A Study on Damping Properties of Cu based on MD

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Abstract: This paper mainly focuses on the damping properties of Cu by simulations based on molecular model of Cu crystal. Through LAMMPS molecular dynamics software, tensile and compressive simulation is carried out. The mechanisms of energy dissipation and damping properties of material are investigated on the molecular level. Hysteretic curve is obtained from the simulation results. In loading process, as shown in the result, energy begins to dissipate when the load reached to the point that crystal produces defects such as dislocations. Then more energy is dissipated along with the dislocations breaking away from the pinning position. Further simulation is carried out, a model of Cu crystal with a crack is established to perform tensile simulation. Result shows that the dislocations are susceptible to crack, which makes crystal have a better damping capacity.

Key-Words: *Damping Properties, Dislocation, Energy Dissipation, Hysteretic Curve, Molecular Dynamics*

1. Introduction

Over the last decades, molecular dynamics (MD) simulation has emerged as a powerful method to develop materials by postulating that material properties are difficult or costly to study experimentally. In MD, macroscopic material properties are aggregations of atomic interactions and dynamics. Many properties, such as energetics, diffusion, crack formation and propagation, the impact of vacancy or atom defects and the load-bearing capacity can be better understood through simulation [1].

The damping mechanism of material is studied during the process of its vibration deformation. It is discovered that before the macroscopic yield stage, with the increase of the strain amplitude, the damping capacity can be divided into four stages: resonated damping during dislocation elastic deformation, static hysteresis damping during dislocation break loose pinning (slip breeding), dislocation line entwisted and the slip band generated [2].

2. Method

Models of Cu crystal is built in LAMMPS molecular software, and tensile and compressive dynamics simulation is performed. The phenomena shown in OVITO visualization software. The hysteretic curve is drawn and energy dissipation is calculated by using ORIGIN.

2.1 Pair potentials

Pair potentials are defined as potentials between atoms pairs that are within a cutoff distance and the set of active interactions typically changes over time. The pair potentials is calculated by the Embedded Atom Method（EAM）.In this method, every atom is considered to be embedded in the electron background density constituted by all other atoms of the system [3]. EAM computes pairwise interactions for metals and metal alloys. The total energy Ei of an atom I is given by

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta(\tau_{ij})\right)+\frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(\tau_{ij}) \qquad (1)$$

2.2 Calculation models of Cu

Two models which including a perfect crystal and a crystal with a crack are built, as shown in Figure 1. The boundary is periodic in the x direction, and non-periodic and shrink-wrapped in the y and z direction.

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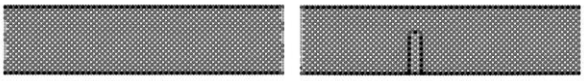

Figure 1 Perfect crystal model and crystal with a crack model

3. Result

The curve of tensile process on perfect crystal modal is drawn, analysis of each of its phases shown as Figure 2.

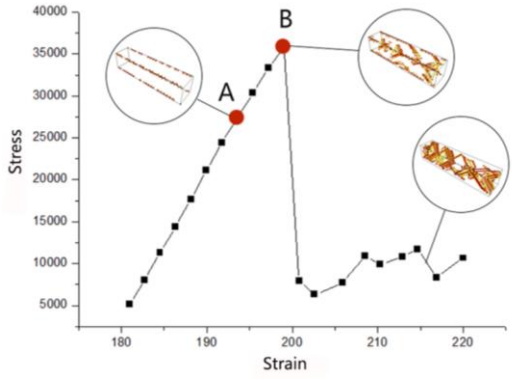

Figure 2 The perfect crystal tensile process curve

No defects appear before point A which is elastic deformation stage. The crystal produce vacancy defects at point A and begins to dissipate energy, and then it produce dislocation defects at point B after which the stage is called yielding deformation stage. With the increase of deformation, more energy is dissipated along with the dislocations breaking away from the pinning position.

Using the crystal after point B, cyclic strain simulation is carried out. The hysteretic curve shown as Figure 3. The yielding deformation stage can be found.

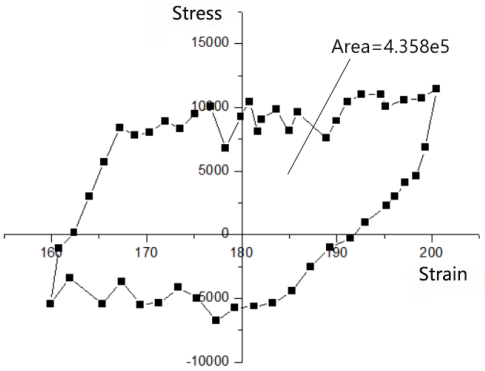

Figure 3 The hysteretic curve of crystal with defects

The model of Cu crystal with a crack is used to perform tensile simulation. The tensile curve that compared with which drawn by perfect crystal is shown in Figure 4.

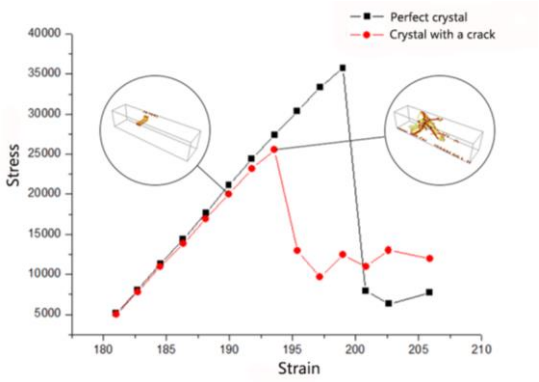

Figure 4 The stretching process curve of perfect crystal and crystal with a crack

Figure 4 shows that the crystal with a crack gets into yielding deformation stage earlier, and the dislocations appear around the crack.

4. Conclusion

According to the simulation results, the conclusion can be described as follows.

(1) In the tensile process, the crystal begins to dissipate the energy when it produces defects such as dislocations.

(2) In the yielding deformation stage, energy dissipated along with the dislocations breaking away from the pinning position.

(3) The dislocation is susceptible to crack, which makes crystal have a better damping capacity.

References:

[1] Ocaya R O, Terblans J J. C-language package for standalone embedded atom method molecular dynamics simulations of fcc structures[J]. Softwarex, 2016.

[2] Mi L, Tian T, Tan W. Damping Characteristics of Magnesium Alloy and Its Testing[J]. Journal of Vibration Measurement & Diagnosis, 2010, 30(1):75-77.

[3] Yin Y, Takahashi K, Yuan X, et al. Dimer Reference Embedded Atom Method (DR-EAM) and Its Application to Vacancy Formation Energy of FCC Metals[J]. Quarterly Journal of the Japan Welding Society, 2005, 23(23):509-514.