Atomic-scale simulations of the interaction between a moving dislocation and a bcc/fcc phase boundary

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Abstract

In the past, molecular dynamics (MD) simulations have shown that grain boundaries are very strong obstacles to dislocation motion. Whereas such studies typically have been performed for boundaries between grains with the same crystal structure, in the present study the interaction of a moving edge dislocation and a boundary between a bcc (Fe) and an fcc (Cu) phase with almost identical lattice distances in the glide planes has been studied using MD. It is found that an edge dislocation can be transmitted from the bcc- into the fcc-regime, but not vice versa. This may be due to the splitting of the edge dislocation into Shockley partials inside the fcc region.

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1. Introduction

The plastic behaviour of polycrystalline materials can only be understood taking into account the interaction between dislocations and phase- or grain boundaries (GBs). Besides point defects, precipitates and other structural defects, GBs provide an important contribution to the strengthening of metallic materials. GBs are usually considered as...
obstacles to dislocation motion but also as sources of dislocations. Transmission of dislocations through interfaces and the macroscopic deformation of polycrystals are strongly correlated [1]. Therefore, the detailed study of interactions of dislocations with GBs using molecular dynamics (MD) simulations is very important for the quantitative understanding of the mechanical behaviour of materials. Such interactions including dislocation pile ups or Hall–Petch effects have been subject of various molecular dynamics (MD) simulations e.g. [2–4]. In these studies, the generation of dislocations at GBs as well as their blocking at GBs has been studied and visualized repeatedly and thoroughly. Investigations whether dislocations are able to penetrate a GB have yielded various answers, which depend on the crystal structure as well as on the type of the GB and of the dislocation. For instance, screw dislocations in fcc-Cu can be transmitted through a GB [5], whereas an edge dislocation in bcc-Fe is stopped at the GB [6]. Generally, up to now the interaction between dislocations and interfaces between grains with the same crystal structure has been studied [2–6], but not yet between unlike crystal structures.

2. Description of the model

For the present study, the interface between Fe and Cu has been chosen as a model case. One advantage of this model system is that the lattice plane distances of the typical preferred glide planes for edge dislocations in Fe and Cu differ only by 3%. The atomic structure of the simulation system used in the present work is represented in Fig. 1. It is a cuboidal aggregate of about 30,000 atoms. The model comprises two types of structures: In the left half it consists of bcc-Fe with crystal orientations [1 1 1], [1 1 0] and [−1 1 2] in the x-, y- and z-direction, respectively while in the right part it consists of fcc-Cu with crystal orientations [1 1 0], [1 1 1] and [−1 1 2] in x-, y- and z-direction, respectively. The preferred glide plane of an edge dislocation in the Fe part therefore is known to be the (1 1 0) plane. In the adjacent Cu part, this plane continues into the (1 1 1) plane, favoured glide plane in the fcc structure, rotated around z-axis by 30°.

The dimensions of the calculational cell in x-, y- and z-directions are 159 Å, 59 Å and 35.26 Å, respectively. According to the anisotropic elasticity theory a displacement field for a perfect edge dislocation is calculated and superimposed to the ideal atomic structure [7,8]. The model setup is subjected to shear loading applying the molecular dynamics program IMD [9,10] and employing Embedded-Atom-Method (EAM)-potentials for the Fe–Fe– [11], Cu–Cu– [12] and Fe–Cu– [13] interactions. Free boundary conditions are applied to the y-direction and periodic boundary conditions are applied to the z-direction, i.e. along the direction of the dislocation line. The atoms within the layers of the cut-off radius $R_{\text{cut}} = 5$ Å to the right and to the left of the specimen are constrained and their movement is prescribed in order to simulate an externally applied shear strain with a stepwise shear deformation of up to $\gamma = 0.4 \times 10^{-5}$. The rate of shear deformation is given by $8 \times 10^{-3}$ ps$^{-1}$.

![Fig. 1. The structural model, containing a $a/2[111](-110)$ edge dislocation, showing the definition of $\gamma$.](image)
3. Results and discussion

3.1. Splitting of an edge dislocation in Cu into two Shockley partials during relaxation of an fcc structure containing an edge dislocation

A Cu crystal with fcc structure was generated with the orientation, represented in Fig. 2a, with [110], [1−11] and [−112] orientations in x-, y- and z-directions correspondingly. Free boundary conditions were applied in the y-direction of the simulation cell, periodic boundary conditions in the x- and z-direction and then the structure was relaxed with the MD program. After relaxation, the MD algorithm yields a new geometrical configuration together with the potential energy and the stress tensor at the position of each atom.

In the present study, the positions of the dislocations are determined by selecting the most energetic atoms of the system; for Cu, e.g., the energy of an atom at the dislocation core is found to amount to −3.4 to −3.47 eV. In order to proof the validity of this detection algorithm, Burgers circuits around dislocations were also investigated for selected cases.

Using the described dislocation detection rule, Fig. 2b shows the evolution of an initially simple edge dislocation as introduced into the fcc model. The atoms at the core of the dislocations are depicted in dark grey. Terminating atom layers on

![Fig. 2. The structure of the fcc lattice of copper with an edge dislocation (a) and the patterns of the splitting of edge dislocation into two Shockley partials (b).](image)
the lateral surfaces of the specimen perpendicular to the $x$-direction of the simulation box [110] within the distance of cut-out radius are depicted with brighter colour.

Fig. 2b shows the splitting of the dislocation in fcc-copper with the aforementioned orientation into two Shockley partials after allowing the model to relax. According to Frank’s criterion [7] it is known that in fcc metals the elastic strain energy in a crystal is reduced by the dissociation of a perfect dislocation into partials.

After splitting of the dislocation into partials the Burgers vector $\frac{1}{2}[110]$ can be represented as a sum of two partials $\frac{1}{2}[110] = \frac{1}{6}[21 \bar{1}] + \frac{1}{6}[121]$. In Fig. 3 the projections of dislocations and Burgers vectors onto the (112) plane are shown before and after splitting as they were identified with the help of the same energy criterion of monitoring the core of the dislocation. The core of the perfect dislocation is marked by a triangle in the surrounding structure which is represented by regular dots.

After splitting, the partials move apart from each other and stop moving after reaching a distance of seven Burgers vectors. The distance $d$ observed in our simulations agrees quite well with the value, derived from [14, Eq. (1)].

\[
d = \frac{Gb^2}{4\pi\gamma}
\]

where $G$ is the shear modulus, $b$ is a Burgers vector and $\gamma$ is the dislocation line energy per unit length (tending to pull dislocations together).

Shown in Fig. 3b are the Burgers circuits around the two partials, both separately as well as together. From the definition of the Burgers vector for each case it can be seen, that the sum of Burgers vectors of the partials is equal to the Burgers vector of the initially generated dislocation.

Analogous calculations have been performed for the bcc-Fe specimen with an edge dislocation located in the center of the specimen. Contrary to the previous case of the fcc-copper specimen, the dislocation did not split into partials likewise it had been expected from theoretical knowledge about bcc structures [7].

3.2. The movement of an edge dislocation from Fe to Cu

Taking the aforementioned behaviour of the dislocation in Fe and Cu into account, the simulation of the movement of a dislocation under the influence of shear deformation for both cases from...
Fe to Cu and from Cu to Fe has been performed. The simulation cell has been generated consisting of two metals bcc-Fe and fcc-Cu with an edge dislocation in the center of Fe, as described in Section 3.1. The glide plane of the edge dislocation in Cu was the continuation of the glide plane of the edge dislocation in Fe, but rotated at an angle of 30° around the z-direction. We consider the inclination of the Cu-crystal because of two reasons: (i) we did not see any dislocation transmissing the interface when no inclination was applied and (ii) we wanted to study the influence of an crystal inclined with respect to Fe. This model specimen was subjected to shear loading in the computer which causes the movement of the dislocation towards the interface.

The simulation results of a moving dislocation from Fe to Cu are shown in Fig. 4. Represented in the figures are the atoms on the vertical surfaces of the simulation cell as well as atoms with the potential energy matching the energy of the dislocation core. The movement of the atoms on the vertical surfaces is constrained and obeys to the given prescribed shear loading conditions. Atoms belonging to the different structures are depicted by different colours (darker—for iron and

![Fig. 4. The patterns of a dislocation core moving from Fe to Cu at different instants of time under external shear loading, showing a stacking fault and partial dislocation moving in Cu.](image-url)
brighter—for copper). It can be seen from the figure that along with the atoms of the dislocation core, the atoms of the interface belonging to iron and to copper are depicted. These atoms were also selected because their potential energy lies in the same range as the energy for the core of the dislocation. This is due to the structural disorder at the GB, which changes during ongoing shear deformation.

As can be seen from Fig. 4, at approximately 4.8 ps the dislocation reaches the phase boundary and only after time step 16.5 ps it passes through it. The shear deformation of the specimen at the late stages of the simulation can be seen from the inclination of the lateral atoms in Fig. 4. At the time 16.5 ps the appearance of one Shockley partial dislocation was detected in Cu at the interface. Shown in Fig. 4 in medium dark colour is the stacking fault, which follows this partial. The detection of the stacking fault was performed by selection of atoms, having hexagonal closed-packed structure (hcp). As far as the Shockley partial dislocation moves ahead towards the lateral surface of the specimen, the region occupied by the stacking fault is enlarging. Thus, the second partial is still kept by the phase boundary, while the first one has already passed it.

The individual results from Fig. 4 are gathered in Fig. 5 showing the position of the dislocation line depending on the shear deformation $\gamma$. It is found that the first partial dislocation is kept at the interface for shear strains from $\gamma = 3\%$ to $13\%$.

3.3. The movement of an edge dislocation from Cu to Fe

The simulations have been repeated analogously to the case of the previous section, but with Cu and a dislocation at the left-hand side of the model and trying to transmit the dislocation to the right-hand side with the Fe. Monitoring the core position in the same way as before allows to determine the dislocation motion. Shown in Fig. 6 are the consecutive patterns of the dislocation core position at definite instants of time.

The same analysis to detect the dislocation position like in the previous section has been performed. The positions of the center (arithmetical average) of two partials in Fig. 6 are gathered in Fig. 7 showing the position of the dislocation line depending on the shear deformation $\gamma$.

As can be seen from the figure, the dislocation in Cu splits into two partials. Both of them are attracted by the phase boundary. However, the dislocation does not penetrate from copper to iron.

3.4. Temperature dependence of the dislocation moving from Fe towards Cu

In order to study the behaviour of the dislocation under the influence of different temperatures, the simulations with the same loading conditions have been performed using the IMD program [9] with constant volume, constant temperature ensemble of atoms, using a Nose–Hoover thermostat [9,10].

The simulations were performed for the temperatures 0 K and 300 K. The simulation shows an insignificant decreasing velocity of the dislocation with temperature increasing from 0 to 300 K (Fig. 8). This result is in agreement with MD calculations of other authors [15,16], who have also described increasing ‘friction’ of dislocation movement with increasing temperature. A smaller change of viscosity in Fe as compared to Cu might be the reason for this insignificant decrease in dislocation speed in Fe than in Cu.
4. Conclusions

The movement of edge dislocations passing through phase boundaries in the Fe/Cu system has been simulated by the molecular dynamics (MD) method using many-body Embedded Atom Method (EAM)-potentials. The position of the dislocation core was derived from the energy data of atoms selecting the atoms with elevated energies. This leads to the observation that a dislocation penetrates through the phase boundary in Fe–Cu direction. The glide plane (1–11) of the dislocation in Cu is inclined at an angle of 30° to the glide plane (1–10) of the edge dislocation in Fe. Edge dislocation dissociates into two partials in both cases—when moving from Fe to Cu and vice versa. When moving from Fe to Cu, the one partial penetrate to Cu, leaving the stacking fault behind it. When initially generated in Cu, the dislocation is split into two Shockley partials and they are absorbed by the phase boundary. The simulation data show an insignificant decreasing velocity of the edge dislocation with increasing temperature.

Fig. 6. Patterns of the dislocation core moving from Cu to Fe at different time steps under shear loading.
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References