Phase-field chemomechanical modeling of dislocation interaction with precipitates and solutes in metallic alloys

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The purpose of the current work is the development and application of continuum thermodynamic models for the effect of solute chemistry and segregation on dislocation-mediated deformation in metallic alloy systems at the nanoscopic scale. Examples of such systems include two-phase γ-γ' nickel-based superalloys or two-phase γ-κ high maganese lightweight steels. Model development is carried out in the framework of a recent phase-field-based approach to the formulation of chemomechanics for multiphase, multicomponent solid systems [3]. In this framework, models for dislocation-solute and -microstructure interaction build in particular on *ab initio*- and atomistics-based Peierls-Nabarro and phase-field models for nanoscopic dislocation processes (e.g., dissociation, core and stacking fault formation) in single-element fcc materials [e.g., 1, 2, 6]. Basic aspects of the extension and generalization of these models to multicomponent, multiphase alloy systems will be discussed, e.g., the effect of solutes on the (generalized) stacking fault energy. In addition, initial simulation results for dislocation-precipitate interaction in Ni-Al alloys will be presented and compared with analogous MD simulation results as well as with related previous work [e.g., 4, 5, 7]. If time permits, preliminary results for the Ni-Al-Co system will also be discussed.

References

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