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Molecular dynamics simulation of tensile deformation of nano-single crystal aluminum

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Abstract

In order to research the mechanisms of tensile deformation at nanometer, molecular dynamics (MD) was employed to simulate the tension process of nano-single crystal aluminum (Al) under different temperatures. The results show that the stress–strain curves decrease after a linear increase up to the maximum abruptly because the first transition from elastic to plastic deformation and the slip take place. Then the multiple slips on the (1 1 1) planes continue to occur after the yield. At last, the plastic deformation causes ductile shear fracture. Atomistic simulations of tension at nanometer give results that agree with the phenomenological attributes of plasticity observed in macroscale experiments. The lower strain rate results in the lower yield stress. The tensile strength decreases at higher temperatures.

Keywords: Molecular dynamics; Tensile deformation; Single crystal aluminum

1. Introduction

Now the emergence of nano-electro-mechanical systems (NEMS) [1] and the development of micro-electro-mechanical systems (MEMS) are urgently required to understand the micro-mechanism of materials deformation behavior at nanometer level. In addition, the micro-structural elements used in micro-electro-mechanical systems (MEMS) are almost devoid of defects [2]. So an investigation of the deformation and fracture process of defect-free materials at nanometer level is indispensable. While tension tests are very common in determining the mechanical properties at macrolevel, such tests at nanoscale are extremely difficult, if not impossible to realize. An alternative approach is molecular dynamics (MD) simulation.

At present, MD simulation has been proposed to study the micro-mechanism of tensile deformation at nanometer. Sasaki et al. [3] adopted the two-dimensional L–J potential to simulate the tensile deformation of α-Fe single crystal under a constant tensile stress. The temperature was controlled by the velocity scaling method and the comparison of deformation mechanisms with or without temperature scaling was investigated. The simulation results showed that brittle fracture started at a notch in the plane perpendicular to the direction of stress. And if no scaling was used, the temperature of the crystal increased during the deformation showed that plastic deformation would occur at the slip plane. The L–J potential was also used to investigate the tensile deformation of some single crystals by Lynden-Bell [4–6]. The results showed that the failure of crystals was due to the void deformation and their growth to nanocracks. Doyama [7] studied the tensile deformation of single crystal Fe and Cu under a constant tensile strain by N-body potential. The free boundary condition was adopted and one notch was designed at the outer surface in the middle of model. They found that notch was the source of crack because of stress concentration. To investigate the effect of different boundary conditions on tensile fracture process, Kitamura et al. [8] used EAM potential to simulate the tensile deformation of single crystal Ni under two boundary conditions: (1) periodic boundary condition and (2) transverse constraint condition. The tensile strain was loaded on boundary atoms and the temperature of total model was controlled at 0 K. The results showed that if tension with constraint of transverse deformation, a cleavage crack initiated and brought brittle fracture. The constraint changed the fracture mode. Heino et al. [9,10] conducted MD simulations of tension on single crystal Cu for different orientations. The differences between the calculated and experimental tensile moduli were reported to be in

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the range of 2–6%. Hu et al. [11] used MD simulation to investigate the effects of different model sizes, boundary conditions, crystal orientations and load speeds on tensile deformation of single crystal α-Fe. Makarov et al. [12] compared the simulation results of tensile deformation and fracture at micro-, meso- and macrolevels. MD simulation was adopted at nanometer level and the elasto-plastic behavior of monocrystals at different orientations was simulated. Komanduri et al. [2] conducted MD simulation of uniaxial tension of some single crystal cubic metals using Morse potential. The boundary was flexible and only the temperature of boundary atoms was controlled. The necking was observed in the simulation. Moreover, Tersoff-type potential was selected to simulate uniaxial tension of two semiconductor materials Si and Ge [13]. The results showed that no necking was found.

The above studies show that the tensile deformation of single crystals at nanometer can be quite different from what continuum plasticity predicts. However, this simple loading configuration, namely nominal uniaxial stretching of a crystal, has generated many uncertainties. Although above simulation models were close to the true system, the load ways were far from the real load. Moreover, the temperature of simulations was almost at 0 K, few simulations of tension process were conducted at different temperatures.

In this paper, molecular dynamics simulation was employed to research the tensile deformation behavior of nano-single crystal aluminum at three different temperatures (10 K, 300 K and 800 K). The velocity scaling method was adopted to keep the temperature of system. Then the mechanisms of tensile deformation of nano-single crystal aluminum at different temperatures under nanometer were analyzed.

2. Model and method of molecular dynamics simulation

2.1. Potential and simulation method

The Morse potential was adopted in the simulation, the potential energy between atom i and j is

$$u(r_{ij}) = D[\exp\{-2\alpha(r_{ij} - R)\} - 2\exp\{-\alpha(r_{ij} - R)\}] \quad (1)$$

where r_{ij} is the distance between particles i and j, the parameters D, α and R are determined by fitting to experimental data of the equilibrium lattice parameter, cohesive energy and bulk modulus of aluminum featuring near-neighbor interactions. The parameters are $D = 0.2703$ eV, $R = 3.253$ Å and $\alpha = 1.650$ Å^{-1}.

After the potential function is determined, the molecules force F_{ij} is given as the derivative of the potential energy, namely

$$F_{ij} = -\frac{\mathrm{d}u(r_{ij})}{\mathrm{d}r_{ij}} \quad (2)$$

The potential interaction is truncated smoothly at a distance of $2.5R$. The time step used in the simulation is 1 fs. The algorithm adopted is velocity Verlet method. The details of the velocity Verlet method see Ref. [14]. The temperature is controlled by the velocity scaling method. For details of the temperature control see Ref. [14].

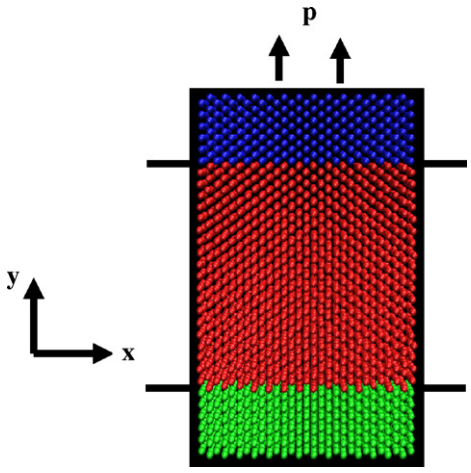

Fig. 1. Initial atoms configuration of nano-single crystal Al.

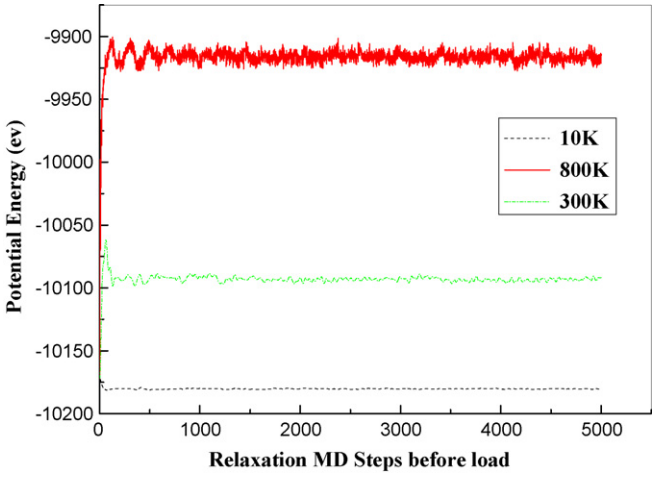

Fig. 2. Potential energy variation during relaxation before load at different temperatures.

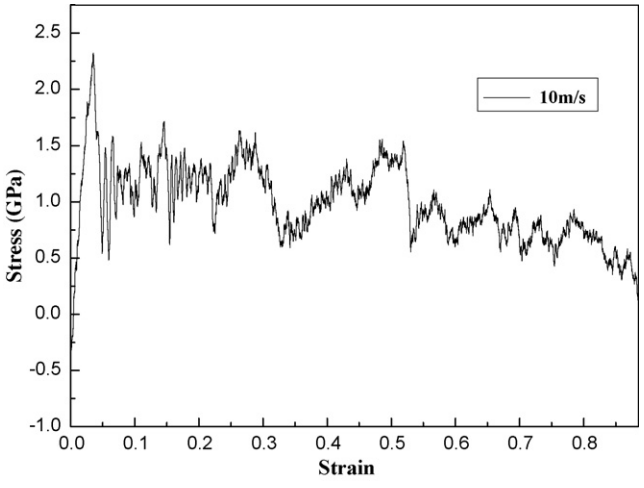

Fig. 3. Stress–strain curve of the tensile deformation of nano-single crystal Al at 300 K and 10 m/s loading rate.

2.2. Model of tensile deformation

The initial atomic configuration of nano-single crystal aluminum is arranged with the ideal lattice as shown in Fig. 1. The total model consists of two parts. One part is designed to as the active zone in which the atoms move according to the interatomic potentials; another part is designed to as the boundary zone where the positions of the atoms are given by the prescribed boundary conditions. A periodic boundary condition is imposed along the z-direction to simulate plane strain conditions. In both x, y directions, the periodic boundary condition is not adopted. The crystal orientation was [1 0 0, 0 1 1, 0 $\bar{1}$ 1]. In order to simulate uniaxial tensile loading in the y-direction, the lower end of the specimen is fixed, and a constant velocity increment is applied to all atoms in the upper end block. In order to avoid the shock which would be induced into the block of material because of the high strain rates, the interior atoms in the model were also given an initial y-velocity that varied linearly from 0.0 to the prescribed velocity at the top atomic plane depending on their y-coordinates in the simulation box. Following initialization, a constant number of atoms, constant volume and constant energy (NVE) simulation was performed with a 1 fs time step until the block of atoms had undergone stain sufficient to create yield and fracture.

Fig. 2 shows atoms potential energy of the system after 5000 molecular dynamics steps at three temperatures (10 K, 300 K, 800 K). As shown in Fig. 2, the systems are stable after 500 molecular dynamics steps under three temperatures. When the

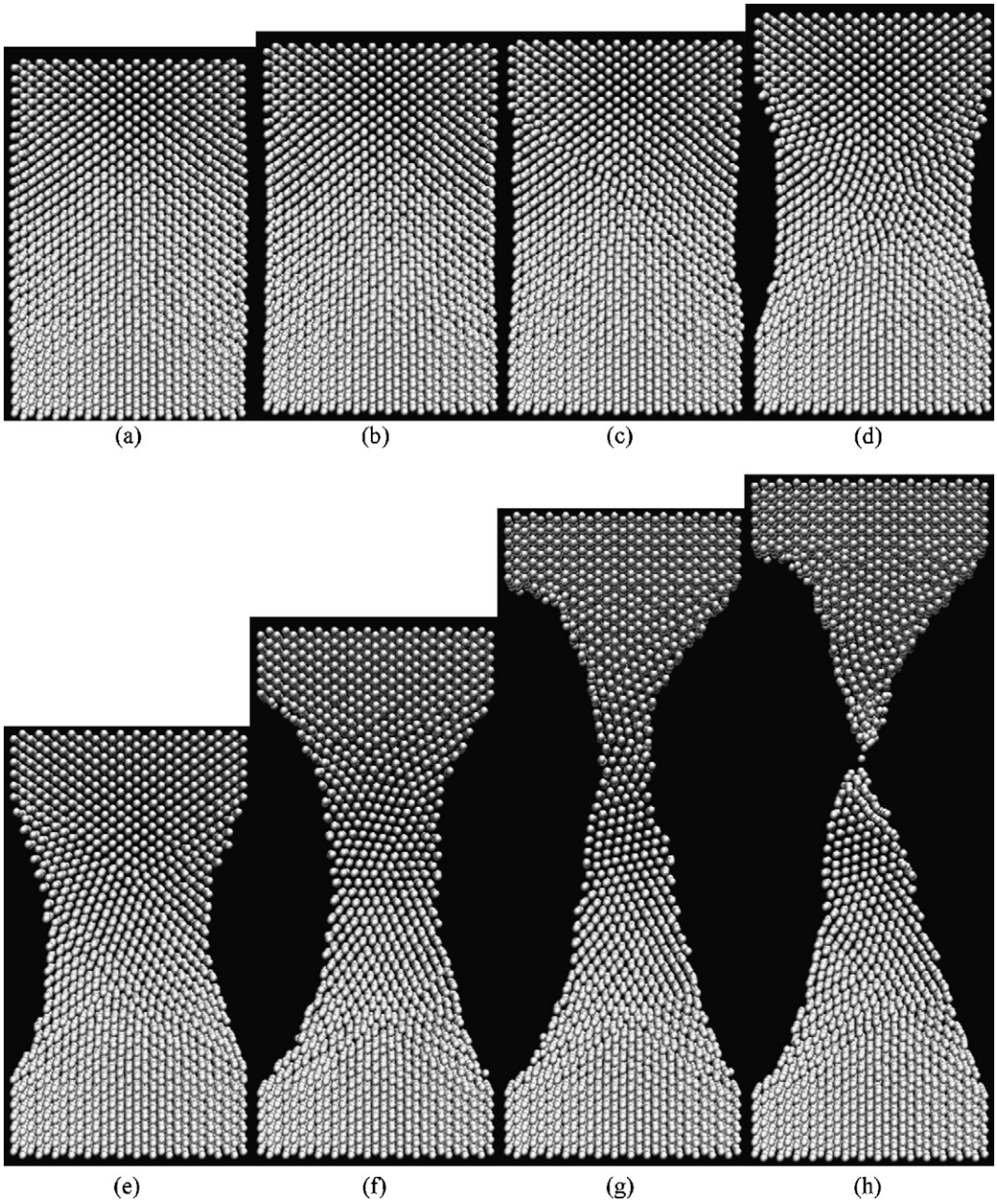

Fig. 4. Snapshots of atomic configurations of nano-single crystal Al at 300 K and strain rate of 10 m/s. The configurations presented correspond to the following strain: (a) 0, (b) 0.035, (c) 0.040, (d) 0.10, (e) 0.17, (f) 0.46, (g) 0.78, (h) 0.89.

system is stable, the potential energy value fluctuates at the equilibrium value.

3. Results and discussion

3.1. Stress–strain curves at 300 K and loading rate 10 m/s

The details of the solution of atomic stress see Ref. [15]. In order to investigate the mechanisms of tensile deformation at nanometer, Fig. 3 presents the stress–strain curve of nano-single crystal Al at 300 K and strain 10 m/s. After relaxation the symmetry of the surface atoms was broken to lead to the surface tension, so the atoms stress when there is no external load is not zero. The deformation is elastic in the initial stage of tensile deformation of nano-single crystal aluminum. The stress rises linearly to the maximum with the strain. The maximum stress is 2.30 GPa at strain of 0.035. Then the stress decreases suddenly, the tensile deformation is in the flow of plasticity. The phenomena can be attributed to the first transition from elastic deformation to plastic deformation. The yield stress of 2.30 GPa, obtained from the stress–strain curve, is far above that of experimental bulk Al. This great difference can be attributed the experimental bulk samples have defects, such as dislocations, voids, and impurities which are advantageous for the deformations process. However, this value is good agreement with the ab initio calculation of Al perfect shear stress. With the further tensile, the stress drops abruptly to 1.57 GPa at strain of 0.040 and the stress–strain relations display a zigzag curve as the strain is increased. When the strain reaches 89%, the stress is close to zero, which means a breaking of the nano-single crystal aluminum.

3.2. Atoms snapshot of tensile deformation

To visualize the process of tensile deformation of nano-single crystal aluminum at 10 K and strain 10 m/s, the snapshots of atoms rearrangements are as shown in Fig. 4. After relaxation, the atoms arrange very regularly as shown in Fig. 4(a) when there is no strain load. Then after the crystal stretches to strain of 0.035 (the peak point of stress–strain curve), the deformation of nano-single crystal aluminum is elastic as shown in Fig. 4(b). When the crystal stretches to strain of 0.040, the first dislocation moves out free surface to create a slip step as displayed in Fig. 4(c). Then dislocations continue to occur and move, propagate, and slips take place with the strain as shown in Fig. 4(d). Fig. 4(d) also shows that the multiple slips on the (1 1 1) planes continue to occur after the yield and the neck appears. From the stress–strain curve, the plastic deformation takes place with the strain. Then the deformation concentrates in the neck region as shown from Fig. 4(e) to (g). At last, the plastic deformation causes ductile shear fracture as shown in Fig. 4(h). From Fig. 4, the tensile mechanisms at nanometer of atomistic simulations give results that agree with the mechanisms of plasticity observed in macroscale experiments.

3.3. Strain rate effects

To study the effects of different strain rates on the tensile deformation at nanometer, Fig. 5 shows the stress–strain

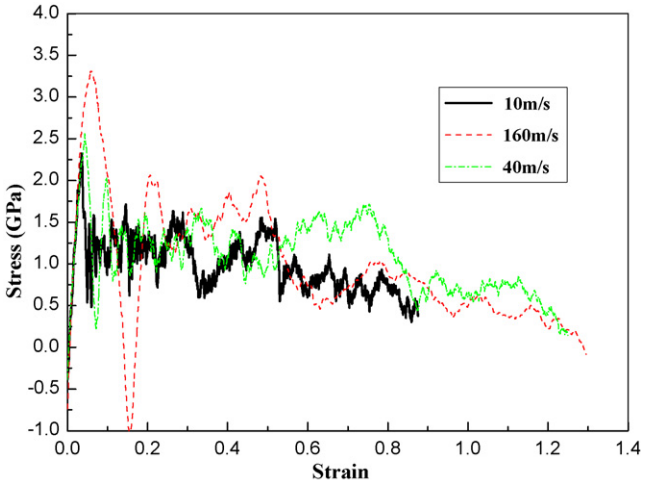

Fig. 5. Stress–strain curves of tensile deformation at different loading rates (10 m/s, 40 m/s, 160 m/s) at 300 K.

curves at 300 K and different strain rates. For all the strain rates employed, the stresses increase linearly with the strain. Below the elastic limit, the stress–strain curves for the three strain rates are different. This implied that the strain rate has effect on the elastic properties of nano-sinlge crystal Al. For the strain of 10 m/s, the first peak of the stress, namely the yield stress is 2.30 GPa at the strain of 0.035, the strain of 40 m/s and 160 m/s, the yield stress is 2.50 GPa and 3.29 GPa (at strain of 0.044 and 0.059), respectively. So we can get the conclusion that atomistic simulations of tension at nanometer give results that agree with the phenomenological attributes of plasticity observed in macro-scale experiments. The lower strain rates results in the lower yield stress.

3.4. Tensile deformation at different temperatures

This section considers the influence of temperature upon the deformation of nano-single crystal aluminum under tension at nanometer. Fig. 6 presents the variation in stress with strain

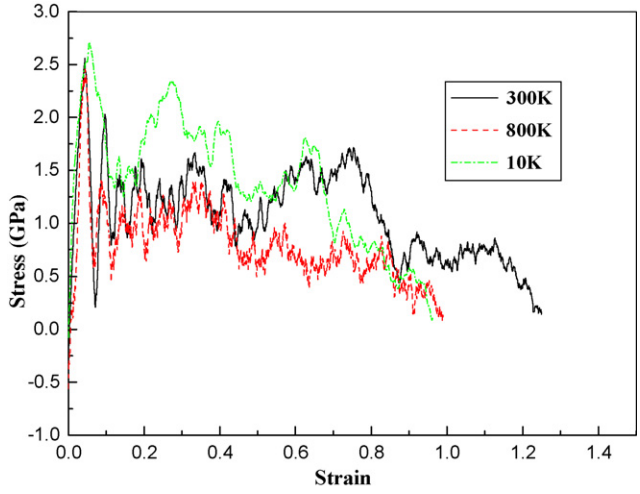

Fig. 6. Stress–strain curves at different temperatures (10 K, 298 K, 800 K) and 40 m/s loading rate.

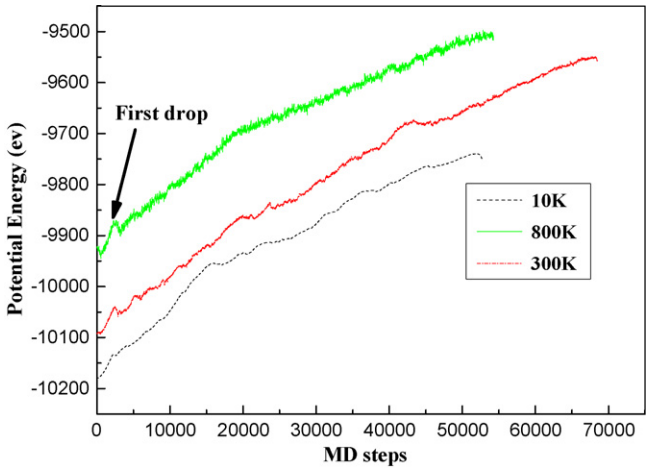

Fig. 7. Potential energy of tensile deformation at different temperatures (10 K, 298 K, 800 K) and 40 m/s loading rate.

at different temperatures and 40 m/s loading rate. The results demonstrate that the tensile strength decreases at higher temperatures. At 10 K, the tensile yield stress is 2.70 GPa at 0.053 strain. But at 300 K, the tensile yield stress is 2.56 GPa when the strain is 0.041. At 800 K, the tensile yield stress is 2.39 GPa when the strain is 0.044. These results clearly demonstrate that tensions at nanometer agree with the temperature effects of plasticity observed in macro-scale experiments. The thermal effects play an important role in tensile deformation of nano-single crystal aluminum at nanometer. The tensile strength decreases at higher temperatures.

3.5. Potential energy curves at different temperatures

Fig. 7 shows the potential energy curves of tensile deformation of single crystal aluminum at different temperatures and 40 m/s loading rate. The potential energy rises linearly in the elastic deformation stage. Then the potential energy drop abruptly like the stress–strain curves. The first drips in potential energy around 1800–2600 steps in each temperature indicate that the first dislocation forms. It is obvious that higher temperature makes it is easier for the dislocation to form.

4. Conclusion

In this study, MD simulation has been employed to investigate the high speed tension process of nano-single crystal aluminum at nanometer. The present study demonstrates the success of modeling in reproducing the essential mechanisms of plasticity and damage on the atomic scale. Based on the above research, the following conclusions can be drawn:

1. The employment of a Morse potential is seen to be able to render an elastic, plastic and fracture behavior for the model crystal under consideration.
2. The stress–strain curves of tensile deformation of nano-single crystal aluminum decrease abruptly because the first transition from elastic to plastic deformation and the first slip take place. Then the multiple slips on the (1 1 1) planes continue to take place after the yield. The plastic deformation causes ductile shear fracture.
3. Atomistic simulations of tension at nanometer give results that agree with the phenomenological attributes of plasticity observed in macroscale experiments. The lower strain rate results in the lower yield stress. The tensile strength decreases at higher temperatures.

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