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**ON THE RELATIONSHIP BETWEEN GRAIN-BOUNDARY  
MIGRATION AND GRAIN-BOUNDARY DIFFUSION BY  
MOLECULAR-DYNAMICS SIMULATION\***

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# On the Relationship between Grain-Boundary Migration and Grain-Boundary Diffusion by Molecular-Dynamics Simulation

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## Abstract

A molecular-dynamics method for the simulation of the intrinsic migration behavior of individual, *flat* grain boundaries is presented. A constant driving force for grain-boundary migration is generated by imposing an anisotropic elastic strain on a bicrystal such that the elastic-energy densities in its two halves are different. For the model case of the large-planar-unit-cell, high-angle (001) twist boundary in Cu we demonstrate that the drift velocity is proportional to the applied driving force, thus enabling determination of the boundary mobility. The activation energy for grain-boundary migration is found to be distinctly lower than that for grain-boundary self-diffusion. A *decrease* in the related activation energies with increasing temperature is shown to arise from a crossover in the underlying mechanisms, from solid-like at low temperatures to liquid-like at high-temperatures that is accompanied by an underlying grain-boundary structural transition.

## 1. Introduction

Grain-boundary (GB) migration is the fundamental mechanism involved in the processes of recrystallization and grain growth. In spite of the importance of these processes during microstructural evolution, the atomic-level mechanism(s) by which GBs move and how the structure of a given GB affects its mobility are still largely unknown [1]. This is not only due to the poorly understood high-temperature structure of GBs but also because experimentally GB migration is very difficult to investigate since (i) the GB mobility is so sensitively affected by minute amounts of impurities, (ii) experiments are typically limited to curved GBs and (iii) quantification of an often inhomogeneous and time-dependent driving force is intrinsically very difficult. [2,3] Extrinsic factors, such as GB pinning, surface drag and thermal grooving are known to play an important role as well. [4] For example, when the displacement of a GB during migration is observed on a surface, the GB motion usually appears jerky rather than continuous [5], an effect presumably caused by thermal grooving on the surface; such a jerky movement therefore probably does not represent the intrinsic mode of GB movement [6].

Phenomenologically grain-boundary migration resembles a continuous, viscous movement of a GB through a crystal under an applied driving force. According to reaction-rate theory, irrespective of the underlying mechanism the GB drift velocity,  $v$ , and the driving force,  $p$ , should be related linearly provided that  $p\Omega/kT \ll 1$  (where  $\Omega$  is the atomic volume,  $k$  is the Boltzmann constant and  $T$  the absolute temperature); i.e., [3,7,8]

$$v = mp \quad , \quad (1)$$

where  $m$  is the GB mobility. The latter depends, for example, on the GB geometry and structure, temperature and the concentration and chemistry of impurities at the GB.

A continuous, viscous movement requires that the GB be subject to a sustained driving force. If a GB segment of area  $A$  moves a distance  $d$  normal to the GB and thus lowers the overall Gibbs free energy of the system by  $\Delta G$  ( $<0$ ), then the driving force,  $p$  (defined to be positive), acting on the GB segment is

$$p = \frac{|\Delta G|}{\Delta V} = \frac{|\Delta G|}{Ad} \quad (2)$$

where  $\Delta V=Ad$  is the volume through which the GB segment has swept during such a migration step of length  $d$  [3]. (The definition in eqn. (2) demonstrates that the driving "force" is actually an energy-density difference, i.e., a force per unit area, or a pressure.)

Computer simulations are ideally suited for the study of impurity-free, individual GBs and to provide atomic-level information on the migration process that can then be compared with the related process of GB self-diffusion. Ideally one would like to simulate the migration behavior of a flat GB under the effect of a time-independent driving force, and hence with a well-characterized atomic structure and GB geometry. While simulations of the dynamical fluctuations of such a GB about its equilibrium position (i.e., in the absence of a driving force) can provide valuable insights into the atomic-level mechanism involved in GB motion [9], like the earlier simulations by Jhan and Bristowe [10] they provide no information on the *mobility* of the boundary. The key problem therefore consists in the development of a simulation method that permits application of a driving force to a *planar* GB; i.e., a boundary with no driving force due to its shape.

The basic idea of our method for the simulation of GB migration is to establish a difference between the Gibbs free-energy densities in the two halves of a given bicrystal by imposing anisotropic elastic strain on the system such that the elastic energies stored in the two grains are different. Such an energy-density difference gives rise to a net driving force for migration, resulting in the energetically favored grain to grow at the expense of the unfavored grain while lowering the overall energy of the system in the swept volume.

Our new simulation method [11] enables us to determine the activation energy for GB migration which can then be compared directly with that for self-diffusion in the same bicrystalline GB. Turnbull [8] and In der Schmitt et al. [12] have suggested that the two processes should involve essentially the same activation barriers for the movements of the atoms, although their jump distances may be somewhat different in the two processes. Following the discussion of our molecular-dynamics method for the study of GB migration, in this paper we hope to demonstrate for the case of a large-unit-cell, high-angle twist GB that the activation barriers for the diffusion jumps of GB atoms are significantly higher than those involved in the collective reshuffling of the atoms during GB migration; i.e., that GB migration and GB self-diffusion are distinct processes.

## 2. Elastic Driving Force for Grain-Boundary Migration

To quantify the elastic driving force to be used to induce GB migration, we define the elastic Gibbs free-energy densities,  $g_A$  and  $g_B$ , in the two grains labeled A and B (assuming that  $g_A > g_B$ ). After the GB has moved by some distance  $d$  into grain A, the Gibbs free energy has decreased by  $\Delta G = -(g_A - g_B)Ad$ , and according to eqn. (2) the driving force becomes

$$p = \frac{|\Delta G|}{Ad} = |g_A - g_B| \quad (3)$$

The concept of an elastic driving force works only for elastically anisotropic materials. In a cubic system, a measure of elastic anisotropy is given by

$$c_a = 2C_{44} - [C_{11} - C_{12}] \quad (4)$$

where the elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  are defined in the principal cubic axes, and Voigt's notation is implied.

As discussed in detail in our original paper [11], for (001) twist GBs the difference in the elastic energy densities stored in the lower and the upper grains is given by

$$p = \Delta E(\theta) = E^B - E^A = c_a \sin(2\theta) \varepsilon_{12} (\varepsilon_{22} - \varepsilon_{11}) , \quad (5)$$

where  $\theta$  is the twist angle. Notice that strains with a component in the direction of the GB normal (i.e.,  $\varepsilon_{13}$ ,  $\varepsilon_{23}$  and  $\varepsilon_{33}$ ) do not produce an elastic energy difference between the grains.

In practice, throughout our simulation we choose

$$\varepsilon_{11} = -\varepsilon_{22} = \pm \varepsilon/2 \text{ and } \varepsilon_{12} = \varepsilon ; \quad (6)$$

equation (5) then reduces to

$$p = \text{Sign}(\varepsilon_{22}) c_a \sin(2\theta) \varepsilon^2 . \quad (7)$$

It is worth noting that, to first order in  $\varepsilon$ , deformations satisfying eqn. (6) conserve the planar unit-cell area of the simulation cell and hence its volume. Because of  $\Delta E \sim \varepsilon^2$ , doubling  $\varepsilon$  will quadruple the driving force; similarly, switching the signs of  $\varepsilon_{11}$  and  $\varepsilon_{22}$  should reverse the direction of GB migration.

It is interesting to estimate the magnitude of the driving force for GB migration that can thus typically be imposed on a bicrystal containing the (001)  $\theta=43.60^\circ$  ( $\Sigma 29$ ) twist GB (see Sec. 3) studied in this paper. For the interatomic potential representing Cu that will be used in our simulations (see Sec. 3),  $c_a=1.239 \times 10^{12}$  dyne/cm<sup>2</sup> at T=0K and  $0.572 \times 10^{12}$  dyne/cm<sup>2</sup> at T=1000K, respectively ( $10^{12}$  dyne/cm<sup>2</sup> = 0.1 TPa). With  $\sin(2\theta) \approx 1$ , a strain of 1% ( $\varepsilon=0.01$ ) gives values for  $\Delta E$  of  $1.239 \times 10^8$  and  $0.572 \times 10^8$  dyne/cm<sup>2</sup> at T=0K and T=1000K, respectively; i.e., at the high end of the experimentally achievable range [3].

### 3. Simulation Method

The molecular-dynamics (MD) method used throughout was described in detail in Ref. [11]. Because the potential function has been used widely for GB simulations [13], we adopt the Lennard-Jones (LJ) potential, with parameters  $\varepsilon=0.167$ eV and  $\sigma=2.3151$ \AA, obtained from a fit to the zero-temperature lattice parameter and approximate melting point of bulk copper. To avoid discontinuities in the energy and forces, the potential and its first derivative are shifted smoothly to zero at the cut-off radius,  $R_c=1.49a_0$ . For this particular parameterization and cut-off procedure, the zero-temperature lattice parameter is  $a_0=3.616$ \AA and the melting temperature  $T_m \approx 1200$ K.

The (001)  $\theta=43.60^\circ$  ( $\Sigma 29$ ) twist boundary chosen for this study, generated by a twist rotation by  $\theta=43.60^\circ$  about the [100] axis, has a square planar unit cell with an area that is  $\Sigma=29$  times larger than that of the related primitive planar unit cell of perfect-crystal (001) planes; it hence contains 29 atoms per plane in the primitive planar CSL unit cell. This particular GB is well-suited for this study for a number of reasons. First, it has a relatively large planar unit cell, thus representing what we consider a "representative" *high-angle* grain boundary. Second, with an interplanar spacing of  $d(001)=0.5a$ , the (001) lattice planes are widely separated, thus permitting a clear distinction between the in-plane and out-of-plane movements of the atoms. Third, two previous simulation studies of this GB, with [10] and without application of a driving force [9], have shown it to be quite mobile at elevated temperatures; these studies also have provided insight into its migration mechanism. Finally, according to eqn. (5) a twist angle near  $45^\circ$  maximizes the driving force.

Throughout, 3d periodic border conditions are imposed on the simulation cell which therefore contains *two* identical GBs, however with opposite rotational sense (labeled GB<sub>1</sub> and GB<sub>2</sub> in Fig. 1). Under the influence of the driving force acting on them they will move towards each other until they annihilate, leaving behind a perfect crystal. To ensure that the GBs do not strongly interact with one another throughout most of the simulation, the number of (001) planes was chosen to differ in grains 1 and 2 (see Fig. 1). Since the simulation cell will be strained such that grain 2 grows at the expense of grain 1, 60 (001) planes are assigned to grain 1 and 24 to grain 2; the

simulation cell then contains a total of 84 planes, or  $84 \times 29 = 2436$  atoms. With this arrangement, even after 20 migration steps of each GB, the two boundaries are still 20 (001) planes apart.

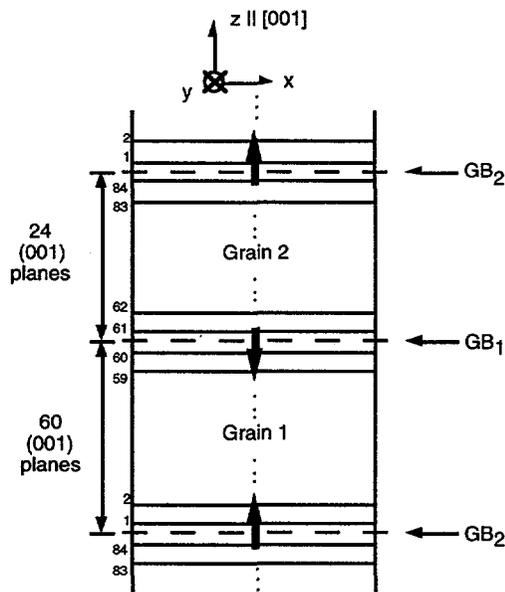


Figure 1. 3d periodic simulation cell. Under the imposed driving force, the two GBs move in the directions indicated by the arrows. Initially, 60 (001) planes form grain 1; 24 planes form grain 2.

#### 4. Simulation Results

Our results focus on three key aspects. First we show that the GB, indeed, migrates under the effect of an elastic strain of reasonable magnitude and that a GB drift velocity can reliably be extracted. Second, we establish the existence of a linear relationship between the magnitude of the applied driving force and the observed drift velocity; according to eqn. (1) this yields the absolute value of the mobility,  $m$ , of an individual, flat GB at a given temperature. Third, the temperature dependence of the mobility is shown to exhibit Arrhenius behavior; however the related activation energy is found to be significantly lower than that for GB self-diffusion.

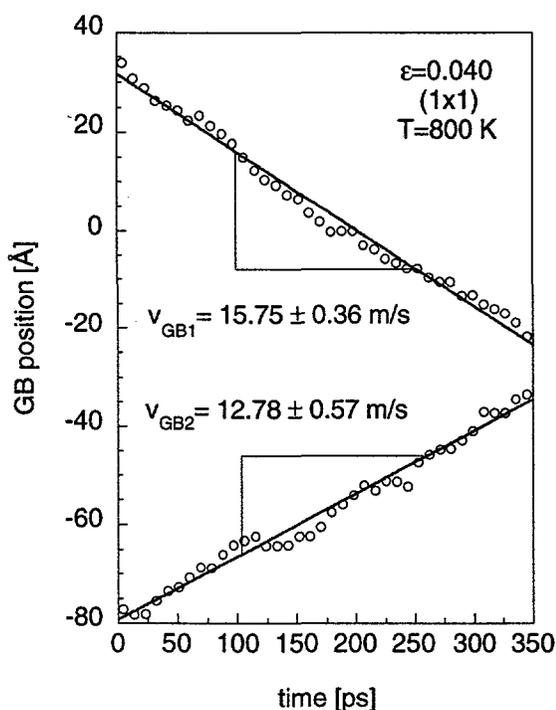


Fig. 2. Average positions of  $GB_1$  and  $GB_2$  versus time at  $T=800K$  and  $\epsilon=0.04$ .

That the two GBs in the simulation cell in Fig. 1, indeed, move under the effect of an elastic driving force and that a GB drift velocity  $v_{GB}$  can be extracted is illustrated in Fig. 2 for a (relatively large [11]) strain of  $\epsilon=0.04$  at  $T=800K$  ( $\sim 2/3 T_m$ ). The figure shows the average  $z$ -positions of the two GBs versus time in the simulation cell containing 84 (001) planes (see also Fig. 1). The two boundaries move towards each other and, after 350ps, are close to annihilating one another. According to the figure, the displacement-time behavior of both GBs can clearly be described by a straight line, giving constant GB drift velocities of  $12.78 \pm 0.57$  m/s and  $15.75 \pm 0.36$  m/s (the average velocity being  $v_{GB} \approx 14.3 \pm 2.1$  m/s).

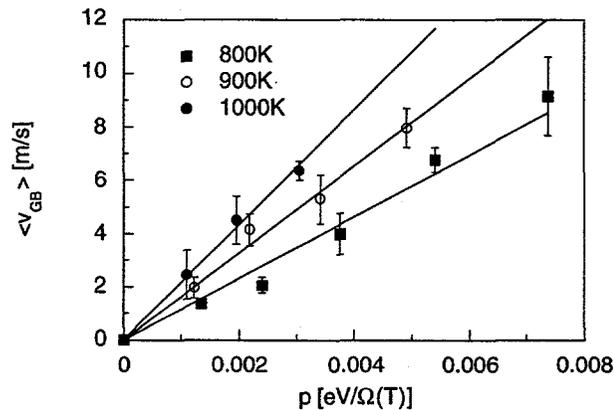


Figure 3. Average GB velocity at 800K, 900K and 1000K versus elastic driving force.

The example shown in Fig. 3 demonstrates that the GB drift velocities thus obtained are reasonable well proportional to the elastic driving force at all temperatures (solid lines) [11]. According to eqn. (1) the slopes of the straight lines yield the mobility,  $m$ , of the GB. This important result represents the foundation of our MD method for the simulation of GB migration.

For a comparison of computed mobilities,  $m$ , with experiments, it is sometimes convenient to consider the *reduced* mobility,  $\mu = m\gamma$ , where  $\gamma$  is the GB energy which in the case of the  $\Sigma=29$  twist GB is  $0.708$  J/m<sup>2</sup> at  $T=0K$  for the LJ potential [14]. The value of  $\mu$  thus obtained, for example, at  $T=800K$  ( $\sim 2/3 T_m$ ) is  $m=9.269 \pm 0.309 \times 10^{-8}$  m<sup>4</sup>/Js, giving  $\mu=6.568 \pm 0.22 \times 10^{-8}$  m<sup>2</sup>/s.

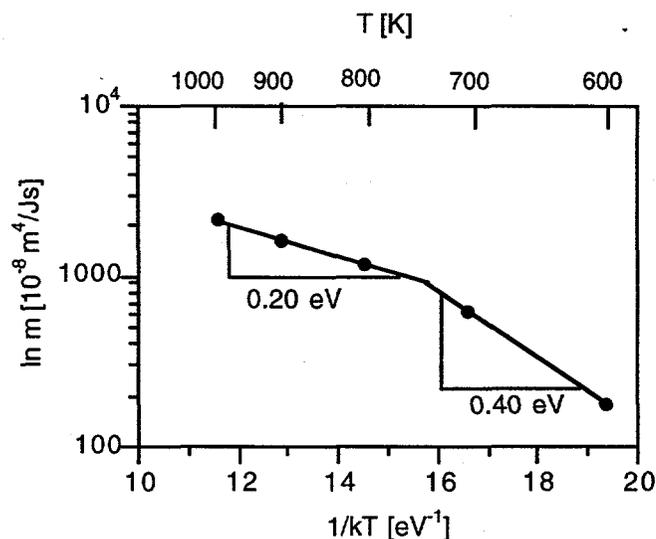


Figure 4. Arrhenius plot of the mobility,  $m$  (in units of  $10^{-8}$  m<sup>4</sup>/Js) for the (001)  $\theta=43.60^\circ$  ( $\Sigma=29$ ) twist GB. The error bars in the data are smaller than the symbol size.

According to Fig. 3, the mobility increases sharply with increasing temperature. If GB migration is a thermally activated process,  $m$  should obey the Arrhenius expression

$$m = m_0 \exp(-Q/kT) \quad , \quad (8)$$

where  $Q$  is the activation energy for the migration process. The related Arrhenius plot in Fig. 4 demonstrates that the mobility is, indeed, thermally activated. However, at  $T \sim 750\text{K}$  the activation energy decreases suddenly, from a low-temperature value of  $\sim 0.40\text{eV}$  to a high-temperature value of only  $\sim 0.2\text{eV}$ .

### 5. Relationship between GB Diffusion and GB Migration

To investigate self-diffusion in the (001)  $\Sigma 29$  twist GB, simulations were performed for the unstrained system (i.e., in the absence of GB migration). Because of the relatively small mobility of atoms in the perfect-crystal regions surrounding the GB, the total measured mean-square-displacement (MSD) is dominated by the in-plane ( $x$ - $y$ ) motions of the GB atoms. In analogy to the Gibbsian excess energy of the GB, the MSD per unit GB area,  $(\langle(\Delta x)^2\rangle + \langle(\Delta y)^2\rangle)/A$ , represents the integrated, Gibbsian excess MSD of the GB, which is related to the GB self-diffusion constant,  $D^{\text{GB}}$ , via the expression

$$\langle(\Delta x)^2\rangle + \langle(\Delta y)^2\rangle / N_{\text{GB}} = 4 t D^{\text{GB}} \quad . \quad (9)$$

For a GB of width  $\delta$  with a planar unit-cell area,  $A$ , the number of GB atoms,  $N_{\text{GB}}$ , may be written as  $N_{\text{GB}} = A\delta / \Omega$ . Inserting into eqn. (9) yields

$$\delta D^{\text{GB}} = \frac{\langle(\Delta x)^2\rangle + \langle(\Delta y)^2\rangle}{A} \frac{\Omega}{4 t} \quad , \quad (10)$$

which has the dimensions of (length)<sup>3</sup>/time. As is well known,  $\delta$  is the effective "diffusion width" probed during GB diffusion; although  $\delta$  is of similar magnitude as the "structural width" of the GB, the two need not necessarily be identical. (For a detailed discussion of this distinction, see [16].)

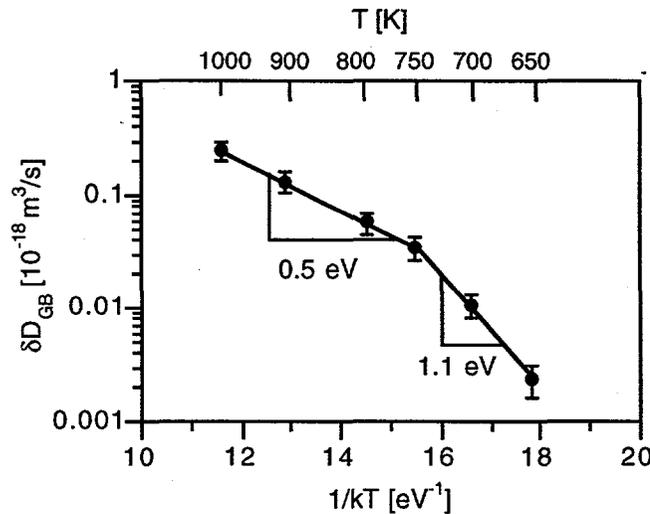


Figure 5. Arrhenius plot of  $\delta D^{\text{GB}}$  (see eqn. (10)).

The linear dependence of the excess GB MSDs with time observed for all simulation temperatures [11] yields the Arrhenius plot shown in Fig. 5. Interestingly, like the Arrhenius plot for GB migration, Fig. 5 reveals a crossover, at  $T \sim 750\text{K}$ , from a low-temperature to a high-

temperature diffusion process. However, the activation energies for GB self-diffusion are more than twice as large as those for GB migration (Fig. 4), suggesting that GB migration and diffusion are distinct processes, contrary to the suggestions of Turnbull [8] and In der Schmitt et al. [12].

To gain a perspective on the magnitudes of these activation energies, we have used zero-temperature lattice-statics relaxation to determine the activation energy for self-diffusion via mono-vacancies in the perfect crystal. Although the vacancy formation and migration energies of  $E_{1V}^f = 1.03\text{eV}$  and  $E_{1V}^m = 0.88\text{eV}$  thus obtained differ by about 20% from the experimental values of  $E_{1V}^f = 1.29\text{eV}$  and  $E_{1V}^m = 0.72\text{eV}$  for Cu [15], the resulting total activation energy of  $E_{SD} = 1.91\text{eV}$  is rather close to the experimental value of  $E_{SD} = 2.01\text{eV}$ . [15] We have also performed constant-pressure molecular-dynamics simulations to determine the self-diffusion constant in the melt in the range of 1300 - 1000K (with the lower temperatures representing the supercooled liquid); these simulations yield an activation energy of 0.39eV [11], close to the experimental value of 0.42eV [17], but different from any of the above activation energies at temperatures close to the melting point.

## 6. Discussion

Intriguingly, both GB migration (Fig. 4) and GB diffusion (Fig. 5) exhibit a crossover from a low-temperature to a high-temperature process at about  $T \sim 750\text{K}$  (or  $\sim 0.62 T_m$ ). This type of behavior has been observed experimentally in a variety of situations during the past three decades, and not only in connection with GB *migration* and GB *diffusion* but also GB *sliding*. For example:

(a) GB migration experiments of Aust on general boundaries in Pb [18] and of Demianczuk and Aust on a  $\langle 100 \rangle 37^\circ$  tilt GB in Al [19] revealed a crossover at about  $0.8 T_m$  similar to that in Fig. 4. Similar experiments of Gleiter in Pb [20] also showed a pronounced decrease in the activation energy at elevated temperatures; this behavior was attributed to a structural transformation in the GB core, and is supported by a discontinuity in the GB free energy at the same temperature [20].

(b) Similar to Fig. 5, recent self- and impurity-diffusion experiments on Cu  $\langle 001 \rangle$  tilt GBs near the  $\Sigma 5$  ( $36.87^\circ$ ) misorientation [21] revealed a crossover between a strongly misorientation dependent low-temperature regime with a high activation energy and a high-temperature regime with a misorientation-*independent*,  $\sim 60\%$  lower activation energy. This transition was interpreted as a structural transition in the GB region from an ordered low-temperature GB structure to a disordered high-temperature structure with atom jump vectors in random directions.

(c) GB sliding experiments by Watanabe et al. on various tilt bicrystals of Zn [22] revealed the existence of a transition temperature,  $T_c \sim 0.7-0.9 T_m$ , above which the activation energy for sliding was significantly lowered from its value below  $T_c$ ; the value of  $T_c$  was found to depend on the GB misorientation. Similarly, sliding experiments of Lagarde and Biscondi on high-angle Cu tilt bicrystals [23] exhibited a sharp decrease (by  $\sim 75\%$ ) in the activation energy for GB sliding for  $T > \sim 0.4 T_m$  which was again interpreted as a GB structural transition.

To investigate the origin of this crossover, we have recently performed extensive simulations of GB diffusion for a variety of high- and intermediate-energy tilt and twist boundaries in Pd. [24] Remarkably, similar to our earlier study of Si GBs [25], at high temperatures all the high-energy boundaries were found to exhibit the same, rather low self-diffusion activation energy and an isotropic, liquid-like diffusion mechanism; i.e., a diffusion behavior that is independent of the boundary misorientation. By contrast, at lower temperatures the activation energy was found to be significantly higher and strongly dependent on the GB energy, with a solid-like diffusion mechanism that involves jump vectors in discrete lattice directions. These simulations [24] not only confirm that a GB structural transition, indeed, takes place in relatively high-energy GBs, but also that (i) the transition proceeds from a solid-like low-temperature to a liquid-like high-temperature structure and (ii) the transition temperature depends strongly on the GB energy. [24]

Consistent with our observation of a liquid-like *high-temperature* structure of the GB, Mott [7] had suggested that local disordering, or "melting" of small groups of atoms at the boundary, is necessary to enable atoms belonging to one grain to reshuffle collectively while aligning themselves with the other grain (see also the description of Mott's concept in Ref. [2]). The moving GB is

therefore viewed as consisting of small islands of alternate fit and misfit between the two crystals [2,7] as small groups of atoms belonging to one crystal "melt locally" and subsequently resolidify onto the other crystal [2,7]. According to Mott's theory the activation energy for migration,  $Q=nH_f$ , should be given by the latent heat of fusion,  $H_f$ , and by the average number of atoms,  $n$ , involved in this local reshuffling. [2,7]

To test this idea, we have used MD simulations to determine the internal energies of the solid and liquid through the melting transition. [11] These simulations revealed approximately linear, parallel curves for the internal energies vs.  $1/kT$  for the liquid and the crystal, giving a value of approximately 0.13eV/atom for  $H_f$  at  $T_m \approx 1200K$  (remarkably close to the experimental value of 0.135eV [26]); i.e., an energy that is, indeed, *lower* than the value of  $Q=0.20eV$  in the high-temperature regime in Fig. 4. This suggests that the migration of the (001)  $\Sigma 29$  GB, indeed, involves the collective reshuffling of the atoms during local melting and recrystallization. Given the ratio of  $n=Q/H_f \approx 1.5$ , one is tempted to conclude that the reshuffling during migration involves typically only 1-2 atoms at a time; i.e., the small "islands" of alternate fit and misfit between the two crystals are extremely small. In practice, the mechanism is probably more appropriately described by a size distribution for these islands, with  $n$  representing the average, albeit very small size. [9]

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