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Microscopic damping mechanism of micro-porous metal films

Guangyu Du[a,*], Zhen Tan[b], Zhuolong Li[a], Kun Liu[a], Zeng Lin[a], Yaoshuai Ba[a], Dechun Ba[a]

[a] Key Laboratory of Vibration and Control of Aeronautical Equipment, Ministry of Education, Northeastern University, Shenyang, 110819, China
[b] Shenyang Radio and TV University, Shenyang, 110003, China

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ABSTRACT

Metal thin films are used widely to solve the vibration problem. However, damping mechanism is still not clear, which limits the further improvement of the damping properties for film and the development of multi-functional damping coating. In this paper, Damping microscopic mechanism of porous metal films was investigated at both macroscopically and microscopically mixed levels. Molecular dynamics simulation method was used to model and simulate the loading-unloading numerical experiment on the micro-pore and vacancy model to get the stress-strain curve and the microstructure diagram of different defects. And damping factor was calculated by the stress-strain curve. The results show that dislocations and new vacancies appear in the micro-pores when metal film is stretched. The energetic consumption from the motion of dislocation is the main reason for the damping properties of materials. Micro-mechanism of damping properties is discussed with the results of in-situ experiment.

1. Introduction

On account of the enhancement of modern mechanical power and speed, the reduction of material reliability caused by harmful vibration of mechanical components has become an important factor for limiting the mechanical development [1,2]. Films and coatings, such as metal films and ceramics coatings, are used to solve vibration problems in the aerospace and other fields due to their good strength, hardness and damping properties. People pay more attention on the influence of microscale changes mechanical properties of material [3].Some of changes can be tested by the method of experiment [4]. However, their damping performance is hard to be explained because small defects are difficult to be observed. Therefore, the numerical simulation of metallic materials has attracted researchers' attention [5–7].

According to the results of Tracy et al. [8], there are many defects in the film. The damping properties of the material under external load are affected by internal defects which cause the energy consumption by the redistribution of atoms in the stress field and lead to additional strain. David R. Clarke et al. [9] demonstrated that the increase of micro-pores is conducive to the improvement of the damping performance of the coating. F. Kroupa and J. Plesek [10] also believe that intra-splat cracks inside the coating is the main source of external energy consumption and supply for damping. In fact, it is easy to find micro-defects, such as micro-cracks and vacancies on copper films prepared by magnetron sputtering. However, it is difficult to observe the change of them during the loading experiment process which is important for understanding the damping law. For that matter, it has been an important trend to understand the changes of the microscopic mechanism of materials through computer simulation [11]. Through the finite element computer simulation method of micro-mechanics, Rashid K [12] found out that the damping performance can be improved by increasing the cracks and controlling the size of them. However, the mechanistic analysis is not enough, such as the explanation of the changes of the micro-cracks and the interdependence of various microcosmic defects on the damping performance because of the scale problem. The molecular dynamics simulation method analyzes the effect of atomic motion and interaction on the model at the atomic scale so that the problems can be avoided effectively. This paper analyzes the copper film with microcosmic defects by molecular dynamics simulation and in-situ tensile-unloading experiments. The damping mechanism of the metal thin film is discussed in order to provide the basis for the research on damping technology of metal thin film.

2. Molecular dynamics simulation

2.1. Model details

The molecular dynamics model was founded by LAMMPS software. Fig. 1 (a) shows integrate copper model with the size of $40a \times 12a \times 8a$ (a is lattice constant, $a = 3.615$ Å). Interaction

* Corresponding author. Northeastern University, NO. 3-11, Wenhua Road, Heping District, Shenyang, China.
E-mail address: gydu@mail.neu.edu.cn (G. Du).

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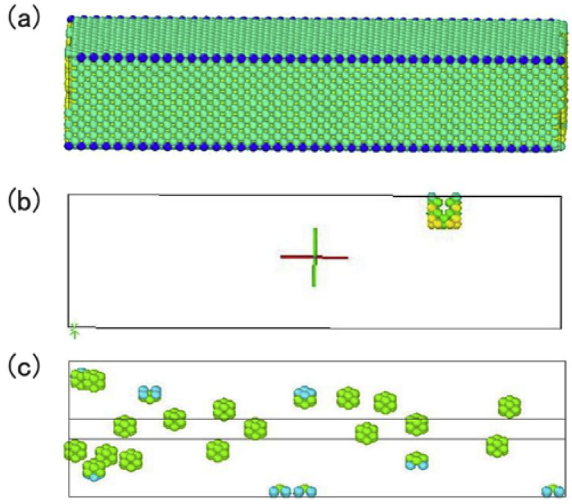

Fig. 1. (a) Integrate Copper Model, (b) Micro-pore Model, (c) Vacancy Model.

between atoms is embedded atom potential (EAM), which was improved by Mishin et al. [13]. Thermodynamic ensemble was regular ensemble (NVT). The boundary condition was periodic-shrink-shrink (PSS) with unidirectional loading direction for the periodic boundaries and free boundary for others.

The atoms of model was marked by the coordination number(CN) with different color. The CN of integrate model atom is 5 and 12, which the atom with 5 at the edge of model (blue atoms). The structure surrounded by atoms with other CN can be judged as defect structure. Hiding the atom of CN 5 and 12 so that the variation of defect micro -structure can be observed by the change of CN color. More exactly, the defects of model can be judged by the locate variation of atom related with the defect.

In this simulation, micro-pore model and vacancy model were studied as a classical defect model. For micro-pore model, the atoms of 1α × 1α × 1α(x(30 31), y(10 12), z(4 5)) were deleted based on the integrate model, as shown in Fig. 1(b). Fig. 1(c) shows vacancy model. 0.2% atoms of full model was deleted by LAMMPS and multiple honeycomb spot defects with a diameter of 2 nm were established.

The balance of the energy was broken because of deleting of atoms. The energy minimization method was used for rebuilding the balance to avoid the influence on initial energy of model. The time-step was 0.02 ps, the relaxation time was 100 ps, and convergence constant (ε) was 10^{-12}eV.

2.2. Simulation details

The Nose-Hoover thermostat was used to maintain the temperature at a constant value of 1 K for excluding the influence of molecular thermal motion in the model [14,15]. Numerical experiments were implemented by stress-displacement control. The load was applied at both sides of the model in the direction of [0 0 1], strain rate was ± 0.001/ps, the load amplitude was 2.8×10^{-8}mm and time step was 1 fs. The step of loading and unloading was both 10000. Fig. 2 shows the stress-strain (σ-ε) curve of integrate copper model. During the loading process, the strain increases from 0 to 0.01 and the step is 100000. The model experienced elastic deformation, and the stress increased linearly with the increase of strain following Hooke's law, the elastic limit reaches at 6.59 GPa. After reach the elastic limit at strain of 0.080, the stress remain stable due to the scale of model. Regardless of the elongation of the sample along the direction of stretching, there is no new defects structure appeared and the micro-structure of model keep stable. In the process of unloading, the stress-strain curve is nearly superposed by that of the loading one. Strain energy stored during loading can be completely released in unloading process. The results of

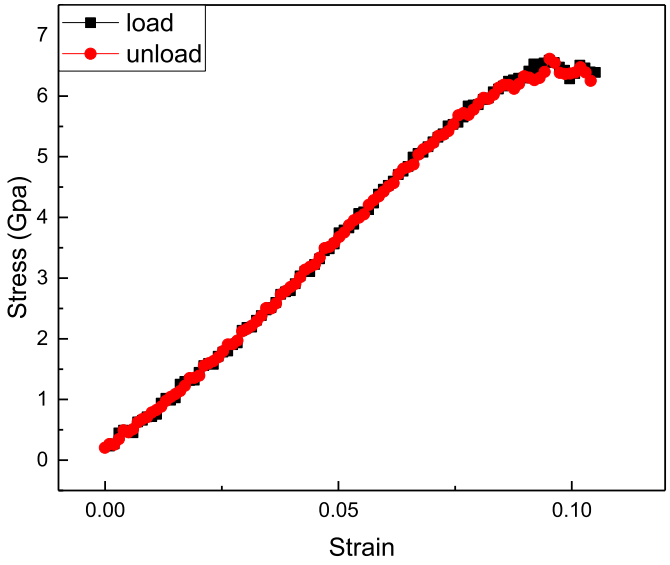

Fig. 2. Strain-stress curve of integrate copper model.

the model are suitable to the theory, which also means the model is correct.

2.3. Results and discussion

Fig. 3 shows Micro-configuration diagram and stress-strain curve of Micro-pore Model in loading and unloading process. Loading process is from (P-A) to (P-C) in Fig. 3. According to Fig. 3(b), strain increases from 0 to 0.08 and stress increases linearly from (P-A) to (P-B). The maximum stress is 5.98 GPa at the strain of 0.008(point B). After that, stress declined to 4.03Gpa rapidly. The color of atom CN showed that dislocations appear around the micro-pores at the point P-B. At Point P-C, the end of the loading, there are a large amount of dislocations in the model with slight moved, which has been approved as the resource of energy consumption according to many researches [16]. From Fig. 3(P-D) and (P-E), the dislocation is almost unchanged during the process of unloading until the strain comes to zero. Only some point defects disappeared. Therefore, the effect of micro-pores on the consumption of the energy is to form dislocation structure [17]. This is a reason for the damping properties of copper film.

Damping properties were evaluated as the difference between the mechanical work provided by the external loading on the model and the distortion energy released during unloading, displayed as the shaded part of Figs. 3(b) and 4(b). Damping factor Q^{-1} can be calculated by Formula (1).

$$\begin{aligned} \Delta W &= \oint \sigma d\varepsilon \\ W &= \int_{wt=0}^{\omega t=\pi/2} \sigma d\varepsilon \\ Q^{-1} &= \frac{1}{2\pi} \cdot \frac{\Delta W}{W} \end{aligned} \tag{1}$$

Fig. 4 shows the micro-configuration diagram and stress-strain curve of vacancy model in loading and unloading process. The micro-cosmic evolution is similar to that of the micro-pore model. There are flocculent vacancies until Period V-B, but they disappear in the process of unloading. And the Q^{-1} of vacancy model is 0.5304, slightly increased compared with 0.5216 of micro-pore model.

23 atoms were deleted from integrate copper model in both models. Micro-pore can be deemed to be defects concentration. On the contrary, vacancy can be regarded as defects dispersion. Therefore, appropriate defect concentration is conducive to enhancing the damping properties of materials. On the one hand, in the process from B to C, transition in the micro-structure occurred in both models. It can consume loading energy to render the material damping properties. On the other hand,