Vertically twinned aluminum nano-pillars under tensile loading: a molecular dynamics study

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Abstract
Nano twinned FCC materials show superior properties comparatively to their single crystal counterparts. The properties of nano-twinned materials are possessed by the interactions of dislocations with the coherent twin boundaries (TBs). In this paper, we describe the fabrication of arrays of vertically aligned aluminum nano-pillars that contain different number of TBs (different twin boundary spacing) and no grain boundaries or other microstructural features. We have investigated the influence of twin boundary (TB) spacing on the mechanical responses of individual nano-pillars under tensile loading. The investigation fabricated with molecular dynamics (MD) simulation reveals that, the yield strength is dependent on number of vertical twins. Yield strength increases with increasing number of twins up to a critical value and then starts to decrease with further increment of twin numbers. An increase of ductility was also found as a result of immobilized dislocation. The deformation process was nucleated by spontaneous dislocation buds and eventually turned into mature partial dislocations. The simulation was done until fracture to give an insight about dislocation behavior.

1. Introduction
Nano-pillar is a type of nano-crystalline material which is extensively researched by material scientists and engineers. These types of materials have established a fundamental base for the next generation devices—as the nominal sizes of modern electronic devices continue to shrink, additionally the demand of strength and ductility continues to increase. State of the art research has been focused on the development and application of next-generation interconnects resulting in increasingly small feature sizes with high performance and greater reliability within a cost-effective manner. Meanwhile conventional lithography may have to deal with a barrier when the critical dimension approaches sub—20 nm [1]. To minimize the upper mentioned barriers, the requirement for the enhancement of mechanical properties of nano-materials for new-generation devices has raised appeal towards the twinned nanopillars. The TB influences multiple mechanical properties, crack resistance improvement [2], higher ductility [3] and enhancement in strain rate sensitivity [4]. When the inexhaustible coherent twin boundaries (CTBs) are introduced into the ultrafine-grained FCC cubic metals with low stacking fault energy, considerable plastic strain is achieved along with ultrahigh tensile strength [5–7].

A strengthening effect developed by the CTBs plays an important role as in their ultrafine-grained counterparts, but greater strength can be achieved mainly in twinned nanowires [8, 9]. By inducing orthogonally oriented CTBs in Au nanowires, the ideal theoretical strength was achieved up to 3.12 GPa [9]. Roos et al investigated the role of longitudinal TB on the deformation mechanism of Au nanowires [10] using in situ transmission electron microscopy. They observed the deposition of partial dislocation in twinned nanowires while twins and stacking faults were observed in single crystal nanowires. The transition of deformation mechanism from twinning in single crystal nanowires to slip in twinned nanowires has been accredited to the pile-up of leading partials against the TB and nucleation of trailing partials [10]. This similar transition in deformation mechanism is observed in this work.
Aluminum nanoparticles are used in many fields including dispersion strengthening, electro deposition [11], material surface coating [12], nano-composites, biomaterials etc. Through experiments along with mathematical analytical methods, researchers have demonstrated that nanowires are quite different than bulk materials regarding the structure and properties because of the effects of large free surfaces in nanomaterials. Materials containing high-density CTBs have been investigated and the findings are satisfying - high strength and hardness without any compromise of ductility, fracture toughness, thermal stability and electrical conductivity. Lu et al. investigated regarding this matter. According to their findings, the source of ultrahigh strength is the constructive blockage of dislocation motion by enormous CTBs which possesses an extremely low electrical resistivity [13].

Incorporating twin is not always the answer to increase strength since the dependency also relies on diameter and length of the nanomaterials which was investigated by Deng et al. They used Au nanopillars and the findings described that the strain-rate sensitivity above 100 K temperature is significantly smaller in twinned NWs of Au with perfectly circular cross-section than in similar NWs without twins [14]. Therefore, to predict the strengthening and other mechanical properties in twinned nanowires, the fundamental understanding on how partial dislocations nucleate from defects in lattice, twinned plane or at free surface is innumerably important. Sanzose et al. studied the effect of nano-enhancement and their explanation implies that the trailing partial dislocation initiated at the beginning stages of deformation demolishes the stable stacking fault formed by the leading partial and consequently empowers both partials to glide as a pair freely away from the nucleation sites [14].

The authors of this paper tried to organize different aspects in a successive way- from describing the simulation methodology through 2 parts: by describing the interatomic potential used and the MD model developed. The result section contains 3 major sub-sections: the ‘stress-strain behavior’ of the model under load, the variation in elastic modulus and maximum strength, the atomic level observation of fracture process. Considering above mentioned different parameters, our investigation was inclined to search for a simple question- how Al nano-pillars containing vertical TBs behave under tensile load. Furthermore, we tried to shed some light on fracture mechanism while the number of twins held as a satisfactory variable.

2. Simulation methodology

2.1. Interatomic potential
MD simulations have been accomplished in LAMMPS package [15] employing an embedded atom method (EAM). LAMMPS uses techniques of spatial decomposition of simulation domain and a message-passing technique [15]. The potential for FCC Al is taken from Mendelev and Kramer [16]. The EAM potential’s validity may be judged by its accuracy with actual experimental data. This potential reproduces melting point and liquid structure accurately. Apart from these properties, this potential is used to find out the crystalline properties which is a major cornerstone of this study. This potential is developed for improving the harmony with the first-principles calculations and new experimental measurements were performed to have reliable results using x-ray diffraction method. Furthermore, liquid-phase diffusivities were calculated to find its correlation with liquid structure which gave satisfying result. This potential was successfully employed to investigate the tensile behavior of Al nanopillars with vertical twins. The post processing operations were undertaken by utilizing OVITO [17].

2.2. Molecular dynamics model
The dimension of the four models under experiment is constant which is 8.3 nm × 8.3 nm × 54.1 nm having a square cross-section. Size is one of the major parameters to accurately simulate dislocation as it interferes on the fracture mechanism of nano-materials. The only variable is the number of vertical TB and that is 0, 1, 2, 3, 4, 5 and 8 respectively. The simulation box contains 243000 atoms. The tensile load is applied on the [1-10] orientation which is considered z axis. The x and y axes are [112], [111] respectively. The twin is created along [111] direction which is visualized in figure 1. For simulating infinitely long nanowire, periodic boundary condition is maintained along the z axis where the load is applied and other two directions are kept independent. From finite temperature Maxwell distribution, the initial velocities were chosen randomly. After the construction of nanowires, minimization of energy was performed by conjugate gradient method to obtain stability in the nanostructures by setting stopping tolerances for force and energy 10⁻¹⁰⁰ and 10⁻¹⁰⁰ respectively. Thermal equilibration at 10 K temperature in canonical ensemble (NVT) was imposed after the energy minimization of the nano-pillars. The model was equilibrated to constant energy for 50 ps. The temperature recalibration was done after every 1 fs. The nano-pillars were equilibrated to constant pressure for 100 ps with a Nose-Hoover isobaric-isothermal (NPT) ensemble. Integration of equation of motion was done by Verlet algorithm with a time-step of 1 fs. After equilibration, a constant strain rate of 3 × 10⁸ s⁻¹ with respect to
the initial box size was applied in the direction of \( z \) axis. The strain rate was much higher than average experimental strain rate, owing to the MD simulation timescale limitations. While straining, the pressure development on the other two orthogonal directions were maintained zero. Dislocation Extraction Algorithm (DXA) was employed to analyze the dislocations, Burger vector of each dislocation type, junctions and their successive line representation [18].

3. Result

3.1. Stress-strain behavior

Engineering stress-strain (\( \sigma - \varepsilon \)) curves of nanotwinned Al nano-pillars with different number of TBs are shown in figure 2 under tensile loading at 10 K temperature. In order to construct the stress-strain curve, the stress is calculated using the virial theorem which is commonly used in MD simulations [19]. All the curves in figure 2 show an abrupt drop of stress after reaching the peak stress (it is defined as yield stress) without considering the variation in TB spacing. Peak stress is the onset of plastic deformation and divides the curve into elastic and plastic deformation region. In the elastic deformation region stress-strain relationship is linear due to the fact

![Figure 1. Atomic model of Al nano-pillars with (a) no twin, (b) one twin, (c) two twin (d) five twin boundary at the initial stage of the tensile loading. This figure is generated using DXA analysis of OVITO.](image-url)
that the atoms of the crystal structure are just flexing. But after the yield point, it starts to deform plastically as the atoms in the crystal structure starts to take a new position relative to each other due to the mechanism of dislocation activation.

3.2. Variation in elastic modulus and yield strength

The modulus of elasticity (i.e. Young’s modulus) is calculated using data points of the elastic region, where the stress-strain curves are linear. Young’s modulus of FCC Al nanopillar without any vertical twin is 74.24 GPa. Meanwhile W.C Oliver found the modulus of elasticity for bulk Al approximately 68 GPa by performing experiments whereas the theoretical value is 70.4 GPa [20] which is less than the current simulation result. The prime reason behind that is the fewer number of surface defects in nano range compared to the bulk material. Therefore, the modulus of elasticity is compatible with the experimental and theoretical values obtained.

The values obtained in this study for modulus of elasticity and yield strength are given at table 1. From the table, it is obvious that there is no significant change in Young’s modulus for the Al nanopillar models with TBs. So, it can be concluded that, there exists no relation between TB spacing and modulus of elasticity as CTBs alter neither modulus nor coherency stress in the neighboring lattice as a highly coherent interface.

The strain at which the sudden drop occurs has been considered as strain to yielding. From the data it can be interpreted that by incorporating TB in Al nanopillars, the strength can be increased which is similar to the experiment orchestrated by Sun et al [21].

From figure 3 it is clear that TB inclusion increases the yield strength of the Al nanopillar upto a certain value, as infinitely strong material cannot be produced. The twin spacing for which the twinned Al nanopillar has the highest yield strength is called the critical twin spacing. After this critical twin spacing, yield stress starts to decrease. 1.66 nm is observed as the critical TB spacing.

| Model   | Young’s modulus (GPa) | Yield strength (GPa) | Strain to yielding (%) | Twin spacing (nm) |
|---------|-----------------------|----------------------|------------------------|-------------------|
| No Twin | 74.24                 | 6.17                 | 8.28                   | 0                 |
| 1 Twin  | 73.39                 | 6.59                 | 9.30                   | 4.15              |
| 2 Twin  | 73.62                 | 6.72                 | 9.39                   | 2.76              |
| 3 Twin  | 73.42                 | 6.75                 | 9.42                   | 2.08              |
| 4 Twin  | 73.64                 | 6.84                 | 9.54                   | 1.66              |
| 5 Twin  | 73.49                 | 6.79                 | 9.51                   | 1.38              |
| 8 Twin  | 73.23                 | 6.57                 | 9.21                   | 0.92              |

Figure 2. The stress-strain graph of Al nano-pillars with and without twin boundaries under tensile loading.

Table 1. Variation of Young’s modulus, Yield strength and Strain to Yielding of the Al nanopillars.
From the plotted data, by fitting a curve we find the Hall-Petch \([22, 23]\) relation as follows-

\[
\sigma_y = 6.19 + \frac{0.828}{\sqrt{d}}
\]

where, \(d\) is in nm and \(\sigma_y\) is in GPa.

The mechanism underlying this strengthening effect of Al nanopillar with vertical TBs is, TBs act as a barrier to dislocation nucleation and dislocation propagation. Using the configuration force resulting from the mismatch of material properties in TB, the interaction between TBs and dislocation can be described \([24]\). This repulsive force which is exerted by the TB to the dislocations moving towards the TB \([25]\), helps to increase the yield strength of nanotwinned material by hindering the glide of dislocations. As a result, dislocations are piled-up and stored inside the twin spacing until it can overcome the repulsive force and can glide through the TB. Variations in TB spacing change the room for dislocation storage and the magnitude of the repulsive force. Decrement in twin interspacing increases the repulsive force and dislocation nucleation sites which result in a dramatic increase in material strength and hardening at the nano-scale \([26]\).

As the twin spacing is reduced below a critical value i.e., into the inverse Hall-Petch regime, the yield strength decreases as there does not exist enough space for dislocation pile-up resulting in the diffusion of the TBs \([27]\).

In contrast, in the twin-free nanopillar steps and jogs are created by the dislocation glide, which are the preferential sites for necking phenomenon \([3]\). From the above investigation, it may be concluded that the TBs can promote high strength and high ductility. Therefore, controlled deformation mechanism regarding the twinned structure has the potential to develop a stronger nanomaterial with improved ductility.

### 3.3. Atomic-level observations of fracture process

The atomic level observations are displayed in figure 4, which visualizes the fracture behavior of the perfect Al nanopillars. It is understood that the nano-pillar yields by nucleation of four leading partials from one of the corners of pillar, followed by another fracture plane from a contemporary nucleation development at figure 4(b). After sufficient rise in yielding the stacking faults transform into twins by the nucleation of Shockley partials on adjacent plane successively.

From figure 3(c), it can be seen that with previously developed twin, another plane of faults arises creating a triplet, which are completely parallel to each other. Deformation process is absolutely dominated by the nucleation and fully development of twins on different planes.

The atomic level observations, displayed in figures 5–7, visualize the fracture behavior of the Al nano-pillars containing TBs 1, 2 and 4 respectively. The twin nano-pillars yield by the nucleation of leading partials from the corners of the planes.

In figure 5(a), the two nucleation sites are developed in the Al nano-pillar model with single twin followed by several other nucleation development while straining further.

In figure 6(a), the nucleation of leading partials is developed in the bottom corner which causes the yielding in nanopillar model with two twins. In figure 7(a), the nucleation of leading partials has several dislocation multiplication sites which result in yielding of nanopillar with 4 twins. The matured dislocations result in a
twinning development among themselves and it’s visible in the atomic structure. With increasing deformation, leading partials originate from both the surface and TB. These leading partials approach to TBs from both sides and get combined to form stair rod $\frac{1}{6}[110]$ dislocation upon the TB shown in figures 5(b), 6(b), 7(b) respectively marked with red circles.

Stair-rod (immobile dislocations) along with TB hinders the movement of leading partials (mobile dislocations), which increases the flow stress. That’s how the dislocations pile-up in between two successive TBs and resist the motion of mobile dislocations which eventually results in increased flow stress. The observed flow stress for different models with different TBs can be presented in the order of ‘4 twin > 3 twin > 2 twin > 1 twin > no twin’.

It is observed that, the fracture mechanism for nanopillars with more than 4 vertical TBs is completely different from the nanopillar models with less than 5 vertical TBs. In figure 8, partial dislocations are formed from the surface followed by the propagation to the TBs. A lot of interaction points between partials and TBs are...
observed in figure 8(b). In some of that interaction points, partial dislocation migration happened instead of deformation twinning. This phenomenon causes the decrement of flow stress after critical twinning space.

4. Conclusion

To unveil the effect of TB on Al nanopillars, MD simulations have been performed. Although similar studies were performed for Fe, Cu, Ni and some other alloys, the increasing application of Al in nanotechnology and materials science makes the current study demanding. The main conclusion can be summarized as below

- The deformation mechanism is mainly caused by twinning in the twin free single crystal Al nanopillar.
In the twinned nanopillars of Al, the deformation process mainly occurs due to leading partial dislocations. As the twin planes hinder the growth of dislocation, the number of dislocations play a crucial role on yield strength, elastic modulus and flow stress.

Although this study fulfills its objectives, there are some other aspects to continue the corresponding research. For instance –

• The mechanical behavior of twinned Al nanopillars subjected to various temperatures.
• The influence of twin orientation on the deformation mechanism.
• The mechanical behavior and deformation mechanism of the nanopillars if subjected to compression.

A detailed study on twinned Al nanopillars is beyond the framework of this paper.

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