

Implementation of the Self-consistent Kröner-Eshelby Model for the Calculation of X-ray Elastic Constants for any Crystal Symmetry

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In this paper, we will report about the implementation of the self-consistent Kröner-Eshelby model for the calculation of X-ray Elastic constants for general, triclinic crystal symmetry. With applying appropriate symmetry relations, the point groups of higher crystal symmetries are covered as well. This simplifies the implementation effort to cover the calculations for any crystal symmetry.

In the literature several models can be found to estimate the polycrystalline elastic properties from single crystal elastic constants. In general, this is an intermediate step towards calculation of the polycrystalline response to different techniques using X-rays, neutrons, or ultrasonic waves. In the case of X-ray residual stress analysis, the final goal is the calculation of X-ray Elastic constants.

Contrary to the models of Reuss, Voigt, and Hill, the Kröner-Eshelby model has the benefit that it can be expanded to cover more complicated systems that exhibit multiple phases, inclusions or pores and/or texture.

We will discuss a recent theoretical development where the approaches of calculating bounds of Reuss and Voigt, the tighter bounds of Hashin-Shtrikman and Dederichs-Zeller are brought together in one unifying model that converges to the self-consistent solution of Kröner-Eshelby.

For the implementation of the Kröner-Eshelby model the well-known Voigt notation is adopted. The 4-rank tensor operations have been rewritten into 2-rank matrix operations. The practical difficulties of the Voigt notation, as usually concealed in the scientific literature, will be discussed.

In addition, we will discuss the required accuracy of the calculations and the consequences of error propagation towards the final results.

We will show some practical examples in which the various models are applied and compared.