Atomic simulation of grain-boundary sliding and migration in copper

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In this study, we present a Monte Carlo investigation, based on the embedded atom method potential, of the $\Sigma 5$ grain-boundary (GB) sliding in copper at elevated temperature. Important aspect of this approach is the implementation of simulated annealing technique. We find a variety of sliding behaviors, including coupling to migration. While our previous results showed that elevated temperature in aluminum $\Sigma 5$ GB increases the rate of migration, we did not find a temperature dependency of interface migration in copper.

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Grain-boundary (GB) sliding and migration at elevated temperature plays an important role in the plastic flow for polycrystalline materials.[1,2] Despite the important role of grain boundaries in this process, our knowledge of how boundaries actually move at the microscopic level is limited. One approach that has provided atomic-level insight into GB in metals is computer simulation.[3] Simulation at atomic level in combination with Monte Carlo (MC) technique[4] enables one to investigate the role of temperature on migration process.[5] Although, the structure and energy of GB for a number of metals can be calculated by *ab initio* methods,[6,7] computational limitations still prevent such methods from being applied to atomic simulation at elevated temperature. Faster methods based on fitting parameters, such as the embedded atom method (EAM) (Ref. 8) are more suitable for this purpose. It has been shown for a number of fcc metals that the EAM technique gives excellent agreement with both *ab initio* and experimental results.[9]

In a recent paper,[10] we addressed the mechanism characterizing the sliding process at the $\Sigma 5$ tilt GB in aluminum. We also evaluated the effect of elevated temperature on GB migration rate. For this we carried out MC simulations using EAM potential constructed by Mishin *et al.*[11] We find that simulated annealing based on MC technique allows the system to gradually anneal to a global-minimum configuration, thus increasing the number of migrations and reducing the GB sliding energy barrier to about factor of 3 compared to the corresponding zero temperature values. We now contrast these results with the study of the microscopic processes that occur during the sliding of copper grains. Copper was chosen here because it is a good candidate for heat sink in the design of ITER plasma facing components.[12] The main function of the heat sink is to transport elevated heat fluxes to the cooling water, thus reducing thermal stress in the structural material. However, high heat loading might invoke mechanical or structural changes in sink material. The goal of the present work is to investigate the thermal effect on polycrystalline copper. In order to achieve this, we have studied the structure and sliding energy of a $\Sigma 5$ [001] (210) tilt perfect GB in copper at elevated temperature. The tilt GB was constructed by bringing together the [001] faces of two crystals, one of which was rotated with respect to the other by 53.13°. The computation supercell consists of 40 (210) atomic layers, corresponding to a separation of 16.49 Å between the two GB planes. There are two atomic planes along the [001] direction. Two-dimensional lattice constant is set to the experimental value of 3.62 Å.[13]

The atomic interaction in copper is described by a semiempirical many-body potential of the EAM. Potential used in this work was developed recently by Mishin *et al.*[14] on a large set of experimental and *ab initio* database. The grain-boundary energy, as an important thermodynamics parameter, is calculated from the difference of the energy of a supercell containing the GB and the energy of a supercell containing an equal number of atoms in the bulk. Simulated annealing (SA) technique[15,16] is used in determining the equilibrium positions of atoms in a supercell. The initial temperature in our simulation was set to 540 K and the system was cooled to 27 K using a stepwise-exponential decrease of temperature involving a total 350×10^3 steps. For a fixed temperature T, the atomic positions were changed using the standard Metropolis technique.[17] Note that the amplitude of the atomic displacements is allowed to vary so that the acceptance rate remains about 0.5 during MC simulations. These amplitudes are typically from 0.01 Å ($T=540$ K) to 0.002 Å ($T=27$ K). In Fig. 1 we show the relaxed supercell of 160 atoms employed in the calculation viewed along the [001] direction. The extrapolated zero-temperature GB energy is 0.946 J/m^2. The accuracy of the least-squares fit of the extrapolated zero-temperature GB energy is 7.32×10^{-3} J/m^2.

The grain-boundary sliding (GBS) is simulated quasistatically, namely the top grain is rigidly shifted over the botom by a series of small specified distances along the interface. The started atomic configuration for each anneal was taken from the previous one. In order to investigate the effect of temperature on the GBS process we have carried out another MC simulation. In this, which we will refer to as ''static,'' the probability of acceptance of any higher-energy configuration is set equal to zero, thus driving the system at zero temperature.

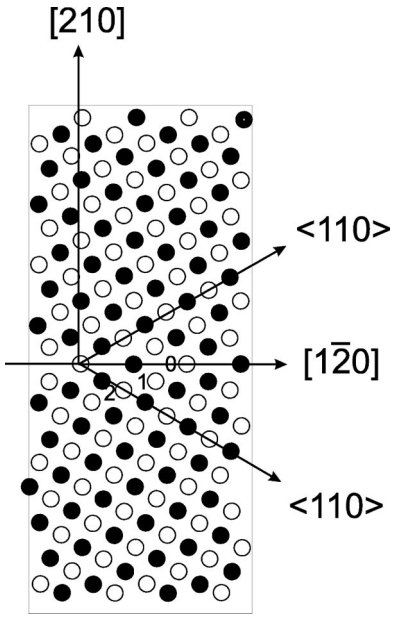

FIG. 1. Relaxed geometry of 160 atoms supercell for the $\Sigma 5$ tilt GB in copper viewed along the [001] direction. Atoms located in different planes perpendicular to the $\langle 110 \rangle$ direction are shown with filled and open circles.

Figure 2(a) shows the variation of the relative GB energy during the sliding of the $\Sigma 5$ Cu tilt GB. The sliding distance is described in percentage a_{CSL} (lattice parameter of the CSL cell along $[1\bar{2}0]$ direction). We plot the energy profiles for both the ''static'' (circles) and SA (triangles) calculations. For both cases, the profile is smooth, exibiting energy peaks and valleys between them, with the latter being associated with the GB migration. The migration rate of GB is independent of annealing temperature. Note that the SA approach reduces the sliding energy barrier by about a factor of 2 compared to the zero temperature (''static'') simulation. The first migration occurs when the shear displacement is about 15% a_{CSL}. This contrasts with our previous results for $\Sigma 5$ Al tilt boundary, where we found that the migration rate depends on temperature [see Fig. 2(b)]. For example, the first migration occur when the shear diplacement is about 40% a_{CSL} in the ''static'' calculation. On the other hand, SA calculation gives the first migration when the shear is about 20% a_{CSL}.

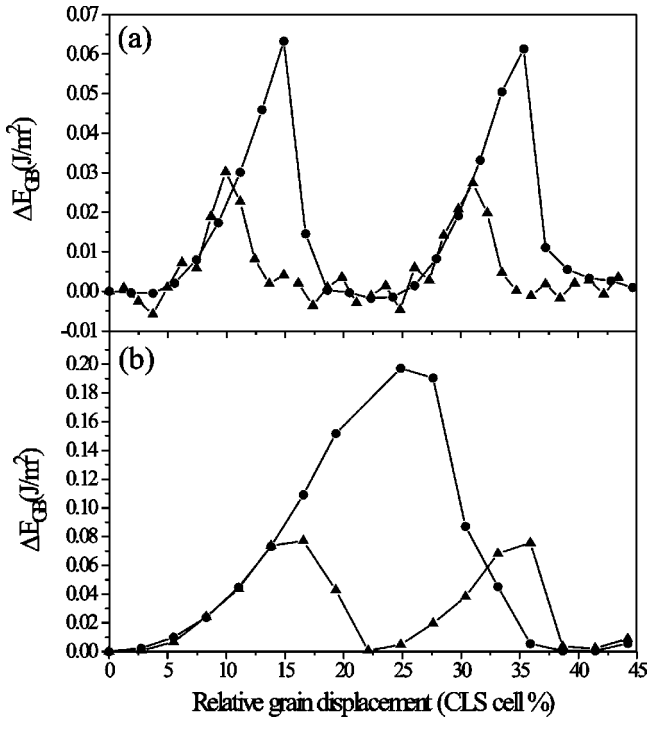

FIG. 2. The variation of the relative GB energy during the sliding of the $\Sigma 5$ tilt GB in copper (a) and aluminium (b). The sliding distance is described in percentage a_{CSL}, of the CSL cell along $[1\bar{2}0]$ direction. The circles and triangles correspond to the ''static'' and the SA simulation, respectively.

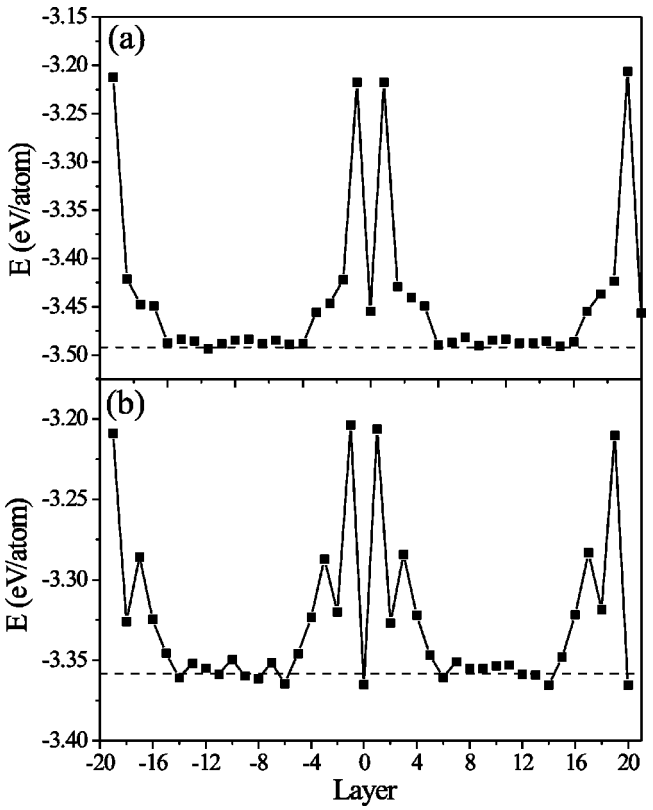

FIG. 3. Energy profile of the GB atoms as a function of the layer away from the interface for copper (a) and aluminium (b). Dashed line denotes the cohesive energy of bulk.

To shed light on the related physical process, we next examine the energy associated with atoms on different layers. Note, that calculations of the energy of an individual atom make sense in the EAM scheme (or other glue model potential) and in total energy calculations cannot be defined correctly. In Fig. 3 we show the energy profile of the grain-boundary atoms as a function of the layer away from the interface for copper (a) and aluminum (b). Both profiles indicate that GB as a plane defect affects atoms localized within a few layers from the interface. The striking feature of the energy profile is the energy penalty for the aluminum atom at the third layer [see Fig. 3(b)]. The atom 2 (see Fig. 1), that controls the GB migration (for more details see Ref.

10), is positioned at an energy minimum. Therefore, in the ''static'' calculations, atom 2 is pinned during the sliding. The atomic configuration coresponding to this process is associated with an energetic barrier and represents the worst configuration of the GB structure. This demonstrates great hindering effect of the atom 2 on the interface mobility. In copper, atoms interacting across the interface experience higher electron density than in aluminum. This, in fact, pushes up the energy of atoms positioned at the second layer and forms monotonic decrease in energy associated with atoms as a function of distance from the GB plane. When comparing the GBS process in copper with that in aluminum, atom 2 is able to relax into the upper grain even at zero temperature. Thus, the effect of thermally independent GB migration in copper can be ascribed to the different energy profiles across the interface in copper and aluminum.

In summary, MC calculations are used in conjunction with EAM interatomic potential to study the sliding and migration of $\Sigma 5$ tilt GB in copper at both elevated and zero temperature. It has been found that the SA approach reduces the GB sliding energy barrier by about a factor of 2 but interface mobility is not sensitive to the annealing temperature. This contrasts with our previous results for aluminum, where we found that the annealing temperature plays an important role in the GB mobility. As has been shown, it is the hindering effect of an atom placed in the second layer from the interface in aluminum for the coupling of annealing temperature and GB migration. Hence, the difference on the energy profile across the interface in copper and aluminum is crucial to thermal effects on GB migration rate.

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