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Scripta Materialia 54 (2006) 1163–1168
Scripta MATERIALIA
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The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals

Z.-H. Jin [a,b,e,*], P. Gumbsch [b,f], E. Ma [c], K. Albe [a], K. Lu [d], H. Hahn [e], H. Gleiter [e]

[a] Institut für Materialwissenschaft, Technische Universität Darmstadt, 64287 Darmstadt, Germany
[b] Institut für Zuverlässigkeit von Bauteilen und Systemen (IZBS), Universität Karlsruhe, 76131 Karlsruhe, Germany
[c] Department of Materials Science and Engineering, Johns Hopkins University, Baltimore, MD 21218, USA
[d] Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, PR China
[e] Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe 76021, Germany
[f] Fraunhofer Institut für Werkstoffmechanik (IWM), 79108 Freiburg, Germany

Received 20 October 2005; received in revised form 17 November 2005; accepted 18 November 2005
Available online 28 December 2005

Abstract

The interaction between screw dislocations and coherent twin boundaries has been studied by means of molecular dynamics simulations for Al, Cu and Ni. Depending on the material and the applied strain, a screw dislocation approaching the coherent twin boundary from one side may either propagate into the adjacent twin grain by cutting through the boundary or it may dissociate within the boundary plane. Which one of these two interaction modes applies seems to depend on the material dependent energy barrier for the nucleation of Shockley partial dislocations.

Keywords: Dislocation; Grain boundary; Twin; Simulation

1. Introduction

It is well established that the mechanical properties of polycrystalline metals depend on the interaction between lattice dislocations and grain boundaries [1–3], but many details of this interaction are not yet understood [4–6].

In order to study the propagation of dislocation glide across a grain boundary (GB) [7–10], we have investigated the interaction of a perfect lattice screw dislocation (Burgers vector $\mathbf{b} = \frac{a_0}{2}\langle 1\,1\,0\rangle$) with a $\{1\,1\,1\}$ coherent twin boundary (CTB) by means of molecular dynamics (MD) simulations. The CTBs are of special interest because they control the deformation behaviour of polycrystalline metals with grown-in nano-twins [11,12] and they are closely relevant to mechanical twinning [7,13–16]. It is of fundamental interest to resolve slip transfer across GBs [17] and to be able to predict the effectiveness of these GBs in blocking and redirecting slip [18,19] in thin films, multilayers and polycrystals.

2. Methods

In the MD cell shown in Fig. 1, periodic boundary conditions (PBCs) are applied in the z-direction with a periodicity length, $L_z = 3\sqrt{2}a_0$, where a_0 is the lattice parameter. Along the other two dimensions, $L_x \approx 50\sqrt{6}a_0$ and $L_y \approx 40\sqrt{3}a_0$, respectively. Several layers of atoms at the two surfaces perpendicular to the y-direction are fixed. The entire MD box consists of more than 150 000 atoms that are allowed to move freely. Larger MD cells do not change our observations.

About 10 outermost layers of atoms at the left side of the specimen are used to create incident dislocations. To create a screw dislocation, e.g., with $\mathbf{b} = \frac{a_0}{2}[1\,\bar{1}\,0]$, rigid

* Corresponding author. Address: Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe 76021, Germany.
E-mail address: zhaohui.jin@int.fzk.de (Z.-H. Jin).

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doi:10.1016/j.scriptamat.2005.11.072

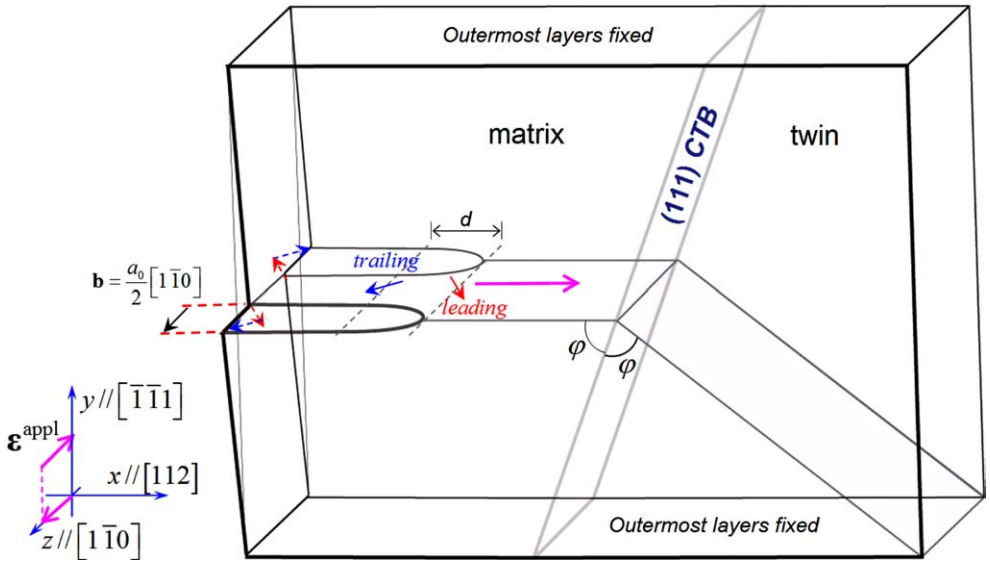

Fig. 1. MD configuration of a twinned bi-crystal for simulating the interactions between an incident screw dislocation and a coherent twin boundary. A unit screw dislocation with a Burgers vector $\mathbf{b}=\frac{a_0}{2}[1\bar{1}0]$ which splits into two Shockley partials at the central glide plane was injected along the central glide plane from the left-hand side of the MD cell. Driven by a homogeneous "out-of-plane" simple shear strain (ε_{appl}), the extended unit dislocation will move toward the CTB. Further slip at the CTB may choose one of two glide planes: either its image plane in the twin lattice or the CTB itself, which are declined to each other at an angle $\varphi = 70.53°$.

displacements (at a speed of $\sim 50\,ms^{-1}$) are introduced above and below the central glide plane (cgp) and in opposite directions. The amount of displacement at the cgp is $b_S = a_0\sqrt{6}/6$ toward the $[2\bar{1}1]$ direction to create the leading partial, followed by another $b_S = a_0\sqrt{6}/6$ but shifted to a different direction, $[1\bar{2}\bar{1}]$, to create the trailing partial. The displacements are strictly confined within the x–z planes and linearly reduced to zero at the two fixed borders in the y-direction. The stacking fault ribbon is automatically formed between the two straight Shockley partials with a splitting width d . After the dislocation has been created, positions of those rigidly displaced atoms are fixed in subsequent MD runs.

Before and after being dislocated, the system was relaxed via energy minimizations. MD-simulations have been carried out in the constant energy ensemble under a constant shear strain (ε_{appl}) applied homogeneously to the entire MD cell at the $(\bar{1}\bar{1}1)[1\bar{1}0]$ (or the y–z) shear plane and MD runs at any specified ε_{appl} are independent to each other. The motion of dislocation is always found to be subsonic. The elastic energy is released by emitting lattice waves (phonons) which lead to an increase of system kinetic energy corresponding to an effective temperature less than 10 K. The MD time step is set to be 2 fs.

Three face-centred cubic (fcc) metals (Al, Cu and Ni) and different applied stresses were used in the simulations in order to study how the dislocation/CTB interaction processes depend on the applied stress and on the chemical nature of the metal. All three metals were modelled by embedded-atom type interatomic potentials well tested [20–22]. Since temperature effects in our simulations remain insignificant, thermally activated processes (such as thermally-driven cross-slips) are suppressed. A constant shear strain ε_{appl}, corresponding to a simple shear stress $\sigma_{appl} = \tau = \mu\varepsilon_{appl}$, was applied to provide a constant driving force [23] for dislocation motion given by $f_{appl} = \tau b$, where $b = a_0\sqrt{2}/2$ is the magnitude of the Burgers vector and $\mu \equiv \frac{1}{3}(C_{11} - C_{12} + C_{44})$, the shear modulus in the $\{1\,1\,1\}\langle 1\,\bar{1}\,0\rangle$ shear plane.

3. Results

The results obtained from these simulations may be summarized as follows. When an incident screw dislocation which is composed of two Shockley partials is forced by an externally applied shear ε_{appl} into a CTB, it was found that two interaction modes exist:

(1) Both partials are redirected into the twin boundary and split in the boundary into two Shockley partials that move along the boundary in opposite directions (Fig. 2, upper panel). In this case the screw dislocation cannot move from one grain across the CTB into the neighbouring grain (twin, Fig. 1) although the resolved driving force ($\approx 0.778 f_{appl}$) acting along such a path is more than twice as large as that along the boundary plane ($\approx 0.333 f_{appl}$). This interaction mode applies to Al.
(2) A second mode of interaction was noted in Cu and Ni. The incident screw dislocation cuts through the CTB without causing any slip in the boundary plane. The cutting process results in a dissociated screw dislocation in the twin crystal (Fig. 2, lower panel).

These two modes of interaction also differ as far as the applied strain, ε_{appl} , is concerned that is required to initiate