Molecular dynamics simulations the effect of temperature on the plastic deformation mechanism in aluminum single crystal

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Abstract: Molecular dynamics simulations are performed to investigate the effect of temperature on the plastic deformation mechanism in aluminum single crystal. It is found that as temperature increases the Yield strength and Young’s modulus of the aluminum under compressive and tensile strain will reduce. Moreover, it is found that the higher temperature is, the easier the dislocation emission is. Under compressive strain, the proportion of 1/6<112> Shockley type of dislocations to total dislocations is found to increase with the temperature increasing. It is also found that only a large amount of dislocation occurring incipiently the strength of the material can be yield.

1. Introduction
The generation and quantitative analysis of dislocation are particularly important for the study on mechanical properties of materials when an external force acts on it [1-3]. The emergence of dislocations, as well as the dislocation types, is influenced by many factors, such as temperature, grain boundaries, secondary phases, vacancies and the mode of external force. Many researchers have kept paying attention to the effect of temperature on generation and evolution of dislocation [4]. For example, a tensile test was performed at different temperatures ranging from 1 to 600 K to assess the yield strength and Young’s modulus of copper-silver nanocomposites. In this study dislocation extraction analysis was implemented to reveal the temperature-based underlying mechanism of plastic deformation [4]. On the other hand, limited researches are reported to study how temperature, at the atomic scale, affect the mechanical properties of materials by the generation and evolution of dislocation in aluminum in detail. In present work, molecular dynamics simulations were employed to investigate the temperature-based plastic deformation mechanism under uniaxial compression/tension in aluminum single crystal.

2. Theory and Method
In this work, the Embedded Atom Model (EAM) potential was utilized to describe the interaction between aluminum atoms. In this method the total energy of a monoatomic system is represented as

$$E_{tot} = \frac{1}{2} \sum V(r_{ij}) + \sum F(\rho_i)$$

(1)
Here $V(r_{ij})$ is a pair potential as a function of the distance $r_{ij}$ between atoms $i$ and $j$, and $F$ is the "embedding energy" as a function of the host "density" $\rho_i$ induced at site $i$ by all other atoms in the system. The unstable stacking fault energy is a crucial parameter of the barrier for partial dislocation nucleation [5]. Thus, the EAM potential employed for atomistic simulations must accurately reproduce pertinent features of the resulted energy curves, especially the unstable stacking fault energy [6]. The accurate characterization of the dislocation nucleation and interaction relies on a qualified EAM potential [7]. The potential for aluminum reported by Mishin et al. [8] describes the characterization of the dislocation nucleation and interaction well and has been widely used for simulation research [7]. Hence, the EAM potential [8,9] for aluminum is chosen in this work to carry out the simulations.

All simulations were performed using the Large-scale Atomic/Molecular Massively parallel simulator (LAMMPS) code [9] developed by Sandia National Laboratory. The calculated supercell containing 256000 atoms with size of $80a_0 \times 80a_0 \times 10a_0$ was built and periodic boundary conditions were applied along $<100>$ (X), $<010>$ (Y), $<001>$ (Z) directions. In order to study the temperature effect on plastic deformation mechanism, simulations were carried out at different temperature of 300, 400, 500, 600, and 700K. The temperature controlling was realized via Nose-Hoover thermostat [10]. According to LAMMPS user manual, the Nose-Hoover thermostat could bring the undesirable oscillation of pressure and temperature to the simulated system [7]. Thus, the uniaxial compressive or tensile simulation can be performed at expected temperature and pressure at a certain rate. In all simulations, energy minimization is realized by the conjugate gradient algorithm to minimize the energy of the simulation system, followed by relaxation to achieve an equilibrium state. Based on above, the compressive or tensile strain were loaded as the increase of time steps along $<100>$ (X) direction, the strain rate ($2e9/s$), within the scope of general adoption and applied in previous work [11-13], was employed in this work. The analysis works were implemented by OVITO software package. Using the OVITO software package, the dislocation extraction algorithm (DXA) developed by Stukowski and Albe [14] was employed to identify the nature of the dislocations, such as the type of dislocations and the dislocation density.

3. Results and Discussion

In order to investigate the effect of temperature on the mechanical properties under uniaxial compression and tension, the curves of stress-strain at different temperatures of 300K, 400K, 500K, 600K, and 700K are shown in Fig.1. According to the presented results in Fig.1 (a), all the stresses at various temperatures have a peak (Yield Point) with the compressive strain loading. At $T=300K$, the compressive strain at Yield Point is about 0.1, and the compressive stress is 6.27GPa. At all considered temperature, the compressive stress increases linearly from the start of the compressive strain loading to the Yield Point and then has a rapidly decline. For uniaxial tension, the similar variation trend is also found. The difference is that the tensile stress and the tensile strain corresponding to the Yield Point are larger than the compressive stress and the compressive strain in magnitude. At the atomistic scale, the Yield strength is defined as the stress corresponding to the Yield Point. Also, the Young’s modulus can be obtained via the slope of linear section of the stress-strain curve at low strain stage. As shown in Fig.1, the Young’s modulus and Yield strength both decrease with the temperature increasing. The Young’s modulus was calculated to be 64.7GPa at 300K, it decreases by 14.5% and drops to 55.3GPa as the temperature rises to 700K. Under compressive strain loading, the Yield strength decreases from 6.27GPa to 4.4GPa as the temperature rises from 300K to 700K. The situation for tensile loading is from 7.7GPa to 4.8GPa. The weakening effect of temperature on the Young’s modulus and Yield strength was also found in Cu single crystal and Cu/Ag nanocomposites in previous works.
Fig. 1 The curves of stress-strain under uniaxial compression and tension at different temperatures of 300K, 400K, 500K, 600K, and 700K.

Fig. 2 Snapshots obtained from (a) compressive and (b) tensile MD simulations at 300K, where the different types of dislocations lines, including screw and edge, at strain of 0.15 are shown. The Green, blue, purple, yellow, and cyan lines are for 1/6<112> Shockley, 1/2<110> Perfect, 1/6<110> Stair-rod, 1/3<001> Hirth, and 1/3<111> Frank dislocations, respectively. The red lines are for other types of dislocations.

As the strain is loaded to the Al, the emergence of dislocation marks the beginning of the strain hardening region. When the strains are loaded continuously the stress increases linearly and reaches an ultimate strength and then the stress drops down rapidly, as shown in Fig. 1. This leads to the yield of strength in the Al. If the strain is not unloaded at this situation the stress will change to keep a stable level (see Fig.1). In fact, during the deformation there are large of dislocations occurring. For example, at strain of 0.15, the distribution of total dislocations in compressed and stretched aluminum single crystal are shown in Fig.2 (a) and (b), respectively. Under a big strain, the dislocations move, accumulate, and interact into net-like structure, as shown in Fig. 2. The similar case is also reported by Kardani et al. [15]. From Fig. 2 it can be seen intuitively that the 1/6<112> Shockley types of dislocations account for a large proportion, while the 1/2<110> perfect types only have a small part. This may be attribute to a most common dislocation reaction (1/2[110] → 1/6[211] + 1/6[121]). As well known, Al is a fcc crystalline where a 1/2[110] perfect dislocation often is produced firstly and then the perfect dislocation is easy to dissolved into two partial dislocations of 1/6[211] and 1/6[121] under a deformation. This also explain why 1/6<112> Shockley types of dislocations occupy a large proportion in a deformed Al crystaline. The existing of a large amount of 1/6<112> partial dislocation in Al also indicates that the 1/6<112> Shockley types of dislocations have a most stable structure in fcc aluminum under external force, as compared with the other types of dislocations. In addition, it is worth noting that the aluminum single crystal under tensile strain loading has a smaller total dislocation density than the compressed one at the strain of 0.15. The total dislocation density at different temperatures was analyzed to investigate the temperature effect on plastic deformation. Fig. 3
shows the variation of total dislocation density vs compressive/tensile strain at different temperatures. For all the conditions of the temperatures it is found that the total dislocation density increases slowly at a small amount level at its incipient deformation stage, and then suddenly increases at its slightly later deformation stage. We call this point as transition point later, where dislocation density varies from slowly to fast with the strain increasing. Compared Fig. 3 with Fig. 1, we can see that the point of strength yield (shown in Fig. 1) is just corresponding to the transition point of variation of dislocation density vs. Strain. This indicate that a large amount of dislocation occurring incipiently the strength of the material can be yield. When such a strain is not unloaded the dislocation density continuously increases till a maximum value and then it falls down rapidly and converges to a stable value as shown in Fig. 3. From Fig. 3 it can be seen that at the incipient and rapidly taking off stages (strain is smaller than 0.10 and 0.14 for compressive and tensile load, respectively) of dislocation concentration increasing, the dislocation density increases with the temperature increasing, while at the convergence stage (strain is larger than 0.11 and 0.15 for compressive and tensile load, respectively) the dislocation density decreases with the increasing of the temperature. Perhaps, it is due to that a higher temperature can provide a larger thermal activation energy and more vacancies for dislocation emission at the former two stages [15,16]. While at the stable stage of the variation of dislocation density vs. strain, the higher temperature, in turn, perhaps is benefit to weaken the resistance of dislocation slipping and make it easier for the annihilation of dislocations [17]. In this situation the dislocation density reduces with the increasing of temperature, as shown at the final stage of variation of dislocation density vs strain in Fig.3. By comparing Fig 1 with Fig 3, it can be seen that the strains corresponding to Yield Point in Fig.1 is identical to the ones where the variation of dislocation density vs. strain takes off incipiently and rapidly in Fig.3. This indicates that only the dislocations accumulate to an enough amount, the yield of a stress in a material takes place.

![Fig.3](image1.png)

**Fig.3** The variation of total dislocation density at different temperatures with (a) the compressive and (b) the tensile strain.

![Fig.4](image2.png)

**Fig.4** The variation of the strain at transition point with the temperature during the compressive/tensile strain loading.
As we know, the large amount of dislocations to form incipiently is a sign of the beginning of strain strengthening. As presented in Fig.3, the strain for the dislocation forming incipiently at large amount is seriously affected by temperature during the compressive and tensile loading. In order to describe this variation trend more clearly and intuitively, the strains, where the dislocations form incipiently at large amount, at the temperatures from 100K to 800K are calculated and shown in Fig.4. It is seen that at the point (we call it transition point, where an amount of dislocations form incipiently) the compressive strain is smaller than the tensile strain at a certain temperature. Due to the higher temperature provides larger thermal activation energy and more vacancies, at the transition point the compressive strain and tensile strain both decrease with the increasing temperature. Moreover, the tensile strain decreases linearly with the temperature increasing while the compressive strain decreases nonlinearly with the temperature increasing.

Conclusion
Molecular dynamics simulations are performed to study the temperature-based effect on plastic deformation mechanism in aluminum single crystal. The Yield strength and Young’s modulus are assessed in the temperature range of 100K-800K. It is also found that they both decrease with the increasing temperature. Based on the analysis of dislocations at different temperatures, it is also found that temperature can promotes the dislocation emission and reduce the strain at the transition point. The compressive strain at transition point has a nonlinear decline, while the tensile strain decreases linearly with the temperature increasing. In turn, at a larger strain loading a high temperature goes against accumulation of dislocations. Moreover, the proportion of 1/6<112> (Shockley) type of dislocations to total dislocations is found to increase as the temperature increasing.

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