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ABSTRACT

The Spectral Model for Grain Boundary Segregation: A Path to Polycrystalline Phase-and-Defect Diagrams

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Alloys with engineered grain boundaries (GBs), specifically those engineered via GB segregation, have crossed into commercial viability in recent years – a trend that promises to accelerate as high throughput computation and theoretical models of GB segregation continue to improve. Many of the recent advances in this area have derived from our improved ability to capture the full distribution of local atomic environments and energetics in the GB network with a spectral representation of GB segregation [1]. Spectral calculations have advanced to consider many complex cases, including solute interactions [2] and vibrational entropy [3]; cases for which we now have large databases of spectral parameters, some of which have been computed with ab-initio accuracy [4]. These efforts have enabled the development of spectral analytical models, from which one can produce phase-and-defect diagrams describing the stable grain sizes and defect states of segregated polycrystalline systems [5]. This talk provides an overview of the development of the spectral GB segregation model, covering the underlying analytical theory, computational modeling and database development, the production of phase-and-defect diagrams, and finishing with a review of recent experimental validations of the spectral model.

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