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The effect of surface step and twin boundary on deformation twinning in nanoscale metallic systems

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ABSTRACT

The effect of surface step and twin boundary on the mechanical twinning process in nanoscale face-centred cubic metallic films was studied using atomistic simulations. Aluminium was considered as a model material but comparisons were made with silver and copper. Surface steps were identified as privileged sites for twin nucleation at lower stresses, leading to the formation of only one large twin in defect-free films. In presence of a coherent twin boundary which acts as a strong barrier to the propagation of dislocations, the extension of nucleated twins is much more limited but the density of secondary twin boundaries is found higher. The key role played by Lomer dislocations, resulting from the interaction between incipient twins and the coherent twin boundary, on the nucleation of new twins was demonstrated. These findings shed light on some elementary mechanisms that can be involved in the elaboration of nanotwinned materials with interesting mechanical properties.

1. Introduction

The plasticity of face-centred cubic (FCC) materials are now well documented and known to be driven in most cases by perfect $1/2\langle 110\rangle$ dislocations dissociated in two $1/6\langle 112\rangle$ Shockley partials in $\{111\}$ slip planes. Mechanical twinning resulting from the glide of Shockley partials in adjacent planes can also contribute to plastic deformation in bulk FCC materials, but only in those with low stacking fault energies that were work-hardened and/or deformed at low-temperature [1–4]. However, it was shown that this elementary plasticity mechanism can also take place in high stacking fault energy materials when their characteristic dimensions decrease up to some nanometers. When the grain size [5], the size of nanowires [6] or the film thickness [7] is decreased, the nucleation of partial dislocations becomes increasingly important and mechanical twinning occurs more frequently. In the case of defect-free nanowires loaded under single slip conditions, it was shown that the external mechanical stress can be fully relaxed by mechanical twinning, leading to remarkable properties, such as super-plasticity [8,9] or pseudo-elasticity [10,11]. More generally, nanostructuring materials with as-grown or mechanically induced nanotwins elaborated using electro-deposition, physical vapour deposition or severe plastic deformation techniques, has recently attracted significant interest regarding the remarkable mechanical properties that such nanotwinned materials can exhibit [12]. Interestingly, whereas mechanical properties are highly affected by the twin density, it was reported for copper that electrical properties are not affected by the presence of nanotwins [13,14].

An important parameter impacting on mechanical twinning is defects. It was found that much higher stresses are required to induce twinning in near perfect materials, such as whiskers, than in less perfect crystals, suggesting that twinning is generally initiated by defects [15]. In bulk materials, many sources can come into play: lattice defects such as dislocations which can induce twinning via a pole mechanism or cross-slip, grain boundaries or surfaces. At the nanoscale, due to closer surfaces (for thin films or nano-objects) or grain boundaries (for nanocrystalline materials), line defects are less frequent, surfaces and grain boundaries acting as sinks for dislocations. But the high density of planar defects (surfaces, grain boundaries) also provides many potential sources for Shockley dislocations nucleation and thus for twinning. For nanocrystalline materials, few twinning models were identified with molecular dynamics (MD) simulations and confirmed experimentally. In all these models, grain boundaries are mainly involved in twin formation as Shockley dislocation sources or because of their migration and splitting [16,17]. For thin films or nano-objects, surfaces are also privileged sites for dislocations or twins nucleation, especially at surface defects which are known to locally concentrate the applied stress [18–22].

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Moreover, defects can also act as obstacles to twinning. Planar defects inside the material, such as high angle grain boundaries, are particularly known to act as strong barriers to dislocations and so to twin propagation [23,24]. In nanotwinned materials, the large amount of pre-existing twin boundaries can give rise to remarkable properties such as both high strength and good ductility, when compared to nanocrystalline counterparts [12–14,25]. In such materials, strength is increased because twin boundaries act as strong obstacles to dislocations, while ductility is improved because twinning partial dislocations are easily formed in order to accommodate the applied strain [26]. Such nanotwinned materials can be synthesized by sputtering techniques producing coherent twin boundaries (CTB) parallel to the substrate during the growth of the film with densities depending on the deposition rate conditions [14,27–29].

The present study aims to investigate, at the atomic-scale, the competitive influences of the surface corrugation and of a pre-existing twin boundary on the formation of secondary twins that can lead to a denser distribution of twins. Because of the small space and time scales involved, it is difficult to observe experimentally the impact of defects on mechanical twinning. Thickening can be observed but only for large twins [30–32] and for large time scales which are inappropriate for the detailed study of twin-defects interactions. Conversely, atomic-scale simulations used here allow for a visualization of plasticity mechanisms at the atomic scale and for short time ranges. The choice has been made to consider thin film geometries that have the advantage, in contrast to nanowires, to consist only in one type of surface whose relief can be easily customized with monoatomic steps and for which secondary twinning has not been extensively studied from a numerical point of view. It is believed that the results obtained could be applicable to other systems with multiple surfaces or interfaces (grain boundaries, twin boundaries) competing as sources or obstacles for the formation of twins. This study focuses on twinning in aluminium which is a good candidate for mechanical twinning at the nanoscale because of its quite low energy barrier for twin thickening [33] in spite of its high stacking fault energy. Other FCC materials such as copper and silver have also been considered in order to figure out how generalizable the results could be.

In that context, we performed MD simulations of a thin FCC film, with and without an initial coherent twin boundary (CTB) at the centre of the film, and with and without steps on the free surfaces. Our model system allows us to highlight separately the impact of these particular defects on the different stages of the mechanical twinning process: nucleation, propagation or thickening. Simulation model and methods are detailed in Section 2. In Section 3 we analyze the influence of a monoatomic surface step on twin nucleation, and then we describe in Section 4 some plasticity mechanisms induced by the introduction of a CTB. In Section 5, the surface steps density is varied for two cases, with and without an initial CTB. Finally, we discuss the influence of different parameters such as the material in Section 6.

2. Model and methods

For this study, a self-supported thin film was constructed, as shown in Fig. 1. Periodic boundary conditions (PBC) were applied in the $X = [0\bar{1}1]$ direction and the $Y = [\bar{2}11]$ loading direction; in the $Z = [\bar{1}\bar{1}\bar{1}]$ direction, free surfaces were introduced (light red atoms in Fig. 1). Some tests with semi-rigid non-periodic boundary conditions along the Y direction were also performed. In that case, the atoms in two zones at the simulation box ends (see Fig. 1) are kept fixed in the Y direction while allowed to move in the two other directions. The dimensions of the film were 17.1 nm × 39.0 nm × 20.6 nm, for approximately 870,000 atoms. A few tests for larger systems and with different aspect ratios were also carried out. Crystallographic orientations were specifically chosen to facilitate twin formation and the introduction of specific surface defects or planar defects inside the film. Indeed, monoatomic surface steps can easily be introduced along the $X = [0\bar{1}1]$ dense direction, for example by removing one atomic layer over a portion of the surface. Because of the periodic boundary conditions, the steps are introduced in dipolar pairs in our systems (red atoms in Fig. 1). A coherent twin boundary (light blue atoms in Fig. 1), can also be introduced by rotating the lower half part of the film around the Y axis by 180° angle. The crystallographic orientations in this bottom half part are then $X = [0\,1\,\bar{1}]$, $Y = [\bar{2}\,1\,1]$and $Z = [1\,1\,1]$ (Fig. 1). For the chosen orientations, the Schmid factor is 0.31 for the $[2\,1\,1](\bar{1}\,1\,1)$ slip system, which corresponds to a leading Shockley partial dislocation under compression (the Schmid factor is 0.16 for the trailing partial). This is the maximum value for slip in conventional $\{1\,1\,1\}$ planes containing the surface steps, so that formation of partial dislocations in these planes is expected and twinning promoted.

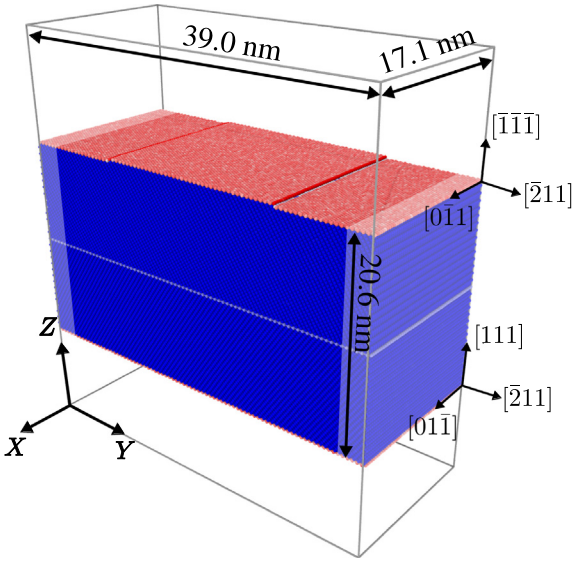

Fig. 1. Geometry of a thin film containing two surface steps spaced by 20 nm each other. A coherent twin boundary has been created at the centre of the film. Atoms are coloured according to the centrosymmetry parameter. The transparency indicates the zones where atoms are kept fixed in the Y direction when semi-rigid non-periodic boundary conditions are used. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

MD calculations were then performed using the LAMMPS code [34]. Atomic interactions were modelled using EAM potentials for aluminium [35], copper [36] and silver [37]. These potentials were chosen to reproduce as closely as possible the elasticity constants and the stacking fault energies, which are key parameters when one is interested in plasticity and twin formation, as discussed in Section 6.3. An energy minimization using a conjugate gradient minimization was first performed. The temperature was next applied by giving initial velocities to all atoms according to the Maxwell-Boltzmann distribution. Most calculations were done at 300 K to mimic experimental conditions. Simulations at 10 K were also carried out in aluminium and are discussed in Section 6.2. The system was then relaxed using an NPT integration according to the Nosé-Hoover thermostat with zero pressure. The system was subsequently deformed in compression along the $Y = [\bar{2}\,1\,1]$ direction, at $\dot{\varepsilon} = 10^8\ s^{-1}$ constant strain rate and using an NVT integration at the chosen temperature. The timestep was $\Delta t = 1$ fs. In LAMMPS,