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Migration energy barriers of symmetric tilt grain boundaries in body-centered cubic metal Fe

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ABSTRACT

Migration energy barriers of two symmetric tilt grain boundaries in body-centered cubic metal Fe are obtained via first-principles calculations in combination with the nudged elastic band methods. Although the two grain boundaries show similar grain boundary energies, the migration energy barriers are different. Based on a homogeneous nucleation theory of grain-boundary dislocation loops, the calculated energy barrier provides a measure of intrinsic grain-boundary mobility and helps to evaluate effects due to vacancy and interstitial atoms such as carbon.

Grain boundaries (GBs) in polycrystalline materials are essentially mobile planar defects and the mobility depends on GB structure, GB energy, temperature, applied strain or stress, as well as a number of other factors, such as grain size, lattice dislocations, vacancies, solute atoms (impurity) and precipitates [1,2]. Understanding the evolution of grain boundaries is crucial for better design of microstructures in order to achieve improved mechanical property and performance for both nanostructured and conventional polycrystalline metals and alloys [3–5]. The motion of a GB can be considered as conservative if the same GB structure is preserved during the motion [6]. Conservative GB motion occurs most likely for symmetric GBs because such GBs consist of identical structural units in terms of the coincidence site lattice (CSL) [1]. The GB mobility is then limited intrinsically by the migration energy barrier when the GB is forced to move from one position to the next by applying shear stresses. In particular, the theoretical shear stress of GB migration can be defined at which the migration energy barrier vanishes at zero temperature conditions, a way similar to the definition of the theoretical shear stress for a perfect lattice [7].

However, to promote GB migration under thermal fluctuations, it is energetically more favorable to form a dislocation loop on a perfect GB plane. Following Frank's homogeneous dislocation nucleation model [7,8], it has been proposed [6,9] that the required free energy to nucleate a GB dislocation loop may be written as

$$\Delta G(R,\tau) = (\gamma - \tau b)A + 2\pi R\frac{\mu b^2}{8\pi}\left(\frac{2-\nu}{1-\nu}\left(\ln\left[\frac{8R}{r_0}\right] - 2\right) + 0.5\right) \quad (1)$$

if a circular loop of dislocation of radius R and an area $A = \pi R^2$ is formed under a shear stress τ applied parallel to the Burgers vector b of the GB dislocation. The last term presents the elastic energy of the dislocation loop [7,10] with a cutoff radius (r_0). Within r_0 the continuum theory breaks down, the core energy of the loop per area is measured merely by the migration energy barrier (γ) where γ is also a function of the applied stress, τ. That is, the migration energy barrier is introduced here in a manner similar to the well-known generalized stacking fault energies for nucleation of lattice dislocations (see, e.g. Ref. [10]). Both γ and b are specific material properties and are closely related the GB structures. With increasing R the energy ΔG increases and a maximum value $\Delta G_{\max}(R_c,\tau)$ can be found numerically from the condition $\partial(\Delta G)/\partial R = 0$ which occurs at a critical radius R_c. Only a loop of radius larger than R_c can expand, so $\Delta G_{\max}$ represents an activation energy for GB migration. Therefore, in the absence of any heterogeneous nucleation site, the homogeneous nucleation model sets an upper limit to measure how difficult an individual GB might migrate under thermal activations and an applied shear stress.

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A number of recent literatures can be found to address the characters of GB dislocations, or namely, GB disconnections [11–16]. Both experiments and molecular dynamics (MD) simulations have also indicated that the nucleation and propagation of GB disconnection dipoles for symmetric tilt GBs can be considered as the elementary migration mechanism under shear [11,12,16]. The intragranular shear is believed to play an important role on GB migration. In particular, the migration of most symmetric GBs has been found to be coupled with grain displacement or sliding parallel to the GB plane [13–15], perhaps also aided by GB disconnections.

To illustrate how GB migrates and to measure the GB mobility, the GB migration energy barrier (MEB) has to be included as an essential physical quantity according to Eq. (1). In this paper, we aimed to obtain MEBs via DFT calculations by taking two symmetric tilt GBs, i.e. Σ5 <001> (210) and Σ5 <001> (310) in bcc iron as examples. Meanwhile, effects due to the presence of point defects have also been examined by considering an interstitial atom (carbon) as well as a vacancy at the two GBs.

Our first-principles calculations are based on spin-polarized density function theory within Blöch's all-electron projector argument wave method (PAW) implemented in VASP [17–20]. The generalized gradient approximation of PBE is used to treat electron exchange and correlations [18]. Through the convergence test, energy cutoff is set to be 450 eV. Monkhorst–Pack method is used to set *k*-point mesh [21]. The equilibrium lattice parameter, bulk module and local magnetic moment for bcc Fe are determined to be 2.84 Å, 175.5 GPa and 2.16 μB at zero temperature and zero pressure conditions, respectively [22].

The (210) or (310) GB is created by putting in contact of two slabs of bcc lattice of identical size but as mirrored images with respect to the GB symmetry plane. Due to the restriction of periodic boundary conditions, two antiparallel GBs would be formed if atoms were filling up the supercell. When a vacuum layer is added to the supercell, a bicrystal configuration containing a single GB can be produced within the supercell (left panels in Fig. 1(a) and (b)). The upper and lower grains are built of 10 atomic layers on each side of the GB. The clean GB structure is relaxed until the force for each atom is less than 0.01 eV/Å. To relax the GB structures with an interstitial atom or a vacancy, the force convergence criterion has been set to 0.03 eV/Å. The Climbing Image Nudged Elastic Band (CINEB) method [23] is used to find the minimum energy paths (MEP) and transition states of the migration process.

The relaxed atomic configurations of Σ5(210) and Σ5(310) show similar GB structures as those in references [24–29]. The GB energy of Σ5(210) is 1515 mJ/m^2, merely ~54 mJ/m^2 or 3.6% higher than that of Σ5(310). As displayed in Figure 1(a) and (b), the two GBs show different combinations of GB units. The GB units across alternative (001) layers (denoted by black and white atoms, respectively) are of the same shape for the Σ5(310) GB. In contrast, the Σ5(210) GB is characterized by two GB units of different shapes, so the GB structure looks more complex.

The MEB of Σ5(310) is found to be 450 mJ/m^2 (γ_{310}), much larger than that of Σ5(210), $\gamma_{210} \sim 89$ mJ/m^2. Atomic configurations along the MEPs of the two GBs have been shown in Figure 1 (upper panels in both (a) and (b)). Obviously, the migration has been achieved by cooperative atomic-shuffling events involving several atoms, as characterized by shape changes of the corresponding GB units.

For Σ5(310) GB, the two identical GB units at neighboring (100) planes, each consisting of five atoms, evolve in the same fashion during the GB migration. As the GB plane moves downward, each GB unit tends to transform into a larger one involving six atoms such that an intermediate GB configuration can be formed, an unstable one corresponding to the saddle point state

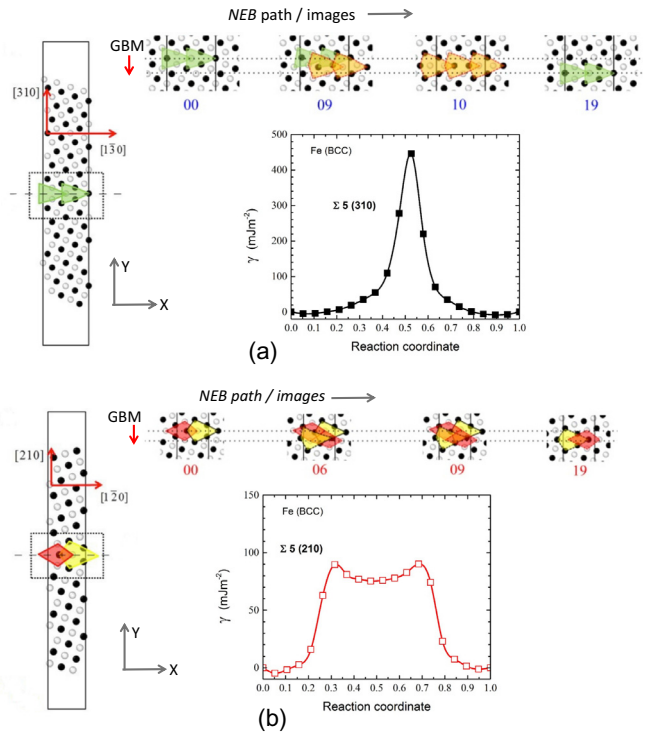

Figure 1. Relaxed configurations of Σ5(210) (a) and Σ5(310) GBs (b) containing 59 and 96 Fe atoms, respectively. The black and white circles distinguish atomic sites in two neighboring (001) planes. Form initial state to final state, 19 NEB images (states "00" to "18") are used to obtain the minimum energy paths (MEPs) for GB migration. Changes of GB structures are marked in transition-state configurations, based on that the stable structure of Σ5(210) GB is characterized by two different GB units, a "4-atom" unit and a "6-atom" unit; and the stable structure of Σ5(310) GB is characterized by two identical GB units, each consisting of 5 atoms.

(image 9). The 6-atom GB unit has to transform back into the 5-atom unit as approaching to the new position of the GB-plane. On the other hand, the Σ5(210) GB is characterized by a "4-atom" unit for one (001) plane and a "6-atom" unit for the other. As the GB plane moves downward to its final-state position, the two GB units evolve in their own fashion such that a metastable intermediate configuration (image 9) can be found. In addition, two unstable saddle-point configurations (images 6 and 13) show up, leading to a "camel-hump" energy profile.

The maximum atomic displacement involved from the initial state to the final state is found to be $\delta \sim 0.95$ Å for Σ5(210) and $\delta \sim 1.1$ Å for Σ5(310), so $\frac{b_p}{3} < \delta < \frac{b_p}{2}$ comparing to the Burgers vector of perfect lattice dislocation in bcc iron, $b_p = \frac{a_0}{2}\langle 111\rangle$ (a_0 = 2.84 Å). The in-plane translational displacement is 1.8 Å for Σ5(310) and 1.27 Å for Σ5(210) GB, from which the Burgers vector of the GB dislocation/disconnection can be determined to be $b = \frac{a_0}{10}[130]$ and $b = \frac{a_0}{10}[120]$, respectively. The migration distance (m) normal to the GB plane is 2.8 Å and 1.27 Å for Σ5(310) and Σ5(210), respectively. The coupling factor [13–15], i.e. $\beta = \frac{b}{m}$, turns out to be ~1.0 for Σ5(210) and ~0.64 for Σ5(310).

The stress-dependence of MEB is required according to Eq. (1). We repeated our NEB calculations by applying homogenous simple shear, to obtain the MEP under the corresponding shear stress, τ. The calculated γ vs τ data has been shown in Figure 2(a). For both GBs, the $\gamma - \tau$ relations are nonlinear and the γ values tend to decrease faster with increasing the shear stress. The MEB tends to vanish at $\tau \approx 5$ GPa for Σ5(310), a critical stress almost twice of that for Σ5(210). They can be fitted with polynomials for example up to the second order in a functional form $\gamma(\tau) = \gamma_\infty f(\tau)$,