Precession Electron Diffraction for the characterization of pseudo-symmetrical crystals: the case of coesite

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Recent developments in electron diffraction call for a reappraisal of the possibilities offered by spot patterns. Among them is the Vincent-Midgley Precession Electron Diffraction (PED) technique [1], which recently became available on many TEM thanks to hardware implementations. Giving the possibility to measure integrated electron diffraction intensities, this technique was originally developed for electron crystallography applications. In this work, we take advantage of the intensity data provided by PED to characterize defects in coesite.

Coesite is a high-pressure polymorph of silica that exhibits a monoclinic symmetry (space group $C12/c1$) with $a \sim c$ and $\beta = 120.34^{\circ}$. While monoclinic in symmetry, the crystal is pseudo-hexagonal, and conventional selected-area electron diffraction (SAED) can easily lead to incorrect indexing. In this study, we have characterized a (021)-twin in a metamorphic coesite from Parigi, Dora Maira Massif, Western Alps. Two techniques have been used to characterize this defect: large angle convergent beam electron diffraction (LACBED) and PED. In LACBED, we take advantage of the large number of hkl Bragg lines to determine absolute orientations. With PED, the absolute indexation of the patterns is made possible through the possibility of measuring spots intensities. PED appears very powerful to investigate crystals with low symmetries.

In both cases, the orientation relationships between adjacent parts of the twin are characterized unambiguously. The twin is described as a rotation of 89.94° around the [100] axis of the monoclinic C12/c1 coesite. This microscopic description is fully consistent with original descriptions of twinning in synthetic coesite.

[1] Vincent R and Midgley P, Ultramicroscopy **53** (1994), p. 271.
[2] Jacob D, Cordier P, Morniroli JP, Schertl HP, European Journal of Mineralogy **20** (2008), p.119.

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