Slip of shuffle screw dislocations through tilt grain boundaries in silicon

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\begin{abstract}
In this paper, molecular dynamics (MD) simulations of the interaction between tilt grain boundaries (GBs) and a shuffle screw dislocation in silicon are performed. Results show that dislocations transmit into the neighboring grain for all GBs in silicon. For \( \Sigma_3 \), \( \Sigma_9 \) and \( \Sigma_19 \) GBs, when a dislocation interacts with a heptagon site, it transmits the GB directly. In contrast, when interacting with a pentagon site, it first cross slips to a plane on the heptagon site and then transmits the GB. The energy barrier is also quantified using the climbing image nudged elastic band (CINEB) method. Results show that \( \Sigma_3 \) GB provides a barrier for dislocation at the same level of the Peierls barrier. For both \( \Sigma_9 \) and \( \Sigma_19 \) GBs, the barrier from the heptagon site is much larger than the pentagon sites. Since the energy barrier for crossing all the GBs at the heptagon sites is only slightly larger than the Peierls barrier, perfect screw dislocations cannot pile up against these GBs. Furthermore, the critical shear stress averaged over the whole sample for the transmission through the \( \Sigma_9 \) and \( \Sigma_19 \) GBs is almost twice on heptagon site for initially equilibrium dislocation comparing with dislocations moving at a constant velocity.
\end{abstract}

1. Introduction

Along with other applications, polycrystalline silicon has been widely used for photovoltaic solar cells. Tremendous efforts have been made to reduce the cost and improve the energy efficiency of polycrystalline Si photovoltaic cells [1,2] due to the vast demand for renewable solar power. The strength and ductility of polycrystalline silicon depend not only on the interaction and multiplication of dislocations, but also are determined by the interaction between dislocations and grain boundaries (GBs). However, many details of the dislocation-GB interactions in silicon are not fully understood. Experiments have shown that dislocations in silicon can either pile-up or transmit the GBs [3]. Atwater and Brown found that amorphous silicon nucleates heterogeneously at the GBs during the irradiation of polycrystalline Si thin films [4]. Using the in situ high-voltage electron microscopy, Ballin et al. observed that dislocation with a common Burgers vector 1/2[011] transmitted from one grain to the neighboring grain [5]. Chen et al. has investigated the interaction between shuffle dislocation loops with \( \Sigma_3 \), \( \Sigma_9 \) and \( \Sigma_19 \) GBs [6]. They found that \( \Sigma_3 \) GB exhibits significantly higher resistance to dislocation transmission than \( \Sigma_9 \) and \( \Sigma_19 \) GBs. However unlike the atomistic simulations for metals [7,8], non-periodic boundary condition along the dislocation line has been applied, which exhibits the free surface effect [6]. In order to isolate the free surface effect and the interactions between dislocations and GBs, periodic boundary condition is applied in this paper.

Also, the dislocation pile up against grain boundary was considered as a key contributors for the drastic reduction of the phase transformation pressure in materials under a large plastic shear [9,10]. It is important to find out whether screw dislocations can pile up against GBs in Si.

This paper aims to provide a fundamental understanding on the interaction between shuffle screw dislocation and (\( \Sigma_3 \), \( \Sigma_9 \) and \( \Sigma_19 \)) GBs. Our next paper would present results on interaction between 60° shuffle dislocations with GBs [11].

2. The computational set-up

Fig. 1 shows the computer models of bi-crystalline silicon, with \( \Sigma_3 \), \( \Sigma_9 \) and \( \Sigma_19 \) GBs in (a), (b) and (c), respectively. These are three most stable GBs among all (110) tilt GBs and make up more than 70% of all possible GBs [6,12,13]. As shown in Fig. 1(a–c), grain-I in all the three models have the same crystallographic orientation with xy plane on the (111) glide plane. Periodic boundary conditions were applied in \( x \) direction with a periodicity length, \( L_x \approx 4 \text{ nm} \). Lengths of \( L_y \) has been varied from 4 nm to 30 nm and results are independent of this length due to periodic boundary conditions. Along the other two directions, \( L_y = 60 \text{ nm} \) and \( L_z = 40 \text{ nm} \). Several layers of atoms at the two surfaces perpendicular to the y-direction are fixed. The model consists of

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GBs, the pentagon sites generate an energy barrier of \( \Sigma \) site, as shown \( \Sigma _{3} \), which is composed of continuous pentagon-heptagon defects as shown in Fig. 1 [12,6]. The perfect screw dislocation transmits the GB at the pentagon site. For a heptagon site, the GB acts as a low energy barrier for the dislocation motion (Fig. 3). For both \( \Sigma 9 \) and \( \Sigma 19 \) GBs, the pentagon sites generate an energy barrier of 1.9 eV/nm while the heptagon sites produce an energy barrier around 0.6 eV/nm. This explains why the screw dislocation always transmits the GB at the pentagon sites rather than the heptagon sites. Since the energy barrier is lower than the pentagon sites, it has another cross-slip in grain II to a plane with the lower critical shear stress and inclination angle [15]. This again demonstrates that the pentagon site imposes a higher energy barrier for the dislocation migration than the heptagon site does.

The climbing image nudged elastic band (CINEB) method was used to determine the energy barrier of the dislocation motion across a stress-free GB [22,23]. In the CINEB calculations, the dislocation was created by adding the screw dislocation displacement into the sample. It can be seen that the energy barrier imposes an almost the same energy barrier as the Peierls barrier for dislocation motion (Fig. 3). For both \( \Sigma 9 \) and \( \Sigma 19 \) GBs, the pentagon sites generate an energy barrier of 1.9 eV/nm while the heptagon sites produce an energy barrier around 0.6 eV/nm. This explains why the screw dislocation always transmits the GB at the pentagon sites rather than the heptagon sites. Since the energy barrier for crossing all the GBs at the heptagon sites is only slightly larger than the Peierls barrier for the dislocation motion in bulk, perfect screw dislocations cannot pile up against these GBs and cannot reduce phase boundaries in silicon

Fig. 2b presents the process of the interaction between a perfect screw dislocation with \( \Sigma 19 \) GB, which is composed of continuous pentagon-heptagon defects as shown in Fig. 1 [12,6]. The perfect screw dislocation can have two different interaction sites with \( \Sigma 19 \) GB, i.e., the pentagon site (designated \( p_1 \) site below) and the heptagon site (designated \( p_2 \)). When a dislocation interacts with \( \Sigma 19 \) GB at \( p_1 \) site as shown in the left side of Fig. 2b, the dislocation switches the glide plane to the (111) plane in the neighboring grain directly, which is similar to a cross-slip behavior. However, when the dislocation interacts with the \( p_2 \) site, as shown in the right side of Fig. 2b, the dislocation first moves into the neighboring grain on the \( p_2 \) site in grain I and then transmits the GB. This results show that the pentagon sites act as higher energy barrier for dislocation motion than the heptagon site does. This can also be seen in the process of an interaction process between perfect screw dislocations and \( \Sigma 9 \) GB shown in Fig. 2c since \( \Sigma 9 \) is also composed of continuous pentagon-heptagon GBs (Fig. 1). For the heptagon sites, the dislocation transmits the GB directly through a similar cross-slip behavior which is similar to that in \( \Sigma 19 \) GB. However, for a pentagon site, the dislocation first moves into the neighboring grain to a plane with 71.3° inclination angle as shown on the right side of Fig. 2c. Thereafter, due to the large critical shear stress, it has another cross-slip in grain II to a plane with the lower critical shear stress and inclination angle [15]. This again demonstrates that the pentagon site imposes a higher energy barrier for the dislocation migration than the heptagon site does.

Simulations were performed at a constant temperature of 300 K using Nosé-Hoover thermostat. Displacement corresponding to a constant shear strain (\( \epsilon_{appl} \)) is applied homogeneously to the external surface of the MD cell in the \( x-z \) shear plane. The atomic interactions are described by the Stillinger-Weber (SW) potential [17], which is capable to capture undissociated shuffle dislocations in silicon. The time step for all simulations is 1 fs. All simulations were conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [18].

3. The interaction between shuffle screw dislocations and grain boundaries in silicon

In this section, we present how perfect screw shuffle dislocations interact with different GBs. The trajectories of dislocations are tracked using the von-Mises shear strain in OVITO [19–21].

Fig. 2a shows how a shuffle screw dislocation transmits the \( \Sigma 3 \) GB directly. In our simulations, as long as the screw dislocation migrates in grain I, it can transmit the GB into grain II, which indicates that the \( \Sigma 3 \) GB also imposes no barrier for a screw dislocation motion. This is consistent with the screw dislocation behavior in bi-crystalline F.C.C. metallic materials [7]. In F.C.C. metals, the full screw dislocation dissociates into two partial dislocations. When the screw dislocations interact with twin boundaries in metal, the dissociated screw dislocations first cross into a full screw dislocation and then transmit the GB. During the transmission procedure, the constriction process imposes the main energy barrier [7]. However, in silicon, since the screw dislocation on the shuffle set is already a full dislocation, the constriction process is not needed, consequently, \( \Sigma 3 \) GB acts as a low energy barrier to shuffle dislocations in silicon.

Fig. 1. Computational models of bicrystalline silicon with (a) \( \Sigma 3 \), (b) \( \Sigma 9 \), and (c) \( \Sigma 19 \) grain boundaries.

~ 400,000 atoms. Additional computer models for large samples were also constructed and it was shown that the results observed in this paper did not change with the size. To create perfect screw dislocations, e.g., with the Burgers vector \( b = 1/2[110] \) [14], a constant ramped velocity \( v \) along \( x \) direction is applied on the several layers of atoms at the left boundary above and below the central glide plane and in opposite directions, as shown in Fig. 1(a) [7,8,15]. In all simulations, \( v = 0.001 \) nm/fs and the central glide plane is put between the shuffle set to generate a perfect screw dislocation. To study the effect of dislocation velocity of the GB resistance, shear stress was applied immediately after dislocation generation near the right side of the sample. Under prescribed shear stress, dislocation in silicon reaches a stationary velocity [16] before it reaches GB. This procedure was repeated with increasing shear strain until dislocation passes through GB. Alternatively, the static screw dislocation is inserted by applying the displacement field of a screw dislocation [15] near the GB, for example, near the heptagon defects in the first grain. The system is relaxed for 100 ps to get the stable dislocation structure. Then shear stress is gradually increased until the dislocation transmits into the neighboring grain.
transformation pressure during plastic deformations [9,10]. At the same time, all GBs produce 60° dislocation pile-up, which essentially reduces the transformation pressure from Si I to Si II under shear [24,25].

In addition, the velocity of a dislocation is also found to play an important role in the process of a dislocation-GB interaction. Here we found that the critical shear stress needed for dislocation transmission through the GB is different for moving and static dislocation. For static dislocation the critical shear stress averaged over sample is \( \tau_s = 5.3 \) GPa and for moving dislocation it is \( \tau_d = 2.9 \) GPa for \( \Sigma 9 \) GB and \( \tau_d = 5.4 \) GPa and \( \tau_d = 2.9 \) GPa for \( \Sigma 9 \) GB on heptagon defects. Here, the dislocation reaches a stationary speed \( v = 3065 \) m/s when it meets the GB under shear stress 2.9 GPa, which is far below the elastic wave speed in silicon [26]. Interestingly, \( \tau_d \) and \( \tau_s \) are almost the same for \( \Sigma 9 \) and \( \Sigma 19 \) GBs, which demonstrates that the energy barrier is determined by the local structure of the GB. Thus, the energy barrier is the same for heptagon sites in \( \Sigma 19 \) and \( \Sigma 9 \) GBs and it is independent of the misorientation angle of the GBs under stress-free state [15,7], which is similar to the screw dislocation behavior in F.C.C. metals.

4. Conclusions

In the paper, the interactions between tilt GBs and a shuffle screw dislocation in silicon are investigated using molecular dynamics. Results show that the dislocation transmits into the neighboring grain for all GBs. For \( \Sigma 3 \) GB, the dislocation goes through the GB directly. For \( \Sigma 9 \) and \( \Sigma 19 \) GBs, when the dislocation is on heptagon site, the dislocation transmits the GB directly as well. However, when the dislocation is on the pentagon site, it first cross slips to a plane on the heptagon site and then transmits the GB. The energy barrier was calculated using the
GBs at the heptagon and dislocations, the barrier for dislocation transmission of heptagon sites is for pentagon defects. Furthermore, we found that the critical shear stress for the transmission is lowered from $1.9 \text{ ev/n}$ to $1.6 \text{ ev/n}$ for pentagon GBs in silicon under stress-free state. For comparison, energy barrier for dislocation motion in bulk (without GB) is shown.

climbing image nudged elastic band method. Results show that $\Sigma 3$ GB generates the barrier at the level of the Peierls barrier. For both $\Sigma 9$ and $\Sigma 19$ GBs, the barrier for dislocation transmission of heptagon sites is $0.6 \text{ ev/n}$, while it is $1.9 \text{ ev/n}$ for pentagon defects. Furthermore, we found that the critical shear stress for the transmission is lowered from $5.3 \text{ GPa}$ to $2.9 \text{ GPa}$ for moving dislocation versus the static dislocation. Since energy barrier for crossing the $\Sigma 3$ is equal to the Peierls barrier for dislocation motion in bulk, and for $\Sigma 9$ and $\Sigma 19$ GBs at the heptagon defects it is only slightly larger than the Peierls barrier, perfect screw dislocations cannot pile up against these GBs and cannot reduce phase transformation pressure during plastic deformations $[9,10]$.  

**References**

11. H. Chen, V. Levitas, L. Xiong, Amorphous phase in silicon induced by 60° dislocations pile-up against different grain boundaries (submitted for publication).