# Chemistry Assisted Phase Differentiation in Automated Electron Backscatter Diffraction

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Automated Electron Backscatter Diffraction (EBSD) is routinely used to map out the crystallographic orientations in polycrystalline materials. In order to map out the orientation in multiphase materials, the system must be able to differentiate the phases during the scanning procedure. To index a pattern various parameters associated with the phase of the material in the diffracting volume must be known *a-priori*. These parameters include the crystal symmetry and lattice parameters of the unit cell and the indices of the strongly diffracting lattice planes. Phase differentiation is generally achieved through an iterative approach [1]. During a scan, each pattern is indexed assuming the required structure parameters for each identified phase in a sample. For each candidate phase various parameters describing the fit of the indexing to the pattern are determined. The phase assigned to the scanned point is that which produces an indexing solution with the best fit to the detected bands in the pattern. When the structure parameters of the candidate phases are very different this procedure generally works q uite well. However, when the structures are similar there are generally specific orientations where the iterative approach has difficulty differentiating correctly. An example is shown in Fig. 1 for a pattern from the Alumina phase of a sample containing both $Al_2O_3$ and $AlTi_3$. Fig. 1(a) shows the pattern and Fig. 1(b) shows the indexing of the pattern in Fig. 1a assuming the $Al_2O_3$ phase parameters (trigonal) and assuming the $AlTi_3$ parameters (hexagonal) in Fig. 1(c). While the software does correctly identif y the phase associated with this pattern it is easy to see that many of the bands are in the same position and that the software could have difficulty distinguishing the phase correctly from a lower quality pattern.

In phase identification [2] a pattern from a given point in the microstructure is obtained along with an X -ray EDS spectrum. The chemical elements present at the point of interest can be identified from the energy spectrum. This information can be used as a filter to a material database to iden tify potential candidate phases. The phases associated with the point of interest are identified based on a match between the structure parameters derived from the database and those derived from the pattern. Phase identification is generally done with considerable user interaction relative to phase differentiation, which is done without any user interaction. In addition, a requirement of phase differentiation is that it must be done rapidly. Fast scanning is desired in order to generate orientation maps with sufficient spatial resolution for good imaging of the microstructure as well as to collect the large numbers of measurements for reliable statistical analysis of the orientations (texture analysis). Thus, generally the resolution (and quality) of incoming patterns during scanning is sacrificed for in order to either increase the density of points in the measurement grid or the number of grains sampled. While the more sophisticated techniques used in analyzing the high -resolution patterns obtained in phas e identification would potentially give more accurate results the time required to performs these techniques makes them impractical for phase differentiation. However, the idea of using chemistry as a filter can be adapted to phase differentiation. This requires that the geometry of the SEM is suited for simultaneous collection of EDS and EBSD information.

An example is shown for a material in which five phases were identified, namely: $Al_2O_3$, $AlTi_3$, $ErO_2$, monoclinic $ZrO_2$ and tetragonal $ZrO_2$. Fig. 2(a) show s the phase map resulting from the standard phase differentiation procedure during scanning. Fig. 2(b) shows the phase map obtained when chemical information obtained via EDS is coupled with the crystallographic information obtained via EBSD. No clean up of the scan data was applied in these images. Details of the approach taken to incorporate the chemistry into the phase differentiation procedure will be presented.

References

[1]    S.I. Wright and D.P. Field, *Microsc. Microanal.* 3 (Suppl. 2) (1997) 561.
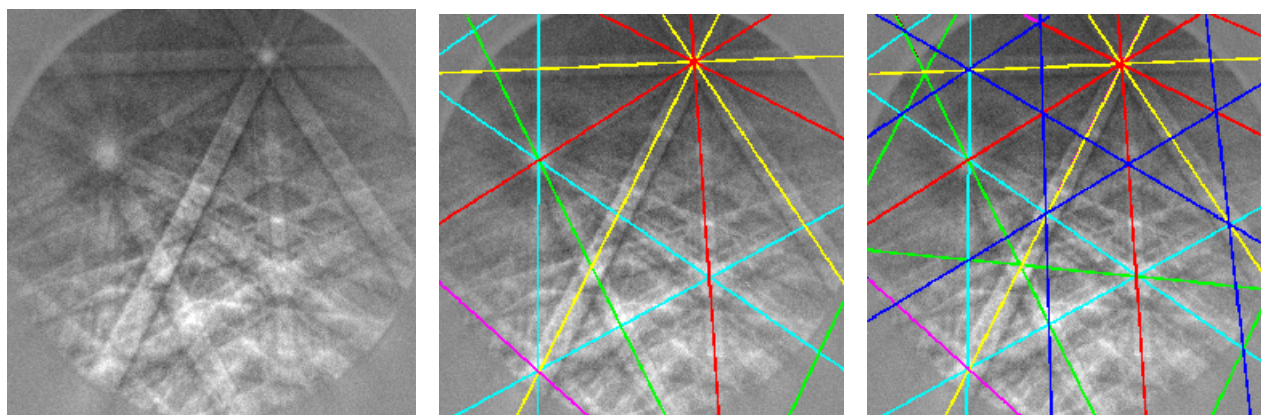[2]    J.R. Michael, *Microsc. Microanal.* 3 (Suppl. 2) (1997) 387.

FIG. 1.  (a) An EBSD pattern from $Al_2O_3$.from a sample containing both $Al_2O_3$ and $AlTi_3$. (b) The pattern in (a) indexed as $Al_2O_3$. (c) The same pattern indexed as $AlTi_3$.
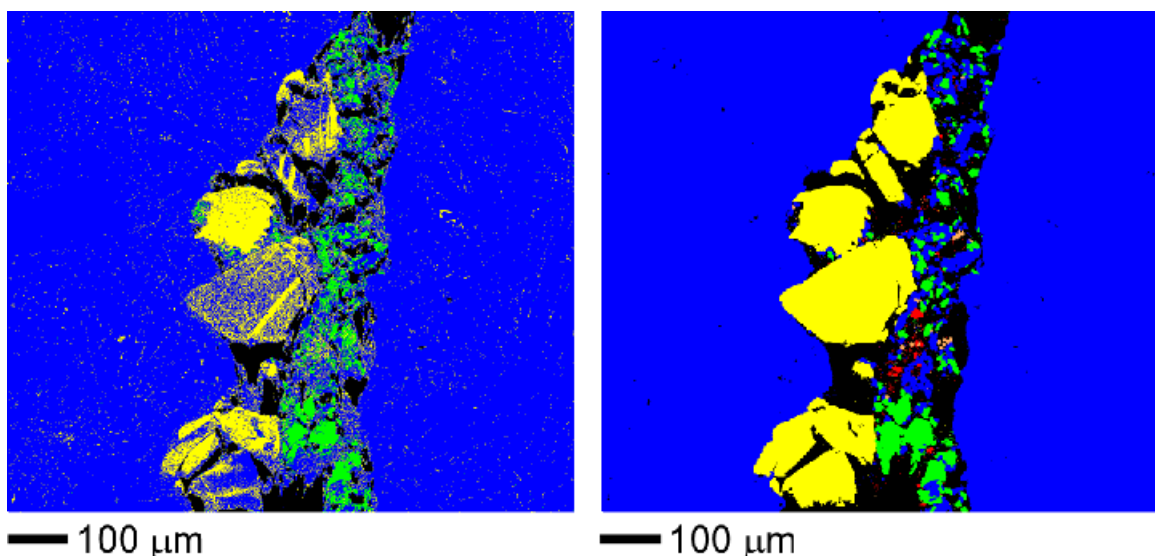


FIG. 2.  (a) A phase map obtained using only EBSD information of a multiphase sample containing $Al_2O_3$ (yellow), $AlTi_3$ (orange), $ErO_2$ (green), monoclinic $ZrO_2$ (red) and tetragonal $ZrO_2$ (red). (b) A phase map from the same sample area obtained using both EBSD and EDS information.