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Deformation criterion for face-centered-cubic metal nanowires

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ABSTRACT

Much of our understanding of the tendency for deformation by dislocation slip (DS) versus deformation twinning (DT) in bulk metals relies on the magnitude of the stacking fault energy (SFE). However, the criterion based only on SFE is insufficient for evaluating the deformation behavior of nanowires (NWs) and possibly nano-grained crystalline metals. Here, by employing fault energy theories and dislocation theory, we have developed a parameter that enables the quantitative analysis of the relative tendency for DS and DT in Al NWs. In situ TEM tensile tests and atomic simulations of Al NWs showed that the competition between DS and DT is sensitive to the misfit energy, crystal size, and loading direction. Additional studies were conducted on Au and Pt NWs to determine the applicability of the proposed theory to other crystals. The theory produces self-consistent results even for metals with different SFE values.

1. Introduction

The competitive relationship between the deformation by dislocation slip (DS) and deformation twinning (DT) in polycrystalline bulk metals has traditionally been assessed only by the magnitude of the stacking fault energy (SFE). This view is based primarily on statistics quantifying the empirical observation that DT is more common in materials with low SFE (typically < 20–$50\,mJ\,m^{-2}$) [1–4]. However, significant scatter accompanies this observation and exceptions to the rule are many. In pure face-centered-cubic (fcc) metals, the variation from the rule is particularly striking in the anomalous behavior of Al. Pure Al is known to favor DS because of its high SFE of $\sim 150\,mJ\,m^{-2}$, but DT is frequently reported [5–9]. The scattering and contradictions in the SFE–twinnability relationship arise from the static nature of the SFE, which does not reflect the intermediate stages of deformation and only describes the structural state of a crystal under static conditions.

Conceptual theories were developed regarding the dynamics associated with the formation of stacking faults and their evolution to either full dislocations or twins. The energy profile associated with the generation of a full dislocation, known as the generalized stacking fault energy (GSFE) curve [10,11], describes the process of DS, while that corresponding to a twin (also known as the generalized planar fault energy (GPFE) curve [12–16]) describes the process of DT. The problem of the tendency for DT (or twinnability) in fcc metals has been extensively studied in the past. Most are made by comparing the relative values of the unstable/stable fault energies evaluated from the GPFE curves [12,15,17–21]. Despite their ability for evaluating the relative tendency for the twinnability of different materials, these parameters developed in the previous studies are unable to predict the competitive relationship between DS and DT in the same material. This is because the twinnability of fcc metals depends not only on the intrinsic properties (as depicted in the GPFE curve) of materials, but also on the external parameters including the loading direction, sample size, etc. Researchers later recognized the significance of the GSFE and GPFE theories in relating them to the tendency for DT occurring in the same fcc metals. Several results on the relative tendency for DS versus DT were reported for Al [5,9,18,21–23]. Chen et al. [5] assumed that the type of deformation is determined by the competition between the full dislocation and partial dislocation and claimed that DT in Al could occur only in grains of less than 10–20 nm in size. Subsequently, Jo et al. [23], by assuming the shape of dislocations as an infinitely long line, reported that $< 110 >$ was the only tensile direction that can promote DT in a perfect Al crystal. However, as will be shown in this study, DT in a perfect Al crystal is feasible along various tensile directions, including $< 110 >$, for any crystal smaller than ~ 250 nm. The discrepancies between the present results and previous analyses [5,23] arise from the inappropriate assumption employed to compare the deformation processes of DS and DT, on one hand and the absence of parameters, such as loading direction and sample size, required to predict the twinnability [17,20], on the other. Much regarding DT remains unsettled, requiring further analysis.

Because DS and DT are both activated by stress, deformation is

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favored by whichever pathway is activated at a lower external stress. Therefore, the twinnability of a crystal can be quantitatively analyzed by directly comparing the magnitudes of the applied stresses required to activate DS and DT. Despite the simplicity of this approach, it has never been attempted because of the complexity in calculating the activation stresses and the delicacy of the experimental validation procedures. In addition, the crystal used to evaluate the twinnability must be monocrystalline and free of defects. Al nanowires (NWs), in addition to being perfectly crystalline, possess a high SFE of $\sim 150\ \mathrm{mJ\,m^{-2}}$. The Al NW is suitable not only for micro-mechanical tensile testing, but also for studying the previously unexplored regime of high-SFE materials. It thereby provides an excellent test material for evaluating the competitive relationship between the DS and DT mechanisms.

In the present study, a feasible evaluation of the twinnability of a crystal is explored by combining the first-principles calculations, classical molecular dynamics (MD) simulations, and micro-mechanical testing using in situ transmission electron microscopy (TEM). This paper addresses three issues and is organized as follows. First, following the Peierls framework on dislocation theory and employing the GSFE and GPFE curves calculated for a perfect Al crystal, we derived equations for evaluating the stresses required to activate DS and DT. We next developed a theory that quantitatively expresses the relative tendencies for DS versus DT in a crystal by simultaneously considering the fault energy, loading direction, and crystal size. The proposed theory was validated via the tensile testing of Al NWs along multiple crystallographic directions, using either quantitative in situ TEM (along the $< 110 >$ direction) or MD simulations (for directions other than $< 110 >$). Finally, the tensile tests were extended to NWs of other metals, specifically Au and Pt, in order to elucidate whether the proposed parameter produced self-consistent results and therefore could be generically extended to other fcc crystals with different SFE values.

2. Materials and methods

2.1. Ab initio calculations

The calculations of the generalized stacking/planar fault energy of Al were performed using the Vienna Ab initio Simulation Package (VASP) [24,25] with the generalized gradient approximation [26] and the projector augmented wave [27] pseudopotential. For the Brillouin zone *k*-point sampling, an $8 \times 8 \times 2$ Monkhorst-Pack grid [28] was used with an energy cutoff of 240.3 eV, sufficient to ensure an energy convergence of 1 meV/atom. The supercell was constructed of ten layers of the (111) plane containing two vacuum layers along the z-axis, with the *x*-, *y*-, and *z*-axes being parallel to the $[2\bar{1}1]$, $[0\bar{1}1]$, and [111] directions, respectively. Since the GSFE curve was constructed with the subsequent slip of the leading and the trailing partials, the upper-half layers of the supercell were forced to glide first along the direction of the Burgers vector of the leading partial, and then along that of the trailing partial. Meanwhile, DT was activated by the successive slip of the twinning partials on the adjacent slip plane. Therefore, after the intrinsic stacking fault was nucleated by sliding the upper-half layers along the direction of the twinning partial, the extrinsic stacking fault and twin were nucleated by the successive slip of the twinning partials. Following these procedures, the GPFE curve was calculated. The supercell was relaxed using the conjugate gradient algorithm throughout the described process.

2.2. MD simulations

The Al, Au, and Pt NWs with circular cross-sections and surfaces parallel to various longitudinal orientations were modeled using MD to eliminate the effects of the preferential orientation and surface geometry on the nucleation of deformation. Approximately 60,000 atoms were packed into each cylindrical cell with dimensions of $8 \times 8 \times 20$ nm. In order to allow the surface effects of the NW, the cell

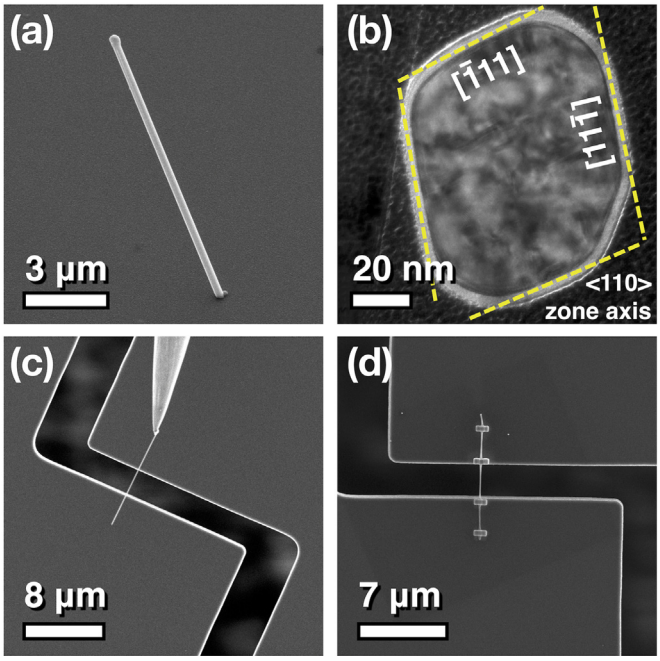

Fig. 1. (a) Al NW grown on the SiO_2 substrate. (b) Rhombus-shaped cross-section of the Al NW with four faceted {111} sides. (c) Al NW sample attached to the W tip of the nanomanipulator using electron-beam (e-beam) assisted Pt deposition. (d) Al NW welded to the upper and lower jigs of the PTP device using e-beam assisted Pt deposition.

was modeled with non-periodic boundary conditions in all three directions. The interaction among the constituent atoms of Al [29], Au [30], and Pt [30] NWs was calculated based on the embedded atom method [31] potential, as implemented in LAMMPS [32]. The NWs were relaxed using conjugate gradient energy minimization and subsequently equilibrated using a Nosé-Hoover thermostat [33,34] at the ambient temperature. This allowed collating with the experimental tensile tests performed at room temperature. To simulate uniaxial tensile testing, a uniform strain loading condition was applied by fixing one end of the NW and applying velocities to the atoms along the loading direction. The velocities varied linearly from zero at the fixed end to a defined maximum value at the opposite end [35], corresponding to a strain rate of $\sim 10^7\ \mathrm{s^{-1}}$.

2.3. Synthesis of Al NWs and in situ TEM tensile testing

Al NWs with long axes parallel to the $< 110 >$ direction were grown by a stress-induced method on an SiO_2 substrate, as reported elsewhere [36] (see Fig. 1(a)). The NWs used for the in situ TEM tensile tests are 5–20 μm in length and oriented along the $< 110 >$ direction (see Fig. 1(b)). When indexing with standard procedures used in diffractometry, these NWs are rhombic in cross-section with four equivalent {111} side facets and an acute angle of 70° (see Fig. S1 in Supplementary materials). The NWs were single-crystalline, nearly defect-free, and covered with a ~6-nm-thick aluminum oxide layer. One side of the NW was attached to the W tip of the nanomanipulator (MM3A, Kleindeck) installed in a focused ion beam (FIB) system (Quanta 3D, FEI) using an electron-beam (e-beam) deposition technique. This NW was then welded to the upper and lower jigs of the push-to-pull (PTP) device (see Fig. 1(c) and (d)). At this welding stage, delicate manipulation of the NW was necessary to align the long axis exactly with the direction of the tensile force. The PTP device, which acquired load-displacement data along with real-time images of the microstructural evolution, was then mounted to a picoindenter (PI-95 TEM, Hysitron) capable of measuring load and displacement. Tensile tests were conducted on the Al NW samples at initial strain rates of