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Separating grain boundary migration mechanisms in molecular dynamics simulations

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ABSTRACT

In molecular dynamics (MD) simulations of grain boundary (GB) migration it is quite common to find a temperature dependence of GB mobility that deviates strongly from an Arrhenius-type dependence. This usually indicates that more than one mechanism is actually active. With the goal to separate different GB migration mechanisms we investigate a Σ7 <111> 38.2° GB by MD using an EAM potential for aluminium. To drive the GB with a well-known and adjustable force, the energy conserving orientational driving force (ECO DF) is used that had been introduced recently. The magnitude of the DF and the temperature are varied. This yielded a high and a low temperature range for the GB velocity, with a transition temperature that depends on the magnitude of the DF. A method is introduced which allows both a visual and a statistical characterization of GB motion on a per atom basis. These analyses reveal that two mechanisms are active in this GB, a shuffling mechanism and its initiation. These mechanisms operate in a sequential, coupled manner. Based on this, a simple model is introduced that describes all simulated GB velocities (and hence the mobility) very well, including the transition between the dominating mechanisms.

1. Introduction

Experimental studies on grain boundaries (GBs) usually find an Arrhenius type dependency of GB mobility on temperature [1], as suggested by theory [2,3]. Many Molecular Dynamics (MD) simulations of GB motion in metal crystals often suggest otherwise, though. For different GBs many different thermal dependencies of mobility have been reported [4,5]. The latter study investigated a huge range of different coincidence site lattice GBs in nickel with respect to GB plane and misorientation angle. It was found that a large fraction of the simulated 388 GBs did in fact show strong deviations from an Arrhenius type temperature dependence. One common result of many simulations across different elements as well as different types of MD potentials is that different types of motion can occur depending on temperature and the magnitude of the force that drives the GB. This is evidenced for instance by the existence of a critical temperature, the so called roughening temperature [6]. Above the roughening temperature the GBs always show a continuous motion and a linear dependency of the GB velocity on the magnitude of the applied driving force. Below this critical temperature the type of GB motion depends on the magnitude of the applied driving force. With high forces a continuous/linear GB motion can be enforced [6,7], but for lower forces the GBs show jerky motion. In this case a distinct jump of the whole GB over a specific distance (several atomic layers) can be clearly separated from the waiting times between the individual jumps. It is not known if such a transition between different types of motion actually occurs in reality as the time scales accessible in simulations are many orders of magnitude smaller than the experimental ones: on the experimental time scale the jerky motion occurring in MD simulations would appear entirely smooth. However, it is important to fully understand this transition in order to be able to extrapolate findings from MD simulations to results relevant for reality. Therefore the present paper aims to derive a coherent way to describe the GB velocity as a function of temperature and driving force across this transition. This may help in future to derive mechanism maps as introduced by Zhou [8] and Deng and Schuh [9] which may, in general, describe several such transitions in the parameter space of temperature and DF magnitude.

2. Simulation setup

For our simulations we use the MD software LAMMPS [10]. The

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setup consists of a simulation box with periodic boundary conditions in all directions, containing 6048 aluminium atoms as described by the EAM potential developed by Zope and Mishin [11]. As suggested earlier [8,12], the atoms are arranged to form two fcc single crystals which are tilted by ±19.1° around the <111> axis. This creates two symmetric Σ7 <111> 38.2° coincidence site lattice GBs, one at the centre and another equivalent one on a border of the fully periodic simulation box. Fig. 1 illustrates the geometry of the simulation cell after a short simulation, so that both GBs are directly visible within the box.

The setup potentially restricts the GB motion because a potential coupling effect is suppressed for reasons of symmetry [8]. The two GBs in the simulation box have opposite signs in respect of the coupling effect, in the sense that they try to enforce opposite grain translation as they move towards each other. Recent experimental studies had observed that Σ7 <111> 38.2° GBs show no indication of a coupling effect in aluminium [13]. However, the same may not be true for computer simulations using synthetic interatomic interactions [8,14]. In fact, Zhou showed [8] that the coupling effect can be so strong in simulations at low temperatures that an enforcement of GB motion by an excessively high DF can actually lead to plastic deformation in one of the grains when the coupling effect is suppressed by the boundary conditions. In grain growth or recrystallization of polycrystals, the coupling effect will in general be suppressed because grain translation would have to cause geometrical incompatibilities (gaps, overlaps). Hence, we consider the chosen fully periodic boundary conditions as essential in order to simulate real-world GB mobilities.

At the beginning of each simulation the temperature is chosen by assigning a random velocity of suitable magnitude to all atoms. Subsequently the temperature is equilibrated to the desired value for 12 ps. Nose-Hoover thermostatting and barostatting are applied during each entire simulation. The investigated temperatures are in the range of 450–800 K in steps of 50 K, the pressure is zero. A time step of 1 fs was used.

After the initialization both GBs are driven by an applied synthetic driving force which tries to enlarge one grain on the expense of the other by adding a potential energy depending on the crystal orientation. For this the energy conserving orientational (ECO) force was used with the parameters $R_c = 4$Å and $\eta = 0.25$ [15]. Unlike earlier implementations of driving forces, the ECO force allows to use the added potential energy directly as the thermodynamic driving force, and it avoids potential artefacts caused by the lack of energy conservation inherent with earlier DF versions (see Ref. [15]).

Since it was found in previous simulations that GB velocity is not necessarily proportional to the applied DF [8,12,16], we also perform each simulation for four different DF magnitudes from $p = 2$ meV/Ω to 8 meV/Ω, where Ω denotes the atomic volume.

Furthermore, all simulations were performed for 12 different random velocity initializations to allow for a statistical variation between simulation runs to estimate the simulation error. In total this results in 384 simulations for the same GB geometry, in a wide temperature and DF range. All simulated velocities are displayed in Fig. 2. Note that due to the random nature of individual motion events, for low temperatures and driving forces the simulated velocities span several orders of magnitude (Fig. 2(a)). This huge variation in velocity is caused by the time constraints imposed on the simulations. During the fixed maximal simulation time it may happen that only a very low number of GB jumps occur, which may be insufficient to calculate a statistically valid average. To retain only reliable data, average velocities below 0.03 m/s were removed from the subsequent evaluation. In Fig. 2(b) all remaining averaged velocities are plotted.

For later statistical analysis each atom position was saved every 100fs during the simulations. In addition, individual identifiers and the orientation parameter χ as defined in the ECO force [15] were saved as well. This allows a clear distinction between atoms belonging to one of the two grains ($\chi = +1$ or -1) or to the GB ($|\chi| < 1$) under the applied parameters. This is very useful in post processing, as used in the subsequent Sections 3 and 4.

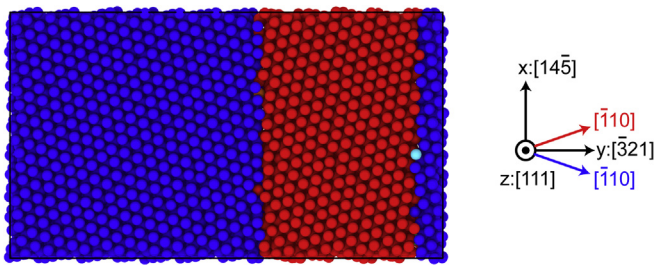

Fig. 1. Fully periodic simulation cell geometry with 6048 atoms after a short simulation at $T = 450$ K. The dimensions are for x: 52.62 Å, y: 93.11 Å, z: 21.10 Å. Red/blue atoms have an increased/lowered potential energy due to the applied driving force. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3. Visual simulation analysis

In general, a GB can be defined as a region between two grains in which the atoms have no unequivocal affiliation with either grain. The growth of one grain and the simultaneous shrinkage of the other one is the process responsible for GB motion. The atoms passing through the GB only have to rearrange themselves locally, traversing much lower distances than the GB itself. The GB moves with a certain velocity, but no mass is transported along its migration front.

However, it is not necessarily clear on which path the individual atoms traverse the GB during its motion. It has been shown that there is a clear minimal energy path for every atom in some cases [17], but this does not mean that every atom always takes the same path. Therefore in the present paper, we track each atomic motion and evaluate all motion in a statistical manner (subsequent section), without concern to which of the two GBs in our simulation box the atom belongs.

In practice, at least for high temperatures, it is a challenge to visualize individual motion mechanisms, even though every atom position is known at every time step. The difficulty arises because each atomic motion in a MD simulation consists of a migrational part and a thermal random part, which can't be distinguished easily. To separate these two atomic motion contributions, we first assume that all atom migration is happening when each atom is in the GB region. This is a valid assumption since no vacancies are included in the simulation, hence bulk diffusion should be very rare.

The orientation parameter χ allows to determine exactly which atoms have been passed by the GB. This is done by checking which atoms had an orientation of $\chi = +1.0$ in the beginning of the simulation (high energy state) and $\chi = -1.0$ at the end (low energy state); only these atoms are considered subsequently. For these, a time averaged position is calculated before and after the GB passed. The time averaging in the bulk removes most of the influence of thermal vibration on these start and end positions, and fluctuations inside the GB ($|\chi|<1$) are excluded entirely. After this filtering of interesting atoms and the almost complete removal of thermal vibration, the distance D between the start and end position is calculated for each atom. This value D is useful during visual representation of the GB migration (Fig. 3) as well as for statistical