Molecular dynamics simulation of twin boundary effect on deformation of Cu nanopillars

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Abstract

Molecular dynamics simulations performed on <110> Cu nanopillars revealed significant difference in deformation behavior of nanopillars with and without twin boundary. The plastic deformation in single crystal Cu nanopillar without twin boundary was dominated by twinning, whereas the introduction of twin boundary changed the deformation mode from twinning to slip consisting of leading partial followed by trailing partial dislocations. This difference in deformation behavior has been attributed to the formation of stair-rod dislocation and its dissociation in the twinned nanopillars.

Keywords: Molecular dynamics simulations, Nanopillar, Twin boundary, Twinning, Slip.

1 Introduction

The requirement to improve the mechanical properties of nanomaterials for advanced applications has raised renewed interest towards the twinned nanopillars. The twin boundaries (TBs) influence the strength as well as the deformation behavior of the nanopillars. It has been demonstrated that the twin boundary enhances the strength coupled with high ductility [1], improves crack resistance [2] and increases strain rate sensitivity [3]. The interaction of TBs with dislocations results in either strengthening or, softening or, has negligible effect on the strength value [4, 5]. In addition to superior properties, the twinned nanopillars show novel deformation mechanisms [6, 7, 8, 9]. It has been shown that the 1/2⟨110⟩ dislocations glide on {100} plane instead of a conventional {111} plane after penetrating the twin boundary (TB) in Cu nanopillar [6]. Based on the experimental results, Wang and Sui [7] have shown that the leading and trailing partials can exchange their order after passing through the TB. TBs can also act as source/sink and glide plane for dislocations [8]. Sinha and Kulkarni [9] have demonstrated that the crack propagation along the twin boundary exhibits directional anisotropy in terms of cleavage in one direction and dislocation emission in the opposite direction. By performing in-situ tensile experiments, Jang et al. [10] observed different mechanisms in Cu nanopillars with orthogonal and slanted twin boundaries. In nanopillar with orthogonal twin boundaries, twin boundary-dislocation interactions dominate plastic flow, whereas detwinning governs deformation in nanopillars with slanted twin boundaries [10].

Most of the studies reported in the literature have been performed on nanopillars containing orthogonal or, slanted twin boundaries. Using in-situ transmission electron microscopy, Roos et al. [11] investigated the role of longitudinal twin boundary on the deformation mechanism of Au nanowires. Under tensile loading, they observed the storage of full dislocations in twinned nanowires, while twins and stacking faults were observed in single crystal nanowires. The transition in deformation mechanism from twinning in single crystal to slip in the twinned nanowire has been attributed to the pile-up of leading partials against the twin boundary and nucleation of trailing partials on the same plane as that of the leading partials in the twinned nanowires [11]. Motivated by this study, we performed molecular dynamics (MD) simulations to investigate the possibility of such transition in the deformation mechanism of <110> Cu nanopillars with and without longitudinal TB. Based on the MD simulation results, we show that the perfect <110> Cu nanopillar deforms by twinning, while the introduction of longitudinal TB changes the deformation mode from twinning to full slip. Further, we explore the atomistic description of the novel deformation mechanism operating in the twinned nanopillars that is responsible for the observed transition.

2 Simulation details

MD simulations have been carried out in LAMMPS package [12] using embedded atom method (EAM) potential for Cu given by Mishin et al. [13]. The visualization was accomplished using AtomEye [14]. Burgers vector of dislocations were determined by dislo-
3 Results

Fig. 1 shows a stress–strain behavior of $\langle 110 \rangle$ axially oriented Cu nanopillars with and without longitudinal twin boundary. The atomic snapshots displaying the deformation behavior of perfect Cu nanopillar along with Thompson tetrahedron are shown in Fig. 2. The Thompson tetrahedron (Fig. 2(e)) is used to index the Burgers vectors and slip planes. It can be seen in Fig. 2(a) that the nanopillar yields by the nucleation of four leading partials from the corners on two different $\{111\}$ planes, $\alpha$ and $\beta$. Following the yielding, the stacking faults on planes $\alpha$ transform into twins (Fig. 2(b)) by the successive nucleation of Shockley partials on adjacent $\alpha$ planes, while on planes $\beta$ they remain as stacking faults. With increasing deformation, one of the twins on planes $\alpha$ grows in width along with twin formation on a plane $\beta$ (Fig. 2(c)). Further deformation is dominated entirely by the growth of twins on both $\alpha$ and $\beta$ planes as shown in Fig. 2(d).

The deformation behavior of a $\langle 110 \rangle$ Cu nanopillar containing a longitudinal TB along with double Thompson tetrahedron is shown in Fig. 3. The double Thompson tetrahedron (Fig. 3(f)) is used to index the Burgers vectors and slip planes activated during the deformation of a twinned nanopillar. As shown in Fig. 3(a), the twinned nanopillar yields by the nucleation of a leading partial with Burger vectors $\beta A$, $A \beta'$ and $\alpha B$ from the corners on the planes $\beta$, $\beta'$ and $\alpha$, respectively. With increasing deformation, the leading partials $\beta A$ and $A \beta'$ meet at TB from the opposite side (Fig. 3(b)) and combine to form a stair-rod dislocation lying on TB with a Burgers vector $\beta \beta'$ as shown in inset in Fig. 3(b). It can be seen that the line of a stair-rod dislocation is parallel to CA, and its Burgers vector $\beta \beta'$ is perpendicular to both dislocation line and TB plane. Therefore, the stair-rod dislocation has an edge character having the magnitude $2a/3\sqrt{3}$ [5]. Since the stair-rod dislocation is sessile on TB plane, with increasing deformation...
Figure 3: The deformation behavior of $<110>$ Cu nanopillar containing a longitudinal twin boundary along with double Thompson tetrahedron. The double Thompson tetrahedron is orientated in such a way that, the direction BA coincides with tensile axis and plane ABC is parallel to twin boundary plane. The alphabets L and T represents the leading and trailing partials, respectively. The white arrow represents the direction of dislocation motion at that instant.

it dissociates into two trailing partials $C\beta$ and $\beta'C$ as shown in Fig. 3(c). These trailing partials eliminate the stacking faults produced by leading partials on planes $\beta$ and $\beta'$. It can also be seen from Fig. 3(c) that the leading partial $Bo'$ also nucleates and interacts with $\alpha B$ at TB. This interaction leads to the formation of another stair-rod dislocation lying on TB with Burgers vector $\alpha'$. The line of this stair-rod dislocation is parallel to BC and is sessile on TB plane. Therefore, any further deformation leads to its dissociation into trailing partials, which eliminates the stacking fault on planes $\alpha$, $\alpha'$. The process of leading partial nucleation on symmetric slip planes, stair-rod formation followed by its dissociation into trailing partials is typically shown in Fig. 4. This process continues to occur at higher strains on different planes (Fig. 3(d)) and leads to the appearance of slip lines on surface of the twinned nanopillar (Fig. 3(e)). Due to the activation of symmetric slip systems, the formation of symmetrical slip lines about TB can be seen in Fig. 3(e).

4 Discussion

The dominant mechanism of plastic deformation in perfect Cu nanopillar is through leading partial nucleation followed by twinning on two distinct twin systems $[\alpha B][\alpha]$ and $[\beta A][\beta]$. In agreement with our observations, many previous atomistic simulation studies [20, 21] have predicted twinning in $<110>$ oriented single crystal fcc metallic nanowires/nanopillars. Since the pillar axis coincides with line BA in Thompson tetrahedron (Fig. 2(e)), the Schmid factor (m) is zero on $\gamma$ and $\delta$ planes and therefore these planes were not expected to participate in deformation. Moreover, the direction DC lying on the planes $\alpha$ and $\beta$ is perpendicular to the tensile axis and the slip will not occur along this direction also. The remaining possibilities are along BD and BC on plane $\alpha$ and AC and AD on plane $\beta$, i.e., a total of 4 systems. For $<110>$ tensile axis, the Schmid factors for leading ($\alpha B$, $\beta A$) and trailing partial dislocations ($Ca$, $D\alpha$, $C\beta$, $D\beta$) are 0.471 and 0.235, respectively. Since, the Schmid factor for leading partial is higher than that of trailing partial, it is apparent that the nucleation of leading partials is easier than the trailing partials [20]. Thus, the yielding in the perfect nanopillar occurs by the nucleation of leading partials alone. With increasing strain beyond yielding, the nucleation of successive leading partials (can be called as twinning partials) on adjacent $\alpha$ and $\beta$ planes leads to deformation by twinning in $<110>$ oriented single crystal Cu nanopillar on two distinct twin systems $[\alpha B][\alpha]$ and $[\beta A][\beta]$. The deformation in Cu nanopillar containing a longitudinal TB is dominated by slip involving both leading and trailing partial dislocations. It is important to mention that the MD simulations on $<110>$ Cu nanopillar containing two and more longitudinal TBs have shown similar deformation behavior dominated by slip. Further simulations and analysis are in progress. Interestingly, no twinning is observed in Cu nanopillar containing longitudinal TBs. The observation of deformation by slip in twinned Cu nanopillar and twinning in perfect Cu nanopillar is similar to experimental results on Au nanowires [11]. In Au nanowires, the deformation by full slip in twinned nanopillar has been attributed to the pile-up of leading partials against the TB and nucleation of trailing partials on the same plane as that of the leading partials at higher stresses [11]. Following an analogy with perfect nanopillar, the trailing partial nucleation should not be observed in twinned nanopillar. However, due to the activation of symmetric slip systems, the two leading partials combine at TB to form a stair-rod dislocation, which dissociates into two trailing partials as observed in the present investigation in the twinned nanopillar (Fig. 4). In double Thomp-
son tetrahedron, these processes can be written as
\[
\beta\beta + A\alpha \rightarrow \beta\beta' \quad \text{stair-rod}
\]
(1)

The \(\beta\beta'\) changes to \(\beta'\beta\) due to twin symmetry (i.e. \(\beta\beta' = (\beta'\beta)_T\))
\[
\beta\beta' \rightarrow C\beta + \beta'C \quad \text{trailing trailing}
\]
(2)

and similarly
\[
\alpha B + B\alpha' \rightarrow \alpha\alpha' \quad \text{stair-rod}
\]
(3)
\[
\alpha\alpha' \rightarrow C\alpha + \alpha'C \quad \text{stair-rod}
\]
(4)

The above process of stair-rod formation and its dissociation into trailing partials (Fig. 4) hinders the occurrence of twinning in twinned nanopillars and effectively results in full slip as described in the following reactions in the one half of nanopillar,
\[
C\beta + \beta A \rightarrow CA \quad \text{trailing leading}
\]
(5)
\[
C\alpha + \alpha B \rightarrow CB \quad \text{trailing leading}
\]
(6)

and in other half as
\[
A\beta' + \beta' C \rightarrow AC \quad \text{leading trailing}
\]
(7)
\[
B\alpha' + \alpha'C \rightarrow BC \quad \text{leading trailing}
\]
(8)

The Burgers vector of a resultant full slip on \(\beta\) and \(\beta'\) planes (or \(\alpha\) and \(\alpha'\)) are related by a twin or mirror symmetry \((CA = (AC)_T, CB = (BC)_T)\) and they are parallel to TB that are shared by both the grains. This equivalence makes sure that both sides of the pillar deform collectively \cite{22}. In twinned Cu nanopillar, the slip occurs on four distinct slip systems, \([CB][\alpha], [CA][\beta]\) and their symmetric counterparts \([BC][\alpha'], [AC][\beta']\). The successive emission of leading partials followed by trailing partials and their escape at the free surface leads to the formation of well defined symmetrical slip steps with respect to the twin boundary on the surface of the twinned nanopillar. The observation of symmetrical slip lines is similar to that observed experimentally in micron sized Cu bicrystals \cite{22}.

5 Conclusions

Molecular dynamics simulations have been performed to understand the effect of longitudinal twin boundary on deformation behavior of \(<110>\) Cu nanopillar. The results showed that the single crystal nanopillar deforms by twinning on two independent twin systems, while the longitudinally twinned Cu nanopillar deforms by full slip with leading and trailing partial dislocations on four independent slip systems. The trailing partial nucleation in twinned nanopillar has been attributed to a novel mechanism of stair-rod formation by two leading partials followed by its dissociation. For the first time using MD simulations, the atomistic description of the effect of longitudinal twin boundary on deformation behavior of \(<110>\) Cu nanopillar has been provided.

References

[1] A.J. Cao, Y.G. Wei, Appl. Phys. Lett. 90 (2007) 151909.
[2] L. Liu, J. Wang, S.K. Gong, S.X. Mao, Sci. Rep. 4 (2014) 4397.
[3] C. Deng, F. Sansoz, Phys. Rev. B 81 (2010) 155430.
[4] C. Deng, F. Sansoz, Appl. Phys. Lett. 95 (2009) 091914.
[5] Y.T. Zhu, X.L. Wu, X.Z. Liao, J. Narayan, L.J. Kocsis, S.N. Mathaudhu, Acta Mater. 59 (2011) 812.
[6] J. Wang, H. Huang, Appl. Phys. Lett. 88 (2006) 203112.
[7] Y.B. Wang, M.L. Sui, Appl. Phys. Lett. 94 (2009) 021909.
[8] J. Sun, L. Fang, K. Sun, J. Han, Scr. Mater. 65 (2011) 501.
[9] T. Sinha, Y. Kulkarni, J. Appl. Phys. 116 (2014) 183505.
[10] D. Jang, X. Li, H. Gao, J.R. Greer, Nat. Nanotechnol. 7 (2012) 594.
[11] B. Roos, B. Kapelle, G. Richter, C.A. Volkert, Appl. Phys. Lett. 103 (2014) 201908.
[12] S.J. Plimpton, J. Comput. Phys. 117 (1995) 1.
[13] Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, J.D. Kress, Phys. Rev. B 63 (2001) 224106.
[14] J. Li, Model. Simul. Mater. Sci. Eng. 11 (2003) 173.
[15] A. Stukowski, K. Albe, Model. Simul. Mater. Sci. Eng. 18 (2010) 025016.
[16] J.A. Zimmerman, E.B. Webb, J.H. Hoyt, R.E. Jones, P.A. Klein, D.J. Bammann, Model. Simul. Mater. Sci. Eng. 12 (2003) S319.
[17] F. Hamami, Y. Kulkarni, J. Appl. Phys. 116 (2014) 033512.
[18] Z. Chen, Z. Jin, H. Gao, Phys. Rev. B 75 (2007) 212104.
[19] J.D. Honeycutt, H.C. Andersen, J. Phys. Chem. 91 (1987) 4950.
[20] H.S. Park, K. Gall, J.A. Zimmerman, J. Mech. Phys. Solids 54 (2006) 1862.
[21] C.R. Weinberger, W. Cai, J. Mater. Chem. 22 (2011) 3277.
[22] P.J. Imrich, C. Kirchlechner, C. Motz, G. Dehm, Acta Mater. 73 (2014) 240.