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Three-dimensional formulation of dislocation climb

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ABSTRACT

We derive a Green's function formulation for the climb of curved dislocations and multiple dislocations in three-dimensions. In this new dislocation climb formulation, the dislocation climb velocity is determined from the Peach–Koehler force on dislocations through vacancy diffusion in a non-local manner. The long-range contribution to the dislocation climb velocity is associated with vacancy diffusion rather than from the climb component of the well-known, long-range elastic effects captured in the Peach–Koehler force. Both long-range effects are important in determining the climb velocity of dislocations. Analytical and numerical examples show that the widely used local climb formula, based on straight infinite dislocations, is not generally applicable, except for a small set of special cases. We also present a numerical discretization method of this Green's function formulation appropriate for implementation in discrete dislocation dynamics (DDD) simulations. In DDD implementations, the long-range Peach–Koehler force is calculated as is commonly done, then a linear system is solved for the climb velocity using these forces. This is also done within the same order of computational cost as existing discrete dislocation dynamics methods.

1. Introduction

Dislocation climb plays important roles in the plastic deformation of crystalline materials at high temperature, e.g., in dislocation creep. Dislocations climb out of their slip planes with the assistance of diffusion and emission and/or absorption of vacancies or interstitials. The theory of vacancy diffusion-controlled dislocation climb has received considerable attention for well over 50 years and is discussed in several standard dislocation texts (e.g., Hirth and Lothe, 1982). The dislocation climb velocity can be expressed in terms of the Peach–Koehler climb force and analytical expressions are well known for several simple cases, such as straight edge dislocations and circular prismatic loops. For three-dimensional discrete dislocation dynamics (DDD) simulations, Raabe (1998) presented a formulation to incorporate the osmotic climb force and vacancy diffusion. In the work of Ghoniem et al. (2000), both the Peach–Koehler climb force and the osmotic climb force due to vacancy diffusion were included in a thermodynamics-based parametric DDD approach, and the total climb force was related to climb velocity by a "resistivity." Xiang et al. (2003) and Xiang and Srolovitz (2006) described the climb velocity in terms of the climb-component of the Peach–Koehler force through a tensor mobility law, and studied dislocations bypassing

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particles by the combined action of both glide and climb. This method was employed by Chen et al. (2010) to study dislocation climb in systems with distributions of immobile obstacles in a parallel implementation. Dislocation climb is also included in the mobility law in the DDD ParaDiS code by Arsenlis et al. (2007). Danas and Deshpande (2013) used a drag-type relation for the climb velocity, similar to that employed for dislocation glide, in their small-strain, two-dimensional dislocation plasticity framework. The effect of climb on dislocation dynamics mechanisms and creep rates in γ–γ' Ni-based superalloy single crystal was examined by Hafez Haghighat et al. (2013) using DDD simulations.

Several recent DDD simulation studies have included a more explicit coupling between dislocation climb and vacancy diffusion. Mordehai et al. (2008) incorporated a climb velocity–force relation derived for straight dislocations which can be applied in cases where the vacancy concentration in the bulk is the same or different from its equilibrium value (e.g., due to irradiation). Bako et al. (2011) proposed a dislocation dynamics formulation in which the dislocation climb mobility includes vacancy diffusion and employed it to study the coarsening of prismatic loops in fcc metals. Their climb velocity–force relation was derived based on straight dislocations and they considered the interaction between different dislocation loops through a parameter c_∞ representing the overall vacancy concentration in the sample which includes changes associated with the condensation of vacancies into loops during coarsening processes. Mordehai and Martin (2011) studied the enhanced rate of annealing of the dislocation network under irradiation including the effect of coordinated climb of dislocations in a network due to the elastic interaction between vacancies and dislocations – again, based on analytical formulations for straight dislocations.

As discussed above, in the dislocation climb literature, the dislocation climb velocity is generally formulated as in Eq. (16) below, where the coupling between dislocation climb and vacancy diffusion is based upon the equilibrium vacancy distribution for a single, straight dislocation, as per Eq. (15) below. However, Eq. (15) is NOT the equilibrium vacancy diffusion solution other than for this special case (a single straight dislocation). Accordingly, the climb velocity in Eq. (16) only applies directly to a single straight dislocation, and does NOT apply in general for dislocation structures with multiple, arbitrarily shaped dislocations. (We will show several examples of this in Section 4.)

Keralavarma et al. (2012) addressed this limitation in their two-dimensional DDD simulations by connecting the far field vacancy concentration c_∞ in the climb velocity in Eq. (16) for each dislocation by solving a vacancy diffusion equation with a source term depending on the dislocation density averaged over a finite volume element (rather than solving for the case where each dislocation is a discrete source/sink). However, this treatment is not necessarily accurate on the scale of DDD—it is insensitive to the arrangement of dislocations within the volume element. In addition, the climb velocity expression used by Keralavarma et al. (2012) with an *ansatz* similar to Eq. (16), below, is likely valid where dislocations are widely separated; in cases where dislocations are close together (relative to the average separation), this will lead to errors that can be large and lead to unphysical effects (see Section 4).

In order to obtain the dislocation climb velocity in DDD accurately, one should solve for the vacancy diffusion in Eq. (4), below, subject to the condition that the vacancy concentration is in equilibrium near each dislocation in Eq. (11) (involving the climb Peach–Koehler force), below, as well as boundary conditions appropriate for the far field or the domain boundary. However, solving such a problem in three dimensions is time consuming. In this paper, we present an alternative formulation based upon Green's functions, in which the calculations are performed only on the dislocations instead of over the full three dimensional domain. This new formulation gives accurate dislocation climb velocity predictions for multiple, arbitrarily curved dislocations in three-dimensions. We show that there is a long-range contribution to the dislocation climb velocity associated with vacancy diffusion, in addition to the well-known, long-range elastic effects captured in the Peach–Koehler force. We also present a numerical discretization method for solving for the climb velocity including these long-range effects appropriate for DDD simulations. Our new approach has the same order of computational complexity as the existing DDD simulation methods.

This paper is organized as follows. In Section 2, we review the basic theory of vacancy diffusion controlled dislocation climb. In Section 3, we present Green's function-based formulation for dislocation climb, in which the climb velocity is determined by solving integral equations depending on the spatial distribution and shapes of all the dislocations and the climb component of the Peach–Koehler force. In Section 4, we present several applications of our Green's function formulation for the climb velocity. The long-range effect of a dislocation climb is examined. The widely used local approximation of using the classical climb velocity formula for straight dislocations is shown in general not to be applicable to multiple or curved dislocations (i.e., it leads to unacceptable errors). In Section 5, we present a numerical discretization method for this Green's function formulation of dislocation climb velocity appropriate for use in DDD simulations. Several generalizations of our new dislocation climb formulation are discussed in Section 6.

2. Formulation of vacancy diffusion controlled dislocation climb

In describing vacancy diffusion controlled dislocation climb, the total free energy can be expressed as

$$G = E_1 + E_2, \tag{1}$$

where E_1 is the free energy associated with the instantaneous distribution of vacancies and E_2 is the energy associated with the dislocation distribution.