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Scale transition using dislocation dynamics and the nudged elastic band method

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ABSTRACT

Microstructural features such as precipitates or irradiation-induced defects impede dislocation motion and directly influence macroscopic mechanical properties such as yield point and ductility. Dislocation-defect interactions involve both atomic scale and long range elastic interactions. Thermally assisted dislocation bypass of obstacles occurs when thermal fluctuations and driving stresses contribute sufficient energy to overcome the energy barrier. The Nudged Elastic Band (NEB) method is typically used in the context of atomistic simulations to quantify the activation barriers for a given reaction. In this work, the NEB method is generalized to coarse-grain continuum representations of evolving microstructure states beyond the discrete particle descriptions of first principles and atomistics. This method enables the calculation of activation energies for a $1/2[111](1\bar{1}0)$ glide dislocation bypassing a [001] self-interstitial atom loop of size in the range of 4–10 nm with a spacing larger than 150 nm in α-iron for a range of applied stresses and interaction geometries. Further, the study is complemented by a comparison between atomistic and continuum based prediction of barriers.

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1. Introduction

Thermally activated phenomena underlie many of the processes leading to material microstructure evolution (e.g. diffusion, defect clustering, dislocation migration etc.). Indeed, thermal fluctuations can assist the applied and internal stresses in driving a system to overcome local energy barriers. The waiting time for thermally activated barrier bypass defines the limiting rate for microstructure evolution. The activation rates of linear Arrhenius-type processes (e.g. grain growth Meyers et al., 2006, climb and cross-slip driven creep in metals Kassner and Perez-Prado, 2000), exhibit an inverse exponential dependence on T, where T is absolute temperature. Within this framework, reaction rates for specific processes, k, can be obtained from the knowledge of both attempt frequency ν and activation barrier E_A, i.e.,

$$k = \nu e^{-\frac{E_A}{k_B T}} \tag{1}$$

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where k_B is the Boltzmann constant. A large body of work relies on Eq. (1) to effectively perform a time scale transition as well as to selectively predict the relative contribution of concomitantly active dissipative processes (Domain et al., 2004; Martin-Bragado et al., 2013). Molecular static simulations based on first principles (e.g., DFT) or empirical potentials are often used to calculate activation energies, and more generally minimum energy pathways (MEP), as they are well-suited to address the length scales associated with atomic scale structure rearrangement processes involving limited volumes, such as dislocation bypass of nm-scale obstacles, or point defect migration.

The computational complexity of MEP methods (high degrees of freedom) has motivated the development of several efficient saddle point energy calculation methods. The dimer method (Henkelman and Jónsson, 1999) uses a pair of images of the system, slightly offset in space, to drive the system towards a saddle point according to the local curvature of the system. The activation relaxation technique (Mousseau and Barkema, 1998) first perturbs a degree of freedom in the system, from which the system is driven up the potential energy surface towards the saddle point. From the saddle point, the system is relaxed to find the final configuration of the system. Another commonly used technique is the nudged elastic band (NEB) method (Jonsson et al., 1998), which determines the minimum energy pathway between two known local energy minima. A series of system images are created (typically linear interpolations between the initial and final states), which are relaxed under the combination of a physical force and a fictitious spring force. The spring force acts to maintain even image spacing across the potential energy surface while the physical force acts to drive the system into a minimum energy configuration. In combination with atomistic simulations, these methods have been used to investigate numerous phenomena such as point defect migration as well as dislocation migration and cross-slip (Bai et al., 2010; Gordon et al., 2011; Rao et al., 2011).

Although atomistic methods provide valuable insight into atomic-scale processes, significant computational requirements limit simulations to processes involving small activation volumes and therefore restrict the possible range of phenomena that can be considered. Furthermore, spatial and temporal coarse-graining atomistic simulation methods that link directly to constitutive models have yet to be firmly established. Recent studies have demonstrated success in several cases such as dislocation nucleation at boundaries (Capolungo et al., 2007) and shear-coupled grain boundary migration (Prieto-Depedro et al., 2015), but the use of NEB based on atomistic simulations to inform continuum descriptions of thermally activated processes has been primarily limited to unit processes with activation volumes comprising up to tens of atoms. A mesoscale continuum phase field modelling approach combined with NEB was used to find the critical nucleus configuration and activation energy in a cubic to tetragonal transformation using a free-end NEB method (Shen et al., 2008). However, larger scale cooperative processes of microstructure rearrangement characteristic of dislocation-obstacle interactions that have both short and long range character have eluded treatment via such methods.

For dislocation-obstacle interactions, this problem can be rendered computationally tractable by employing discrete dislocation dynamics (DDD) to represent the energy landscape based on the continuum elastic theory of defects. When the necessary approximations are valid, simulations described using a continuum theory are desirable in terms of low computational requirements and offer a more direct connection to constitutive models. With such significant reductions in computation time, it is possible to compute the MEP and saddle point energies for transition not only for a single reaction, but for more complex many-body dislocation-obstacle field interactions to map a more comprehensive energy landscape for obstacle interactions; this potentially represents a significant advancement in coarse-graining techniques to achieve what one of the authors had referred to as activation volume averaging of collective evolving microstructure events (McDowell, 1997; 1999) as an alternative to classical homogenization approaches for effective properties of stationary (non-evolving) microstructures in micromechanics. In the present work, we demonstrate the capabilities of a novel DDD-NEB method to investigate the size and stress dependence of dislocation bypass activation energy with self-interstitial atom (SIA) loops induced by irradiation for activation volumes comprised of several hundreds of atoms. Results are used to inform a constitutive harmonic transition state theory model (Kocks et al., 1975) as well as to create a complete activation energy map for different interaction geometries. Perspectives and limitations of DDD-NEB are directly addressed with comparisons to atomistic calculations for a dislocation-SIA loop bypass process.

We emphasize the premise of this approach to continuum rather than discrete descriptions of evolving microstructure is that NEB can be applied to any coarse-grained continuum description that includes the following essential features:

- Dominant kinematic degrees of freedom for evolving attributes of microstructure are included.
- Various self- and interaction (potential) energies of evolving microstructure attributes are included, as necessary to coarse-grain the energy landscape, including short and long range interactions.
- A continuous representation of the state of the system is available from the continuum representation as microstructure evolves during state transitions, as opposed to distinct sets of states that evolve as per assigned prescription.

The latter two requirements are particularly demanding for continuum theories, particularly of many body theories (e.g., metal viscoplasticity), both in terms of approximation of long range elastic fields and the continuity of evolution of the sequence of states in a complex reaction pathway. It is immediately recognized that DDD is a continuum theory construct with the necessary features above. Moreover, it is apparent that phase field theory has these essential features and is therefore also amenable to the extended NEB methodology outlined here. What might not be as evident is that internal state variable (ISV) models are also amenable to this methodology provided they assert these key three requirements of state transitions. Such ISV models include evolving state parameters within the context of a thermodynamically consistent formulation; they must be enriched with sufficient kinematics of evolution to accompany the energetic formulation to allow for the above requirements, which is typically not the case. More often, probability distributions of transition states describe by ISV mod-