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Investigation of coherency loss by prismatic punching with a nonlinear elastic model

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Abstract

Coherency loss of misfitting precipitates by nucleation of dislocations at the interface is investigated using a nonlinear elastic model. This is made possible because the model inherently takes into account, in addition to long-range elastic interactions, phenomena involving dislocation cores such as dislocation nucleation and cross-slip. It is also shown that the model naturally delivers viscous motion laws above a threshold stress. The mechanism of prismatic punching proposed by Ashby and Johnson is confirmed by the present work for small precipitates. For larger precipitates, more complex situations are predicted which involve several dislocations, beyond the scope of the available analyses, but often observed experimentally.

Keywords: Nonlinear elasticity; Dislocations; Coherency loss; 3-D Peierls–Nabarro

1. Introduction

In the solid state, the coexistence of different phases often generates internal stresses which influence mechanical and physical properties. Hence, understanding how these stresses can be accommodated is an important step in predicting the properties of materials. While, in several systems, accommodation can proceed by solute redistribution in the precipitate vicinity (e.g. [1]), coherency loss processes involving interface dislocations and plastic relaxation of the matrix phase are most frequently encountered.

In diffusion-controlled phase transformation, coherency loss can have a significant influence on the precipitate growth regime. For instance in Ref. [2], the authors show that the lengthening rate of platelet-like η and θ' precipitates in Al–Au and Al–Cu alloys is slowed down when precipitates become semicoherent. The presence of interface dislocations reduces the stress field generated by the misfitting precipitate, which provokes a decrease in the driving force, slowing down the precipitate growth. An opposite situation is encountered for the coarsening behavior of Al_3Sc precipitates in Al–Sc alloys [3], where the appearance of interface dislocations increases the precipitate surface energy and increases the coarsening rate.

Generally, the onset of coherency loss is assessed in terms of a simple free energy balance between the contributions from misfit dislocations and the interface energy [4,5]. This is due to the complexity and the variety of the mechanisms proposed so far, often based on early post-mortem observations: (i) nucleation and growth of dislocations by the condensation of point defects within the precipitate [6–8]; (ii) attraction of dislocations at interfaces from the bulk matrix [7,9]; and (iii) formation and emission of dislocation loops of prismatic nature (i.e. purely edge loops with their normal parallel to the Burgers vector), also called prismatic punching [10,8,11]. As noted in Ref. [12], this last

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process is likely to prevail for small precipitates with strong misfit, in particular when the dislocation density in the matrix is low. Indeed, prismatic punching has been observed in many multiphase materials. This is the case, for example, during precipitation of hydrides in zirconium alloys due to the misfit-generated stresses [13,14], or in metal matrix composites (MMCs) with the build-up of thermal stresses during non-isothermal treatments [15,16]. It has been noted in Ref. [17] that a significant hardening can be achieved by such a process in MMCs.

The very first models proposed for coherency loss by prismatic punching are based on analytical expressions for the elastic interactions between a single precipitate and static dislocation loops with simplified geometries [10,18,19]. Among them, the model of Ashby and Johnson [10] is the most appealing as testified by its recurrent use in subsequent studies [12,13,20,21]. Unfortunately, it relies on a particular sequence of events which is assumed rather than proved: first, a shear dislocation loop nucleates at the interface, expands into the matrix and forms a prismatic loop by cross-slip of its screw segments. Hence, validating this sequence requires a dynamic modeling approach. This would also be beneficial for investigating more complex situations such as rows of loops as observed in, for example, Refs. [14,15,22] or tangles ensuing from the interaction between prismatic loops [12,14].

However, very few attempts to tackle coherency loss have been made with the current modeling techniques. Prismatic punching around an inclusion has recently been obtained with a molecular statics approach in Ref. [23]. However, due to the small length scales available in atomistic simulations, the observed processes are likely to be influenced by the boundary conditions. In Ref. [24], a level-set method accounting for dislocation dynamics has been used to investigate the by-pass mechanisms of dislocations around a misfitting inclusion and the resulting coherency loss of the precipitates. However, this method does not take into account dislocation nucleation and thus cannot be used to investigate prismatic punching mechanisms. Although the phase field modeling in Ref. [25] attempted to account for a change in the nature of the interface with some effective eigenstrain, the actual process was unfortunately not described.

In the present work, we propose a continuum modeling of dislocation dynamics able to describe nucleation, glide and cross-slip of dislocations based on nonlinear elasticity, which is subsequently used to investigate loss of coherency of a misfitting precipitate. This model can be seen as an extension to three dimensions of the Peierls–Nabarro model [26,27].

The paper is organized as follows. We describe the model in Section 2 before presenting its validation in static and dynamic conditions in Section 3. Then, results concerning the loss of coherency by prismatic punching are discussed in Section 4, demonstrating the relevance of our model and bringing new insights into the physical process.

2. Nonlinear elastic model

Our model relies on an elastic energy which is periodic with respect to the shear components of the strain tensor. It is comparable to the models of Carpio and Bonilla [28,29] and Onuki and Minami [30,31]. Whereas the former authors resort to a discrete atomic lattice, the latter consider a continuous framework, as followed in the present work. Nonetheless, both approaches yield similar equations after discretization. The major advantages of this kind of model over standard phase-field models of dislocations [32,33] are the following: (i) it incorporates naturally dislocation nucleation, a necessary feature for investigating coherency loss mechanisms and (ii) it does not resort to some gradient term which artificially smooths dislocation cores. Finally, it incorporates naturally cross-slip of screw dislocations which is absent in previous phase-field models of dislocations.

Assuming isotropic elasticity, the total elastic energy of the system is written as follows:

$$\mathcal{F} = \int dx \left[\frac{\lambda + 2\mu}{2} \sum_i (\varepsilon_{ii} - \varepsilon_{ii}^0)^2 + \frac{\lambda}{2} \sum_{i \neq j} (\varepsilon_{ii} - \varepsilon_{ii}^0)(\varepsilon_{jj} - \varepsilon_{jj}^0) + \frac{\mu b^2}{8\pi^2 d^2} \left(3 - \sum_{i \neq j} \cos\left(\frac{4\pi}{b/d} (\varepsilon_{ij} - \varepsilon_{ij}^0) \right) \right) \right] \quad (1)$$

where λ and μ are the Lamé coefficients which may be position dependent, ε_{ij} denote the strain tensor components, ε_{ij}^0 are eigenstrain components associated with the microstructure, and b and d are respectively the norm of Burgers vector and the grid spacing. This elastic energy contains the usual harmonic contributions of the diagonal components of the strain tensor, whereas the shear components are embedded into nonlinear periodic potentials accounting for lattice periodicity. For example, if we consider a perfect crystal which is sheared by the quantity $b/2d$ on a platelet of height d and normal $n = z$, the expression (1) recovers a minimum energy because of these periodic functions. On its glide plane, a dislocation can then be seen as a frontier between a sheared and an unsheared part of the crystal, both stabilized as minimum energy states (see Fig. 1). The prefactors of the periodic terms are chosen such that, for small deformations, the elastic energy of a linear elastic solid is recovered. Cosines have been chosen for simplicity and generality reasons but they can easily be replaced by more complicated forms such as the γ-surfaces obtained from

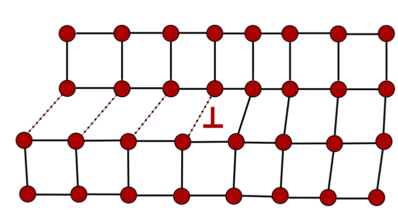

Fig. 1. Edge dislocation seen as a frontier between sheared and unsheared parts of the crystal.