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Atomic-scale features of grain boundaries in metals: from atomistic to the continuum

Houssam Kharouji, Vincent Taupin, Julien Guénolé

Université de Lorraine, CNRS, Arts et Métiers, LEM3, F-57000 Metz, France

houssam.kharouji@univ-lorraine.fr

Polycrystalline metallic materials lie at the heart of many important engineering applications, including aerospace, automotive, aeronautic and energy industries. Their mechanical properties depend not only on the grain size, grain morphology and textures, but also more specifically on the grain boundary types and structures themselves. Therefore, a fundamental understanding of the structures of grain boundaries (GBs) is necessary to improve our understanding of their impact on the mechanical properties of polycrystalline metallic materials. In the present work, we focus first on the atomic scale features of GBs. We propose to use molecular dynamic simulations based on semi-empirical potentials, in order to obtain physical features of selected grain boundaries and interfaces of metallic alloys. In particular, various intrinsic properties will be computed, such as the optimal microscopic degrees of freedom for the GB, the GB defects content and the interfacial GB-energy. Recently, a new framework has been developed to derive a continuous representation of the defected structure and plasticity of grain boundaries from atomic-scale modelling [1,2]. The obtained interfacial atomistic configurations will thus be employed in a “bottom-up” approach to determine an accurate continuum field description of interfaces, which aims at building the foundation of a generalized discrete-to-continuum crossover for the meso-scale continuum modelling of interfacial plasticity in high performance materials.

Keywords: Polycrystalline metallic materials, Grain boundaries, Molecular dynamics, Plasticity.

References:

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