

## Electron Backscattering Diffraction (EBSD) as a Tool to Evaluate the Topotactic and Epitactic Growth of Minerals: The Example of the Magnetite and Hematite

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Under equilibrium growth conditions, a mineral will be formed in the direction perpendicular to a substrate. This direction is perpendicular to the face of the highest surface energy of the crystal and the consequence of this crystallographic-controlled growth is a reduction in the overall surface energy of the crystal [1]. Epitaxy is the elegant term for this kind of growth of solids. On the other hand, the chemical reaction of a crystal may be formed in one or several crystallographic equivalent orientations relative to the parent mineral, defining the well-know topotaxy. Both phenomenons may be described in the natural system of growth of hematite and magnetite through EBSD. In previous works with minerals and other substances, the correlation of intergrowing was frequently displayed by the coinciding lines of X-ray diffraction analyzes [2]. However, with the EBSD, not only the coincidence planes or axes between a pair of minerals can be evaluated, but also the related microstructure of the chemical reaction. The aim of this work is to show, through an example of two natural iron oxide phases, how EBSD can be used during the study of topotactic and epitactic intergrowing of solids.

Three octahedral crystals of magnetite were analyzed each one in one different plane  $\{111\}$ ,  $\{110\}$  and  $\{100\}$  as shown in the figure 1. The plane  $\{111\}$  is one face of the octahedral and the  $\{110\}$  and  $\{100\}$  were observed in a surface generated after cutting a crystal of magnetite in two halves. that divided into two pieces the crystal of magnetite. After polishing with diamond paste and colloidal silica, the faces of the selected planes were analyzed in an EBSD (Oxford/HKL system) and the data were processed in the Channel 5 software package. A phase and an inverse pole figure maps were generated to one area of each surface in the XY plane. Afterwards, pole figures of the  $\{111\}$  and  $\{110\}$  of magnetite (Mgt) were compared to the pole figures of  $\{0001\}$  and  $\{11-20\}$  of hematite (Hm), to evaluate the degree of coincidence between these planes according to the different analyzed surfaces. On the surface  $\{111\}_{\text{Mgt}}$ , of magnetite crystals hematite grew with more or less lamellar habits. (just a suggestion) there is a large amount of hematite (Fig.1, phase map, in blue) that is growing on the surface of the magnetite with a lamellar form probably. There are small relicts of magnetite (Fig. 1, phase map, in red). The crystallographic orientation of the minerals can be observed in relation to the Z plane (or XY) through the inverse pole figure map (Fig.1). There is an coincidence between the poles of the planes  $\{111\}_{\text{Mgt}}$  and  $\{0001\}_{\text{Hm}}$  in their respective pole figures (PF) . On the surfaces  $\{100\}_{\text{Mgt}}$  and  $\{110\}_{\text{Mgt}}$ , the magnetite predominate over hematite crystals and the transformation can be observed, that is the minerals are distributed in a texture of phase transformation. It is not possible to visualize a grain of hematite while the magnetite is still a monocrystal. The PFs of  $\{0001\}_{\text{Hm}}$  and  $\{11-20\}_{\text{Hm}}$  are diffuse and this is an evidence of a polycrystalline texture. There is not a conspicuous coincidence between poles of hematite and magnetite on the  $\{100\}_{\text{Mgt}}$  surface. On the other hand, the coincidence between the geometric distribution of  $\{110\}_{\text{Mgt}}$  and  $\{11-20\}_{\text{Hm}}$  in the  $[110]_{\text{Mgt}}$  is clear.

The coincidence of planes and poles during the growth of hematite in a magnetite substrate or through a magnetite transformation was systematically described in previous studies [e.g., 3, 4]. We assume that the growing of hematite on the  $\{111\}_{Mgt}$  substrate is an example of an epitaxy instead of topotaxy that is clearly present in the transformation of magnetite to hematite in the  $[110]_{Mgt}$  and  $[100]_{Mgt}$ . The development of a defined morphology of the hematite crystals in the case of  $[111]_{Mgt}$  induces to believe that the mineral growth is not due to the oxidation of the surface of magnetite. The surface of the mineral acts as substrate for epitactic nucleations of hematite outside the octahedral planes of magnetite crystals. Therefore, the use of EBSD may be a powerful tool to evaluate the topotactic and epitactic reactions in minerals due to its capacity to join the crystallographic analyzes and the textural evaluations.

References:

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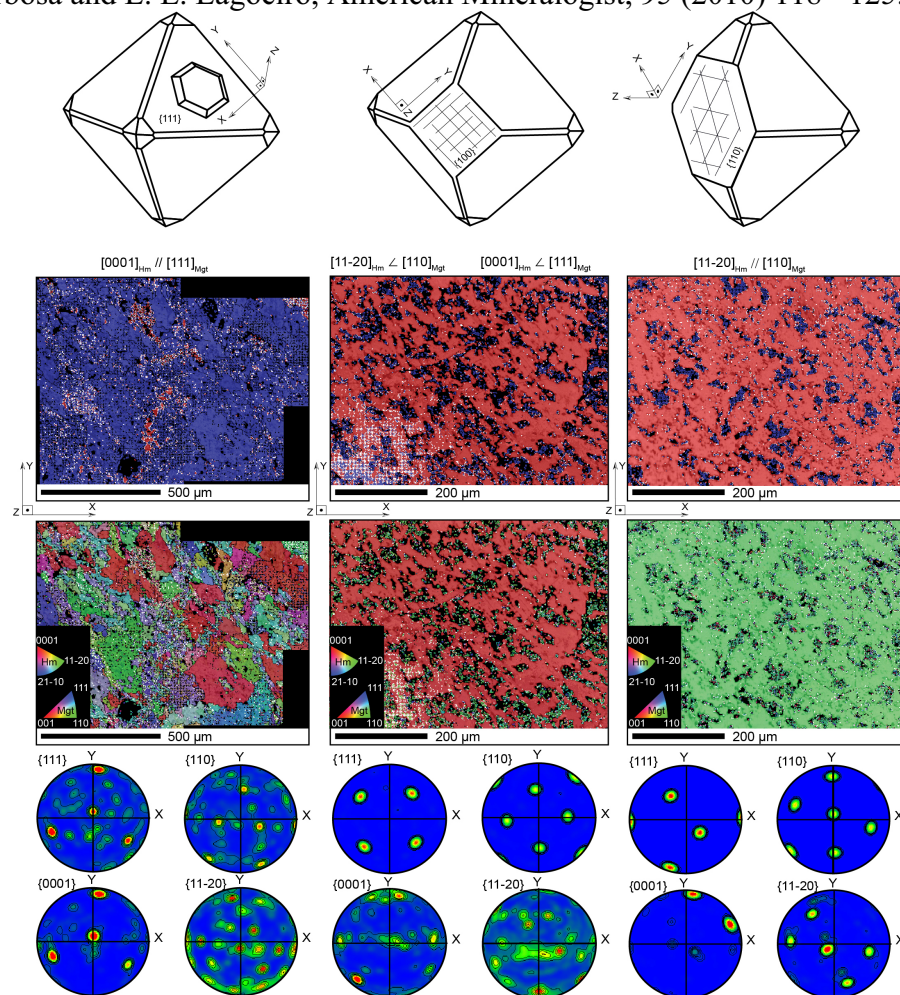


FIG1: Three analyzed surfaces of the planes  $\{111\}$ ,  $\{100\}$  and  $\{110\}$  and their respective phase maps; inverse pole figure maps and pole figures.