Computational Materials Science 142 (2018) 59–71

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Deformation twinning and dislocation processes in nanotwinned copper by molecular dynamics simulations

Xing Zhao [a,b], Cheng Lu [a,*], Anh Kiet Tieu [a], Lihua Zhan [b], Minghui Huang [b], Lihong Su [a], Linqing Pei [a], Liang Zhang [a]

[a] School of Mechanical, Materials and Mechatronic Engineering, University of Wollongong, Wollongong, NSW 2522, Australia
[b] State Key Laboratory of High Performance Complex Manufacturing, Central South University, Changsha 410083, People's Republic of China

ARTICLE INFO

Article history:
Received 3 June 2017
Received in revised form 27 September 2017
Accepted 28 September 2017

Keywords:
Deformation twinning
Dislocation
Nanotwinned Cu
Molecular dynamics
Slip transfer

ABSTRACT

Nanotwinned materials exhibit a combination of high strength and good ductility which is attributed to the interactions between dislocations and twin boundaries. But no attempt has been made to explore the possibility for deformation twinning in nanotwinned face-centered cubic materials. Here we use large scale molecular dynamics simulations to elucidate the mechanical behaviour of nanotwinned Cu. We demonstrate that deformation twinning plays an important role in the deformation of nanotwinned Cu with specific twin orientations, in addition to conventional dislocation slip. Deformation twins are formed through the glide of Shockley partials on adjacent {1 1 1} slip planes and two twinning mechanisms are identified based on the arrangement of Shockley partials. The first mechanism involves the successive motion of Shockley partials of different types, named as double-Shockley partials, which forms unstable thin twin plates. The second process involves the successive passage of the same twinning dislocations on neighbouring slip planes, which forms stable deformation twins along one primary twinning system or symmetric twinning systems. The dislocation processes involved in the dislocation-twin reactions are analysed at atomic level. The orientation dependence of deformation twinning is discussed and compared with available experimental results.

1. Introduction

Deformation twinning has been widely observed in coarse-grained face-centered cubic (fcc) metals and alloys, which plays an important role in plastic deformation in addition to dislocation slip [1–3]. Twinning propensity is strongly affected by stacking fault energy [4,5]. Deformation twinning takes place easily in metals with low stacking fault energies, such as brass, Cu-Al alloys and stainless steels; in contrast twinning hardly occurs in materials with high stacking fault energies. Deformation twinning is also promoted by high strain rates and/or low temperatures, where slip activities are restricted because the number of operable slip systems is reduced. Grain size also influences the twinning tendency in fcc metals. Twin formation is restricted with decreasing grain size. But when grain size is reduced to nanometer level, deformation twinning is greatly enhanced [6]. Metals that normally do not twin are found to twin in nanocrystalline form [7,8]. Molecular dynamics (MD) simulation revealed extensive deformation twinning in the deformation of nanocrystalline Al [7], which was verified by later transmission electron microscopy (TEM) observations [8]. The change in twinning propensity is attributed to twin nucleation from grain boundaries [9]. The role of grain boundaries needs to be incorporated to develop new models for deformation twinning [10].

A number of models have been proposed to rationalize the formation of deformation twins in fcc materials [1,11,12]. Twin nucleation involves two essential processes: the nucleation of twin embryos and their subsequent growth to large twins [1]. It is assumed that the formation of twins requires dislocations and the twinning source can be categorized into two types: prismatic and glide [13]. In prismatic models, the primary slip does not lie on the twinning plane. Cottrell and Bilby [14] proposed the pole mechanism which involved the dissociation of a full dislocation into a Shockley partial and a sessile Frank dislocation. But only monolayer stacking fault was produced. Venables [15] extended the pole mechanism and explained how mechanical twins grew. Cohen and Weertman [16] suggested that the overlap of stacking faults formed imperfect deformation twins. These stacking faults resulted from glide of Shockley partials dissociated from

* Corresponding author.
E-mail address: chenglu@uow.edu.au (C. Lu).

https://doi.org/10.1016/j.commatsci.2017.09.055
0927-0256/

piling-up dislocations near Lomer-Cottrell locks. Fujita and Mori [17] presented a similar model involving the cross-slip of stair-rod dislocations. Mahajan and Chin [18] described a simple glide model, in which the interaction between two coplanar perfect dislocations led to the nucleation of a three-layer twin. We can see that there is a lack of consensus for twin nucleation at the moment [12,13,19].

Recent studies on high manganese steels reveal that deformation twinning plays a significant role in the strain-hardening behaviour of twinning-induced plasticity (TWIP) steels [20–26]. The evolution of twin structure has been extensively characterized using advanced experimental techniques [11,25,27]. Ueji et al. [23] reported that deformation twinning was restricted by grain refinement and strongly depended on grain orientation. Gutierrez-Urrutia and Raabe [25] systematically distinguished three types of twin substructure at high tensile strains. A low deformation twinning activity was observed in grains oriented close to ⟨0 0 1⟩ directions; twin substructure was developed along one primary twinning system in grains oriented between ⟨0 0 1⟩ and ⟨1 1 1⟩ directions; and a multiple twin substructure was built up along the primary and secondary twinning system in grains close to ⟨1 1 1⟩ directions. Karaman et al. [28] introduced a new dislocation model to explain the formation of extrinsic stacking faults and deformation twins in theoretically untwinning directions, such as ⟨0 0 1⟩ under tension and ⟨1 1 1⟩ under compression. The nature of dislocations was identified by the advanced characterization tools, which provided evidence for earlier proposed twinning mechanisms [11,27]. Recently Casillas et al. [27] reported that extrinsic stacking faults served as twin nuclei in TWIP steels using aberration corrected scanning TEM. However, it is difficult to obtain the detailed evolution of dislocation structures based on TEM studies. Little is known about the specific deformation mechanisms involved in deformation twinning.

Nanotwinned materials exhibit simultaneous ultrahigh strength and increased ductility, as well as high electrical conductivity [29,30], which make them attractive for numerous applications. However, no attempt has been made to explore the possibility for deformation twinning in nanotwinned fcc materials until now, because twin formation cannot be controlled in nanotwinned materials despite that multiple twin structures have been extensively observed in twin-free materials [25]. Moreover, it is not easy to distinguish deformation twins and growth twins in experiments, which are identical from a crystallographic view. In this study, we use large scale MD simulations to elucidate the mechanical behaviour of nanotwinned Cu. Our simulations reveal that deformation twinning occurs in the deformation of nanotwinned Cu with specific twin orientations. The atomistic mechanisms involved in the formation of deformation twins and the dislocation-twin reactions are analysed in detail.

2. Methods

The simulation cells contained parallel growth twin boundaryies (TBs) with different orientations. The nanotwinned structure was constructed by continuous atomic displacements on adjacent (1 1 1) planes to get a symmetric twin while keeping the matrix unchanged [31]. Atoms above one (1 1 1) plane were shifted along $[1\,1\,\bar{2}]$ direction by the magnitude of a partial dislocation, which was repeated to produce a specific twin spacing. Then the nanotwinned model was rotated about the $[1\,\bar{1}\,0]$ direction to obtain samples with different orientations. The sample dimensions are around 100 nm × 50 nm × 2 nm and the total atom number is approximately 850,000. Fig. 1 shows the cross-sectional view of fabricated samples T4A19, T4A75 and T4A90. The letters T and A in the sample names indicate the twin spacing and inclination angle.

MD simulations were performed using the large-scale parallel molecular dynamics package LAMMPS [32]. The embedded atom method potential for Cu by Mishin et al. [33] was used to describe the atomic interactions between Cu atoms. This potential was fit to experimental data and ab initio calculations and accurately reproduced many material properties, including the stacking fault energy that is important for deformation simulations. Periodic boundary conditions were imposed in all three directions to model the behaviour of bulk materials. The samples were first equilibrated at 300 K for 100 ps, using a Nose-Hoover thermostat and a Parrinello-Rahman barostat (an NPT ensemble). The tensile deformation was applied by continuously scaling the atomic coordinates and box size along the *X* direction in Fig. 1 at a constant strain rate of 5×10^8 s^{-1}, while along the other two directions, stresses were kept at zero using an NPT ensemble.

The atomic configurations were visualized using the scientific software package Open Visualization Tool (OVITO) [34]. Common neighbour analysis (CNA) was used to visualize the defects. Three types of atoms are defined: grey represents perfect fcc atoms, red stands for hexagonal close-packed (hcp) atoms (corresponding to stacking faults and TBs), and green indicates defected atoms (corresponding to GBs, dislocation cores, and other defects). Moreover, the relative shear strain of each atom with respect to its original position was calculated (embedded in OVITO) to trace the evolution of dislocation structures. Perfect fcc atoms that are not involved in the plastic deformation were eliminated for the sake of clarity in the analysis of the dislocation structures [35]. This procedure was carried out by deleting atoms with shear strain of less than 0.15, as calculated by OVITO. In this way, the atoms that experience slip and still retain the fcc structure are coloured in grey. The dislocations were characterized using dislocation extraction algorithm Crystal Analysis [36].

The slip system in nanotwinned fcc materials can be described by the double Thompson tetrahedron [1,6,37] as shown in Fig. 2a. Twin boundary is shared by the twin and the matrix. The lower Thompson tetrahedron represents matrix slip systems, while the symmetric upper tetrahedron shows twin slip systems. Although the slip directions on the twin plane are common, the slip planes ABC(d) or (1 1 1) plane in the matrix and ABC(d′) or $(\bar{1}\,\bar{1}\,\bar{1})$ plane in the twin are opposite. From the cross-sectional view (Fig. 2b), the slip activities can be catalogued into three groups: dislocations on slip planes (d) or (d′) are parallel to the twin plane; dislocations on slip planes (c) or (c′) are inclined 70.5° to twin plane; and dislocations on other slip planes (a), (b), (0 0 1) or (a′), (b′), $(0\,0\,1)^T$ are inclined 54.7° to twin plane. The nature of the dislocations was in agreement with the results from Crystal Analysis. In this study, the dislocation reactions are represented by Burgers vector equations expressed in terms of the double Thompson tetrahedron, and the same equation in vector form is also given [1]. Indices relative to the twin lattice are given the superscript *T*. The conservation of Burgers vector is fulfilled for all the dislocation reactions.

3. Results

3.1. General observation

Fig. 3 shows three typical atomic configurations after tensile deformation, where deformation twinning occurs in addition to dislocation slip. In sample T4A19 (Fig. 3a), the dislocation processes dominated by slip transmission are accompanied by a small amount of deformation twinning. Mechanical twins are formed along one twinning system in the twinned grains, while slip activities dominate the plastic deformation in the matrix grains. These