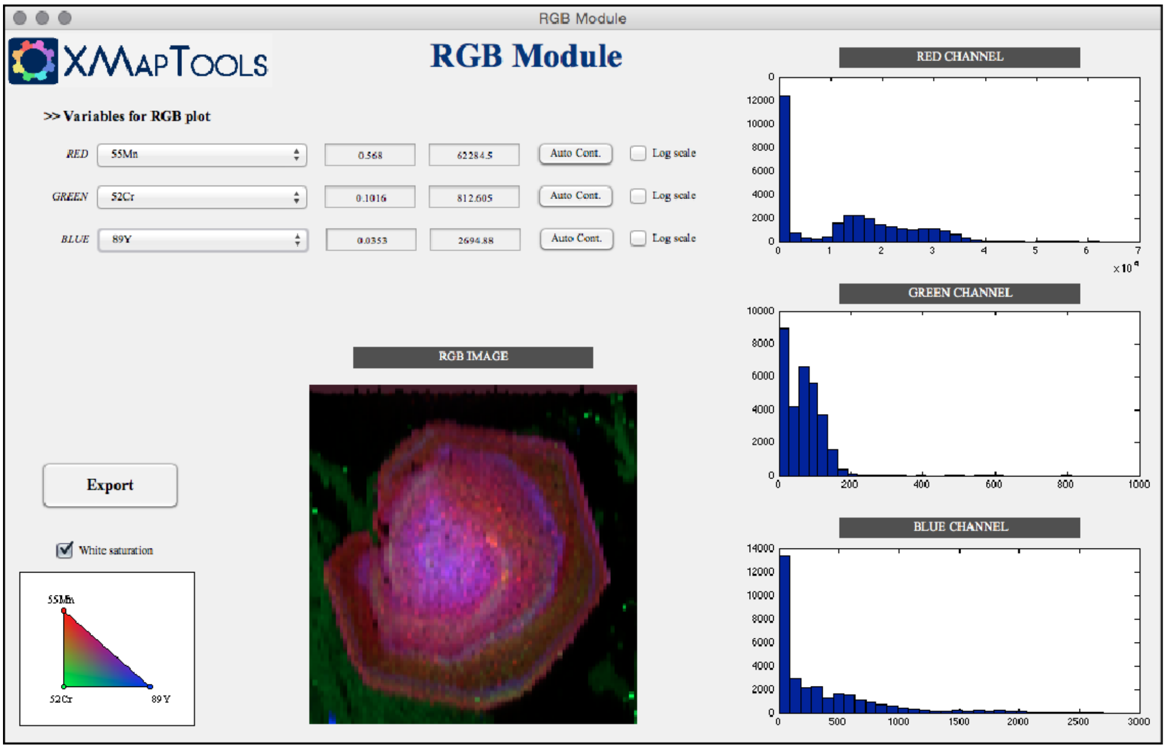
[3] Line: The button *Line* enables selecting two pixels and plotting the composition of the pixels along the line. An example of selection of line from garnet core to the rim is provided in figure **??**. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram.

[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 3.39. Note that the colors of the spot corresponds to the colors of the lines in the spider diagram. In this case the standard deviation (1σ) envelopes are displayed together with the average. This mode can be activated using the option below the button *Area(s)*. The envelope is not displayed if $(mean - std) < 0$ or $(mean - std) = 0$.

The map figure can be managed using the following functions:

- *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*)

The button export allows exporting the two figures in new MATLAB© windows (see [B5102] for details).



RGB Module

>> Variables for RGB plot

RED 55Mn 0.568 62284.5 ☐ Log scale

GREEN 52Cr 0.1016 812.605 ☐ Log scale

BLUE 89Y 0.0353 2694.88 ☐ Log scale

☑ White saturation

Figure 3.35 – *Chemical modules RGB (see text for details)*

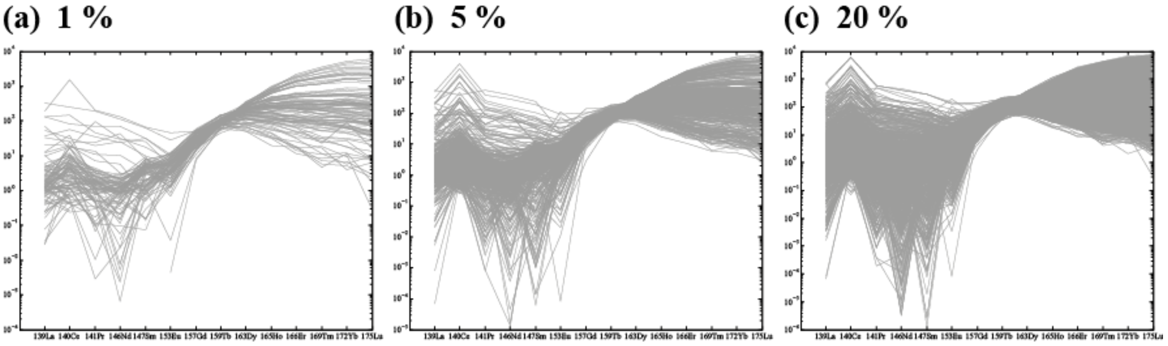


Figure 3.36 – *Spider diagram of REE in garnet using (a) 1%, (b) 5% and (c) 20% of the pixels of the map. See Fig. 3.37 for x labels.*

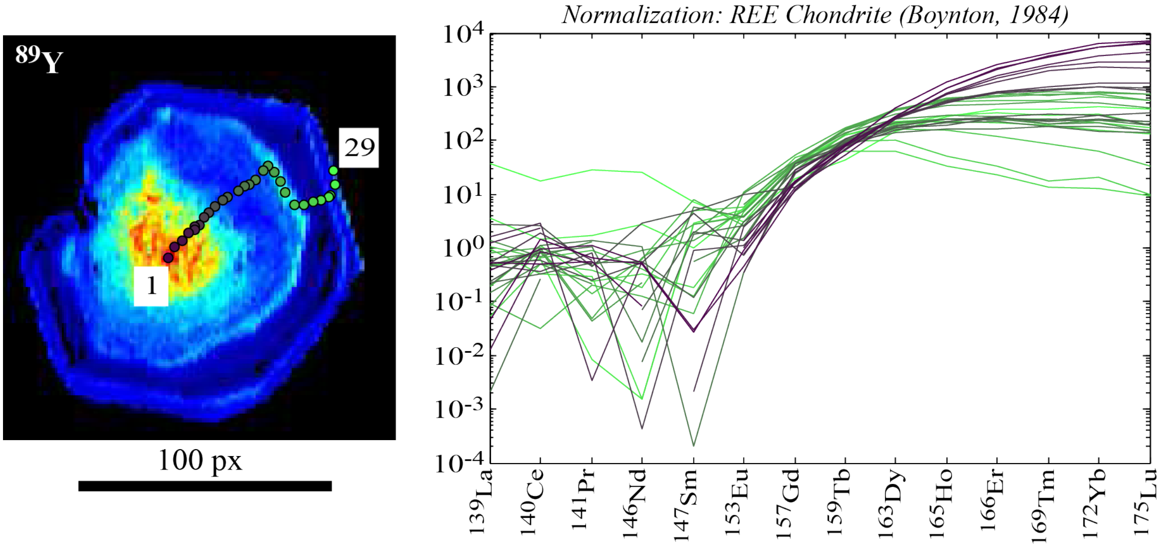
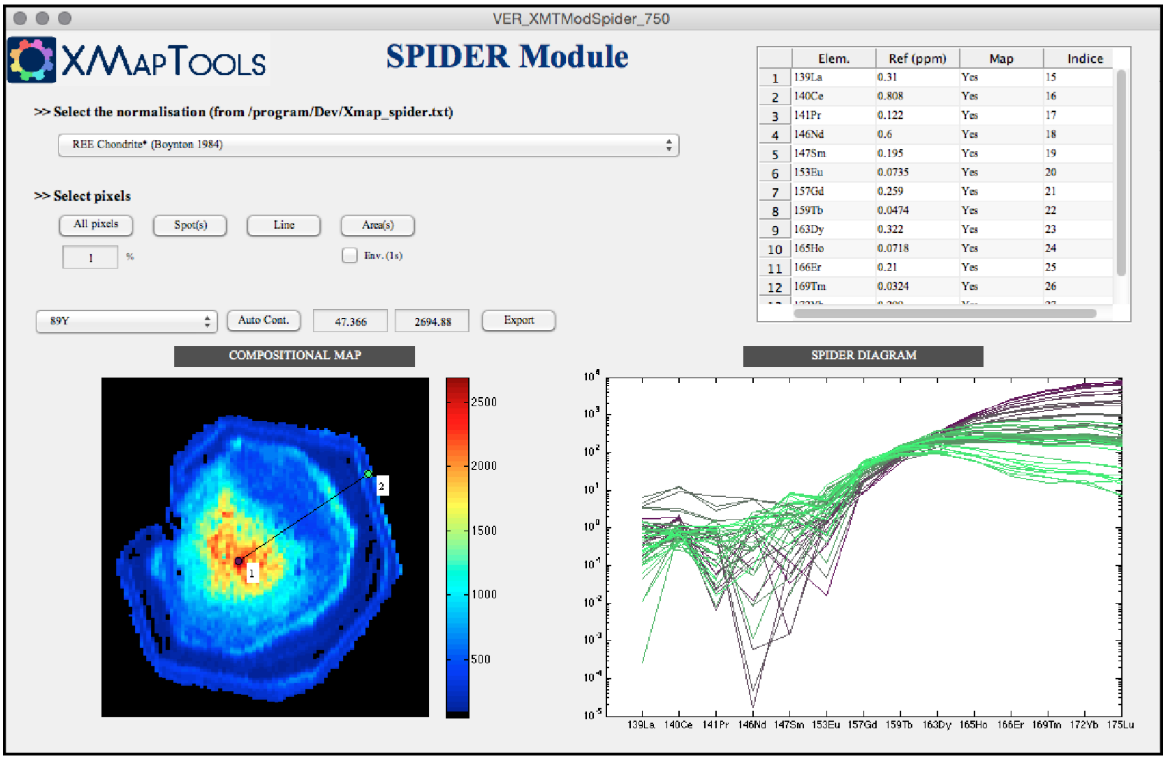


Figure 3.37 – *Spider diagram of REE in garnet using the sampling method: spot analyses. Map: ^{89}Y (red high concentration, blue low concentration, in ppm, see Fig.* **??** *for color scale)*



\>> Select the normalisation (from /program/Dev/Xmap_spider.txt)

REE Chondrite* (Boynton 1984)

\>> Select pixels

1 %

☐ Env. (1s)

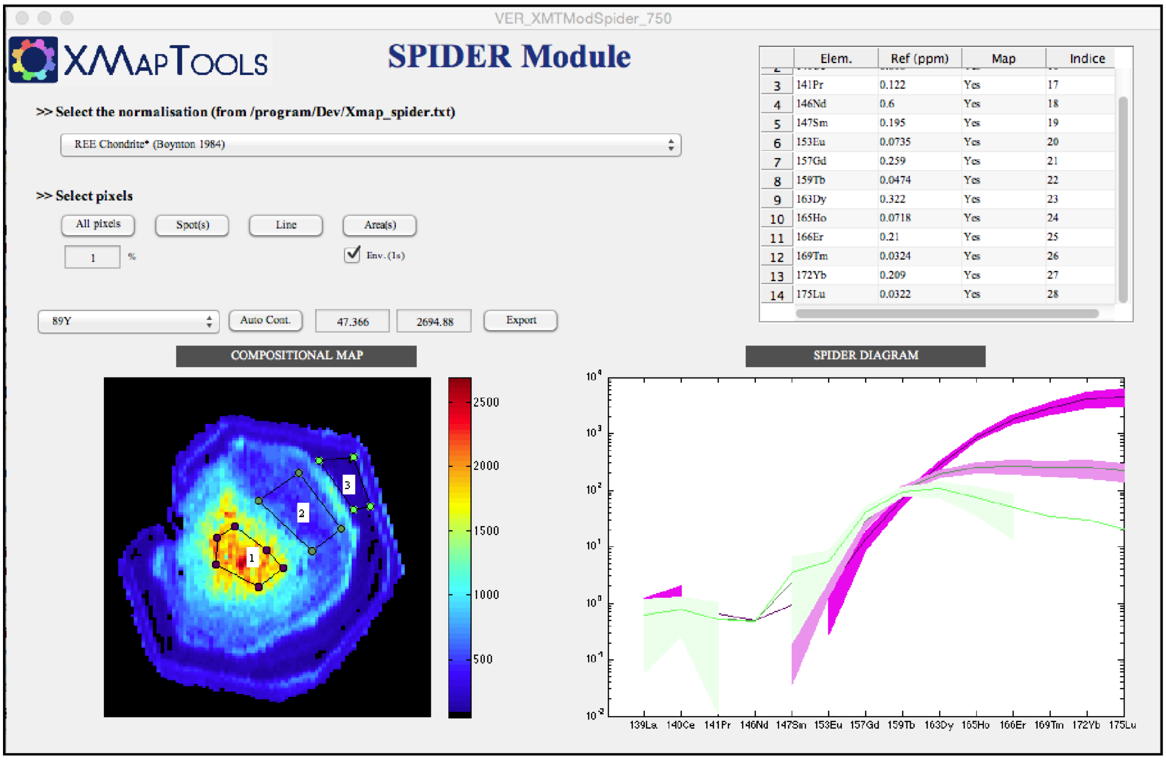
89Y

47.366

2694.88

	Elem.	Ref (ppm)	Map	Indice
1	139La	0.31	Yes	15
2	140Ce	0.808	Yes	16
3	141Pr	0.122	Yes	17
4	146Nd	0.6	Yes	18
5	147Sm	0.195	Yes	19
6	153Eu	0.0735	Yes	20
7	157Gd	0.259	Yes	21
8	159Tb	0.0474	Yes	22
9	163Dy	0.322	Yes	23
10	165Ho	0.0718	Yes	24
11	166Er	0.21	Yes	25
12	169Tm	0.0324	Yes	26

Figure 3.38 – *Spider diagram module; sampling mode: line.*



>> Select the normalisation (from /program/Dev/Xmap_spider.txt)

REE Chondrite* (Boynton 1984)

>> Select pixels

1 %

☑ Env. (1s)

89Y

47.366

2694.88

	Elem.	Ref (ppm)	Map	Indice
3	141Pr	0.122	Yes	17
4	146Nd	0.6	Yes	18
5	147Sm	0.195	Yes	19
6	153Eu	0.0735	Yes	20
7	157Gd	0.259	Yes	21
8	159Tb	0.0474	Yes	22
9	163Dy	0.322	Yes	23
10	165Ho	0.0718	Yes	24
11	166Er	0.21	Yes	25
12	169Tm	0.0324	Yes	26
13	172Yb	0.209	Yes	27
14	175Lu	0.0322	Yes	28

Figure 3.39 – *Spider diagram module; sampling mode: area(s)*

ADVANCED FUNCTIONALITIES

4

4.1 EXPORT MASK IMAGES WITH PERSONALIZED COLORS

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

[1] Export a mask image (Fig. 7.1-1) using the button The button *export mask image* in the workspace *Xray*. An example of mask image is reported in figure 4.1.

[2] Functions are available and can be activated using the icons available below the menu. Press the last one *Show plot tools and Dock figure*. MATLAB© turns the figure window into editing mode (Fig. 4.2).

[3] With pop-up menu color map, select *Custom*. A new window *Colormap editor* opens (Fig. 4.3) and you can select the colors for each mineral by pressing on the color arrows (see examples in Fig. 4.3).

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

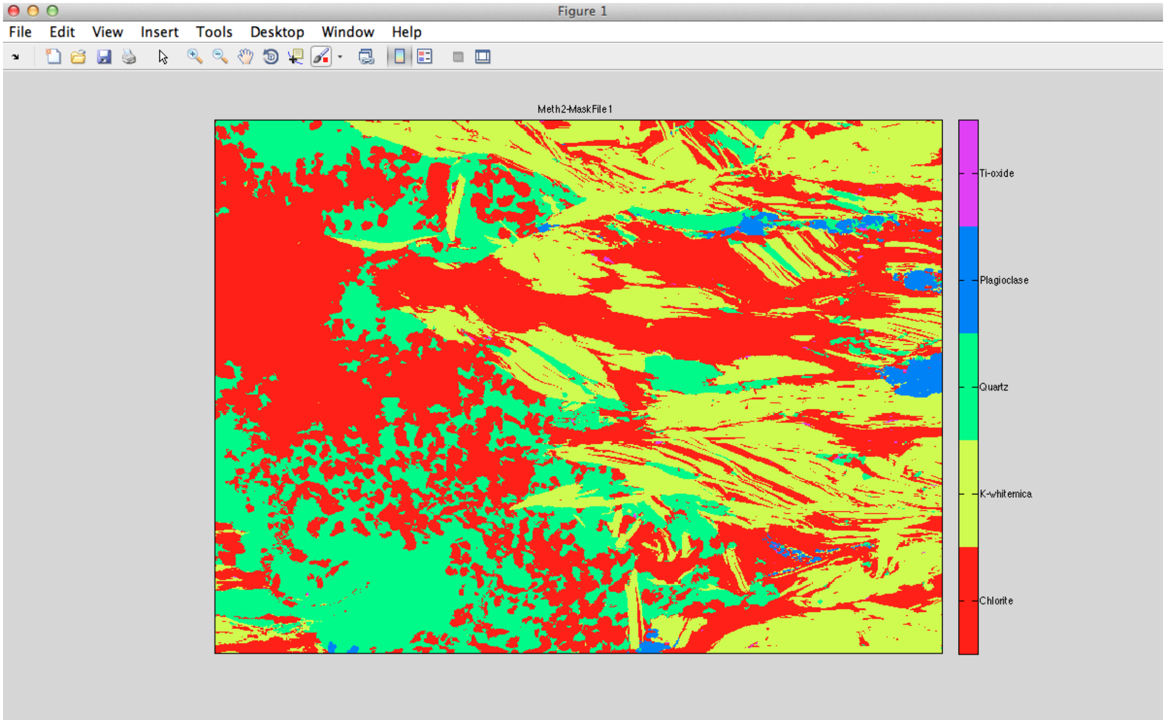
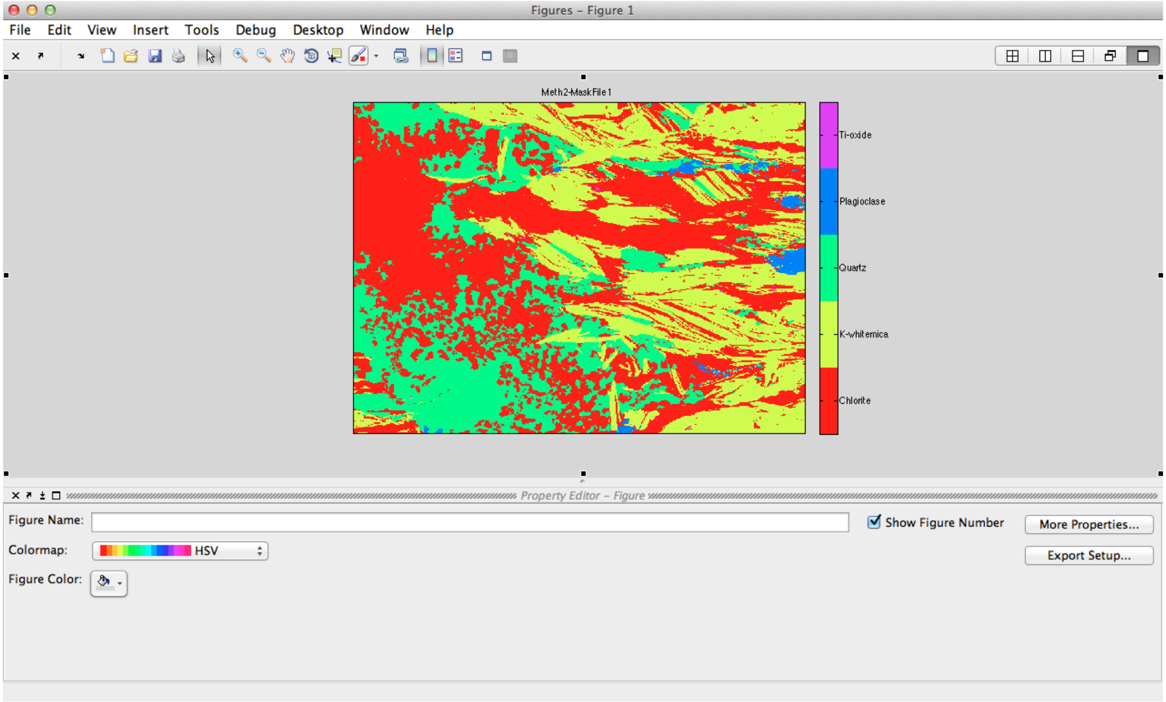


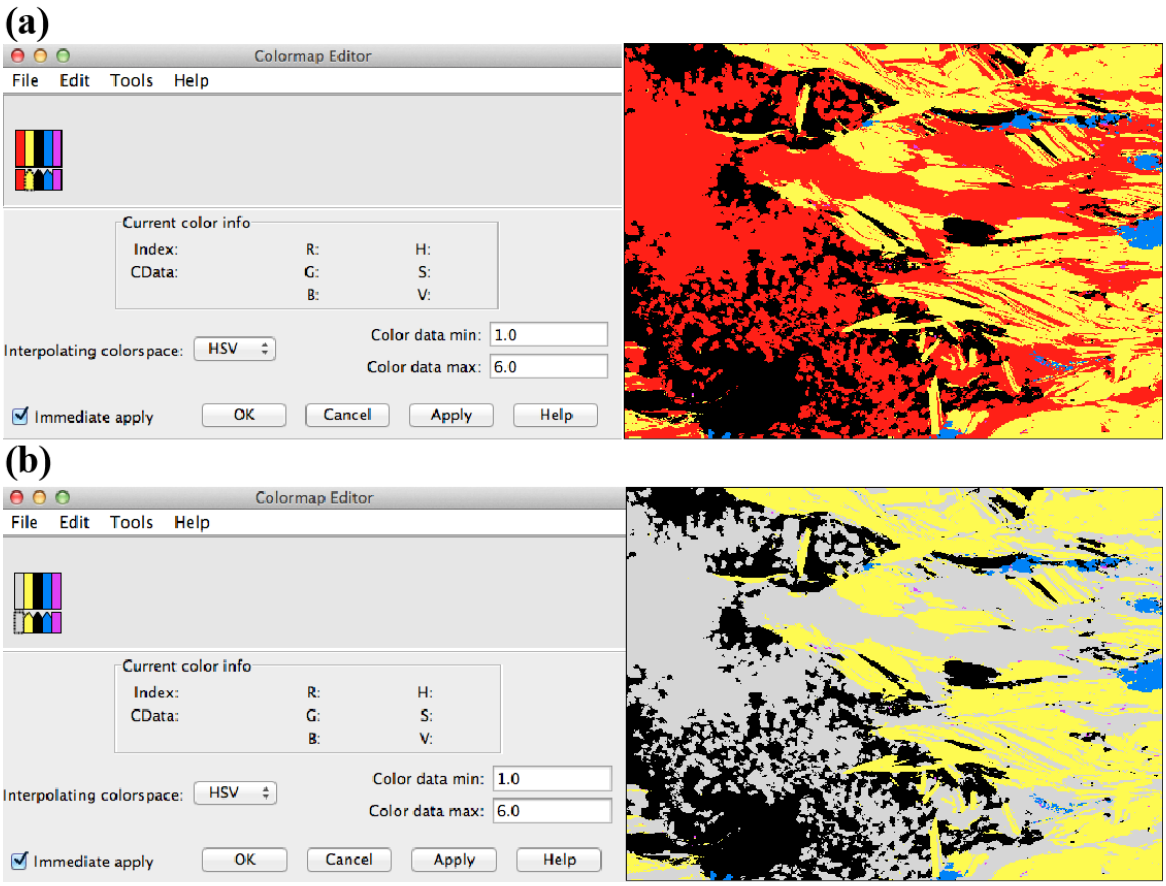
Figure 4.1 – *Mask image exported using the function* export mask image *(see text)*



Colormap: HSV

☑ Show Figure Number

Figure 4.2 – *Mask-image with the Figure editor*



(a)

Interpolating colorspace: HSV

Color data min: 1.0

Color data max: 6.0

☑ Immediate apply

(b)

Interpolating colorspace: HSV

Color data min: 1.0

Color data max: 6.0

☑ Immediate apply

Figure 4.3 – *Colormap Editor with the new colors*

4.2 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.

4.2.1 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:

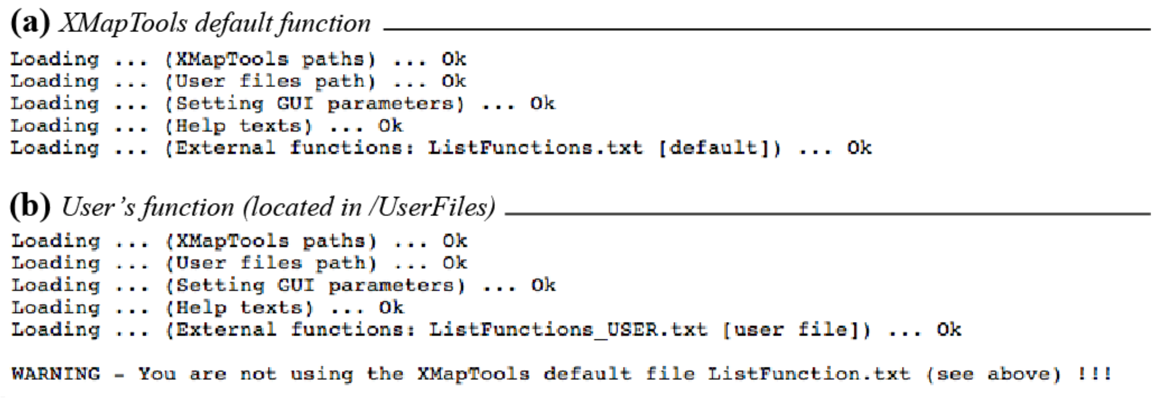
- **Function type** that correspond to the function category. Possible indexes are: [1] Structural formulae; [2] P, T and P-T map mode; [3] P, T and P-T spot mode; [4] General Functions.
- **Mineral(s)** that correspond to the name(s) of mineral phase(s) for which the function may be applied. For example, 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© functions files (**.m*). For example, the function name *StructFctChlorite* is reported for the file *StructFctChlorite.m*.
- **Output variables** is the list of output variable names.
- **Input variables** is the list of input variable names that are the names of the standardized maps generated by XMAPTOOLS. The oxide names available are: Na2O, MgO, Al2O3, SiO2, P2O5, SO2, Cl2O, K2O, CaO, TiO2, V2O5, Cr2O3, MnO, FeO, CoO, NiO, CuO, ZnO, ZrO2, AgO, CdO, SnO2, Ce2O3, As2O5, Sb2O3, Cs2O, La2O3, Nd2O3, PbO, SrO, ThO2, UO2, Y2O3, Sm2O3, Gd2O3, Dy2O3, Pr2O3. The metalloids names available are: Fe_ms, Cu_ms.
- **External variables** (optional for function of type [3]) are variables that can be edited by the user at each iteration. Such variables must be provided together with a default value, for example: *PressureKbar(10)*.

All these options are separated by the delimiter >.

This file *ListFunctions.txt* should never be edited by any user. If additional functions are needed, the following procedure can be applied:

[1] Close XMAPTOOLS and go to the setup directory (*/program*).

[2] Copy the file *ListFunctions.txt* into the repertory */UserFiles*.



(a) *XMapTools default function*

```
Loading ... (XMapTools paths) ... Ok
Loading ... (User files path) ... Ok
Loading ... (Setting GUI parameters) ... Ok
Loading ... (Help texts) ... Ok
Loading ... (External functions: ListFunctions.txt [default]) ... Ok
```

(b) *User's function (located in /UserFiles)*

```
Loading ... (XMapTools paths) ... Ok
Loading ... (User files path) ... Ok
Loading ... (Setting GUI parameters) ... Ok
Loading ... (Help texts) ... Ok
Loading ... (External functions: ListFunctions_USER.txt [user file]) ... Ok

WARNING - You are not using the XMapTools default file ListFunction.txt (see above) !!!
```

Figure 4.4 – *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* UserFuntions *and the default file is loaded and a warning message displayed. (b) The file ListFunctions_USER.txt exists and has been loaded.*

[3] Rename *ListFunctions.txt* as *ListFunctions_USER.txt* (case sensitive).

[4] Come back to the working directory and restart XMAPTOOLS. If the user's function is read by the program a warning message is displayed in the Command Window when XMapTools is launching (Fig. 4.4b). If this warning is not displayed (Fig. 4.4a) the default file has been loaded by the program. Check the external function name in */UserFiles* that must be *ListFunctions_USER.txt*.

4.2.2 Procedure to add an external function to XMapTools

Not yet available...

4.2.3 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 4.2.1, this file reports all the characteristics of the external functions. This file provides the list of input and output parameters for each functions.

4.2.3.1 Two names functions (P, T and P-T functions)

In this example, we can test the thermometer chlorite-chloritoïd of Vidal et al. (1999). The setup line in *ListFunctions.txt* corresponding to this external function is:

3>Chlorite+Chloritoid>T- Vidal etal 1999>NThermoCCVidal1999>T lnKd>SiO2 TiO2 Al2O3 FeO MnO MgO CaO Na2O K2O>

- **Function type** [3] corresponds to P, T and P-T spot mode
- **Mineral(s)** The thermometer is indexed in the group *Chlorite+Chloritoid*

- **Name** displayed is *T- Vidal etal 1999*
- **Function name** is *NThermoCCVidal1999.m*
- **Output variables** are: T and lnKd
- **Input variables** are SiO2, TiO2, Al2O3, FeO, MnO, MgO, CaO, Na2O, K2O
- **External variables** are not used in this case (no pressure dependency).

the input data are organized as a matrix in which the first line is the composition of the chlorite and the second line the composition of the chloritoid (same order of the name: Chlorite+Chloritoid). The compositions order is given by the input variables: [SiO2, TiO2, Al2O3, FeO, MnO, MgO, CaO, Na2O, K2O].

The following analyses of chlorite and chloritoid PSB9210b are used from Table 2 in Vidal et al. (1999).

- **Chlorite:** 25.63 0.03 23.37 22.82 0.22 15.13 0.06 0.02 0.02
- **Chloritoid:** 24.15 0 40.80 22.81 0.16 3.02 0.04 0.01 0.02

[2] Open the directory */program/Functions* with the MATLAB© *Current Folder* tool. Use the following code into the *Command Window* to test the function:

Code 4.1 – *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).

4.2.3.2 One 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© 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.

4.3 XMAPTOOLS ADD-ONS

4.3.1 List of compatible add-on

There is no official add-on published so far.

4.3.2 How to install and use the XMapTools' add-on

[1] Download and unzip the add-on package.

[2] Cut the add-on folder.

[3] Close XMAPTOOLS and 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 to the add-on.

4.3.3 Procedure to create a new add-on

Not yet available...

Please contact me if you are interesting in developing a XMAPTOOLS' add-on.

5

GENERAL ERRORS AND SOLUTIONS

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

6

TUTORIAL 1: ELECTRON MICROPROBE X-RAY MAPS PROCESSING

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).

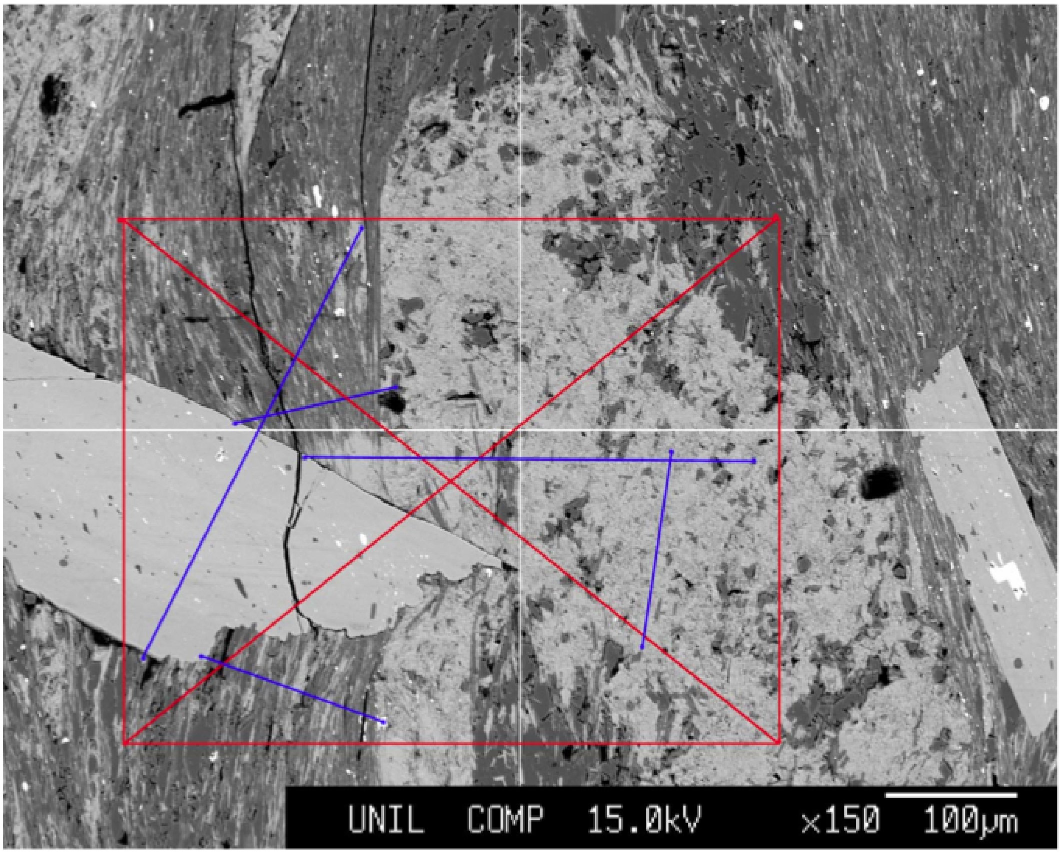


Figure 6.1 – *BSE image of the studied area (red rectangle) with transect of spot analyses (blue lines) from Bernier (2011).*

6.1.1 How to get started

XMapTools is a software that can only be executed from the MATLAB© environment. The following steps explain how to run XMapTools in you computer.

(1) Run MATLAB©

(2) Go to the data example repertory using the *Current Folder* window in the MATLAB© window. This step is critical as many files will be generated by XMapTools and stored in the working directory. Make sure that the current path is *.../Example* as in Figure 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© 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).

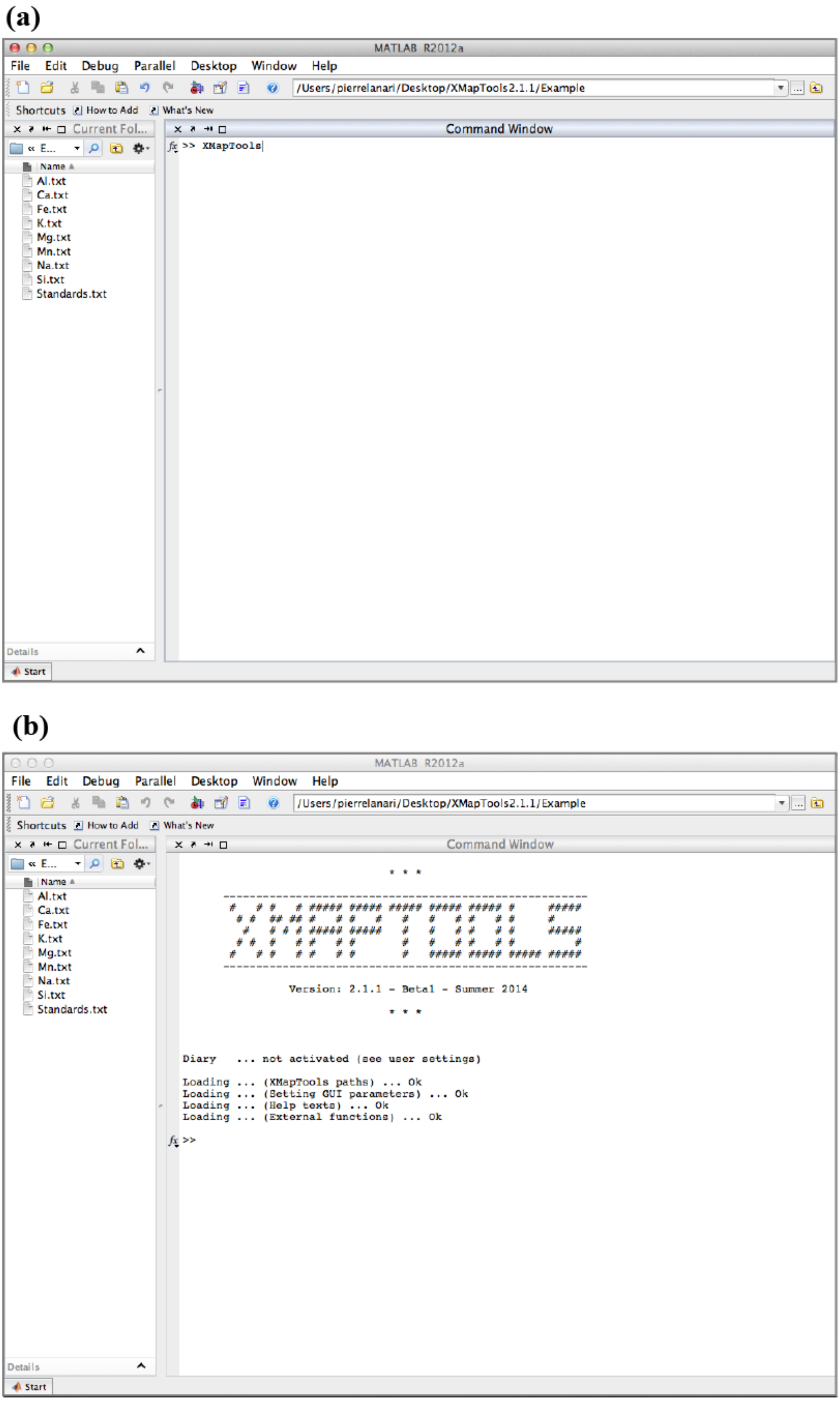
(2) A dialog box opens in which files can be selected (6.4a). Select all the files together (i.e. Al.txt, Ca.txt, Fe.txt, K.txt, Mg.txt, Mn.txt Na.txt and Ti.txt) using the *maj* button. Press the button *open* and XMapTools reads and imports the selected files.

(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.

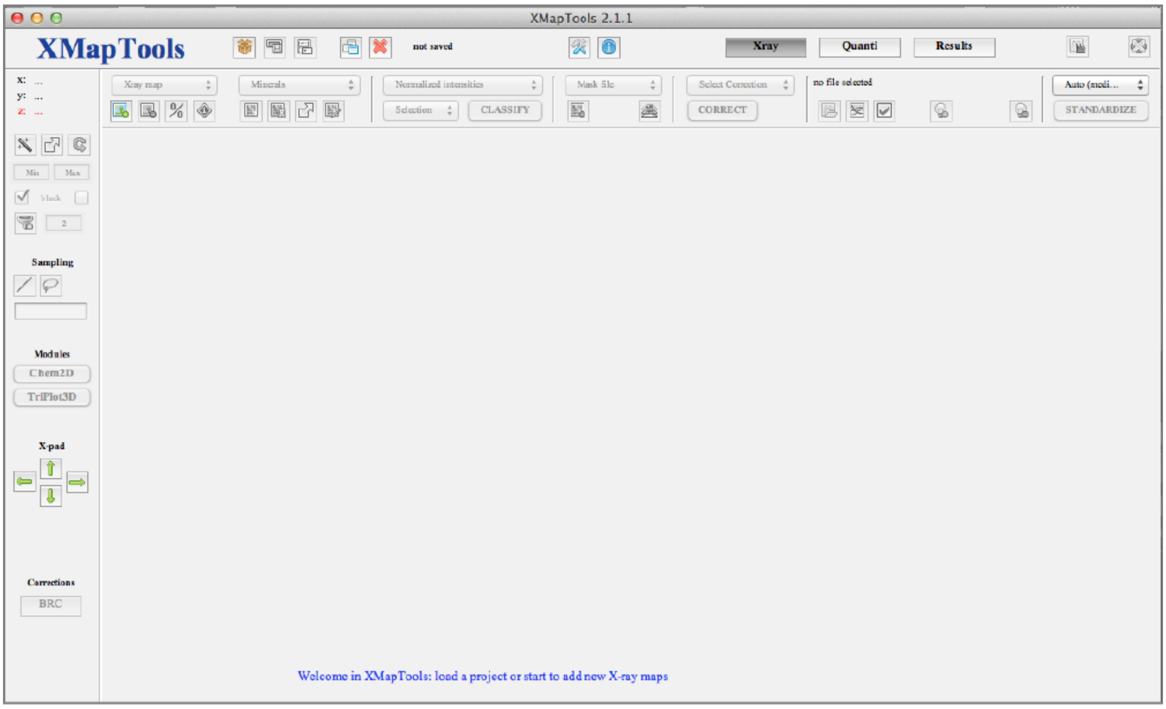
Warning: Do not apply any transformation such as rotation to EPMA maps, otherwise the map coordinates in Standard.txt will not work anymore. The rotation correction should only be used with standardized maps such as LA-ICP-MS maps.



```
>> XMapTools
```

```
                        * * *

    ------------------------------------------------------
     #   # #   # ##### ##### ##### ##### ##### #     #####
      # #  ## ## #   # #   #   #   #   # #   # #     #
       #   # # # ##### #####   #   #   # #   # #     #####
      # #  #   # #   # #       #   #   # #   # #         #
     #   # #   # #   # #       #   ##### ##### ##### #####
    ------------------------------------------------------

            Version: 2.1.1 - Beta1 - Summer 2014

                        * * *


Diary   ... not activated (see user settings)

Loading ... (XMapTools paths) ... Ok
Loading ... (Setting GUI parameters) ... Ok
Loading ... (Help texts) ... Ok
Loading ... (External functions) ... Ok

>>
```

Figure 6.2 – *Procedure to run XmapTools from the MATLAB© command window*



Welcome in XMapTools: load a project or start to add new X-ray maps

Figure 6.3 – *XMapTools main window*

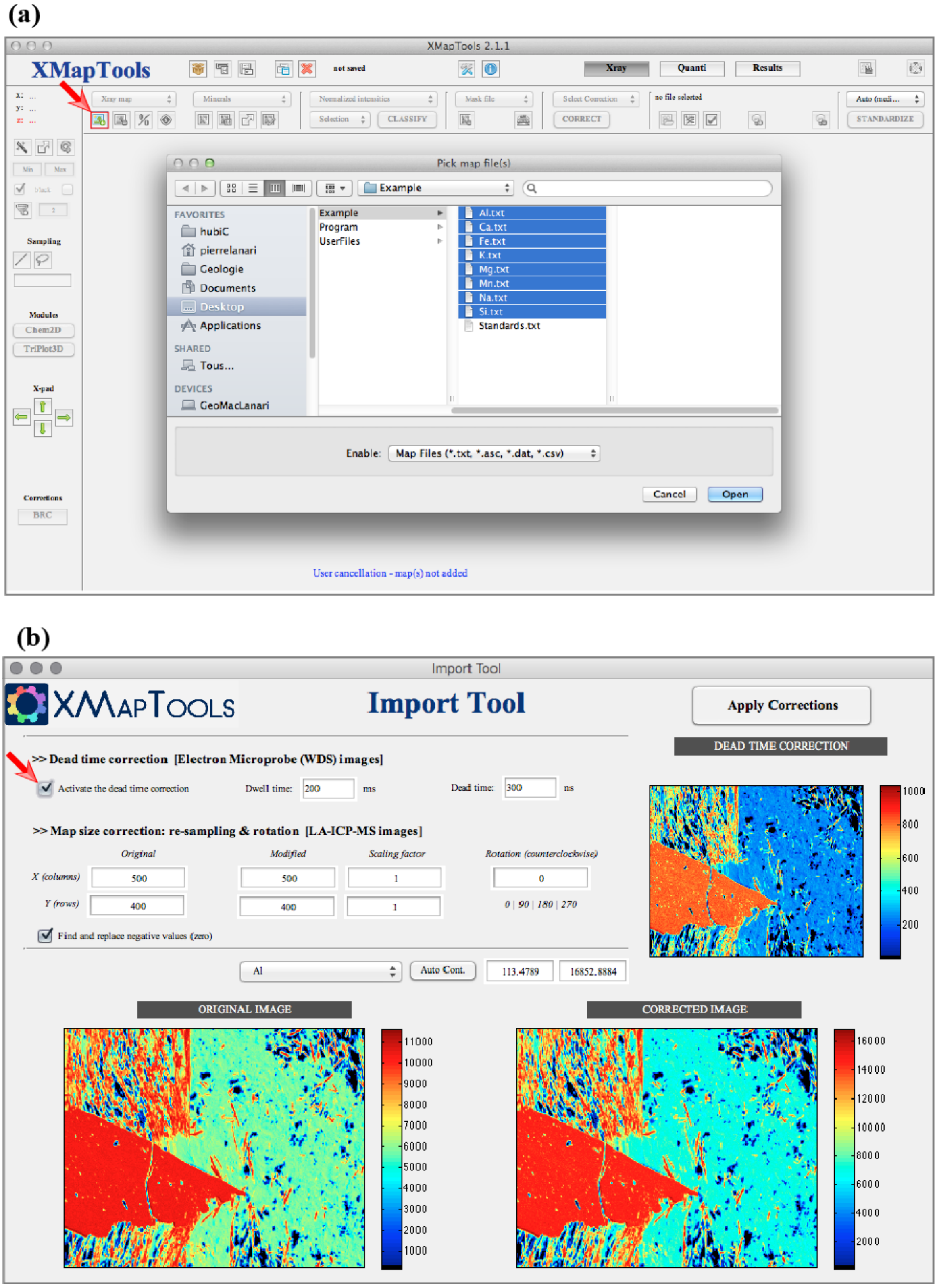
(6) When all the corrected files have been imported, XMAPTOOLS displays the first map in the main figure area (Fig. 6.5). The details about the maps and the corrections are displayed in the MATLAB© *Command Window* (see insert 6.1).

```
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.



Enable: Map Files (*.txt, *.asc, *.dat, *.csv)

User cancellation - map(s) not added

>> Dead time correction [Electron Microprobe (WDS) images]

☑ Activate the dead time correction Dwell time: 200 ms Dead time: 300 ns

>> Map size correction: re-sampling & rotation [LA-ICP-MS images]

	Original	Modified	Scaling factor	Rotation (counterclockwise)
X (columns)	500	500	1	0
Y (rows)	400	400	1	0 | 90 | 180 | 270

☑ Find and replace negative values (zero)

Al 113.4789 16852.8884

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

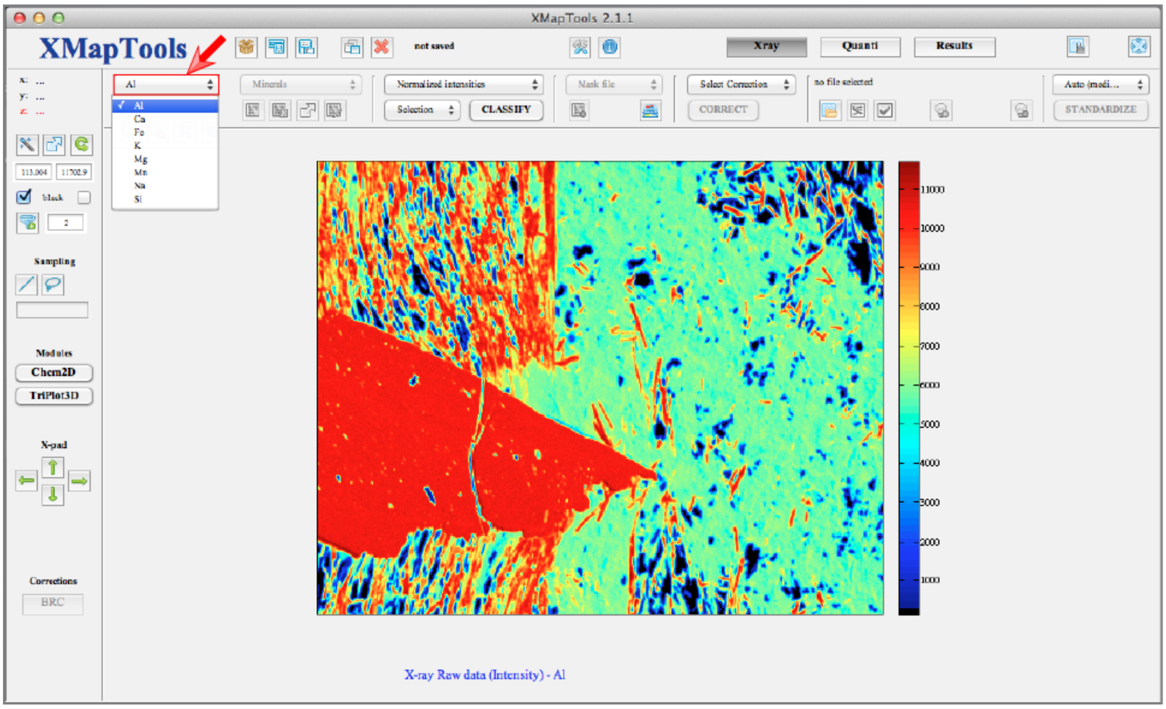


Figure 6.5 – *X-ray menu is available to display X-ray images*

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)

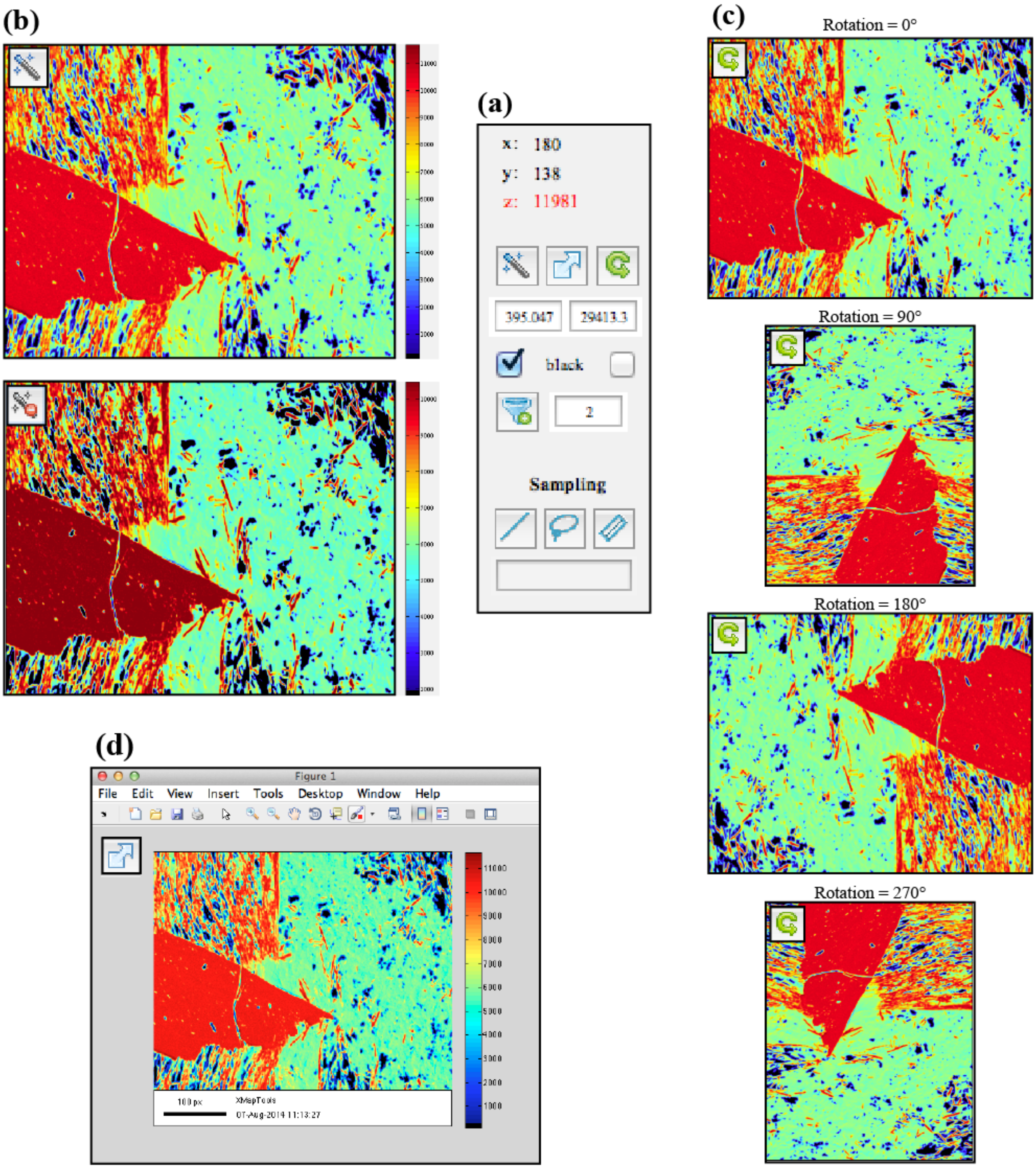
(2) In the figure option window, the live coordinate screen displays X, Y and Z coordinates corresponding to the mouse position on the X-ray map. The Z value is the value of the overflew pixel located at (X,Y) position. Try to displace your mouse above the map in order to get Z values, here corresponding 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).



x: 180
y: 138
z: 11981

395.047 29413.3

☑ black ☐

2

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° (counterclockwise). Four positions corresponding to 0°, 90°, 180° and 270° 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° 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©

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).

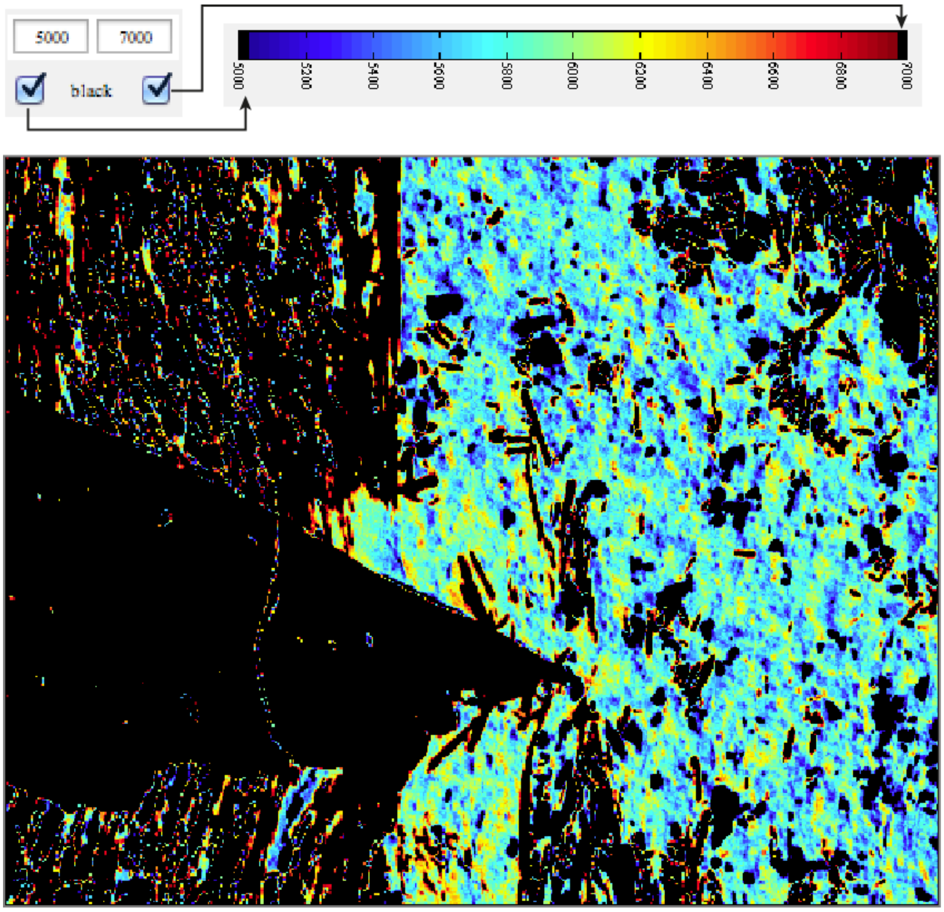


Figure 6.7 – *Display options. (a) Display option menu; (b) auto-contrast mode enabled (down), disabled (up); (c) rotation mode for different rotation angles.*

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.

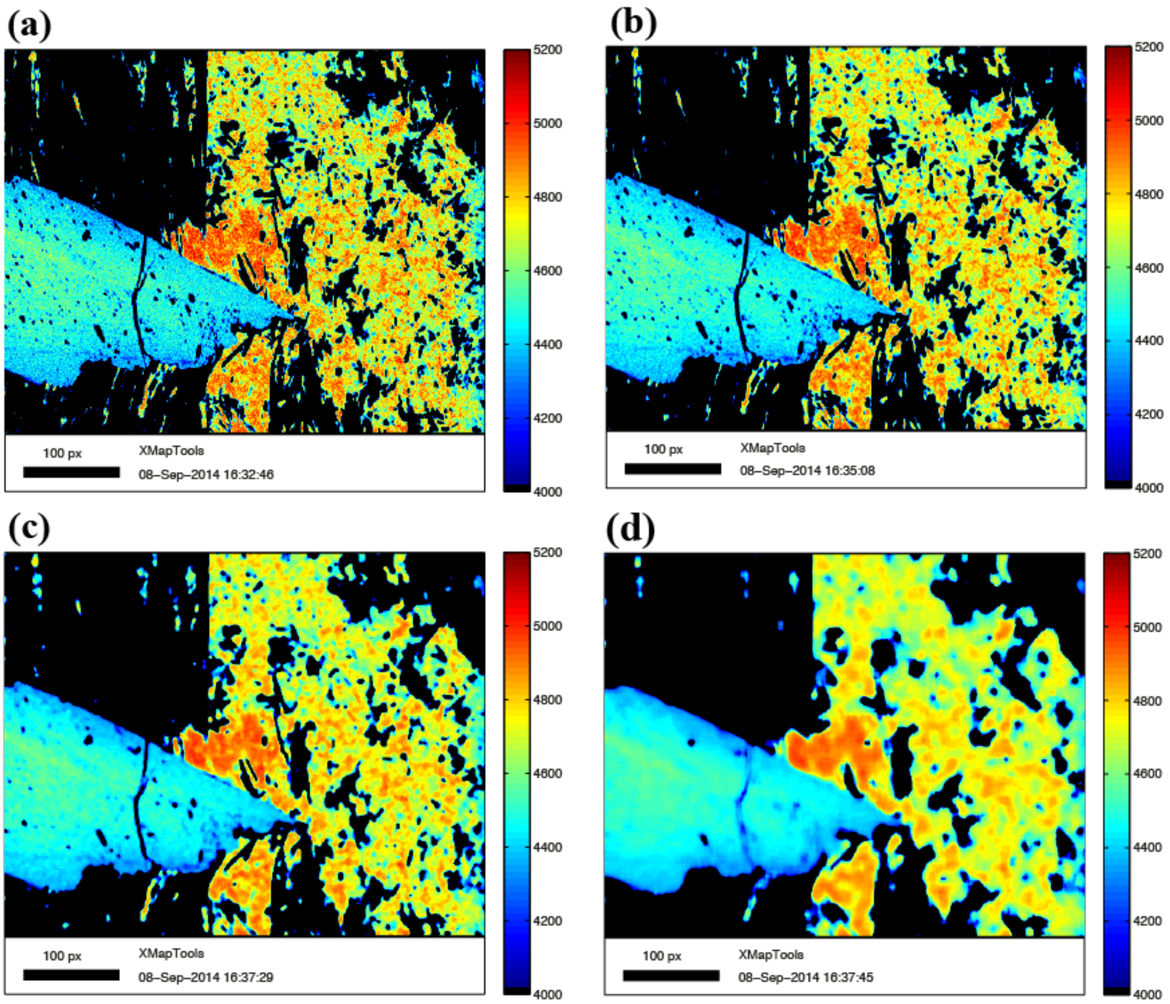


Figure 6.8 – *Median Filter. (a) not used; (b) size = 2; (c) size = 5; (d) size = 10;*

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© 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*.

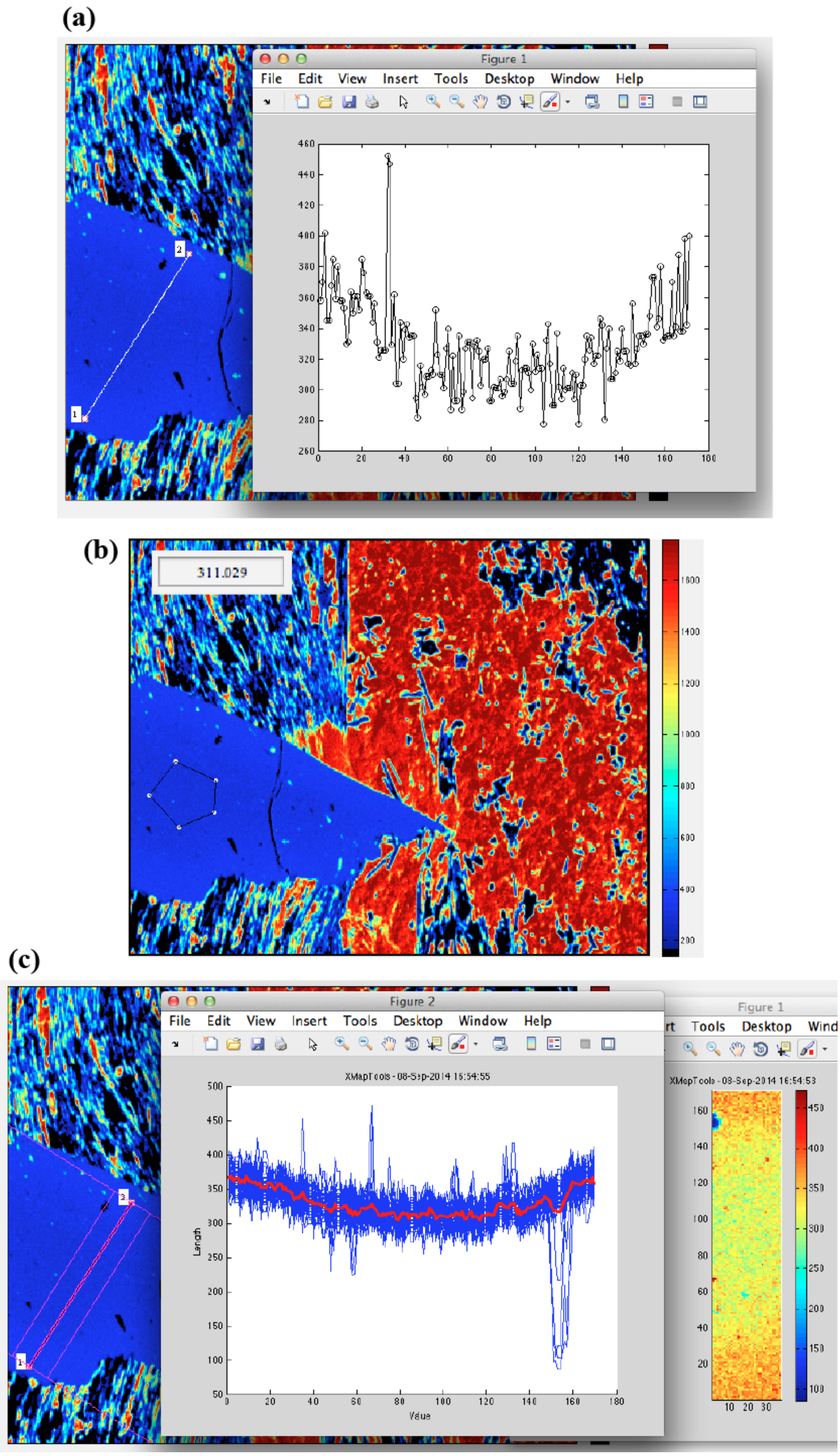


Figure 6.9 – *Sampling functions. (a) mode: line; (b) mode: area (c) mode: integrated lines.*

(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 ± 18 counts (1σ).

(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 % 2σ) 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© 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

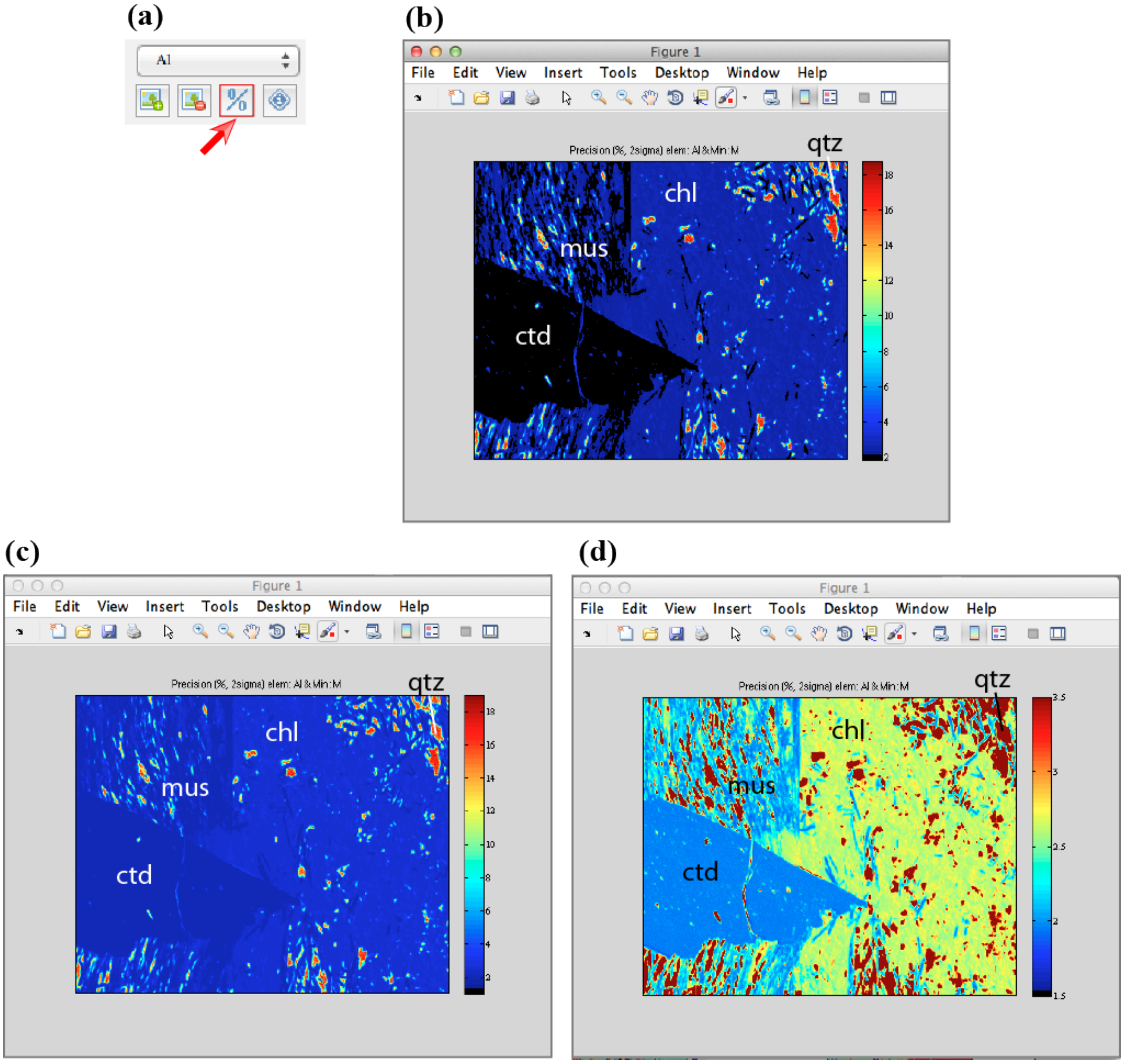
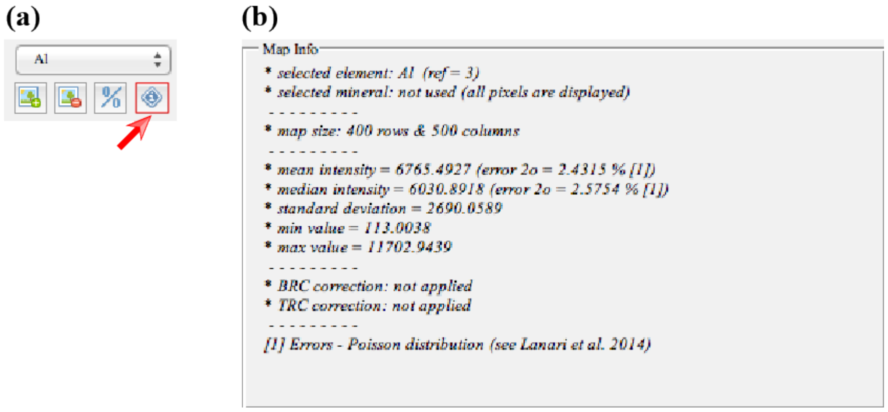


Figure 6.10 – *Precision image in % calculated from the X-ray map of Al. (b), (c) and (d) are the same data (precision image for Al in %) plotted with different color bar axis values (see text)*

```
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*



```
* 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)
```

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)

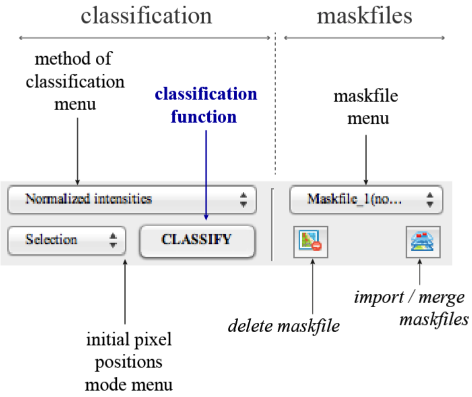


Figure 6.12 – *Classification and mask file menus and buttons*

(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).

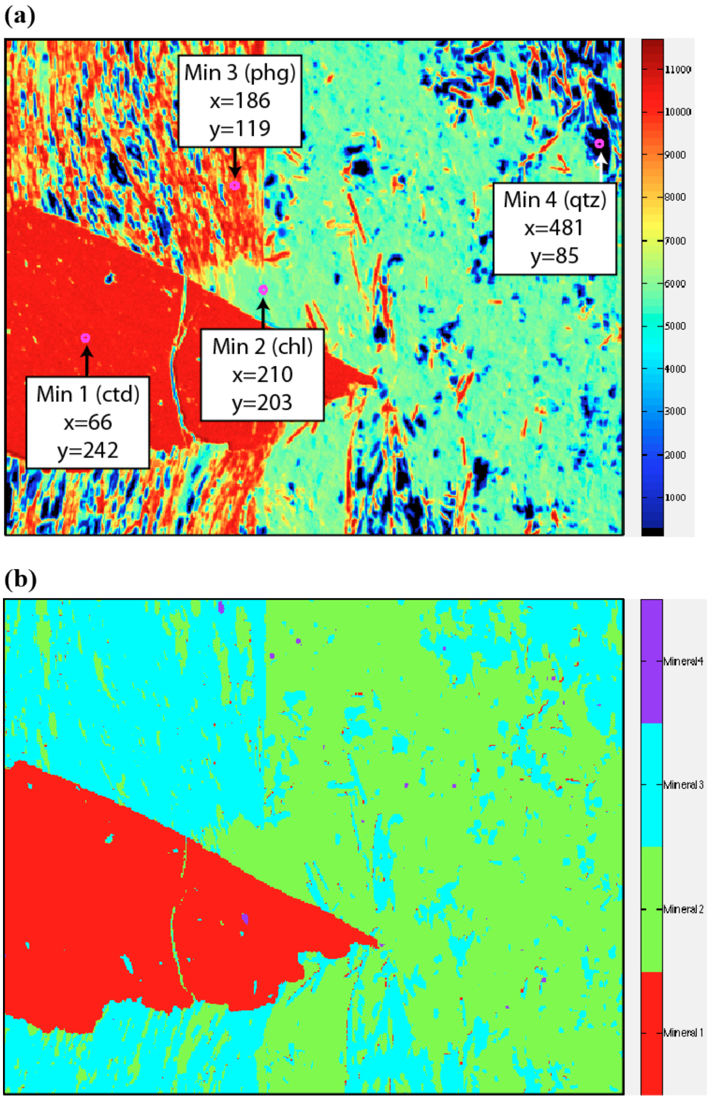


Figure 6.13 – *Classification: (a) Coordinates and position of the input pixels selected by the user in order to define the compositions of the minerals (map: Al in number of counts). (b) Mask image generated using the mode* Normalized intensities *and the mode* Selection *(see [6])*

(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.

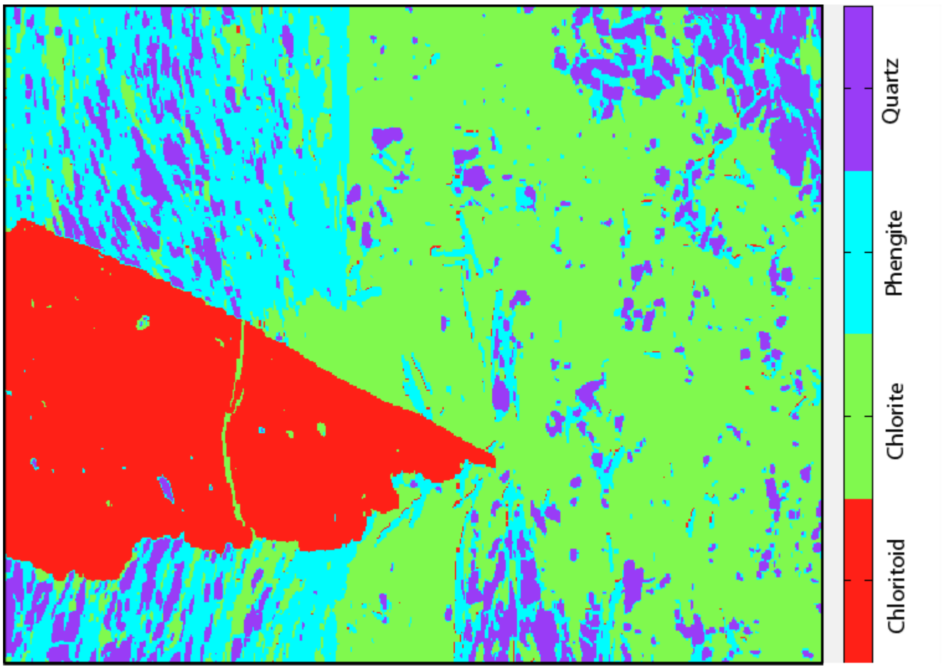


Figure 6.14 – *Classification: Mask image generated using the mode* Classical computation *and the mode* File *(see [8])*

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 Chem2D and TriPlot3D modules

The manual classification option has been developed in the framework of XMAPTOOLS 2. This new method consists of defining groups of pixels (i.e. masks) in chemical diagrams using the two modules *Chem2D* and *TriPlot3D* and importing and merging them into a new mask file (see 6.2.5.1). In this section only the way do generate a masks using the *Chem2D* module is described. *TriPlot3D* module is described later in the tutorial (see section **??**).

(1) In the *X-ray workspace*, display the map *Al* using the X-ray menu (first map) and select the phase *none* in the mask menu.

(2) The chemical module may be launched by pressing the button *Chem2D*.

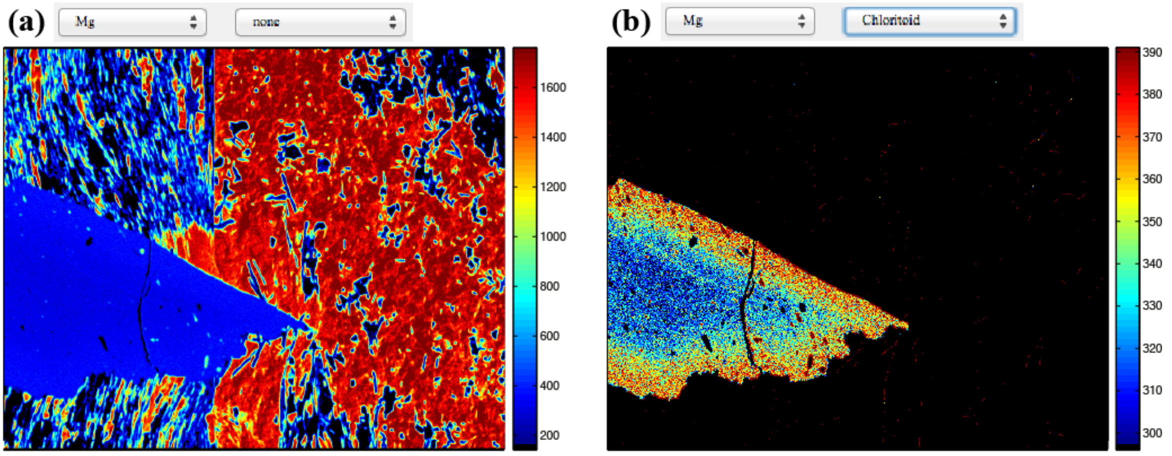


Figure 6.15 – *Display X-ray image Mg (a) with none selected in the mask menu and (b) with chloritoid selected in the mask menu. The auto-contrast function has been used before to generate the images.*

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

In the diagram displayed in figure 6.16, the blue dots correspond to X-ray counts values of pixels directly taken from the maps. In this example, three groups of pixels can be identified in this *Fe vs Mg* diagram (Fig. 6.17). The first group with high Fe and Mg content is the chlorite. A second groups shows high Mg-content but is Fe-poor; this group belongs to chloritoid which has typical low XMg. The group showing both low-Fe and Mg content contains pixels of phengite and quartz. Between two groups mixing analyses are visible.

One of the most important tool of *Chem2D* module is the *Identify pixels* function. User can select a group of pixel compositions in the binary plot (rectangle) and display the corresponding pixels in a map. This function selects the pixels within a rectangle defined by two points. Statistical information is displayed in a small window on the right hand side.

(4) Select the points belonging to the group chloritoid using the function *Identify pixels*. 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 a subfolder *MaskFiles/*.
The same procedure is repeated for the phases identified above.

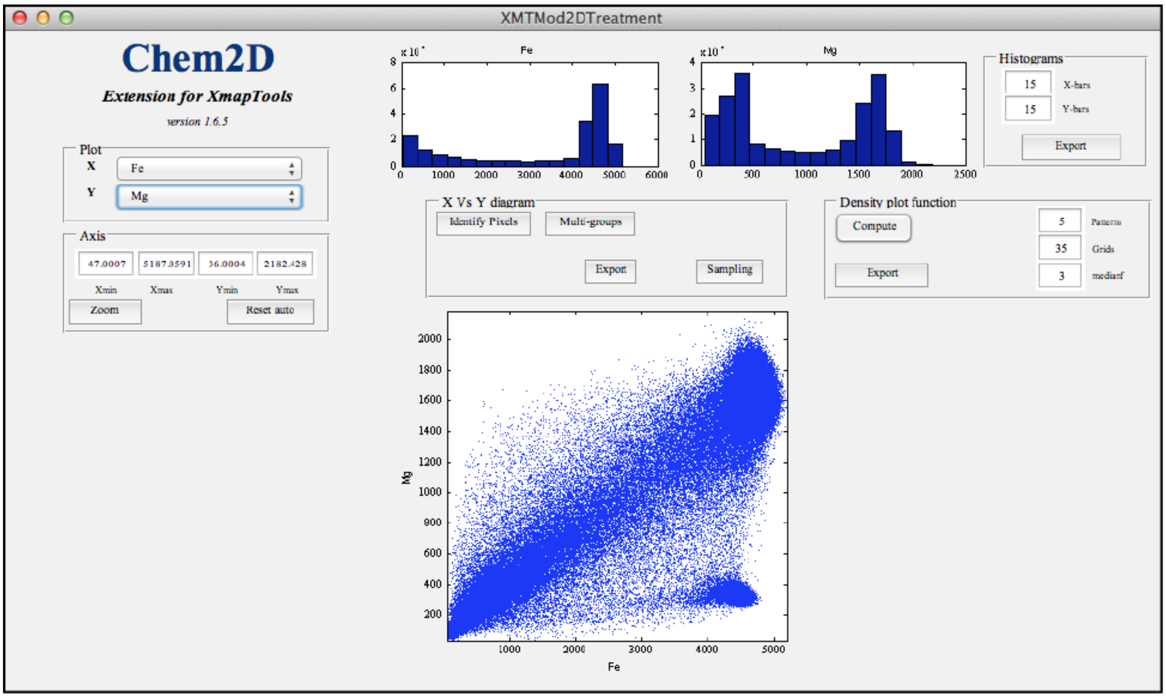
(6) In a diagram *Fe vs Mg* select the points belonging to the groupe chlorite and generate a mask file named *Chlorite.txt* (Fig. 6.18b).

(7) In a diagram *K vs Al* select the points belonging to the groupe 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 groupe quartz and generate a mask file named *Quartz.txt* (Fig. 6.18d).

Individual or merged Mask files can be imported in XMapTools.

(9) Close the module *Chem2D*.



X: Fe

Y: Mg

Xmin: 47.0007

Xmax: 5187.0591

Ymin: 36.0004

Ymax: 2182.428

X-bars: 15

Y-bars: 15

Patterns: 5

Grids: 35

medianf: 3

Figure 6.16 – Chem2D *module with the diagram Fe vs Mg*

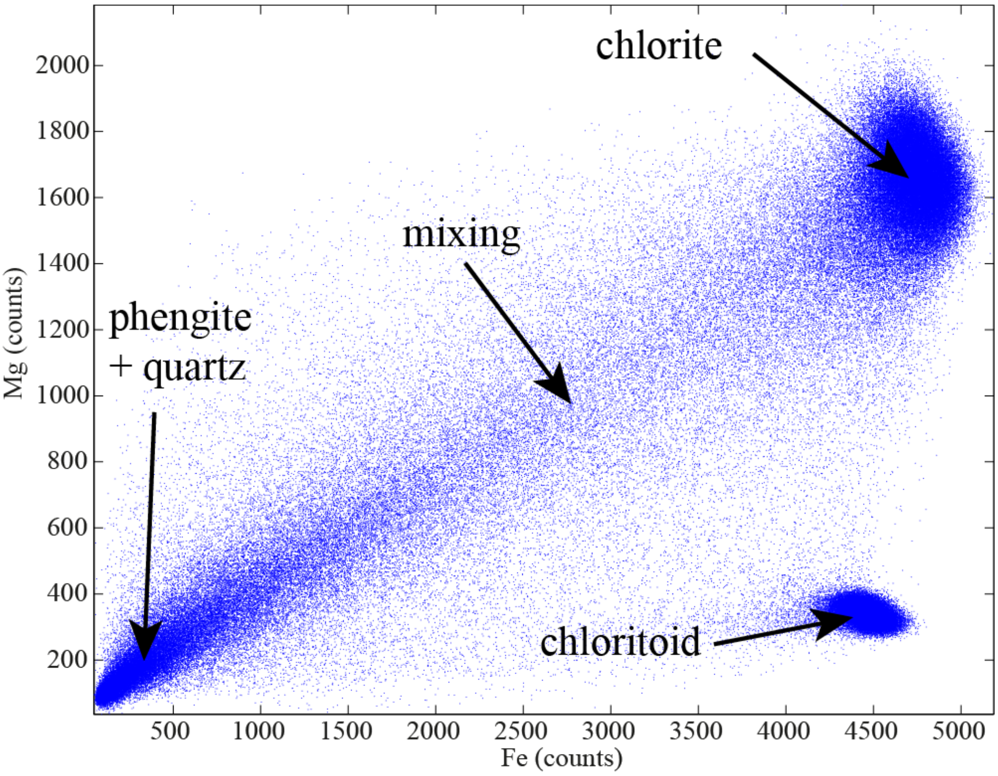
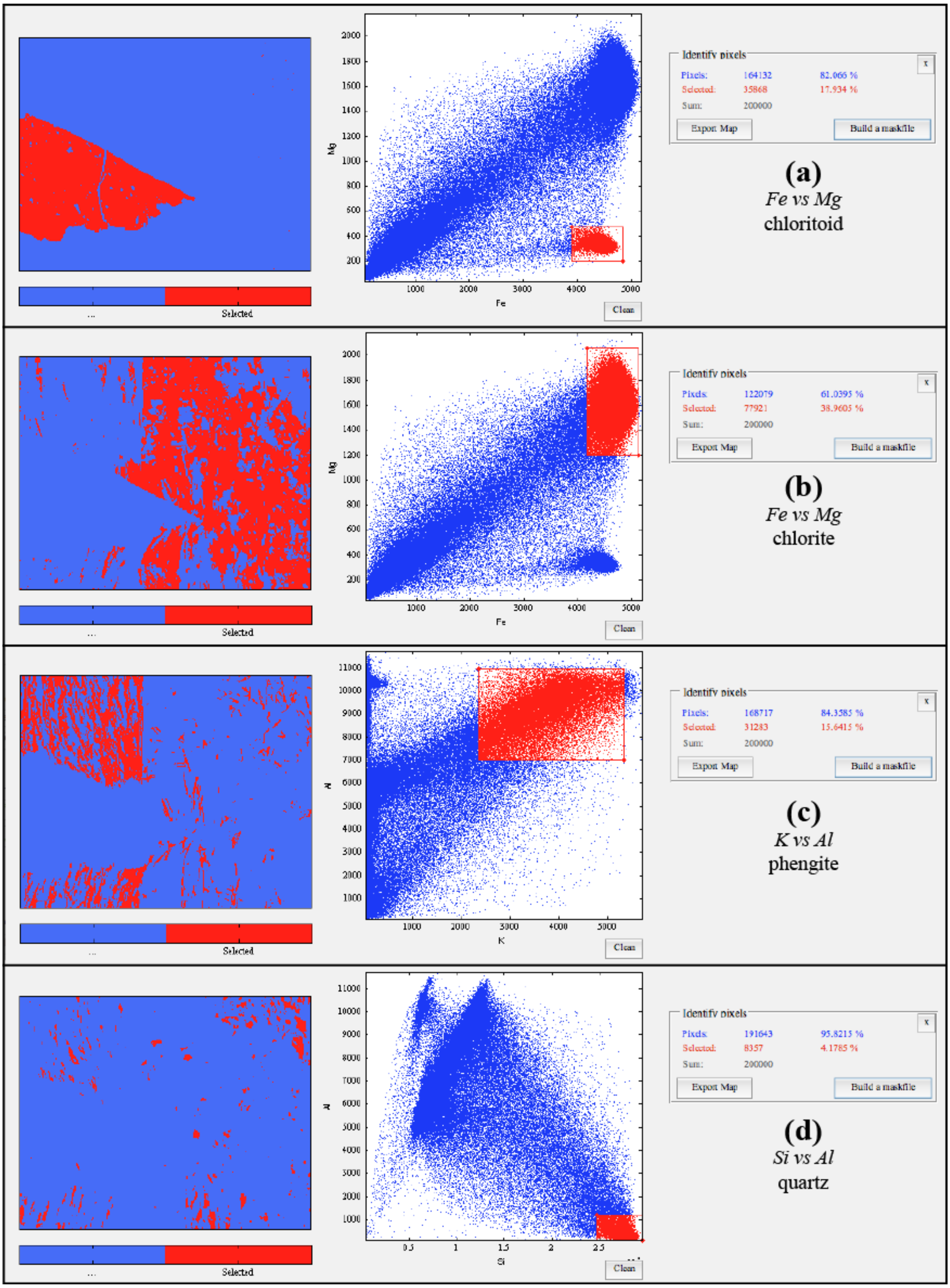


Figure 6.17 – Dhem2D *module with the diagram Fe vs Mg*



Identify pixels
Pixels: 164132 82.066 %
Selected: 35868 17.934 %
Sum: 200000

(a)
Fe vs Mg
chloritoid

Identify pixels
Pixels: 122079 61.0395 %
Selected: 77921 38.9605 %
Sum: 200000

(b)
Fe vs Mg
chlorite

Identify pixels
Pixels: 168717 84.3585 %
Selected: 31283 15.6415 %
Sum: 200000

(c)
K vs Al
phengite

Identify pixels
Pixels: 191643 95.8215 %
Selected: 8357 4.1785 %
Sum: 200000

(d)
Si vs Al
quartz

Figure 6.18 – Dhem2D *module with the diagram Fe vs Mg*

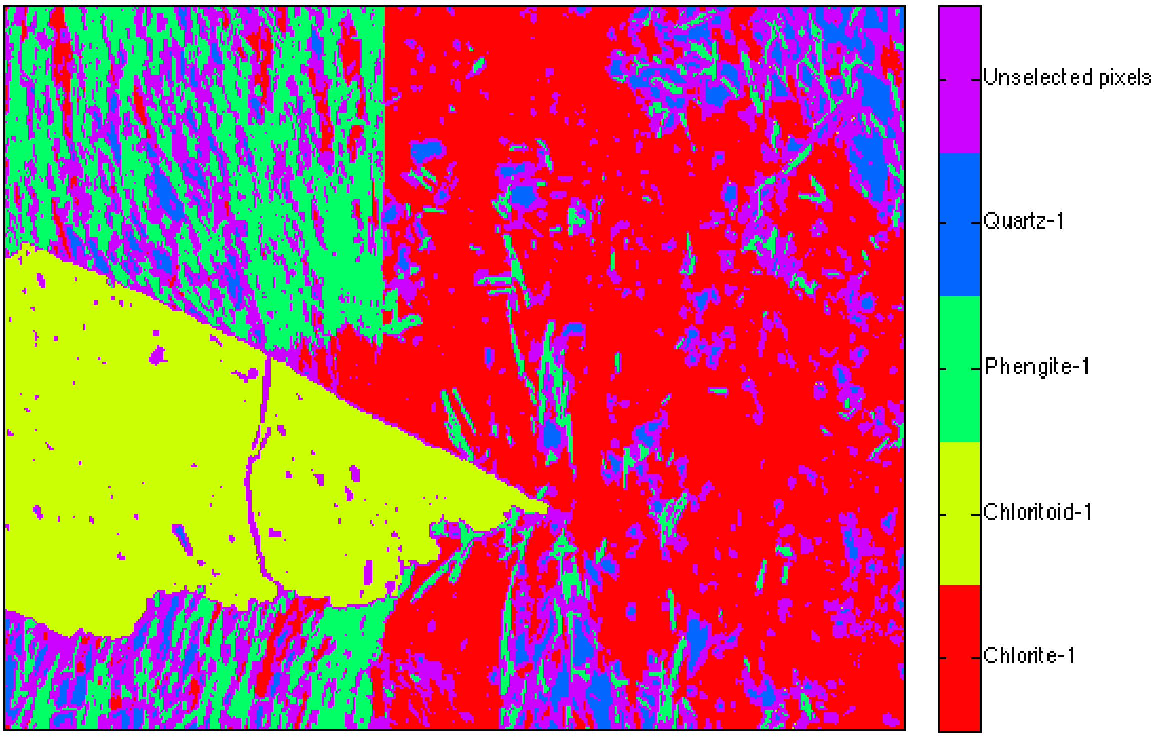


Figure 6.19 – *Mask image of the mask file: Merged-Maskfile*

(10) In XMAPTOOLS main GUI, 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 the XMAPTOOLS paper Lanari et al. (2014b) and references therein.

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 2.6.5 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_2 (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).

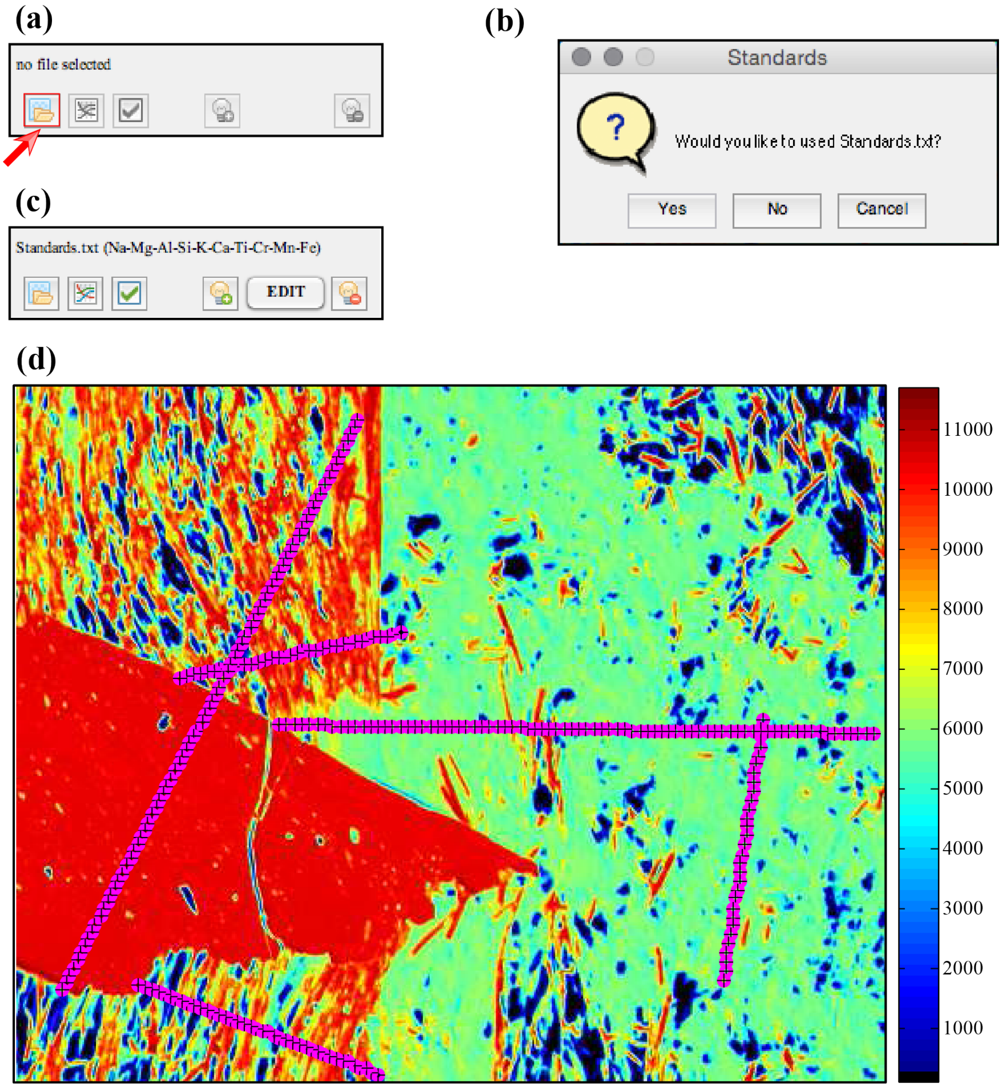
```
Standards testing ... (Element: Si) ...
Standards testing ... (Correlation: 0.77956)
Standards testing ... (Element: Si) .... Ok
```

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

(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 × 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 $Y = +2$.



Would you like to used Standards.txt?

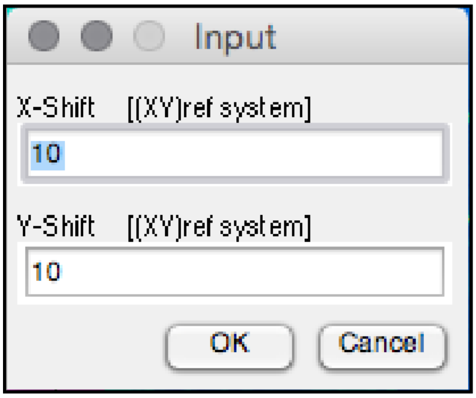
Figure 6.20 – *Procedure to load standards. (a) Group of buttons for internal standards (no standard file) (b) If a file Standards.txt exists in the working directory, the program proposes to open that file. (c) Group of buttons for internal standards (standard file loaded). (d) Map of Al with the spot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

(5) Select the correction *SPC* in the correction menu and press *activate* to enable the correction mode. Press *No*, because you do not need to check again the quality of std/maps positions (see step 4). Use the X-pad navigator (left hand side) to move the spot analyses of *one* pixel rightward and *two* pixels downward. Please wait for figure update before to press again on of the arrow button.

(6) Press *Apply* button located below the X-pad navigator in order to apply the correction. The correction is printed in the MATLAB© Command Window (see Code 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)*



X-Shift [(XY)ref system]

10

Y-Shift [(XY)ref system]

10

Figure 6.21 – *Window to define X and Y shifts*

(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 SiO2 spectra is 0.94.

(8) Save the project.

The new positions of spot analyses are saved. If you want to retrieve the original positions, you must load again the file *Standards.txt* or apply a inverse correction.

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*

(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 enable 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.

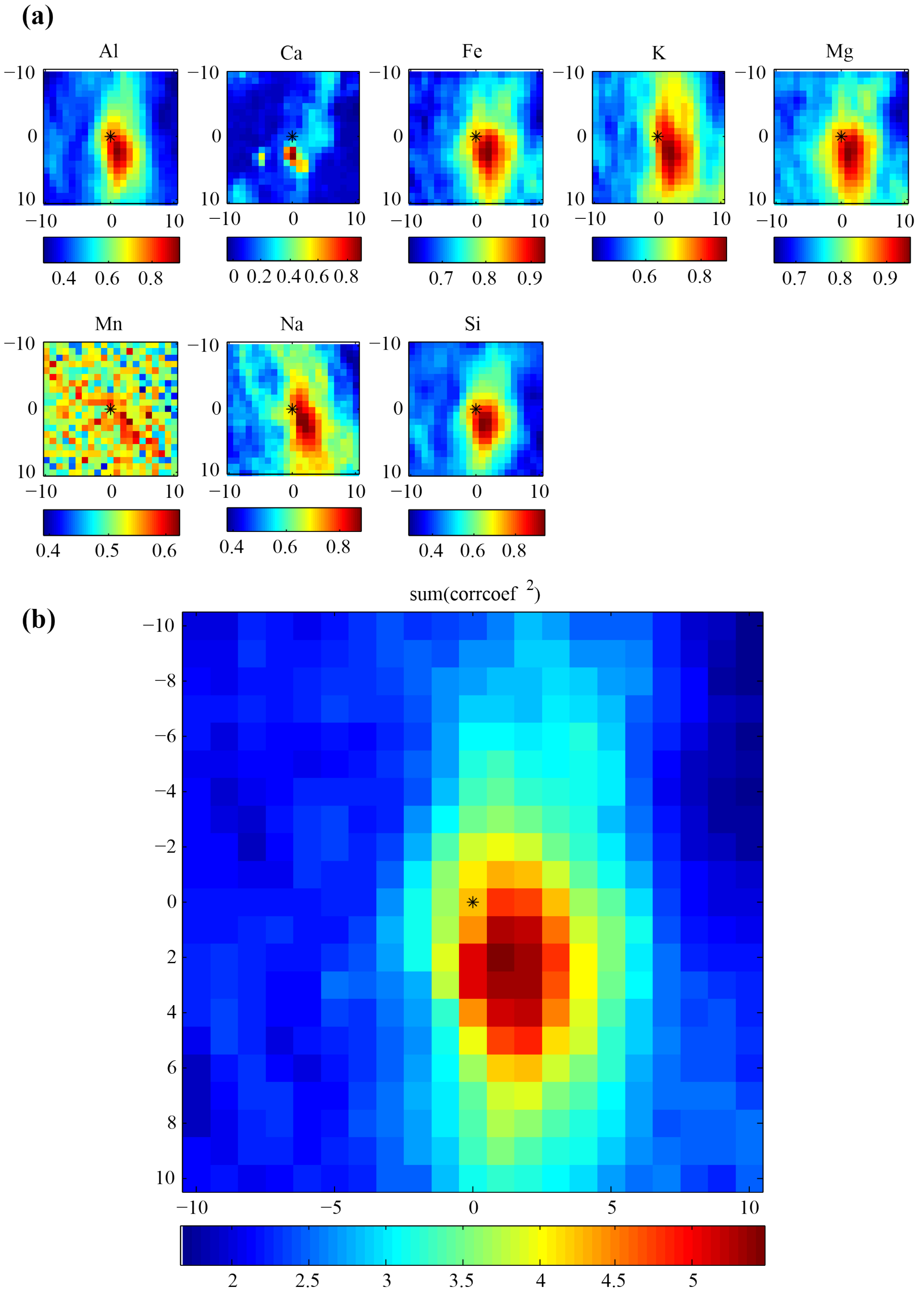


Figure 6.22 – *Results of the check quality of std/maps positions*

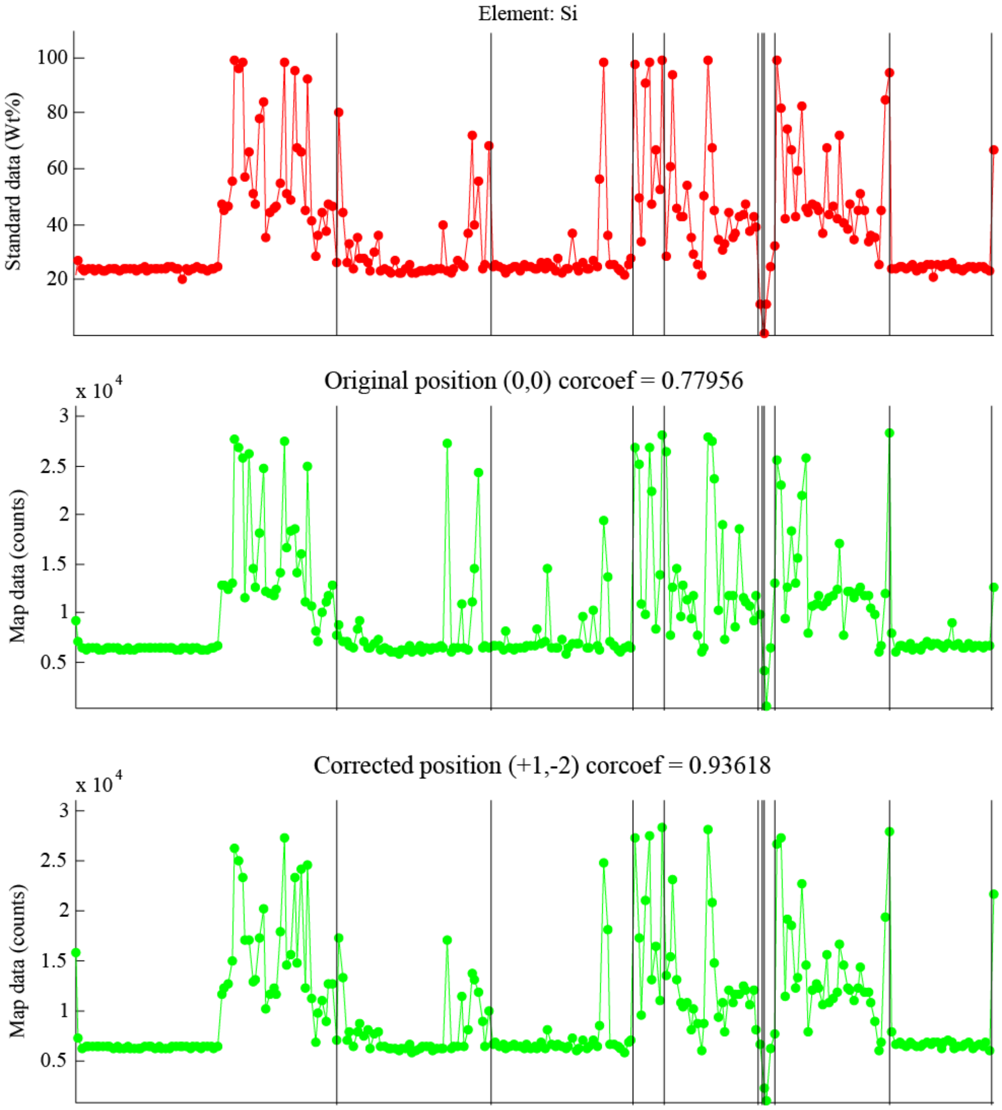


Figure 6.23 – *Results of display intensity vs composition chart for the original and corrected positions*

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 enable the selection mode

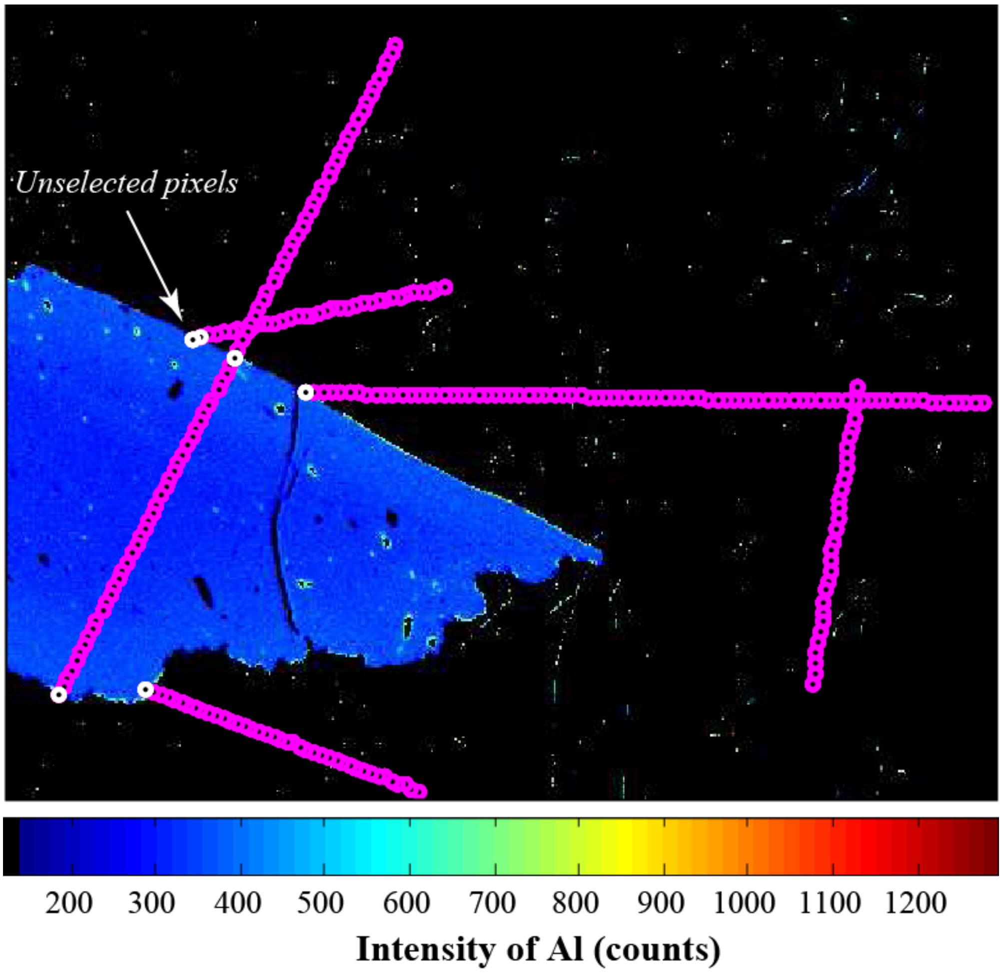


Figure 6.24 – *Internal standards for chloritoid. Note that the spot analyses near the grain boundaries are unselected (white circles)*

(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).

(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.

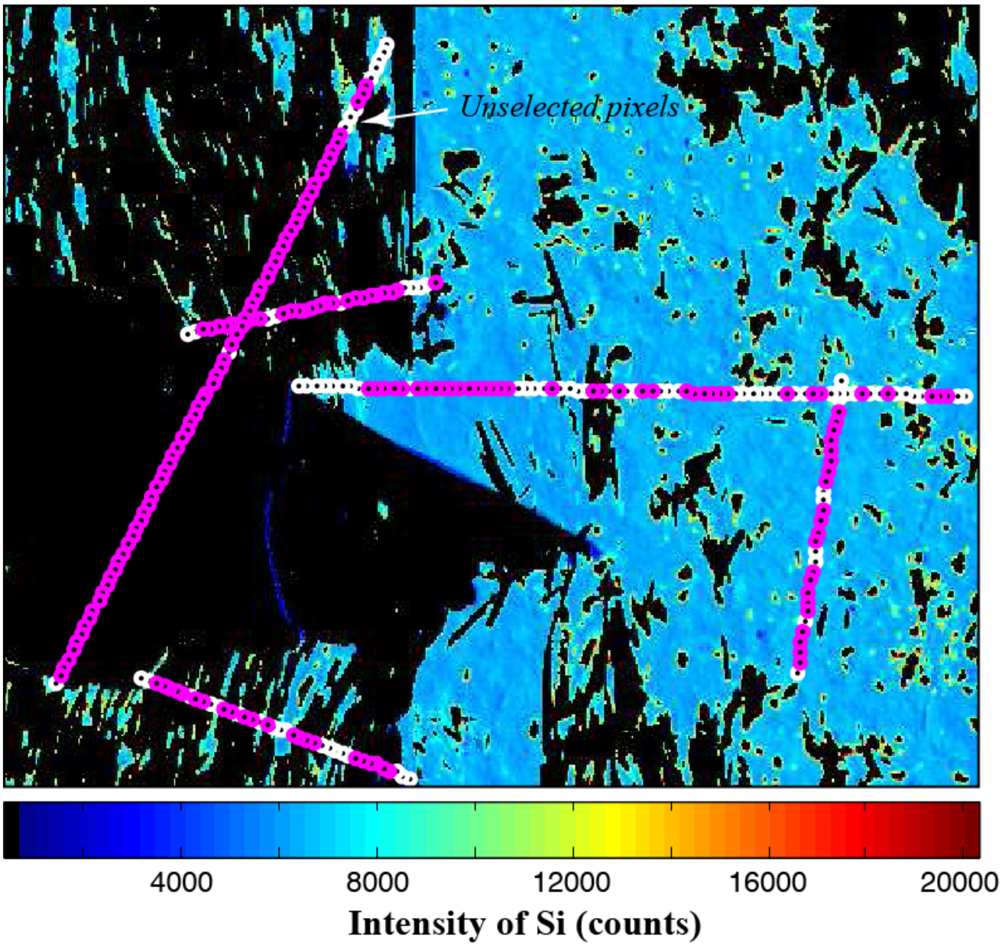


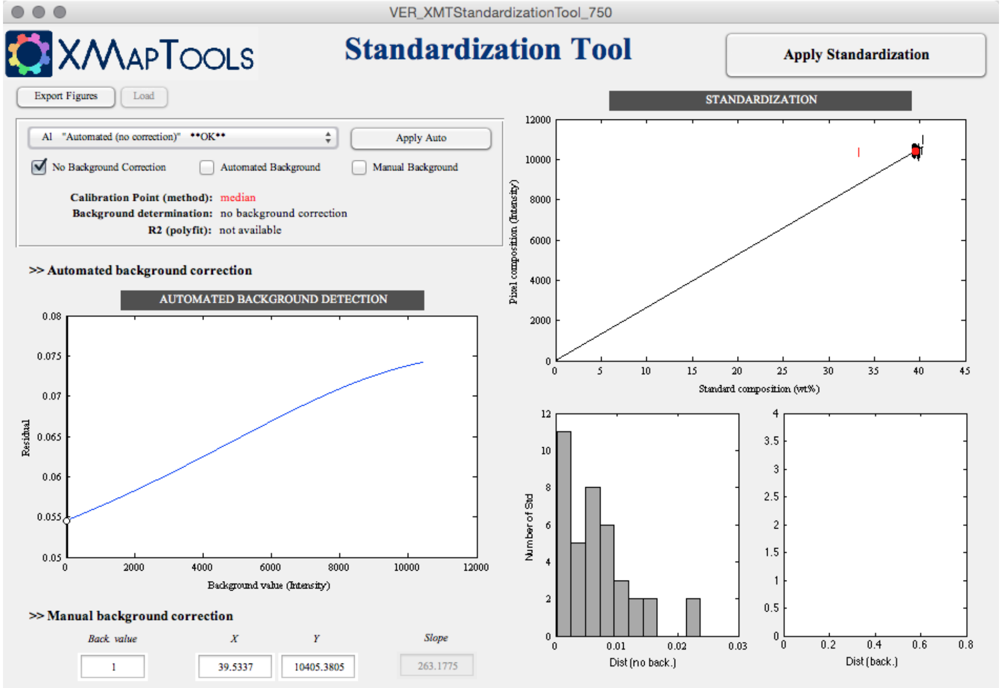
Figure 6.25 – *Internal standards for chlorite. Note that the spot analyses near the grain boundaries are unselected (white circles)*

(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 of the sum of the square of distances between the curve and the model) with the background value. The two diagrams on the lower right panel show the distribution of the residuals.

(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 = 39.5 wt%; Y = 10405 counts (Figs. 6.26 & 6.27).

(4) Select the next element Ca and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point X = 0.35 wt%; Y = 103 counts; a background value of 109 counts is estimated (Fig 6.27).

(5) Select the next element Fe and press the button *Apply Auto*. Automated detection: the calibration curve is defined by the point X = 26.3 wt%; Y = 4471 counts; no background correction needed (Fig. 6.27).



Al "Automated (no correction)" **OK**

☑ No Background Correction ☐ Automated Background ☐ Manual Background

Calibration Point (method): median
Background determination: no background correction
R2 (polyfit): not available

>> Automated background correction

>> Manual background correction

Back. value	*X*	*Y*	*Slope*
1	39.5337	10405.3805	263.1775

Figure 6.26 – *Advanced standardization tool*

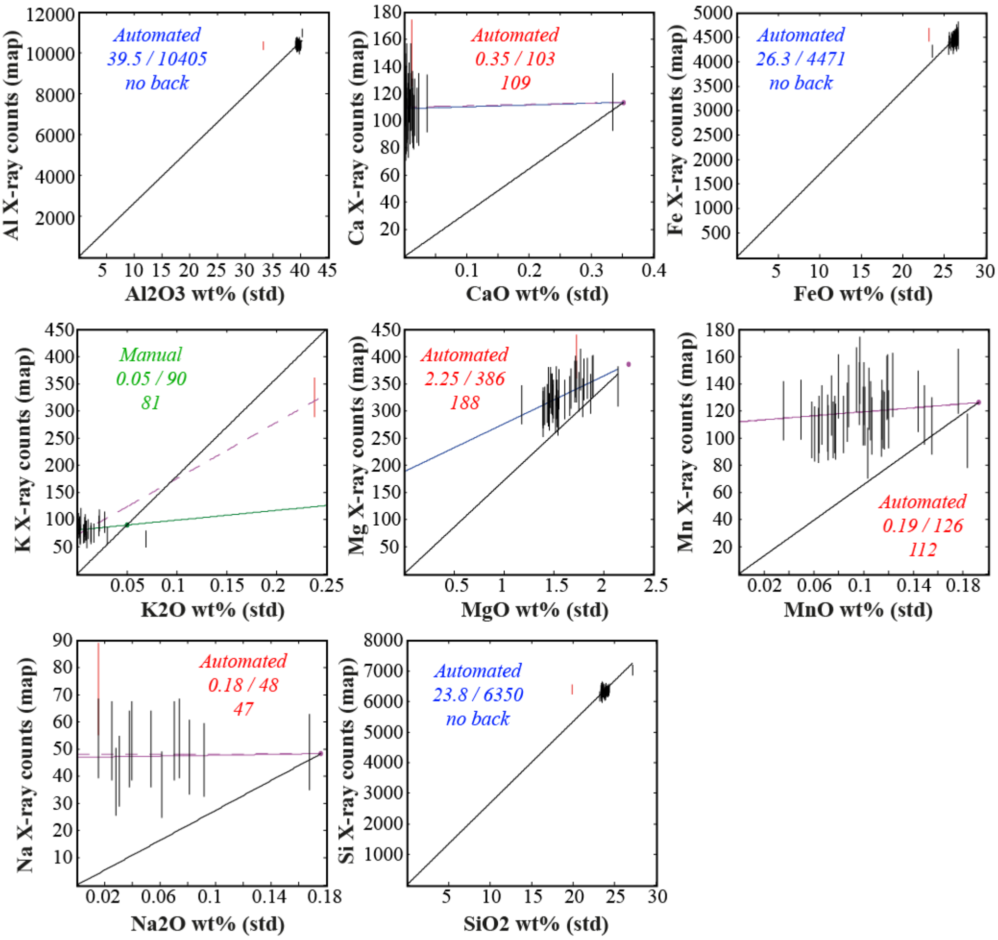


Figure 6.27 – *Standardization diagrams for chloritoid*

(6) Select the next element K and press the button *Apply Auto*. In this case, the automated detection: fails because of the presence of an outlier point ($K_2O = 0.23wt\%$) that was not detected by the program. Note that more than 95% of the cases are correctly corrected by the automated method; the other cases requires to use the manual standardization. Select the option manual standardization and set the calibration curve using the following parameters: X = 0.05 wt%; Y = 90 counts; background = 81 counts (see Fig. 6.27).

(7) Apply the automated technique to define the calibration curves of the next elements (Mg, Mn, Na, Si) and compare the results with Figure 6.27.

(8) Apply the automated technique to define the calibration curves of the next elements (Mg, Mn, Na, Si) and compare the results with 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. submitted). The spot analyses used as internal standards are indeed already corrected for background and the ma 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).

(9) Once all the calibration curves haven been defined, press the button *Apply Standardization* (Fig. 6.26).

(10) 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/*.

(11) The program applies the calibration to the X-ray maps and generate a map of oxide weight percentage that is displayed in the workspace *Quanti*.

(12) Save the project.

(13) Check the quality of standardization using the function *Generate the oxide wt% sum map* Σ

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.

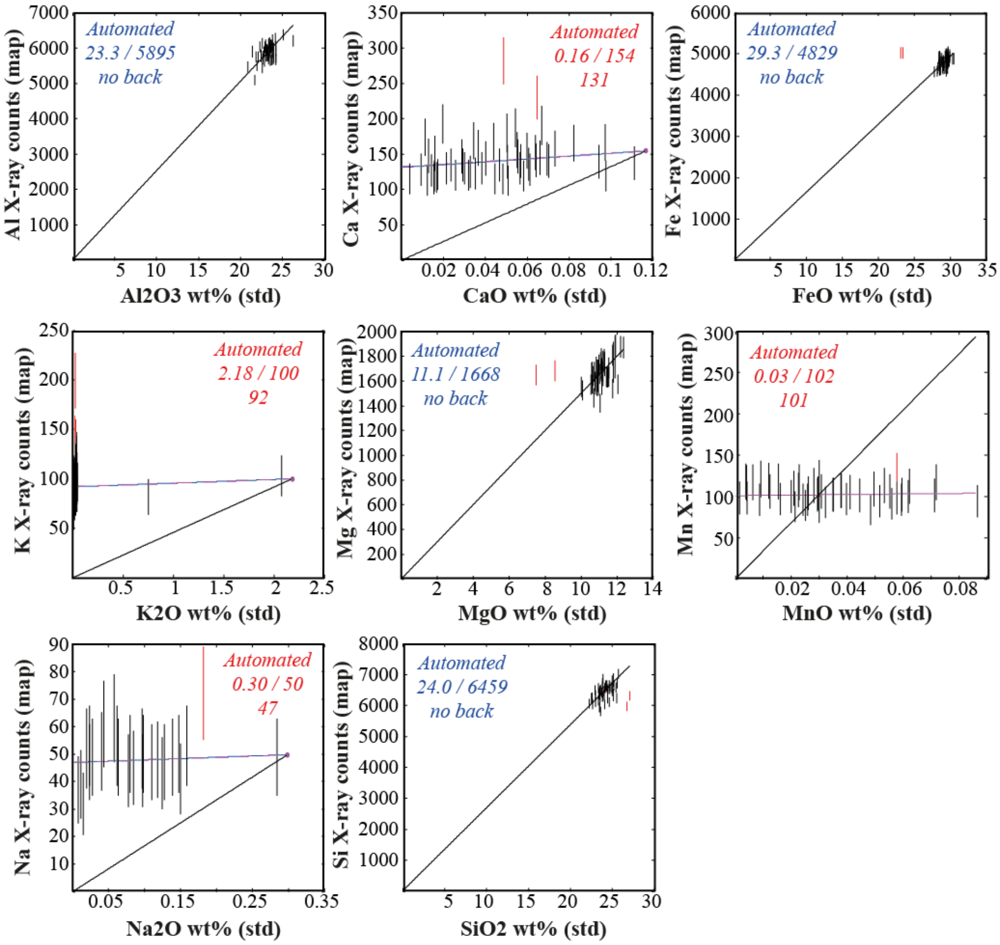


Figure 6.28 – *Standardization diagrams for chlorite*

(4) Check the quality of standardization using the function *Generate the oxide wt% sum map* Σ

In this case, the problem comes from the calibration of K in chlorite. It appears from Figure 6.28 that K in chlorite is below detection limit. However the grain boundaries with phengite have a high intensity of K because of multi-phase sampling or secondary fluorescence effects. To avoid this high apparent K_2O concentration we can calibrate K using the parameters from phengite, here 10 wt% of K_2O and 5400 counts.

(5) Delete the *Quanti* file *Chlorite-advanced* using the function *Delete Quanti file* ⛔

(6) Use the manual standardization for K with the following parameters: $X = 10\ wt\%$; $Y = 5400$; background $= 1$ and the automated procedure to define the calibration curves of all the other elements (Fig. 6.28).

(7) Check the quality of standardization using the function *Generate the oxide wt% sum map* Σ

(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_2 and press *OK*.

The program used a calibration point of X = 100 (wt%), Y = 24123 counts (median value of the Si for the mask quartz) and a background of 0 to calibrate the map. Note that this value can be obtained using the function *Display "Info" window* ℹ 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 SiO2 concentration of these interiors is overestimated by 5-10 %. To solve this issue with are going to lower the calibration value of quartz.

(3) Delete the standardized map *Quartz-homog* using the function *Delete Quanti file* ⛔

(4) Come back to the workspace *X-ray*, select the phase *quartz*, the standardization method *Manual (homogeneous phase)* and press again the button *STANDARDIZE*. Use the name proposed by the program for the standardized phase; Select all the elements to be standardized.

(5) In the input windows, set a value of 85 (wt%) for SiO_2 and press *OK*.

(6) In the worspace *Quanti*, check the concentration of SiO_2 in quartz.

(7) Save the project.

6.2.7.8 The problem of white mica

In this exemple, 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_2O range between 4 and 6 $wt\%$ whereas they should be around 10 $wt\%$. The map cannot be accurately standardized if the internal standards are not accurately measured.
- The compositional zoning in white mica occurs on a very small scale ($< 2\ \mu m$) and the position of the spot analyses measured along the transects is not accurate enough to ensure a good standardization. In this case it is important to use BSE images to locate a few spot analyses in specific areas inclusion free and showing more homogeneous composition.

Try to filter the spot analyses in phengite (see §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. 3.16).

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.

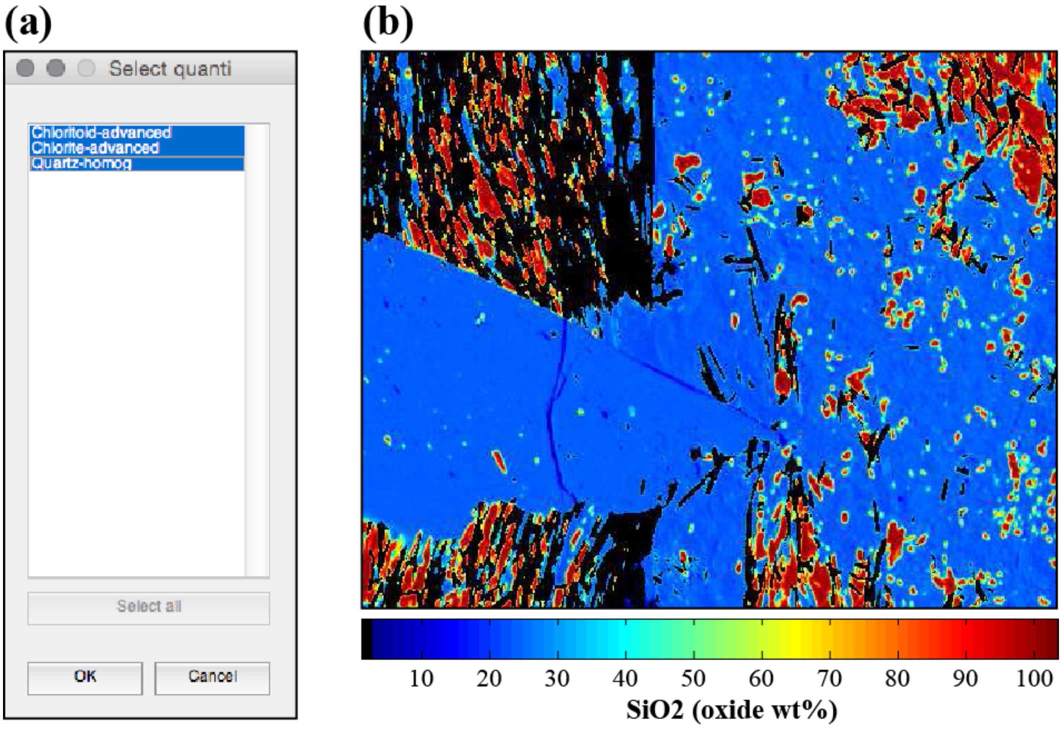


Figure 6.29 – *Merge 'Quanti' files. (a) Select the maps. (b) map of silica*

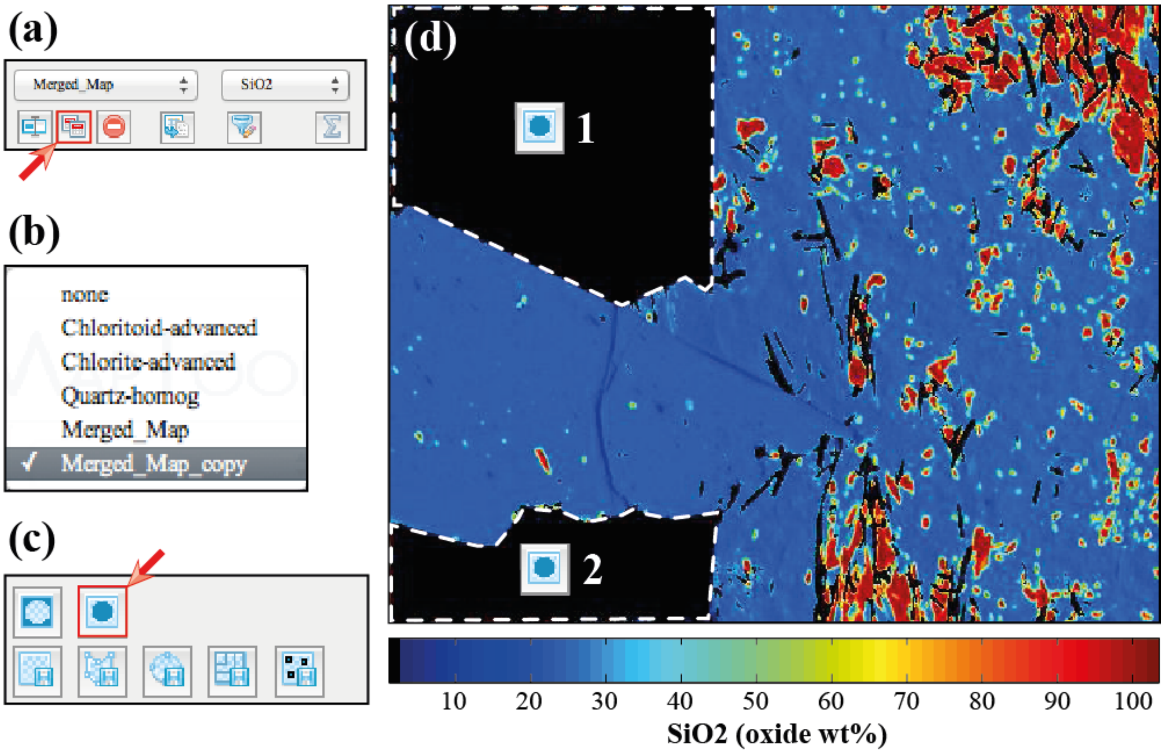
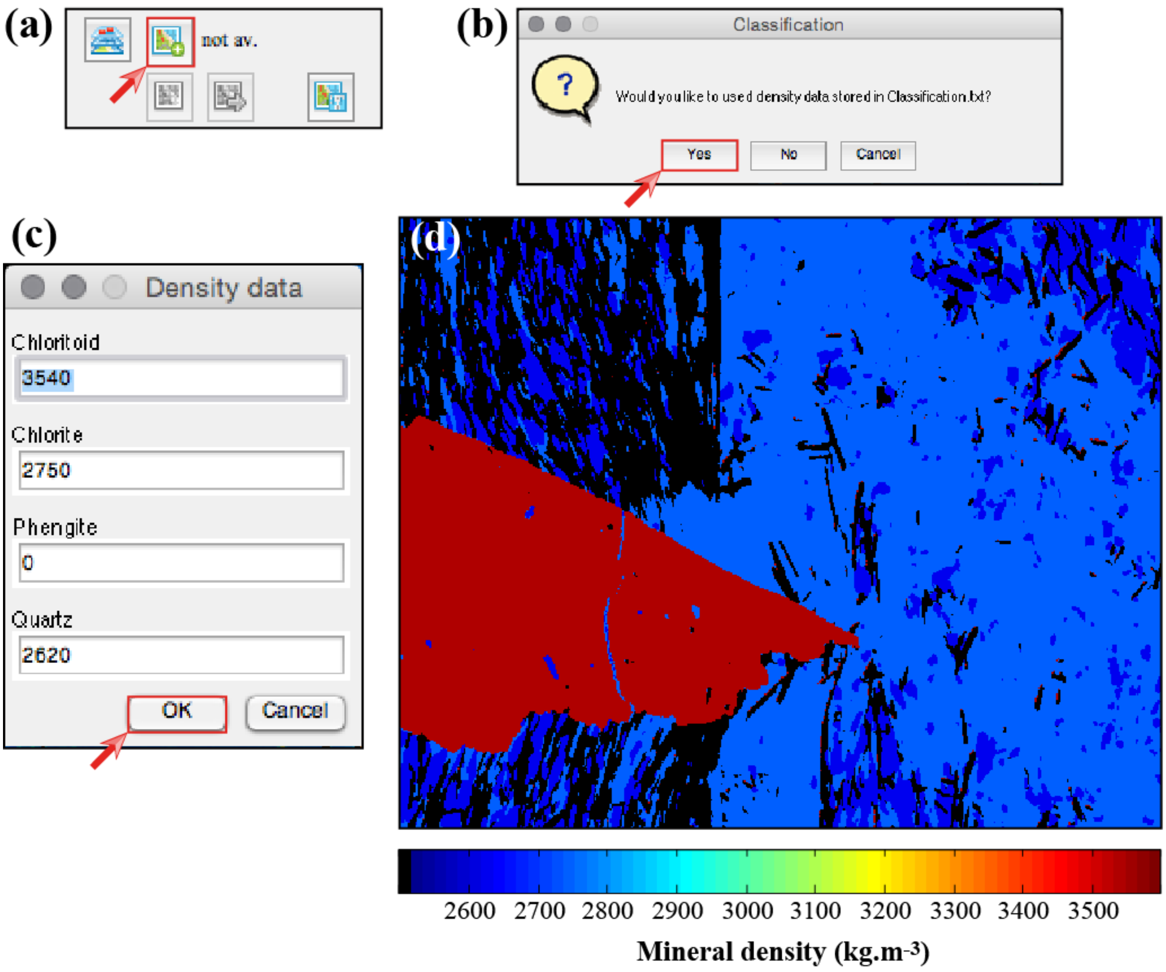


Figure 6.30 – *(a) Duplicate the Quanti file 'Merged map'. (b) The 'Quanti' file 'Merged_Map' has been duplicated. (c) Function used to delete the selected pixels of an area. (d) The pixels of two domains (labeled 1 and 2) have been deleted, i.e. they will not be used to extract the local bulk composition.*



Classification

Would you like to used density data stored in Classification.txt?

Density data

Chloritoid: 3540

Chlorite: 2750

Phengite: 0

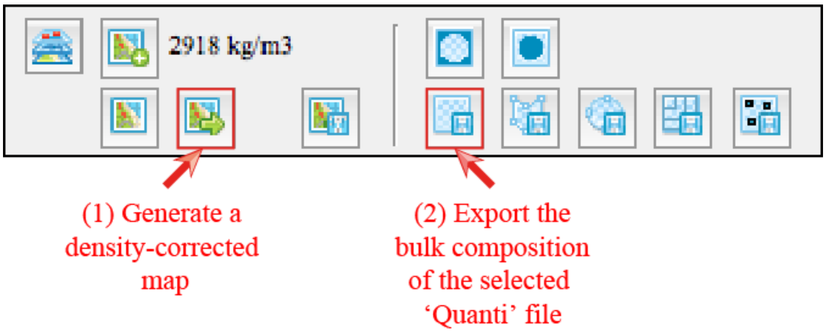
Quartz: 2620

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 selected mask file (in X-ray) 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.



(1) Generate a density-corrected map

(2) Export the bulk composition of the selected 'Quanti' file

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*

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
Al2O3    25.7     22.8
CaO      0.36     0.32
FeO      24.3     22.4
K2O      0.29     0.28
MgO      6.73     6.57
MnO      0.07     0.07
Na2O     0.52     0.48
SiO2     30.8     29.4
```

Code 6.8 – *Comparisons between local bulk composition determined for* *DCM_Merged_Map_Copy *(DCM) and* Merged_Map_Copy *(noDCM).*

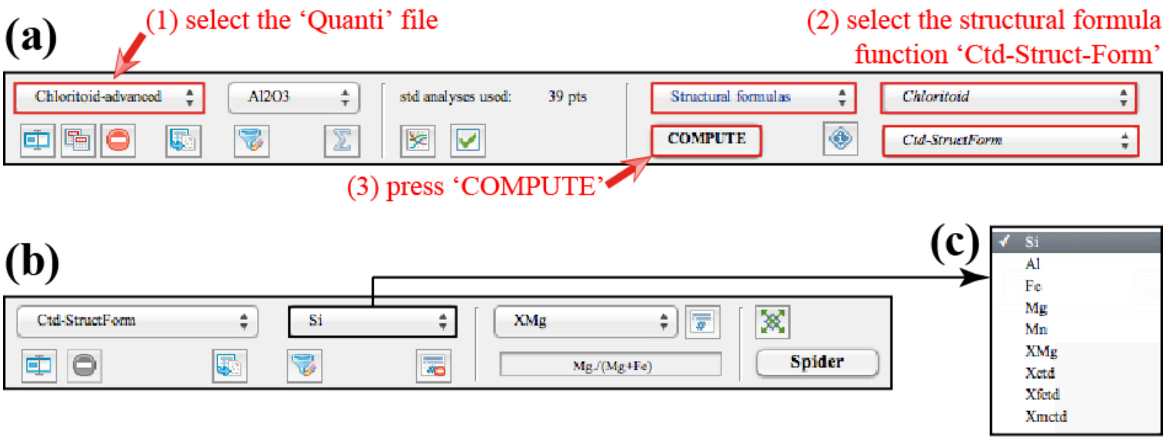


Figure 6.33 – *Computation of structural formula maps: chloritoid. (a) select the 'Quanti' file and the external function Ctd-Struct-Form. (b, c) Buttons and menu of in the workspace* Results.

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?

work in progress

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