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Phase field microelasticity model of dislocation climb: Methodology and applications

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Abstract

We develop a dislocation climb model based on a phase field description that couples non-conservative dislocation motion and vacancy diffusion. A reaction–diffusion model is incorporated where vacancy transport is governed by the Cahn–Hilliard equation, while the binding of vacancies to dislocation cores is described as adsorptive reaction. The model extends the previously developed phase field microelasticity theory of dislocations to consider the osmotic force associated with non-equilibrium vacancy concentration. We first present quantitative validations of diffusion-controlled and quasi-steady-state dislocation climb with and without dislocation–vacancy interaction. The capability of the model is then demonstrated by simulations of Nabarro diffusional creep and the Kirkendall effect, both showing excellent agreement with classical descriptions of dislocation climb plasticity and interdiffusion. Straightforward applications to irradiation and climb-dominated deformation of crystals are possible, as long as multiple climb systems and vacancy thermodynamic databases are taken into account.

Keywords: Vacancy diffusion; Dislocation creep; Kirkendall effect; Reaction–diffusion model; Computer simulation

1. Introduction

The non-conservative motion of dislocations climbing out of their slip planes and the consequential vacancy adsorption/emission at the dislocation cores play important roles in many materials processes, including high-temperature deformation or creep [1], boundary migration during phase transformations and grain growth [2] and the Kirkendall effect during interdiffusion [3], to name a few. The climb velocity is controlled by long-range vacancy diffusion to/from dislocation lines and adsorption/emission at the core. The driving forces for dislocation climb include the climb component of Peach–Koehler forces arising from internal or external sources of stress and the osmotic (or chemical) force due to deviation of vacancy concentration from equilibrium at a given temperature and stress state. Climb is not only important in creep deformation, but also essential for promoting interdiffusion and keeping vacancy concentration in crystals close to thermodynamic equilibrium, such as that of lattice and grain boundary dislocations acting as vacancy sources/sinks.

The interplay among vacancy sources/sinks, diffusion and creep was rationalized by several models [4–11]. Most of them take into account long-range elastic interactions among point defects and sources/sinks of vacancies, but do not emphasize the mesoscopic mechanisms such as short-range interactions and dynamic motion of sources/sinks together with vacancy generation/annihilation. The treatments are acceptable for large-scale simulations in

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which the short-range interactions are difficult to resolve. However, without the consideration of mesoscopic effects, some simplifications had to be introduced, such as isotropic inelastic strain of sources/sinks, equilibrium vacancy concentration, dense and ideal sources/sinks of vacancies or the Newtonian fluid model for the deformation of solids. Accordingly, the development of mesoscopic modeling of dislocations is important for clarifying the short-range coupling mechanisms of sources/sinks dynamics and vacancies.

Dislocation climb coupled with vacancy diffusion was incorporated into dislocation dynamics models for the simulations of Frank-type prismatic loops [12,13], climb-assisted dislocation glide [14,15] and power-law creep [16]. In addition to the climb-assisted glide of pure edge dislocations studied in Refs. [14,15], the glide of screw dislocations with jogs also requires a non-conservative process or climb. Equilibrium vacancy concentration was usually assumed along the dislocation line when considering the climb component of the Peach–Koehler force and the climb velocity was determined by a drag-type relation based on mass conservation and the steady-state condition of climb [17]. These methods require steady-state analytical solutions of vacancy diffusion as the model input and interactions among diffusion fields from each segment were neglected. This limitation was resolved very recently by Ayas et al. [18], who solved the boundary value problem with a superposition method for vacancy diffusion. Nevertheless, the requirement of analytical solutions constrains the application to certain simple situations, such as single-component systems and the assumed linear diffusion equation.

We present a dislocation climb model based on the phase field method, which allows us to remove some of the assumptions. The phase field model of dislocation dynamics [19,20] was developed based on Khachaturyan and Shatalov's (KS) microelasticity theory [21], and was further improved to model dislocation networks and core structures [22,23]. The dislocation configurations were described by the phase fields characterizing the amount of shear with respect to a perfect crystal. Topological changes during dislocation reactions and interactions can be modeled naturally by introducing appropriate energy formulations based on crystal symmetry. The prior pioneering work, however, was mainly focused on the conservative motion (i.e., glide) of dislocations. It is thus highly desirable to extend the model to simulate diffusion-mediated dislocation climb processes as well,[1] taking full advantages of the phase field method in treating coupled diffusional–displacive processes [23]. Compared to the analytical approach and discrete dislocation dynamics models, the main advantage of the phase field approach is its ability to incorporate directly long- and short-range dislocation–dislocation and dislocation–vacancy interactions, osmotic force, diffusion and external applied stress into a single mathematical framework, without the need for simplified analytical solutions. The paper is organized as follows. In Section 2 we present the formulation of the phase field microelasticity theory of dislocation climb combined with the reaction–diffusion model. In Section 3 we show validations of the model against analytical solutions of quasi-steady-state dislocation climb both with and without consideration of elastic interaction between vacancies and dislocations, followed by demonstration of the model capabilities by simple two-dimensional (2-D) plane strain simulations, including Nabarro diffusional creep and Kirkendall effect in unitary and binary systems. In Section 4 we compare our results with the work presented by Geslin et al. [24]. We also address limitations of the model and possible extensions to elastically inhomogeneous systems, multicomponent systems and systems large enough to include dislocation sources. Finally, we summarize some of the promising features of the model in Section 5 based on the simulation results.

2. Model description

2.1. Phase field description of dislocation climb

The phase field model of dislocations [19,20,22] considers a glide dislocation loop on a slip plane as a coherent misfitting platelet inclusion with a stress-free transformation strain (i.e., eigenstrain) of simple shear. The analogy can be traced back to Nabarro's renowned description on dislocation loops [25]. On the slip plane, a set of non-conserved field variables were introduced to distinguish the sheared and unsheared regions, and to describe the amount of shear with respect to a perfect crystal. Such a phase field description of dislocations is suitable for modeling conservative motions of dislocations (i.e., glide). However, dislocation climb is a non-conservative motion out of the slip plane. In this regard, a field description of incomplete atomic planes should be a more natural way to model climb, e.g., a climbing dislocation can be described as shrinking or expanding of a platelet inclusion (either atom- or vacancy-type Frank loops of arbitrary geometry) with a tensile or compressive eigenstrain. The description was first mentioned by Hu and Chen [26] and applied to simulate the evolution of Frank-type dislocation loops by Li et al. [27] and Boyne et al. [28].

Similar to the previous work [27], we introduce a set of non-conserved field variables (i.e., order parameters), η_p, on climb planes (incomplete atomic planes) to characterize the amount of normal displacements resulted from "missing" atomic layers (i.e., vacancy disks), where p indicates the specific climb system. The non-conserved nature of the order parameters is due to the fact that the total number of missing atomic planes is not required to be constant.

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[1] Note added during revision: it should be noted that while our manuscript was submitted for publication, another research group independently introduced a similar dislocation climb model via the phase field approach [24]. Accordingly we have compared some of the features of the two methods.