SciEn

Proceedings of 8th International Conference on Mechanical, Industrial and Energy Engineering 2024
02-04 January, 2025, Khulna, BANGLADESH

SciEn Conference Series: Engineering Vol. 3, 2025, pp 164-169 https://doi.org/10.38032/scse.2025.3.41

Tensile Mechanical Performance of Horizontally Twinned Al Nanopillar by Molecular Dynamics Analysis

Mohammad Samiul Hasan and Zinia Sultana Joti*

Department of Mechanical Engineering, Shahjalal University of Science & Technology, Sylhet-3114, Bangladesh

ABSTRACT

Twin boundaries are known for their strengthening influence and elevation of ductility in metallic nanopillars. They function both as a source of dislocation nucleation and as impediments to dislocation mobility. This study employs molecular dynamics simulations to examine the tensile properties, specifically strength, and ductility, of a twinned Al nanopillar featuring a horizontally orientated [111] twin boundary subjected to uniaxial tensile loading. Five models were constructed using Atomsk by varying the number of twin boundaries ranging from 1 up to 7, and an additional Al sample free of twins was also created to compare the changes in twin boundaries. The tensile deformation was performed at the room temperature using a constant strain rate of 1010 s-1 for 30 ps. From the results, the ultimate tensile strength of Al without twins was 5.72 GPa, whereas UTS increased in each model and stood at 5.91 GPa in the 7-twin model, an almost 3.5% increase. Though the yield strength peaks at 4.17 GPa in the no twin model and reaches its lowest at 1.85 GPa in the 7-twin model. The findings indicated that reduced inter-twin spacing resulted in reduced yield strength, elucidating the anomalous Hall-Petch relationship. The post-processing of the simulation data was conducted by dislocation extraction analysis (DXA) provided by OVITO.

Keywords: Molecular dynamics, Twin boundaries, Stress-Strain behavior, Tensile properties, Dislocation analysis.

1. Introduction

The physical properties of metal nanowires, a crucial component of nanoscale electronics, have been meticulously examined by nanomechanical experiments [1,2] and molecular dynamics simulations [3,4]. Understanding these characteristics is crucial for evaluating the structural strength and integrity of nanowires under different loading conditions. Molecular dynamics simulations provide exhaustive understanding into mechanical characteristics, deformation, and failure behavior through the capability of visual observation and tracking of molecular configurations. Experimental studies have demonstrated that attaining high yield strength in nanocrystalline materials tend to weaken ductility [5]. Researchers have been painstakingly seeking methods to achieve an agreement between high strength and adequate ductility [6,7]. Twin boundaries, a type of crystal defect, are undergoing vigorous study because of their capacity to markedly impact the physical properties of materials. Nano-twinned metals have attracted considerable attention due to their distinctive combinations of elevated strength along with exceptional ductility, characteristics typically regarded as incompatible. [8–10].

Studies have shown that the incorporation of twin boundaries (TBs) in nanocrystalline copper and gold materials can yield an exceptional combination of enhanced strength and excellent ductility [11,12]. Xie et al. [13] utilized in-situ experiments and atomic simulations to illustrate the increased yield strength in twinned Au nanowires, revealing that the existence of coherent TBs can alter the dominant mechanism from twinning-mediated deformation to highly localized deformation in single-crystalline nanowires. Sainath et al. [14] examined the effect of twin boundary positioning on the yield strength of copper nanopillars and showed that it considerably affects their mechanical properties. The maximum strength of nanopillars with a single twin border was reported when the boundary was centrally located.

While these findings demonstrate substantial boost in material properties with the incorporation of twin boundaries, it is important to note that certain research have established that altering the size, shape, and orientations can yield comparable improvements in mechanical properties. Zhang et al. [15] altered the cross-sectional area of Cu nanowires with twin boundaries from square to circular, resulting in the disappearance of the ultimate effect of the twin boundary in the latter configuration. Deng et al. [16] demonstrated that the interaction between nanowire diameter and twin border spacing markedly improves strain hardening. This is ascribed to the distinctive dislocation nucleation and cross-slip mechanisms at particular locations. Guo et al. [17] indicated that the TB spacing governs two competing mechanisms in the initial yield of gold NWs: the number of dislocation sources vs repulsive force, resulting in a transition from softening to strengthening, contingent upon the prevailing mechanism of plastic deformation. Song et al. [18] have shown that the yield strength of a material correlates with its dislocation storage capacity and the repulsive force between twin boundaries and dislocations. In a separate investigation, Song et al. [19] discovered that TB spacing significantly influences strength and also noted the essential TB spacing for copper nanowires.

Jonsson et al. [20] demonstrated that the dynamic strength of Al was significantly influenced by the dislocation density. It is certain that the physical properties of nanowires are significantly influenced by twin boundaries. Rahman et el. [21] demonstrated the effect of longitudinal twin

*Corresponding Author Email Address: samiulhasan823@gmail.com

boundaries on Al nanopillars. Their studies have shown that a critical twin spacing dominates the yield strength of [111] oriented Al. To date, numerous studies have investigated various face-centered cubic (FCC) metals with twin boundaries in different orientations. However, the influence of a horizontally oriented twin boundary on aluminum nanopillars remains unexplored. The primary goal of this research is to better understand how horizontally oriented twin boundaries affect the strength and ductility of aluminum nanopillars while the tension is applied perpendicularly. Furthermore, it provides insights into the role of dislocations, as seen by the dislocation density curve and its distribution throughout various stages of plastic deformation.

2. Methodology

Molecular dynamics simulations were conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [22] to analyze the tensile behavior of Al models with pre-prepared models of TBs. Atomsk [23] is a prominent software for modelling crystal structures. All samples were made using Atomsk with a lattice constant of Al set at 0.405 nm. The crystal structures are aligned along the [11-2], [-110], and [111] directions, corresponding to the x-, y-, and z-axes, respectively. The dimensions in the xy- plane are 6.94 nm and 6.87 nm, while the height along the z- axis is approximately 16.84 nm.

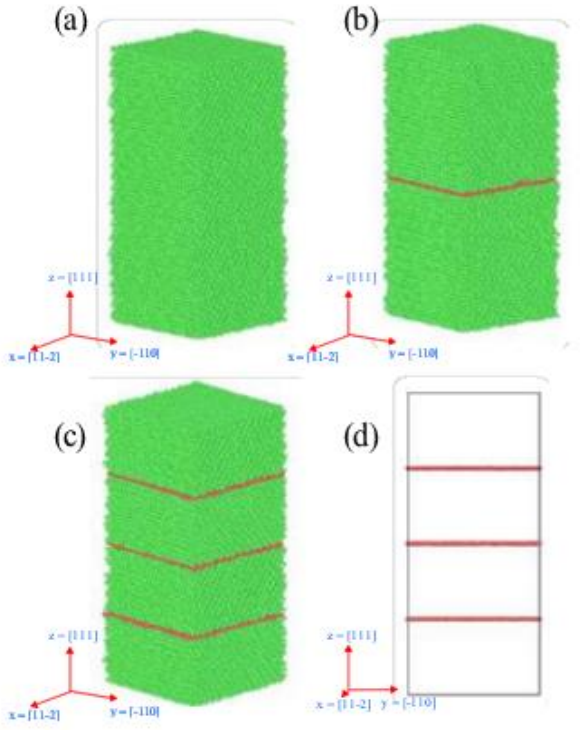

Fig.1 Atomic model of Al nano-pillars with a) no twin, b) 1 twin, c) 3 twin, d) 3 twin model without FCC atoms.

To investigate the influence of horizontal TBs on the mechanical characteristics of Al, models were developed by altering the quantity of TBs present along the [111] direction. The quantity of TBs varied at 1, 2, 3, 5, and 7 for the samples, with uniform spacing preserved across each model. Each model comprises 48,384 atoms within the simulation box. Fig.1 represents the models with no twin, 1 twin and 3 twins. The calculations of molecular dynamics simulations are heavily relied on the interatomic potential to provide validity and reliability. Therefore, this paper uses embedded-atom- all three dimensions to simulate infinitely long nanopillars. An Al sample free of any TB was also prepared with identical orientation, dimensions, and boundary conditions for comparison. The Maxwell-Boltzmann distribution was utilized for the initial velocities of the system. Before applying tension loading, energy minimization was conducted utilizing the conjugate gradient relaxation algorithm to ensure system stability and optimization, with the stopping tolerance for energy and force consistently set at 10^{-25}. Upon completion of minimization, the system was heated from room temperature to 625K for a duration of 50 ps. The process was succeeded by quenching at a cooling rate of $6.25 \times 10^{12}\ K/s$ to 300 K.

Thereafter, equilibration was conducted utilizing the canonical ensemble (NVT) and the Nose-Hoover isothermal-isobaric (NPT) ensemble at constant pressure for 50 ps. The Verlet technique was applied to integrate the motion equation using a timestep of 1 fs. The model was exposed to a tensile stress in the [111] direction, designated as the z-axis, with a constant strain rate of $10^{10}\ s^{-1}$. This strain rate allowed the simulation to run fast enough and produce the results on per with existing literature [28], thus it was selected to run all the simulation. However, as the focus of this study was not to investigate the effect of strain rate on the nanopillars no further strain rate was applied. The post-processing analysis was conducted using the visualization software OVITO [25]. Additionally, to examine the microstructure variations and dislocations generated during loading, the dislocation analysis method (DXA) [26] and common neighbor analysis (CNA) [27] were utilized.

3. Results and Discussion

3.1 Stress Strain Response

Tensile deformation simulations were conducted in order to explore the correlation between twin boundaries and the mechanical characteristics of aluminum. Fig.2 illustrates the elongation of 1 Twin model at the z axis.

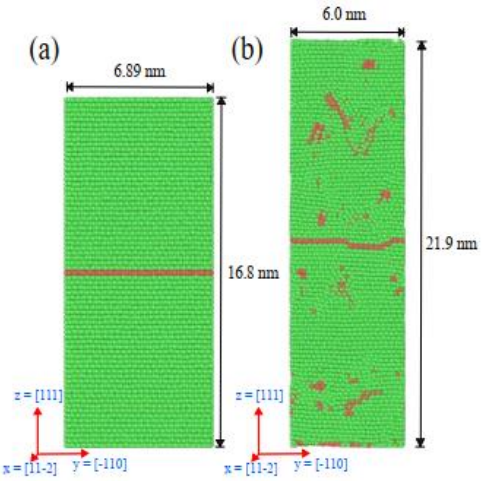

Fig.2 (a) Initial length and (b) Final elongated length

The stress-strain curves for models with various twin numbers are illustrated in Fig.3. The simulations were run at room temperature using a constant strain rate. The stress-strain curve conforms with the existing literature [28]. The initial linear segment of the curve denotes the elastic area, where the stress is proportional to the strain. This study found the Young's Modulus of single crystal FCC Al, with no

of twins, is 69.86 GPa, aligning with values documented by other researchers [28].

The calculated properties obtained from the stress-strain curve are presented in Table 1. The comparison of calculated results indicates that the total number of twin boundaries has little to no correlation with Young's Modulus. Rahman et al. [21] and Zhang et al. [29] similarly indicated that the overall number of twin boundaries is unrelated to the modulus of elasticity. The strain hardening region, when the materials deform plastically, ends when the yield strength reaches a maximum stress, also referred to as ultimate tensile strength (UTS), after which the stress reduces sharply. Because to atom rearrangements within the crystal structure and the activation of dislocations, metals in this region are unable to return to their previous shape. The necking region begins immediately following maximum strength

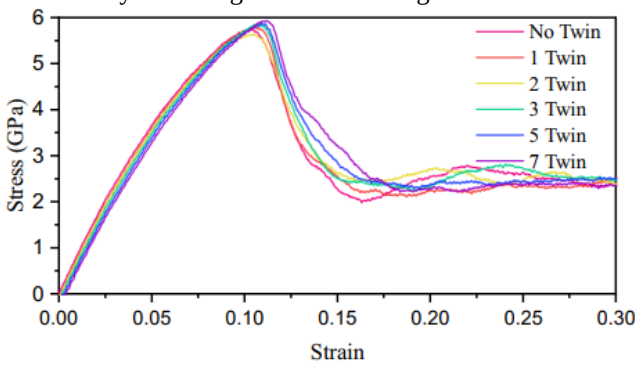

Fig.3 The Stress Strain Behavior of Al Nano-pillars under Tensile load

Table 1 indicates that the UTS increases as the twin spacing reduces with increasing twin number. In the study of twinned Cu nanowires, Sun et al showed the twin boundary spacing have an unfavorable effect on ductility and fracture behavior [30]. While this study found an increasing UTS corresponding to the number of twin boundaries, there was an inverse relation with the yield strength to twin boundary density.

Table 1: Variation of Youngs' Modulus, Yield Strength, UTS

Model	Twin Spacing (nm)	Youngs' Modulus (GPa)	Yield Strength (GPa)	Ultimate Tensile Strength (GPa)
No Twin	0	69.86	4.16	5.72
Twin 1	8.42	70.16	3.87	5.76
Twin 2	5.61	69.76	3.85	5.63
Twin 3	4.21	69.90	3.15	5.83
Twin 5	2.81	69.67	1.99	5.85
Twin 7	2.10	69.27	1.85	5.91

Although Rahman et al. [21] found Hall Petch relation using the twin spacing and the yield strength for vertically positioned twin in Al, this study with horizontally oriented twins found anomalous Hall-Petch relationship [31,32] where the yield strength decreases as the twin spacing reduces, shown in Fig.4(a). The discrepancy may be attributed to the difference in loading condition, simulation temperature and different model sizes. The characteristics of the material vary dramatically with a progression toward lower yield strength and higher UTS. As yield strength decreases, a narrower elastic zone develops that leaves the material more prone to collateral damage from shocks.

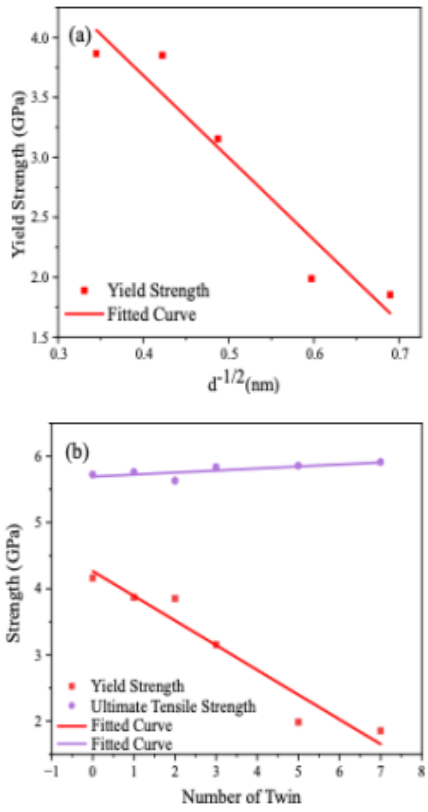

Fig.4 (a) Yield strength wrt twin spacing and (b) Relation between strength and number of twin

Conversely, the model gets more ductile as the plastic deformation region expands. This leads to improved formability, which facilitates the manufacturing process. From Fig.4(b), it can be concluded that with increasing number of twin boundaries the ductility increases. The least yield strength is found in 7 Twin boundary model where the density of the twin boundary is maximum. It is demonstrated enhanced UTS as compared to the no twin Al model. The yield behavior relies on the correlation of number of dislocations and the repulsive force generated by the twin dislocations. [17,33] Dislocation nucleated inside the twin boundaries tends to move towards it. However, the increased twin boundaries provide smaller area for the dislocation creating a blockage of dislocations by the coherent twin boundaries; this results in high tensile strength.

3.2. Dislocation Analysis

Studies have revealed that the presence of pre-existing twin boundaries in FCC nanowires led to outstanding strengthening effects [1]. Konstantic et al. [11] discovered that a decrease in twin interspacing led to a considerable increase in ultimate strength.

Using Common Neighbor Analysis and Dislocation Extraction Analysis in OVITO, the nucleation of dislocations were observed. For FCC systems, Ovito visualizes a line of dislocations, finds the Burger vectors, and finds all the defects. Shockley, Stair Rod, Hirth, Frank, and Perfect are the names of each color-coded dislocation; Ovito categorized the undetermined dislocations as "Other." Fig.5 illustrates the different types of dislocations identified by OVITO for no Twin Al nanopillar. The dislocation density was computed after the dislocation length was extracted using the dislocation extraction algorithm. During the

deformation process, dislocations circulate around the materials, resulting in an elevated dislocation density. Fig.6 demonstrates the total dislocations density in each model with increasing strain.

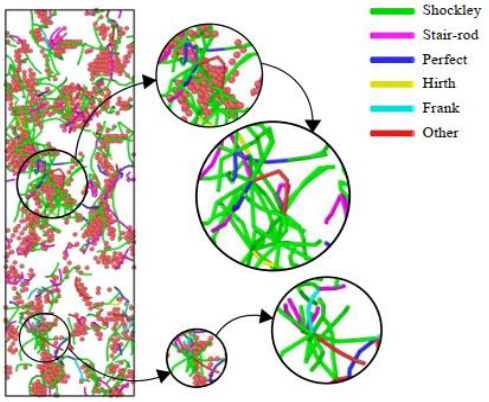

Fig.5 Atomic configuration and detailed view of dislocation distribution recognized by DXA algorithm

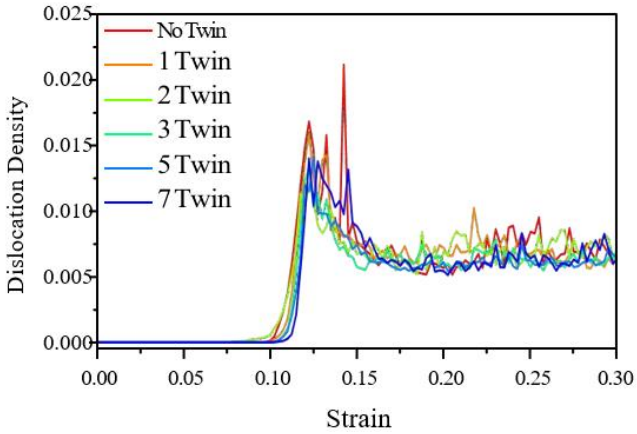

Fig.6 Variation in total Dislocation Density for all models.

During the initial stages, while the system remained within the elastic region, no dislocations were generated. Fig.6 also indicates that dislocation nucleation commences just prior to yielding and progressively escalates with strain. The evolution of different types of dislocation for each model has been demonstrated in Fig.7. Within the strain interval of 35% to 45%, stair-rod dislocations governed over other dislocation types, apart from the 2 Twin model. In pure Al free of any twin model, both Stair-rods and Shockley dislocations appeared to increase at an equivalent rate; yet the density of Shockley dislocations reached its maximum at 43% strain which displayed on in Fig.7(a).

The dislocation mechanism at the twin boundary facilitates the formation of stair-rod configurations. The increasing number of twins lowers intertwin spaces, hence impeding dislocation movement and ultimately leading to enhanced maximal strength. Fig.7(f) depicts a significantly greater density of Stair rods, yielding the highest Ultimate Tensile Strength (UTS) among all of the models. However, Fig.7(c), which indicates 2 Twin model, shows an inverse relation with dominating density of Shockley dislocations. It deviates from the other twinned nanopillar having a UTS of 5.63 GPa; which is the least value showed in this study. Three additional forms of dislocation were also documented to correlate with the increasing strain: Perfect, Hirth, and Other.

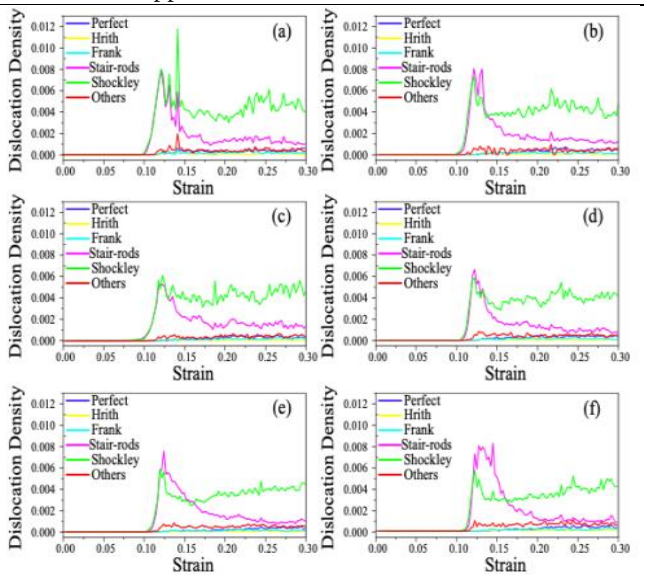

Fig.7 Evolution of different types of dislocation for (a) no twin, (b) 1 twin, (c) 2 twin, (d) 3 twin, (e) 5 twin and (f) 7 twin

3.3 Dislocation Distribution

Fig.8 shows the dislocation distribution diagrams of Al with no twin at three different strain rates: elasticity, plasticity and fracture. The dislocations begin to nucleate from the corners of the nanopillar. The dislocations converge towards the center of the pillar with the increasing strain. At this stage, the dislocations intersect with each other and forms mobile and immobile junctions. In Fig.8 at 43% strain, Shockley dislocations are forming several junctions which breaks after ultimate strength is achieved. If the dislocation density is high, the dislocation will cross each other during motion, forming a cut order, causing dislocation entanglement, which will cause obstacles to the movement of dislocations.

For twinned Al nanopillars, the dislocations start to originate around the twin boundary. Fig.8(b) shows the dislocations starts at the middle area around the twin. It should be noted that for 2 twin model, the dislocation starts at 27% strain, much earlier than the other twinned pillars, which can be inferred from Fig.7(c). For 7 Twin model, as shown on Fig.7(f), the dislocations start around 30% strain. The dislocation nucleation starts in the interspace of the twin boundary and the surface as shown in Fig.8(c).

The dislocation density develops with increasing strain up until the model attains its ultimate tensile strength (UTS). A sudden decline in the density curve in the Fig.6 takes place as a result of material failure, which diminishes the dislocation density in the graph, resulting dislocation breakage visualized in 60% strain at Fig.8.

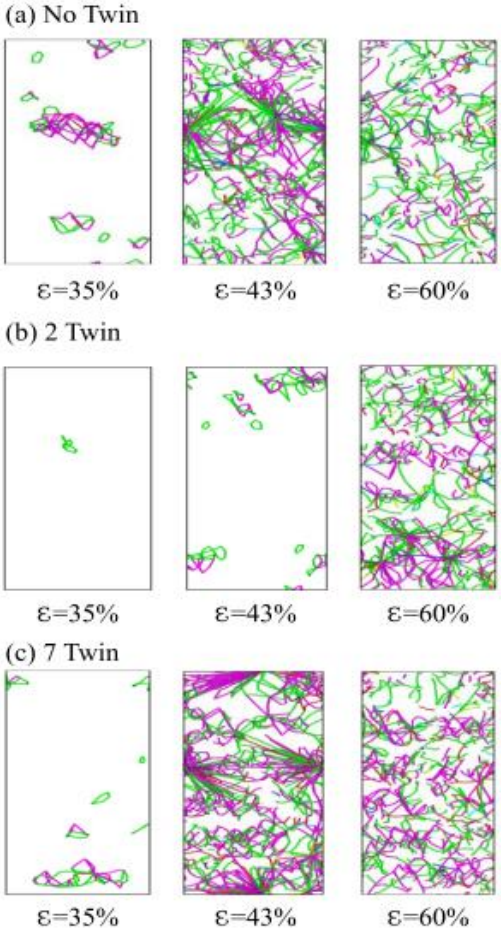

Fig.8 Dislocation distribution snapshots of Al at different strain (35%, 43% and 60%) for (a) no twin, (b) 2 twin and (c) 7 twin

4. Conclusion

This paper elucidates on the effect of twin boundary on mechanical properties of Al nanopillars at atomistic level modelling by using molecular dynamics simulations. The progression of dislocations during tensile loading deformation process, subsequent to a dislocation extraction analysis, was thoroughly studied and deliberated. The findings of this study can be conveyed as follows:

The number of TBs exhibits a positive correlation with the ultimate tensile strength, but the yield strength demonstrates an inverse relationship. Further, it has been proven that the density of TBs does not influence the modulus of elasticity, which corresponds with existing literature.

The dislocation density has been observed to be the factor contributing to the enhancement of maximum strength in the nanopillars. The deformation mainly occurs due to the high density of the Stair-rods and Shockley dislocations, which governs the ductile behavior of the twinned nanopillars.

The nucleation of the dislocations occurs around the corners of the nanopillars; an irregularity is observed in the case of 2 twin nanopillar, where the dislocations begin around the middle part. The distribution of dislocation provides information on how the dislocations breaks at necking stage. Overall, the paper sheds light on the advancement of high-performance ductile aluminum by introducing twin boundary defects in it. There are still certain aspects that require further investigation, such as the mechanical characteristics and deformation behavior under compression. A thorough investigation of these facets, however, was outside the framework of this paper.

References

[1] Wu B, Heidelberg A, Boland JJ. Mechanical properties of ultrahigh-strength gold nanowires. Nat Mater.4(7), 2005.

[2] Wu B, Heidelberg A, Boland JJ, Sader JE, Sun XM, Li YD. Microstructure-hardened silver nanowires. Nano Lett. 2006;6(3).

[3] Deng C, Sansoz F. Near-ideal strength in gold nanowires achieved through microstructural design. ACS Nano. 2009;3(10).

[4] Park HS, Gall K, Zimmerman JA. Deformation of FCC nanowires by twinning and slip. J Mech Phys Solids. 2006;54(9).

[5] Ovid'ko IA, Sheinerman AG. Mechanical properties of nanotwinned metals: A review. Reviews on Advanced Materials Science. 2016;44(1).

[6] Gall K, Diao J, Dunn ML. The strength of gold nanowires. Nano Lett. 2004;4(12).

[7] Hyde B, Espinosa HD, Farkas D. An atomistic investigation of elastic and plastic properties of Au nanowires. JOM. 2005;57(9).

[8] Lu L, Shen Y, Chen X, Qian L, Lu K. Ultrahigh Strength and High Electrical Conductivity in Copper. Science (1979). 2004;304(5669).

[9] Lu K. Stabilizing nanostructures in metals using grain and twin boundary architectures. Nat Rev Mater. 2016;1.

[10] Lu K, Lu L, Suresh S. Strengthening materials by engineering coherent internal boundaries at the nanoscale. Science (1979). 2009;324(5925).

[11] Afanasyev KA, Sansoz F. Strengthening in gold nanopillars with nanoscale twins. Nano Lett. 2007;7(7).

[12] Shen YF, Lu L, Lu QH, Jin ZH, Lu K. Tensile properties of copper with nano-scale twins. Scr Mater. 2005;52(10).

[13] Xie Z, Shin J, Renner J, Prakash A, Gianola DS, Bitzek E. Origins of strengthening and failure in twinned Au nanowires: Insights from in-situ experiments and atomistic simulations. Acta Mater. 2020;187:166-175.

[14] Sainath G, Rohith P, Nagesha A. Role of twin boundary position on the yield strength of Cu nanopillars. Comput Mater Sci. 2021;197.

[15] Zhang Y, Huang H. Do twin boundaries always strengthen metal nanowires? Nanoscale Res Lett. 2009;4(1).

[16] Deng C, Sansoz F. Effects of twin and surface facet on strain-rate sensitivity of gold nanowires at different temperatures. Phys Rev B Condens Matter Mater Phys. 2010;81(15).

[17] Guo X, Xia Y. Repulsive force vs. source number: Competing mechanisms in the yield of twinned gold nanowires of finite length. Acta Mater. 2011;59(6).

[18] Song HY, Li YL. Effect of twin boundary spacing on deformation behavior of nanotwinned magnesium. Physics Letters, Section A: General, Atomic and Solid State Physics. 2012;376(4).

[19] Song HY, Sun Y. Effect of coherent twin boundary and stacking fault on deformation behaviors of copper nanowires. Comput Mater Sci. 2015;104.

[20] Jonsson JC, Chapman DJ, Farbaniec L, Escauriza EM, Smith LC, Eakins DE. Effect of Dislocation Density on the Dynamic Strength of Aluminium. Journal of Dynamic Behavior of Materials. Published online August 6, 2024:1- 15.

[21] Rahman MM, Sakib N, Ashikuzzaman AKM, Alam MF. Vertically twinned aluminum nano-pillars under tensile loading: a molecular dynamics study. Mater Res Express. 2020;6(12):1250b4.

[22] Thompson AP, Aktulga HM, Berger R, et al. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. Comput Phys Commun. 2022;271:108171.

[23] Hirel P. Atomsk: A tool for manipulating and converting atomic data files. Comput Phys Commun. 2015;197:212-219.

[24] Mishin Y, Farkas D, Mehl MJ, Papaconstantopoulos DA. Interatomic potentials for monoatomic metals from experimental data and ab initio calculations. Phys Rev B. 1999;59(5):3393.

[25] Stukowski A. Visualization and analysis of atomistic simulation data with OVITO-the Open Visualization Tool. Model Simul Mat Sci Eng. 2010;18(1).

[26] Stukowski A, Bulatov V V., Arsenlis A. Automated identification and indexing of dislocations in crystal interfaces. Model Simul Mat Sci Eng. 2012;20(8):085007.

[27] Stukowski A. Structure identification methods for atomistic simulations of crystalline materials. Model Simul Mat Sci Eng. 2012;20(4):045021.

[28] Oliver WC, Pharr GM. An improved technique for determining hardness and elastic modulus using load and displacement sensing indentation experiments. J Mater Res. 1992;7(6).

[29] Zhang L, Xin H, Zhao D, Li Z, Ma S. Effect of Twin Boundary Density on Mechanical Behavior of Al0.1CoCrFeNi High-Entropy Alloy by Molecular Dynamics Simulation. Front Mater. 2022;9.

[30] Sun J, Fang L, Ma A, et al. The fracture behavior of twinned Cu nanowires: A molecular dynamics simulation. Materials Science and Engineering: A. 2015;634.

[31] Hall EO. The deformation and ageing of mild steel: III Discussion of results. Proceedings of the Physical Society Section B. 1951;64(9).

[32] Carlton CE, Ferreira PJ. What is behind the inverse HallPetch effect in nanocrystalline materials? Acta Mater. 2007;55(11).

[33] Chen Z, Jin Z, Gao H. Repulsive force between screw dislocation and coherent twin boundary in aluminum and copper. Phys Rev B. 2007;75(21).