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# Atomistic simulation of shear-coupled motion of [1 1 0] symmetric tilt grain boundary in α-iron

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ABSTRACT

Shear-coupled grain boundary (GB) motion (SCGBM) is an important and efficacious plasticity mechanism in the deformation of metals, especially nanocrystalline metals. In this work, molecular dynamic (MD) simulation has been performed to investigate the SCGBM of two [1 1 0] symmetric tilt GBs, Σ9 [1 1 0](2 2 1) and Σ17[1 1 0](2 2 3), in α-iron, and the effects of temperature and strain rate on SCGBM have been studied. The coupling factor $\beta$ which is defined as the ratio of the velocities of GB lateral translation and migration was calculated, and a geometric model of $\beta$ depending on the misorientation angle was constructed in [1 1 0] symmetric tilt GBs of BCC metals. The model was branched into two modes (⟨1 0 0⟩ and ⟨1 1 1⟩) corresponding to the perfect dislocation Burgers vectors in BCC metals. The $\beta$ values calculated in the ⟨1 1 1⟩ mode were in good agreement with the MD simulation results for both the GBs. Further, the atomistic mechanisms of the SCGBM processes were also investigated. A same structural unit transformation was observed for the two GBs, which confirmed that both Σ9[1 1 0](2 2 1) and Σ17[1 1 0](2 2 3) GBs moved in the ⟨1 1 1⟩ mode during the SCGBM process.



## 1. Introduction

Grain boundaries (GBs) play an important role in the mechanical properties of materials, especially for nanocrystalline materials. GB motion properties have a significant influence on recrystallization, grain growth and plastic deformation. The GB motion includes normal motion (migration), relative translation parallel to the GB plane coupled to migration, GB sliding, and grain rotation [1]. Under applied shear stress, the coupling of GB migration with lateral translation is observed in experiments [2–4]. This behavior is called shear-coupled grain boundary motion (SCGBM), and it is an important and efficacious plasticity mechanism in the deformation of metals, especially grain growth and recrystallization [5]. The coupling factor, $\beta$, is defined as the ratio of the velocity of GB translation, $v_p$, to GB migration, $v_n$ [1], and it is indicated that its value depends on the GB structure (including tilt axis and misorientation angle) and perfect dislocation slipping direction. A geometric model of $\beta$ was proposed by Cahn et al. [1,6] for FCC metals. The model is branched into two modes (⟨1 0 0⟩ and ⟨1 1 0⟩) corresponding to the perfect dislocation burgers vectors in FCC metals (⟨1 0 0⟩ and 1/2 ⟨1 1 0⟩).

Due to the challenge and limitations in the direct measurements of GB mobility via experiments, molecular dynamic (MD) simulation has been widely used for researching GB migrations [7,8]. The process of SCGBM is convenient to carry out using MD simulation and the elementary atomic mechanisms can be investigated and analyzed from the MD results. Zhang et al. [9] examined the SCGBM of symmetric and asymmetric tilt GBs in copper using MD simulation and found that the SCGBM could be regarded as sliding of GB dislocations along the boundary plane. Frolov [10] and Zhang et al. [11] demonstrated the influence of temperature and local boundary structural transition [12] on SCGBM, and found that the motion and atomic mechanisms are sensitive to these factors.

Most MD simulation researches for SCGBM focused on FCC metals such as copper, aluminum, and nickel [1,9–11,13–20] and confirmed that the model proposed by Cahn [1] was appropriate for both [1 0 0] and [1 1 0] symmetrical tilt GBs in FCC metals. In recent years, SCGBM has been investigated for [1 0 0] symmetrical tilt GBs of BCC metals such as Nb [21] and W [22,23] as well. It is suggested that the SCGBM plasticity mechanism exists in the plastic deformation of both FCC and BCC metals. Moreover Niu et al. [23] improved the geometric model of $\beta$ in [1 0 0] symmetrical tilt GBs of BCC metals according to the perfect dislocation Burgers vectors in BCC (1/2 ⟨1 1 1⟩ and ⟨1 0 0⟩) which is different from FCC metals. The geometric model for [1 0 0] symmetrical tilt GBs in

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BCC metals has the same expression as that of FCC metals. However, the SCGBM mechanism and coupling factor model of [1 1 0] symmetrical tilt GBs of BCC metals are still unclear.

In this work, the SCGBM of two [1 1 0] symmetrical tilt GBs in BCC Fe is investigated using MD simulation. In Section 2, the general atomistic simulation method is described, and the simulation results are presented in Section 3. In Section 4, structural units of equilibrium GB structures and unit transformation in SCGBM are discussed, and a model for coupling factor $\beta$ is constructed. Finally, the conclusion of this work is presented in Section 5.

## 2. Computational model

In this work, MD simulation was carried out using the large-scale atomic/molecular massively parallel simulator (LAMMPS) code [24]. The embedded atom method (EAM) interatomic potential of iron [25] was used to describe the interaction between atoms, and the atomic configurations were visualized using the Ovito software [26].

Two [1 1 0] symmetric tilt GBs, Σ9[1 1 0](2 2 1) with a misorientation angle of 141.06° and Σ17[1 1 0](2 2 3) with a misorientation angle of 86.63° in α-iron (in this paper the misorientation angle is the angle between [1 0 0] directions in both the crystals in the GB model), were constructed [27,28]. The simulation model with three dimension of 230.16 Å × 291.57 Å × 20.19 Å for Σ9(2 2 1) GB and 233.09 Å × 306.60 Å × 20.19 Å for Σ17(2 2 3) GB approximately to $80a_0 \times 100a_0 \times 7a_0$ ($a_0$ is the lattice constant of iron) is shown in Fig. 1(a). The initial GB structure was energy minimized using conjugate gradient (CG) algorithm and relaxed sufficiently for calculating the GB energy, while periodic boundary conditions were applied along all the three directions. The GB energies calculated by Eq. (1) are 1289.3 mJ/m$^2$ and 1623.1 mJ/m$^2$ for Σ9[1 1 0](2 2 1) and Σ17[1 1 0](2 2 3) GBs, respectively.

$$E_{GB} = \frac{E_{tot} - N\varepsilon}{2S_{GB}}, \tag{1}$$

where $E_{tot}$ is the total system energy after minimization and relaxation, $N$ is the total atom number, $\varepsilon$ is the cohesive energy and $S_{GB}$ is the area of the GB interface.

Periodic boundary conditions were applied along $x$ and $z$ directions and free-surface boundary condition was applied for $y$ direction in the SCGBM simulation. Two thin slabs of atoms ($y$ direction) with 4–5 atom layers (the black blocks in Fig. 1(a)) were fixed, and another slab of atoms (red atoms in Fig. 1(a)) perpendicular to GB interface was selected for marking the movement of atoms in SCGBM. The simulations were performed in isothermal-isobaric NPT ensemble at five different temperatures (10, 100, 300, 600, 900 K), while pressures along the $x$ and $z$ directions were controlled to be around 0 GPa. We first relaxed the initial GB model for 40 ps to obtain the equilibrium structures of GBs at a given temperature. Then, a constant velocity (10 m/s) was applied to the top slab along the positive $x$ direction and the bottom slab was fixed invariably. The equilibrium structures of both GBs at 10 K are presented in Fig. 1(b) and (c). The position of the GB plane is represented by the average coordinates of the defect atoms.

## 3. Results

### 3.1. SCGBM at 10 K

The simulations of SCGBM of two [1 1 0] symmetric tilt GBs were carried out at 10 K to avoid thermal effects. Fig. 2(a) and (b) are the MD snapshots at about 400 ps for Σ9(2 2 1) and Σ17

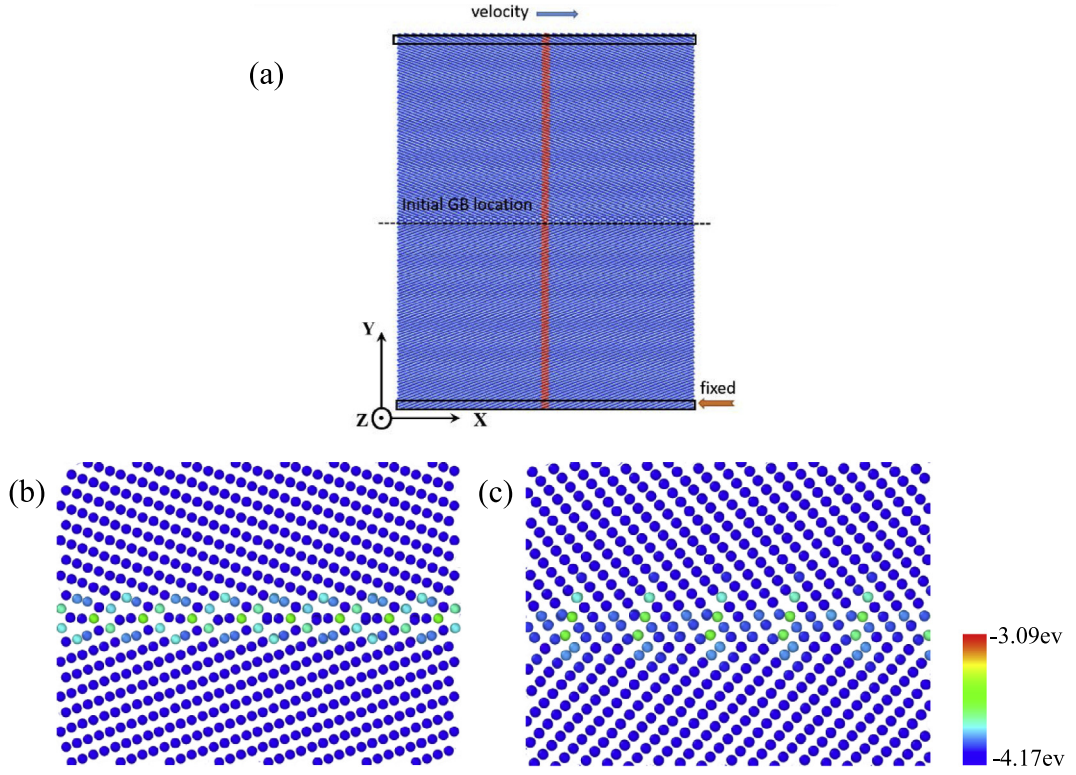


**Fig. 1.** (a) Model of MD simulation. Top and bottom slabs of atoms are fixed, and top slab is used for applying constant strain. Red atoms initially perpendicular to GB interface in the middle of the box along $x$ direction are selected for marking SCGBM. (b) and (c) are equilibrium structures of Σ9(2 2 1) and Σ17(2 2 3), respectively. Atoms are colored according to potential energy, and the color bar is presented for reference. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)