Understanding grain boundary resistivity – A multiscale approach for electrical conductors

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Abstract

The macroscopic electrical properties of metals are significantly influenced by the underlying microstructure, with grain boundaries being one of the key factors in determining electrical conductivity. Accordingly, various phenomenological models, such as the Andrews method (1), have been developed over the past decades to evaluate grain boundary resistivity in experiments. While these models offer simplified approaches, they often rely on ad-hoc assumptions that may not fully capture the intricate relationship between microstructure and conductivity.

To address these limitations, this work employs computational homogenisation techniques to systematically analyse the Andrews method, building on recent developments of computational multiscale methods for electrical conductors with material interfaces (2). In particular, we derive the governing multiscale relations for microstructures with cohesive-type interfaces, and demonstrate that the effective macroscopic conductivity tensor can be extracted from the underlying microstructure.

By a systematic comparison between the Andrews method and the proposed homogenisation approach, we show the fundamental connection between them (3). To this end, one-dimensional analytical expressions are examined, first, so as to uncover the underlying physics. The investigation of primitive anisotropic and isotropic microstructures highlights the importance of grain alignment and morphology influence resistivity in a second step. This crucial understanding of the microstructure-property-relation eventually manifests itself in scaling laws for the effective macroscopic resistivity that are derived thereafter. Finally, the analysis extends to polycrystalline microstructures and is validated against the experimental data. **References**

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