Determination of contrast factors for cubic slip-systems and their application in the microstructural characterization of binary Fm-3m materials

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To effectively decouple the size and strain contributions simultaneously embedded within a sample's diffractogram (see Fig. 1A), a scale transformation to modify the Williamson-Hall (WH) and Warren-Averbach (WA) methods was proposed by Ungár and Borbély using contrast factors (Chkl). These parameters are often interpreted as the visibilities for each dislocation and directly quantify the elastic anisotropy present in materials. A proper implementation of the modified WH and WA methods enhances the accuracy of the microstructural parameters estimated by diffraction techniques, which can even be compared to direct measurements carried out by transmission electron microscopy.

The fundamental step to implement the modified WH and WA methods relies on the calculation of individual contrast factors for each dislocation. A parametric evaluation of such parameters was previously reported for cubic metallic structures (e.g., Cu, Ni), then followed by numerical approximations in hexagonal metals and some low-symmetry mineral phases. Because alkali halides impose additional symmetry restrictions due to their ionic bonds, the use of a first principles approach to calculate individual contrast factors for such materials is necessary. In this study, we report the use of a first principles approach to calculate individual contrast factors with examples of KCl and NaCl.

In this study, closed-form expressions for the displacement field, the distortion displacement, and the distortion tensor were obtained by introducing a dislocation dependent coordinate system (see Fig 1B) that allowed a straightforward evaluation of the contrast factors in binary Fm-3m materials. Crystalline samples of KCl and NaCl were prepared by hand-milling and X-ray diffraction measurements were performed on a Bruker X-ray D2 Phaser powder diffractometer using β-filtered, Cu-Kα radiation (λ= 0.154 nm; 30kV, 10mA). Within the initial WH analysis, the measured integral breadths showed a lesser monotonic behavior as evidenced in a lower coefficient of determination in NaCl (R2 = 0.940) and more particularly for KCl (R2 = 0.692). The evaluated displacement fields for the edge and screw dislocations also showed a behavior which can be explained by elastic anisotropy. Overall, the primary slip-system <110> {110} allows only screw dislocations, while the secondary slip-system <100> {110} only permits edge dislocations to occur. Accordingly, the contrast factors for KCl and NaCl were calculated for the first time and used to characterize their microstructure through the modified WH analysis. This approach significantly reduced the integral breadths dispersion for the KCl case, thus indicating the relevance of the strain anisotropy contribution to the breaths distribution (see Fig 1C). Interestingly, the calculated contrast factors for NaCl showed very small variations on their (hkl) dependence. This effect does not allow to distinguish the broadening contributions from different dislocations, suggesting a possible shortcoming for the modified WH method. Therefore, lattice defects beyond long range strain fields should be considered in a subsequent microstructural study of NaCl.

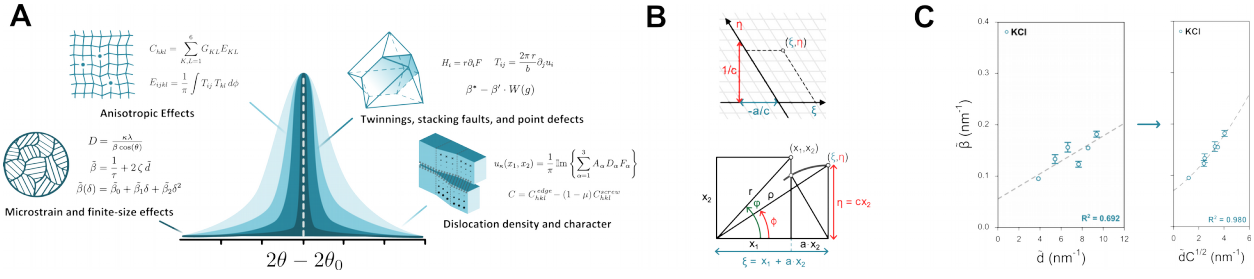

Figure 1. (A) Different peak broadening contributions studied by X-ray line profile analysis techniques. (B) Dislocation-dependent coordinate system introduced in this study. (C) Classical and modified WH analysis implemented for KCl.