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The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature

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ABSTRACT

The mechanisms associated with grain boundary motion induced by synthetic, crystal-orientation-dependent driving forces are investigated for a large-angle [001] Ni symmetric tilt grain boundary. The application of non-physical forces by this method brings legitimate concern that it could lead to non-physical results. This concern is especially relevant below the interface roughening transition temperature where there is a substantial drop in grain boundary mobility and large driving force dependence. Using slip-vector analysis and examining continuum metrics for microrotation and strain, this work shows that the application of synthetic-driving forces does not alter the fundamental mechanisms leading to grain boundary motion. Results in this work are compared directly to shear driven simulations which reveal that the path and deformation history of grain boundary motion is unbiased by the non-physical nature of the driving force acting on the boundary. Nudged elastic band calculations show that the transition path for grain boundary motion is independent of the driving force magnitude and the energy barriers for motion are not appreciably altered by the application of the synthetic driving force.

1. Introduction

A fundamental understanding of grain boundary motion and mobility is necessary to advance mesoscale predictive models of grain growth in polycrystalline materials [1]. Grain boundary motion has been simulated in recent years using synthetic driving force molecular dynamics simulations, first introduced by Janssens et al. in 2006 [2]. In these simulations [2], flat grain boundaries constructed from bicrystal models are driven by a crystal-orientation-dependent driving force superimposed on an embedded atom method (EAM) potential. This driving force stems from a continuous potential energy term that is added to all atoms which varies in magnitude based on the relative orientation of neighboring atoms as compared to a reference grain. Using this method, extra potential energy is added to the atoms of the reference grain resulting in a synthetic driving force that biases the motion of the grain boundary towards the higher energy grain in order to reduce the total system potential energy. The synthetic driving force stimulates motion of flat grain boundaries within the timescale of molecular dynamics simulations and allows any grain boundary misorientation to be studied independently. This facilitates high-throughput studies of grain boundary motion as a function of grain boundary crystallography and temperature such as the study by Olmsted et al. [3].

Prior studies have applied the synthetic driving force method to a variety of grain boundaries spanning a wide misorientation range, with researchers limiting their analysis to the collective motion of the atoms at the grain boundary [2–7]. Here we include studies [4–6] which utilized the adapted interface-random-walk method introduced by Deng and Schuh in 2011 [4] as a hybrid method that combines synthetic driving force and statistical analysis of boundary fluctuations in order to analyze slow moving grain boundaries. By focusing the analysis on the collective motion of the atoms at the grain boundary, prior researchers [2–7] were able to compute grain boundary velocity and mobility as well as compare their results to experimental values [3,5] and conventional molecular dynamics simulations with physically based driving forces such as shear and strain [6,7].

Studies of grain boundary motion have also reported an interface roughening transition which significantly impacts the motion of grain boundaries. Interfacial roughening is a thermodynamic phase transition where the spatial variation of the position of the

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interfacial plane is finite below the transition temperature and diverges with the interfacial area above the transition temperature. The transition temperature reflects the energy cost of a local fluctuation of the interfacial position normal to the interface. It has been shown that there is an abrupt increase in grain boundary mobility as the temperature is increased above the transition temperature for that interface [7]. Simulations that applied synthetic driving force methods revealed large driving force dependence for the smooth grain boundary configurations below the roughening transition temperature [3,7]. Since the synthetic driving force method applies non-physical forces, there is a legitimate concern that this approach might lead to non-physical results, especially below the roughening transition temperature.

While prior work [7] shows that the computed mobility agrees with physical driving force simulations, studies have not yet analyzed the effect of synthetic driving forces on the atomic mechanisms associated with the motion of smooth interfaces, nor has any study examined the effect of synthetic driving forces on the transition energy barriers for grain boundary motion. The purpose of the synthetic driving force method is to bias the system such that the grain boundary will move from its current position towards a region with artificially added energy without purposely raising the basins on the potential energy surface in an attempt to lower the transition energy barriers, as is done in the hyperdynamics method [8]. In this work, we investigate the effect of synthetic driving forces on the atomic mechanisms associated with low-temperature grain boundary motion and compare these mechanisms to those observed in simulations driven by shear. In addition, we study the effect of applied synthetic driving forces on the potential energy surfaces revealing how transition energy barriers are affected by the synthetic driving force method.

2. Methods

The $\sum$37 (5 7 0) [0 0 1] symmetric tilt grain boundary (STGB) modeled in this study was constructed originally by Olmsted et al. as part of their large survey of grain boundary energy and mobility [3,9]. The interface was chosen as a representative large-angle STGB constructed from sets of C type kite structural units [10] that zigzag at the interface. The initial studies by Olmsted et al. on this boundary provided evidence of grain boundary roughening at elevated temperatures and demonstrated motion-coupled shear when applying synthetic driving forces. Motion-coupled shear is the phenomenon whereby atoms in the neighboring grains collectively move parallel to the grain boundary plane in response to the synthetic driving force acting normal to the interface [11]. This phenomena is analogous to shear-coupled motion recently described in detail by Cahn et al. [12]. Boundaries experiencing motion-coupled shear are likely candidates for shear driven grain boundary motion, and would allow for direct mechanistic comparison.

The simulations conducted throughout this study use the LAMMPS molecular dynamics simulator [13] with the Foiles and Hoyt EAM potential for Ni [14]. To determine the roughening transition temperature, mobility calculations for the $\sum$37 (5 7 0) [0 0 1] STGB are performed at 300–1200 K using synthetic driving forces of 0.001–0.025 eV/atom. In this study, we are able to extend into lower temperature and driving force regimes than originally studied by Olmsted et al. [3] by increasing the effective statistical sampling size in order to reduce error in the computed mobility. Increased statistical sampling is achieved by using 25 independent simulations and offsetting initial conditions in a similar manner as described by Deng and Schuh [4]. For each temperature and driving force, grain boundary displacement data are collected every 1 ps using an 2 fs offset. The combined 12,500 displacement data points collected are fit to a Gaussian distribution to determine the mean grain boundary displacement for each time interval. Using enhanced effective sampling, the minimum 10 Å grain boundary displacement criteria used by Olmsted et al. is relaxed in this study such that all simulations with computed grain boundary mobility greater than 1 GPa^{-1} m/s are analyzed.

The effects of the synthetic driving forces below the roughening transition temperature are explored through direct comparisons with shear driven grain boundary motion simulations. Simple shear simulations are constructed at 300 and 400 K such that the normal grain boundary velocities closely match those of the simulations using synthetic driving forces of 0.025 and 0.005 eV/atom. The shear simulations are designed similar to those by Tucker et al. [15], where grain boundary motion is induced by moving rigid edges on both sides of the bicrystal model at a constant (opposing) velocity parallel to the grain boundary plane. To avoid shock wave generation, a linearly ramped velocity profile is imposed on the atoms positioned between the rigid edges. Low-temperature simulations driven by shear and the synthetic driving force method are analyzed and compared using slip-vector analysis and continuum metrics of microrotation and strain as described by Zimmerman et al. [16] and Tucker et al. [17] respectively.

The energy barriers and transition states associated with the motion of the smooth $\sum$37 (5 7 0) [0 0 1] Ni STGB are investigated using the nudged elastic band (NEB) method extracting data from climbing images [18]. NEB calculations determine the 0 K minimum energy configurations along the path from an initial to a final state. In this study, a series of six NEB calculations are performed applying synthetic driving forces in the range of 0.000–0.025 eV/atom. It is important to note that the NEB calculations with no applied driving force are comparable to conditions observed for shear driven simulations; thus, providing a baseline for comparing the synthetically driven methods.

3. Results and discussion

Fig. 1 displays an Arrhenius plot of log(mobility) versus inverse temperature for the $\sum$37 (5 7 0) [0 0 1] STGB revealing an interface roughening transition between 400 and 500 K. From 500–1200 K, synthetic driving forces have minimal effect on the grain boundary mobility and log(mobility) remains nearly constant between 5.5–6.9 log(GPa^{-1} m/s). However, from 300 to 400 K the mobility decreases significantly with application of lower driving forces, which is indicative of a transition into a smooth grain boundary configuration. Mobility data for the 300 K simulations driven by

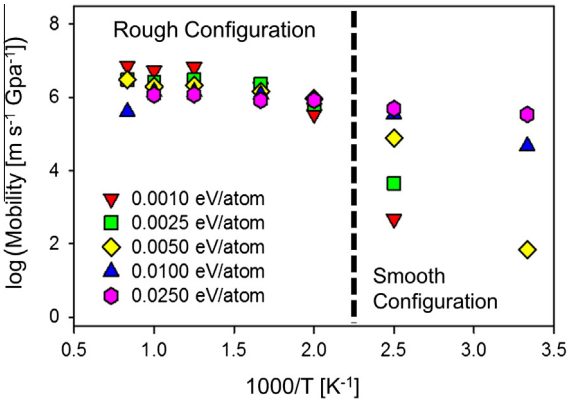

Fig. 1. Arrhenius plot of log(mobility) versus inverse temperature for a $\sum$37 (5 7 0) [0 0 1] STGB computed with various driving forces. Grain boundary roughening occurs between 400 and 500 K as identified by a substantial drop in driving force dependence.