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Short note

A mathematica code to produce phase maps from two element maps ☆

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1. Introduction

The modal abundance of phases and their combined bulk chemical composition are often required as basic information when rocks are studied. Phase maps are false colour images that are produced from the combination of two or more element maps. The results are images in which each phase is designated a different colour and modal abundances of the phases are calculated. Element maps are nowadays quickly obtained using an electron microscope or microprobe equipped with either an energy dispersive or wave-length dispersive spectrometer. The technique of phase maps is not applied frequently (e.g. Simon and Grossman, 2004; Berlin et al., 2006; Hezel and Palme, 2008), although it is a very simple, quick and powerful tool to obtain modal abundances and together with the chemical composition of the phases allows the determination of 2-dimensional bulk composition of the sample. The latter technique is called 'modal recombination' and is the most precise technique for obtaining 2-dimensional bulk compositions (e.g. Albee et al., 1977; Berlin et al., 2006).

Rocks are commonly studied in thin sections, i.e. in a 2-dimensional slice of the rock. It is noted that a 2-dimensional bulk composition is usually not representative of the true 3-dimensional object and hence, has an error (e.g. Chayes, 1956; Underwood, 1970; Eisenhour, 1996; Hezel, 2007). This error can, however, be quantified (Hezel and Kießwetter, 2010).

Phase map programs are sometimes available as part of electron microprobe software packages (e.g. JEOL microprobes). Commercial software that includes a phase map package is available from Oxford Instruments or Bruker. Freely available software for MS Windows systems that allows to produce phase maps is Lispix. Here I provide a phase map program called PHAPS that is freely available and platform independent. It has the advantage that it is quick and simple to use, as its only purpose is to produce phase maps. It is programmed using Mathematica and should run using the Mathematica Pro player. A version that can be used without any kind of Mathematica licence is in the works. The latest version of PHAPS and more detailed information about the program can be found on the web.[1]

2. PHAPS

A phase map is a false colour image of a sample that displays each phase in a different colour. In the first step the different phases of the sample are identified. This is done using the phase's different chemical compositions. Two element maps of the sample are required as input files (Fig. 1a and b). If only a certain area is of interest, this can be selected by drawing a polygon around it. The element maps must be in the form of a text-file that contains a 2×2 matrix, representing the x- and y-coordinates of the element map. The value of each cell represents the element intensity of a pixel at its $\{x,y\}$-coordinate. The intensities (int) of the same $\{x,y\}$-coordinates of both element
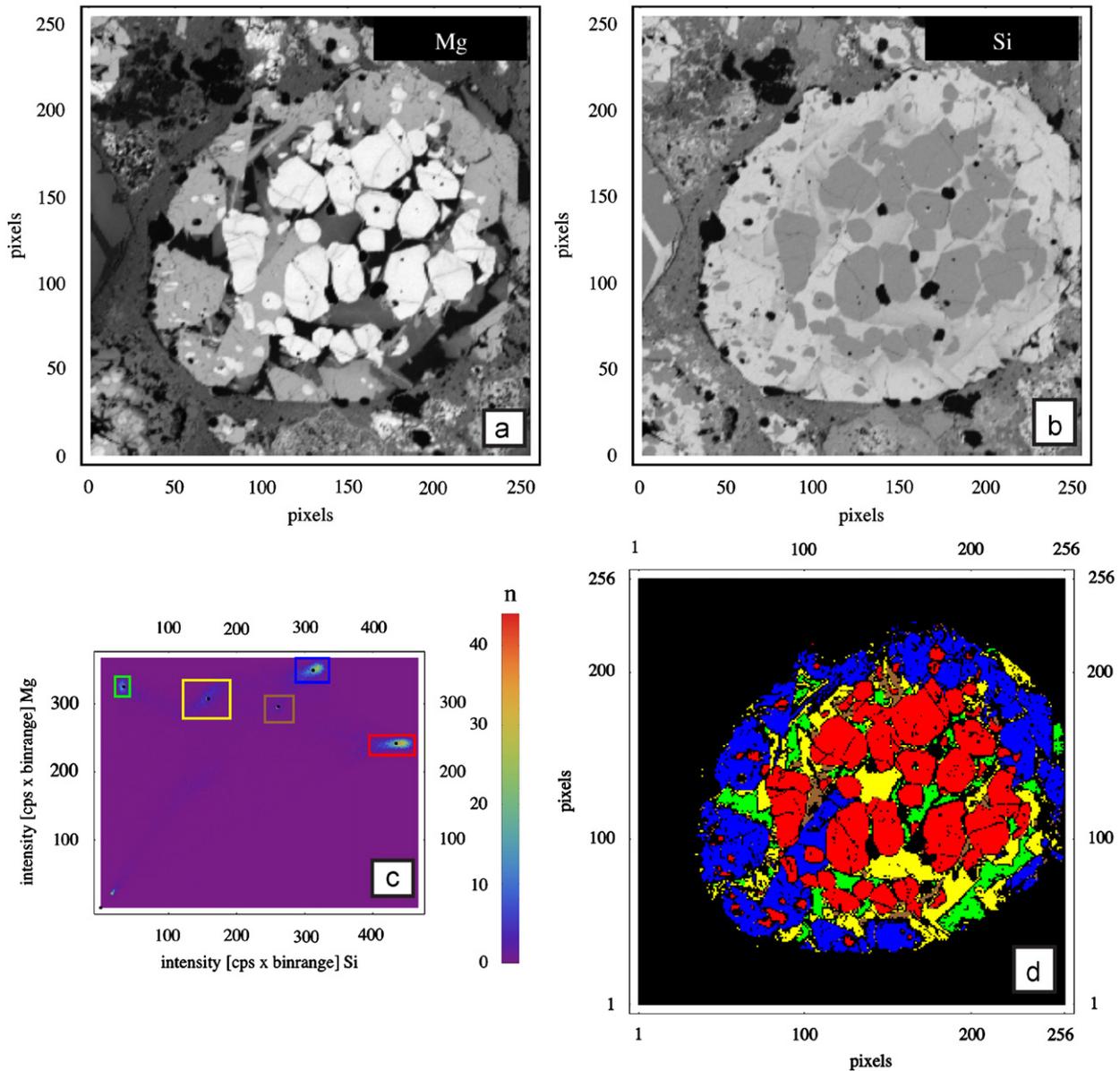
[1] www.cosmoprograms.com

Fig. 1. Plates (a) and (b): input element maps of the sample. Plate (c): projected 2-dimensional histogram of element intensities with rectangles drawn around phase hot spots. White dots represent the average intensities [cps] of all intensity pairs within a box. Black dots represent the average intensities [cps] of intensity pairs that occur at least n times. Plate (d): final phase map: ol (red): olivine; lCa-px 1 (blue), lCa-px 2 (red-brown): low-Ca pyroxene; cpx (yellow): clinopyroxene; mes (green): mesostasis. The colours of the phases correspond to the colours of the rectangles in plate (c). Element maps were obtained with a CAMECA SX100 electron microprobe, equipped with 5 wave-length dispersive detectors used for minor elements and an energy dispersive drift detector used for major elements. The accelerating voltage was set to 15 kV and the beam current to 20 nA. No correction was applied, as only qualitative maps are required for this technique. The maps were stored as text-files. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

maps (e.g. Mg and Si, cf. Fig. 1a and b) are combined to form intensity pairs {int_{Mg}, int_{Si}}, where int_{Mg} and int_{Si} represent the intensities of Mg and Si at the same {x,y}-coordinate. This will produce a list of 64,516 intensity pairs for element maps with a size of 254×254 pixels and a list of 262,144 intensity pairs for element maps with a size of 512×512 pixels. This list of intensity pairs are plotted in a new diagram, with the intensities of e.g. Mg plotted along the x- and the intensities of e.g. Si plotted along the y-axis (Fig. 1c). Phases with similar Mg- and Si-concentrations will have similar Mg- and Si-intensities, i.e. these phases will plot in a narrow field of the newly produced plot. Many intensity pairs will have the same values, i.e. they will plot on the same point. In a 3-dimensional graph, the latter points are stacked on each other, forming a 3-dimensional histogram. This 3-dimensional histogram is projected on a 2-dimensional plane and the heights

of the stacks are colour coded. A bar at the side of the diagram correlates the colour with the number of pixels that have the same {int_{Mg}, int_{Si}} pairs (Fig. 1c). Phases are easily discriminated in this histogram, provided that all phases have different concentrations of the two elements used to produce the histogram. This means one must be careful not to choose elements that might have the same concentrations in different phases, or to produce more than one phase map of the sample using different element pairs to discriminate between different phases.

In the second step, the phase maps are produced. The areas on the histogram of Fig. 1c representing individual phases are called 'phase hot spots'. Rectangles of different colours are drawn around each phase hot spot of interest (Fig. 1c). All pixels of the studied sample which intensities plot inside an individual rectangle are designated the colour of this rectangle. The result

is the phase map, displayed in Fig. 1d. The modal abundance of each phase is calculated by counting the number of pixels of each phase and given as area%.

The size and positioning of the rectangles are partly subjective. This is a problem, as a different size and position of a rectangle will result in a slightly different modal abundance of the represented phase, i.e. the modal abundance itself becomes partly subjective. The scatter of the intensity pairs across the histogram of Fig. 1c has 3 reasons: (i) analytical uncertainties that are comparatively high for element maps ($\sim$10%), (ii) chemical zoning across a phase and (iii) mix analyses at the border of two phases or close to cracks or holes. If there were only analytical uncertainties, Fig. 1c would contain well defined phase hot spots and rectangles could be objectively sized around them. Element zoning systematically changes the shape of the phase hot spot, e.g. elongates them. It is still possible to draw objective rectangles around such elongated hot spots. For such an ideal case the program calculates an element intensity average of all intensity pairs inside a rectangle (white dots in Fig. 1c). Such an average automatically accounts for any existing element zoning. These averages can be matched with intensities obtained from quantitative analyses of the phases, and the latter will then represent an accurate quantitative average of this phase.

However, the rectangles around the phases will also include the mix analyses. These scatter between all phase hot spots, covering a large area of the histogram. The number of mix analyses inside a rectangle depends on how large the rectangle is drawn around a phase hot spot, which is subjective. This subjective measure can be corrected. The number how often a single intensity pair occurs is called n and displayed in the scale bar of Fig. 1c. The intensity pairs of mix analyses are rarely the same, i.e. their n is typically small, usually close to 1. In contrast, the intensity pairs of phase analyses are often the same, i.e. their n is typically very large. It is therefore possible to discriminate between mix analyses and phase analyses by excluding all intensity pairs below a certain threshold. The program allows to input such thresholds for each phase and then calculates modal abundances without any mix analyses. In addition an element intensity average is calculated that does not include the mix analyses (black dots in Fig. 1c). These averages can be used in the same way as above to identify an appropriate quantitative chemical composition for each phase.

Removing the mix analyses results in well constrained modal abundances. However, choosing the thresholds is still subjective to some extent, although much less than the sizing of the rectangles. I recommend to apply a range of thresholds for each phase and provide a range of modal abundances, which, from experience, will vary by less than 5–10 rel.%.

Acknowledgements

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cageo.2010.02.0026.

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