MS14-O6 Energy dispersive white beam diffraction: Translating photon energy into the 3rd dimension for one-shot texture analysis

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Biomineralized tissues and poly-crystalline bio-inspired materials often exhibit complex architectures involving sub-structures with preferred crystallite orientation (crystallographic texture). The crystallographic texture is intimately linked with crystal growth and therefore teaches us important lessons about biomineralization and is often also associated with material functionality. Examples are bone, teeth, sea shells, crustacean cuticle, etc. Unfortunately 3D information about crystallite orientation is particularly difficult to obtain in such complex materials, since diffraction patterns recorded with state-of-the-art area detectors are inherently 2-dimensional. 3D information requires rotation of the sample that which leads to different volume elements being irradiated at every angle and therefore obscuring of the signal. This obstacle can be overcome in an elegant way by a novel approach using multiple wavelengths (white beam) to collect information on differently oriented crystallites. The approach is similar to traditional Laue diffraction, but with the important difference of using an energy dispersive area detector for recording the scattering patterns (energy dispersive Laue diffraction, EDLD). In this way, the x-ray energy becomes the missing 3rd dimension in space. We have, for the very first time, demonstrated the feasibility of such an approach for 3D texture measurements in general and analysis of complex materials in particular. For this purpose we employed EDLD on carbon fiber samples containing different fiber orientations and showed that the new method allows direct 3D reconstruction of crystallite texture and the acquisition of "one-shot" pole figures without sample rotation. Proof of principle was also obtained for biomineralized tissue. The major potential of this method lies in the direct 3D information that could allow texture scanning of larger sample with complex sub-structures or following texture changes in-situ during mineralization processes due to its inherent "one-shot" nature.

Keywords: Laue diffraction, energy-dispersive 2D detector, crystallographic texture, biomineralized tissue

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MS15 Minerals and materials

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MS15-O1 How crystallography can assist process mineralogy – two metallurgical examples

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Process mineralogy can be considered a special branch of applied mineralogy. It combines *process*ing of minerals with traditional *mineral*ogical knowledge in order to assist mineral exploration and to predict and optimize how the relevant ores can be best mined and processed. Process mineralogy is not only an indispensable tool for ore characterization but in also of vital importance for the design and tailoring of the whole manufacturing including refining of semi-finished products. A thorough understanding of the relevant reactions involved is a necessity not only from an engineering point of view but also to meet the constantly growing demands to reduce operational costs and to account for environmental aspects.

The production processes related to metallurgy are frequently based on complex high-temperature reactions which are far away from equilibrium. Analysis of the resulting multi-phase assemblages is usually also rather complex because they may depend not only temperature but on other parameters such as oxygen fugacity as well. In order the characterize the specific compounds completely and to understand their formation conditions and stabilities chemical analysis using microprobe techniques alone are frequently not sufficient and crystallographic information obtained from single-crystal or powder diffraction data can be of great help. Furthermore, crystallographic input can be used to do ab-initio calculation of thermodynamic properties of less-common compounds encountered.

In the present contribution two examples from an ongoing collaboration between the Universities in Innsbruck (Austria) and Pretoria (South Africa) will be presented. They are related to (i) iron-ore sintering involving so-called SFCA-phases as well as (ii) producing low carbon ferrochrome from chromite using aluminothermic reduction.

Keywords: process mineralogy, SFCA-phases, beta-alumina compounds