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Implementation of the nudged elastic band method in a dislocation dynamics formalism: Application to dislocation nucleation

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ABSTRACT

We propose a framework to study thermally-activated processes in dislocation glide. This approach is based on an implementation of the nudged elastic band method in a nodal mesoscale dislocation dynamics formalism. Special care is paid to develop a variational formulation to ensure convergence to well-defined minimum energy paths. We also propose a methodology to rigorously parametrize the model on atomistic data, including elastic, core and stacking fault contributions. To assess the validity of the model, we investigate the homogeneous nucleation of partial dislocation loops in aluminum, recovering the activation energies and loop shapes obtained with atomistic calculations and extending these calculations to lower applied stresses. The present method is also applied to heterogeneous nucleation on spherical inclusions.

1. Introduction

The plastic behavior of metals and alloys depends strongly on temperature because of the role played by thermally-activated processes in dislocation movement. Examples include the nucleation of kink pairs on high Peierls stress dislocations, the cross-slip of screw dislocations and the climb of edge dislocations in creep conditions (Caillard and Martin, 2003; Kassner, 2015; Kubin, 2013). The temperature dependence is even stronger in nanostructures, because in absence of bulk sources, dislocations are nucleated from interfaces (Li et al., 2010; Zhu et al., 2007), revealing another example of thermally-activated process.

So far, thermally-activated processes involving dislocations have been studied numerically mainly at the atomic scale, using saddle point search methods, such as the nudged elastic band (NEB) method (Jónsson et al., 1998; Mills and Jónsson, 1994; Mills et al., 1995) or the activation-relaxation technique (Barkema and Mousseau, 1996; Mousseau and Barkema, 1998; Mousseau et al., 2012). The case of dislocation nucleation has been particularly studied (Aubry et al., 2011; Jennings et al., 2013; Maras et al., 2016; Ryu et al., 2011; Zhu et al., 2008, 2004) to better understand the plastic behavior of nanostructures. As an example, we show in Fig. 1 the activation energy as a function of an applied shear stress computed for the homogeneous nucleation of a Shockley partial dislocation loop in aluminum, modeled with the interatomic potential developed by Mishin et al. (1999). The inset shows the atomistic saddle configuration found at an applied stress $\sigma^a = 1.4$ GPa.

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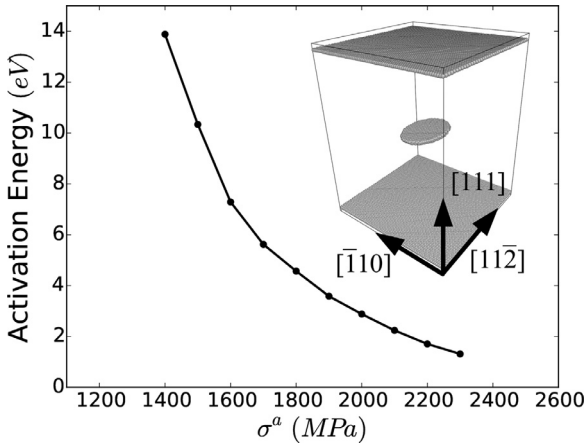

Fig. 1. Activation energy function of applied shear stress obtained from atomistic free-end NEB calculations of the homogeneous nucleation of a Shockley partial dislocation loop in aluminum. The inset shows the saddle configuration at an applied shear stress $\sigma^a = 1.4$ GPa (only the defected atoms in the upper and lower free surfaces and in the stacking fault of the loop are shown).

The calculations in Fig. 1 used the free-end NEB method, which is briefly recalled here. The degrees of freedom are the atomic positions stored in configuration vectors noted $\boldsymbol{R}$ (of dimension $3 \times N_{at}$ where N_{at} is the number of atoms in the system); $E_{at}(\boldsymbol{R})$ is the corresponding energy. The NEB method consists in building a chain of replicas interpolated between an initial and a final state. In the present case, the initial path is formed of circular loops of increasing radius, created using their elastic displacement field (Ohr, 1972). The replicas are linked between first neighbors using springs in configuration space. The degrees of freedom of a replica i are therefore subjected to (i) the forces $\boldsymbol{F}_i^r$ derived from the replica potential energy and projected on the hyperplane perpendicular to the chain of replicas and (ii) $\boldsymbol{F}_i^s$, the contribution of the spring forces associated to the NEB method:

$$\boldsymbol{F}_i^r = -\left(\nabla E_{at}(\boldsymbol{R}_i) - \nabla E_{at}(\boldsymbol{R}_i) \cdot \boldsymbol{\tau}_i\right), \tag{1}$$

$$\boldsymbol{F}_i^S = k_{NEB}(|\boldsymbol{R}_{i+1} - \boldsymbol{R}_i| - |\boldsymbol{R}_i - \boldsymbol{R}_{i-1}|)\boldsymbol{\tau}_i, \tag{2}$$

where k_{NEB} is the elastic constant of the springs between replicas and $\boldsymbol{\tau}_i$ the tangent to the path defined using the improved tangent method (Henkelman and Jónsson, 2000). A quenched dynamics is used to relax the chain of replicas subjected to the forces in Eqs. (1) and (2), to obtain the minimum energy path (MEP) between the initial and final configurations. For dislocation nucleation, the last replica representing the largest loop is not a local energy minimum. We have therefore used the free-end NEB method (Zhu et al., 2007), where this last image evolves at constant energy, while being subjected to the spring force from its neighboring replica. The replica of maximum energy can be treated differently with the climbing image method (Henkelman et al., 2000) to ensure its convergence to the saddle point configuration. The applied stress is controlled by imposing external forces to the atoms within the cut-off radius distance from the upper and lower free surfaces shown in the inset of Fig. 1. The activation energy is then the energy difference between this maximum energy image and the initial configuration. We note that the convergence of the NEB method to a valid minimum energy path relies on the fact that the atomic forces derive from a well-defined energy, i.e. from the variational character of atomistic calculations.

Such calculations are highly informative but are also very limited in term of size scale. The convergence time of the NEB method increases drastically with the number of degrees of freedom (DoFs) in the system, usually limiting its use to volumes smaller than $10^4\,\text{nm}^3$ for dislocation-mediated events. As a consequence, only stresses larger than 1.4 GPa were considered in the example above. This size-scale issue also prevents from modeling complex heterogeneous fields emerging from a surrounding microstructure, for example, of dislocations and/or precipitates. Moreover, atomistic calculations can only give the minimum energy path and activation energy at $T = 0\,\text{K}$, while material parameters such as the lattice spacing, elastic constants and stacking fault energy vary significantly with temperature and affect the activation energy, as shown by Ryu et al. (2011) in the case of dislocation nucleation. Temperature effects can be included in atomistic saddle-point search calculations but at a large computational cost (Gilbert et al., 2013).

It is therefore highly desirable to perform saddle-point searches in higher-scale models, with a limited number of degrees of freedom, to allow for faster calculations in large-scale systems, but also to be able to include temperature effects in an effective way, by varying the model parameters. In this spirit, the NEB method has been incorporated in continuous phase-field models to investigate the nucleation barrier against martensitic transformation (Shen et al., 2008), shape transitions of vesicles (Kusumaatmaja, 2015) and the wetting of patterned surfaces (Semprebon et al., 2016). This type of mesoscale approaches has also the advantage of averaging out the small energy barriers related to subtle atomic rearrangements, allowing to focus on the most relevant energy barriers for macroscopic phenomena.