Geophysical Research Abstracts
Vol. 18, EGU2016-15387, 2016
EGU General Assembly 2016

Tackling pseudosymmetry problems in electron backscatter diffraction (EBSD) analyses of perovskite structures

Elisabetta Mariani (1), Pamela Kaercher (1), Julian Mecklenburgh (2), and John Wheeler (1)

(1) University of Liverpool, School of Environmental Sciences, Liverpool, United Kingdom (mariani@liverpool.ac.uk), (2) University of Manchester, School of Earth, Atmospheric and Environmental Sciences, Manchester, United Kingdom

Perovskite minerals form an important mineral group that has applications in Earth science and emerging alternative energy technologies, however crystallographic quantification of these minerals with electron backscatter diffraction (EBSD) is not accurate due to pseudosymmetry problems.
The silicate perovskite Bridgmanite, (Mg,Fe)SiO_3, is understood to be the dominant phase in the Earth's lower mantle. Gaining insight into its physical and rheological properties is therefore vital to understand the dynamics of the Earth's deep interior. Rock deformation experiments on analogue perovskite phases, for example (Ca,Sr)TiO_3, combined with quantitative microstructural analyses of the recovered samples by EBSD, yield datasets that can reveal what deformation mechanisms may dominate the flow of perovskite in the lower mantle. Additionally, perovskite structures have important technological applications as new, suitable cathodes for the operation of more efficient and environmentally-friendly solid oxide fuel cells (SOFC). In recent years they have also been recognised as a potential substitute for silicon in the next generation of photovoltaic cells for the construction of economic and energy efficient solar panels.
EBSD has the potential to be a valuable tool for the study of crystal orientations achieved in perovskite substrates as crystal alignment has a direct control on the properties of these materials. However, perovskite structures currently present us with challenges during the automated indexing of Kikuchi bands in electron backscatter diffraction patterns (EBSPs). Such challenges are represented by the pseudosymmetric character of perovskites, where atoms are subtly displaced (0.005 nm to 0.05 nm) from their higher symmetry positions. In orthorhombic Pbnm perovskites, for example, pseudosymmetry may be evaluated from the c/a unit cell parameter ratio, which is very close to 1. Two main types of distortions from the higher symmetry structure are recognised: a tilt and a deformation of the anion octahedron. These distortions may occur together. Common misidentifications observed in EBSD data are [100] and [001] seen as equivalent solutions, whereby these dyad symmetry axes are misidentified as tetrad axes of the cubic symmetry. In this study we investigate methods that could be applied to the EBSP automated indexing algorithm to solve the pseudosymmetry problem in perovskite structures. Attention is given to subtle angular deviations between bands and to differences in pseudosymmetric Kikuchi patterns.