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Co-Chairs: Miroslav Urbanek, COMTES FHT; Yunzhi Wang, The Ohio State University

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A combined experimental and simulation study of deformation mechanisms of order precipitates in Ni-based superalloys

Duchao Lv; Don McAllister; Stephen Niezgoda; Mike J. Mills; Yunzhi Wang, The Ohio State University

ABSTRACT

High-temperature alloys in general and superalloys in particular are strengthened by ordered intermetallic phases that possess high-temperature stability and strength. However, their low symmetry and complicated structures impose difficult challenges on detailed understanding of their deformation mechanisms at service conditions. In this study, motivated by detailed TEM observations, we use a combination of *ab initio* calculations of the generalized stacking fault energy surfaces and microscopic phase field model of dislocations to illustrate how dislocations interact with g′ ($L1^0$, cubic) and g″ ($D0^{22}$, tetragonal) precipitates in Ni-based superalloys. The simulations reveal a rich variety of interesting dislocation reactions, leading to various stacking faults and dislocation configurations (including stacking-fault ribbons) actually observed in the experiments. These findings shed light on operating deformation mechanisms of these precipitates during creep and the corresponding strengthening of the superalloys. Incorporation of these detailed deformation mechanisms into continuum level FEM modeling through intermediate level image- and dislocation-density-based crystal plasticity modeling for the development of location-specific, microstructure-, and mechanism-sensitive deformation models will also be discussed.

KEYWORDS: high-temperature alloys, microstructure, dislocation, phase transformation, *ab initio* calculation, phase field modeling, crystal plasticity