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An atomistic study of the correlation between the migration of planar and curved grain boundaries

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ABSTRACT

Molecular dynamics simulations were performed to investigate the migration of curved and planar boundaries. The reduced mobilities of capillarity driven U-shaped half-loop twin boundaries in b.c.c iron (Fe) were computed between 800 and 1200 K. To rationalize these results, simulations were also performed for planar twin boundaries of different inclination to determine their absolute mobilities and grain boundary energies. The variation of these properties with inclination was integrated into a continuum model which was found to produce the steady-state shapes of curved boundaries consistent with those from simulations. A further extension of the continuum model enabled estimations of the reduced mobility that were in good agreement with simulation results. It was also identified that atomistic events governing the migration of curved and planar boundaries shared a number of similarities. Overall, the analyses of the shapes, mobilities and atomic-scale migration mechanisms of curved and planar boundaries presented here provide a correlation between the migration of these types of twin boundaries.

1. Introduction

A key property controlling the microstructural evolution of materials is grain boundary mobility [1]. The mobility is typically assumed to be independent of the magnitude and type of driving pressure P, provided that $P \ll k_B T/\Omega$ where $k_B T$ is the product of Boltzmann constant and absolute temperature and Ω is the bulk atomic volume [2–4]. In this regime, the boundary velocity is proportional to the driving pressure, as confirmed with experiments where the driving pressure is applied, for example, via external magnetic field [5–7] or capillarity pressure [8–10]. The type of reported mobilities depend on the boundary geometry. Planar boundaries (e.g. driven by magnetic field [6]) are associated with absolute mobilities M, while curved boundaries are associated with reduced mobilities M^*, a product of M and stiffness Γ [11]. Experimentally, both types of mobilities have been reported to typically follow an Arrhenius behavior, each being associated with a different activation energy [6–10]. There is also evidence from recent atomistic studies that a number of grain boundaries has non-Arrhenius mobilities [12].

For the thermally activated migration of grain boundaries in a material, it is not clear if there is any correlation between the mobilities of planar and curved boundaries having the same misorientation. A recent experimental study evaluated the migration of magnetically driven planar boundaries in Zn and the capillarity driven migration of quarter loop boundaries of similar misorientations [7]. Different migration energies were found for both types of boundaries and interpreted as an indication that a curved boundary may migrate under a different mechanism than a planar boundary [7]. This interpretation, also made in [8], would suggest that the migration mechanism depends on the type of driving pressure and boundary geometry [1,13].

Experimental measurements of mobilities are challenging. A minor level of impurities can, for example, significantly affect measured mobilities [14]. Molecular dynamics (MD) simulations, prove to be a valuable tool in providing insights to the problems of boundary migration [15] because they allow for all variables to be carefully controlled, even those that are difficult to control experimentally. Several MD techniques for extracting the mobility have been developed, e.g. the capillarity technique [16–18], the artificial driving force (ADF) technique [19–21], the stress-driven technique [22–24], and the random-walk (RW) technique [25–28]. Recent reviews have surveyed their applications and limitations [29,30].

The capillarity technique offers arguably the most direct analysis compared to other driven techniques since it involves no artificial assumptions about the manner by which driving pressures are applied. Reduced mobilities of curved boundaries have been extracted using this technique [17,18]. The shape evolution of

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curved boundaries has also been used to deduce the absolute mobilities of planar boundaries of the same misorientation [16].

The ADF [19] and the stress-driven techniques [22] were designed to examine the migration of planar boundaries. Both techniques have been applied to several f.c.c metals, e.g. Al [19,28] and Ni [24,20,21], and have further been found to produce consistent results in terms of the absolute mobilities [29]. Recent studies pointed to a need for considerable care in analyzing the absolute mobilities determined from the ADF technique [28,31]. For example, difficulties have been experienced in analyzing the mobility of low misorientation angle boundaries [28], thus necessitating a post-simulation correction to the mobility analysis [31].

In contrast to the driven boundary techniques (i.e. the capillary, the ADF and the stress-driven techniques), the RW technique [26], or equivalently the boundary fluctuation technique [32], computes the absolute mobility of a planar grain boundary in a non-driven bicrystal. Above the roughening temperature [33], boundaries undergo uncorrelated spatial fluctuations indicative of a random walk process. The mean-squared displacement of such a boundary can be recorded over time to extract the absolute mobility [26]. While the absolute mobility computed via this technique may not be derived in a conventional manner, i.e. via the migration of a grain boundary, the RW technique provides the benefit of being in the limit of zero driving pressure. One strong limitation to this technique is that the mobility computation is only possible when the temperature is higher than the roughening transition temperature [30].

Previous studies have shown that the same absolute mobilities were found (within the simulation error) from the ADF, the stress-driven and the RW techniques [28,29]. There are, however, no systematic MD simulations that investigate whether the mobilities of planar and curved boundaries, for the same boundary misorientation, can be related to one another. In this study, a direct correlation is established between the mobilities of curved and planar boundaries for a specific boundary misorientation in a b.c.c crystal.

The migration of $\langle 1\bar{1}0 \rangle$ curved twin boundaries in pure b.c.c Fe is first examined in terms of boundary shape and reduced mobility. Planar inclined segments that make up the curved boundaries are then simulated, to quantify their energies and absolute mobilities. Finally, the properties of planar boundaries are incorporated into continuum models that allow for the prediction of the shape and mobility of a curved boundary having the same misorientation. The findings are discussed in terms of atomistic mechanisms underlying the migration of both types of boundaries.

2. Simulation methodology

Simulations were carried out using LAMMPS [34] with a time step of 1 fs. Visuals were produced using AtomEye [35] and OVITO [36]. The Ackland-04 EAM potential was used to model the interaction among Fe atoms [37], since it has been extensively benchmarked with MD simulations of b.c.c Fe.

Two types of simulation cells were prepared, i.e. the type-1 cell, a bicrystal whose grains are separated by a U-shaped half-loop grain boundary (Fig. 1(a)) and the type-2 cell, a bicrystal with two planar boundaries (Fig. 1(b)).

The type-1 cell was constructed by first creating a single b.c.c crystal with orthogonal axes of ($\mathbf{X_A}, \mathbf{Y_A}, \mathbf{Z_A}$). Atoms in the dark-shaded region in Fig. 1(a) were removed and replaced by atoms occupying b.c.c lattice sites of different orientation, i.e. ($\mathbf{X_B}, \mathbf{Y_B}, \mathbf{Z_B}$). The resulting grain boundary is a U-shaped half-loop boundary, consisting of a curved end cap and planar sides, i.e. the $\theta_\perp$ and $\theta_\parallel$ sides, see Fig. 1(a). In this work, two different type-1 cells were prepared, their axes being defined in Table 1. The planar sides of both cells are symmetric coherent and incoherent twin boundaries. The twofold symmetry of $\langle 1\bar{1}0 \rangle$-axis renders the planar sides complementary to each other, e.g. if the $\theta_\perp$ side is the coherent twin, the $\theta_\parallel$ side will be the incoherent twin. To simplify the nomenclature, the curved portion in a type-1 cell will be referred to based on the segment at the tip, e.g. "the coherent loop" is a curved boundary with the symmetric coherent twin at its tip.

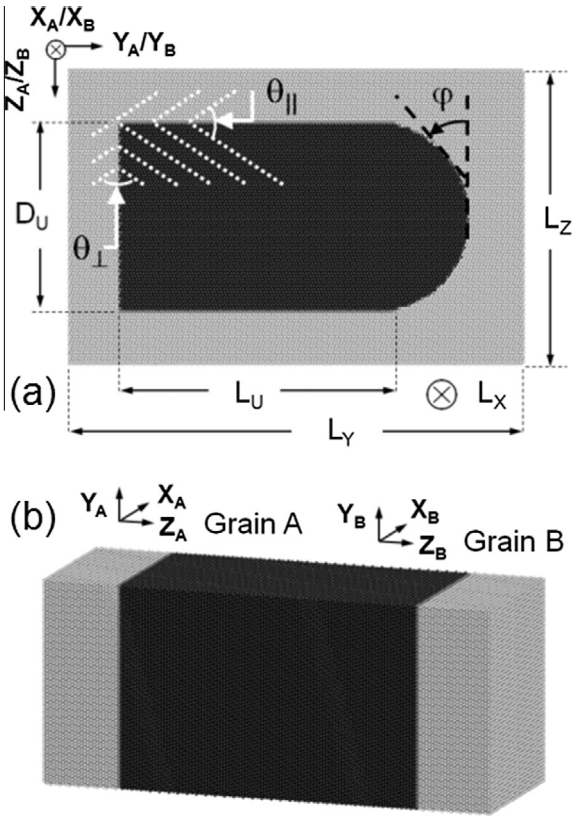

Fig. 1. Two types of bicrystal cells prepared in this study, (a) type-1 cell containing a U-shaped half-loop boundary, and (b) type-2 cell containing two planar boundaries.

Table 1
Crystallographic axes of bicrystals containing a U-shaped grain boundary (the type-1 cell) investigated in this study, see Fig. 1(a) for symbol definition.

Orthogonal axes	Designation	
	Coherent loop	Incoherent loop
$\mathbf{X_A}, \mathbf{X_B}$	$\langle 1\bar{1}0 \rangle$	
$\mathbf{Y_A}$	$\langle 11\bar{2} \rangle$	$\langle 11\bar{1} \rangle$
$\mathbf{Z_A}$	$\langle 111 \rangle$	$\langle 112 \rangle$
$\mathbf{Y_B}$	$\langle \bar{1}\bar{1}2 \rangle$	$\langle \bar{1}\bar{1}\bar{1} \rangle$
$\mathbf{Z_B}$	$\langle 11\bar{1} \rangle$	$\langle 11\bar{2} \rangle$

Periodic boundary conditions were applied to walls normal to the *X*- and *Z*-axes. A shrink-wrapped boundary condition was imposed to walls normal to the *Y*-axis such that two free surfaces were created. Atomic planes within a distance of 1 nm from the free surface were fixed to prevent grain rotation [18]. Molecular statics were then performed to the cells while the cell volume was modified (using the "box/relax" technique on LAMMPS [34]) in order to find the minimum energy configuration at zero pressure.

The type-2 cell was constructed by populating the light- and dark-shaded region in Fig. 1(b) with atoms occupying b.c.c lattice