Molecular dynamics simulation of lattice vibration and elastic properties in nanoparticles

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Abstract. Elastic response and atomistic vibration of these materials are simulated by means of molecular dynamics simulation. The embedded atom method potential for copper is used to express the interaction of atoms. About 37000 atoms are contained in a simulation system. As an initial condition, atomic systems are kept in high temperature molten states (1800 K), and the systems are quenched to 0 K and relaxed to make a particle of amorphous state. The particle of crystalline state is also produced by slowly cooling the molten particles. The structure of the systems is examined through the cross sectional view and the radial distribution function. An Elastic sinusoidal displacement are applied and the vibration of atoms are monitored. Propagation of phonons thorough the nanoparticles is also simulated.

1. Introduction
Recently, strongly enhanced thermal conductivity of fluids containing nanoparticles has been discovered and attracting varieties of interests in the fields of fundamental science and engineering application. These fluid is called as ‘nanofluid’[1-3]. To investigate the mechanism of heat conduction in nanofluid the knowledge of phonon properties and phonon propagation in nanoparticles is essential.

The molecular dynamics simulation is one of the most useful methods in the study of dynamics of disordered and nanomaterials and it can be used in the study of phonons in nanoparticles. A complete atomic configuration at every time steps can be monitored during simulation. We have been developing a simple functional form for the EAM potential [4]. The potential function has successfully been applied on the simulation of the defects [5-7] and the phonon propagation [8]. Then, it can be applied on the present study.

2. Method of simulation
Molecular dynamics simulation has been performed by using an EAM potential. Potential functions are developed by the present authors. The potential energy for $i$-th atom is expressed as

$$E_i = F\left(\rho_i\right) + \left(1/2\right) \sum \phi\left(r_{ij}\right)$$

where $F(\rho_i)$ is the embedding energy for $i$-th atom, and $\rho_i$ is the electron density function, which is a sum of the density of the neighbour atoms labelled by $j$. These are expressed as

$$F\left(\rho_i\right) = D \quad \rho_i \ln \rho_i$$

(2-a)
\[ \rho_i = \sum f(r_{ij}) \] (2-b)

and \( \phi(r_{ij}) \) is the two body interaction between atom \( i \) and \( j \). The functional forms of \( \phi(r_{ij}) \) and \( f(r_{ij}) \) are

\[ \phi(r) = A (r_{c1} - r)^2 \exp(-c_1 r) \] (3)

\[ f(r) = B (r_{c2} - r)^2 \exp(-c_2 r) \] (4)

where \( r_{c1} = 1.6 \ r_0 \) and \( r_{c2} = 1.9 \ r_0 \) are the truncation distance of the potential, and \( r_0 \) is the nearest neighbour distance. The Potential parameters for Cu are determined to reproduce the material properties such as the cohesive energy, the elastic constants, and vacancy formation energy [4].

The time interval \( \Delta t \) for the simulation is chosen to be \( 1 \times 10^{-15} \) s, which is about \( 1/100 \) of the period of the maximum atomic vibrational frequency. Initially atoms were arranged in fcc crystalline structure surrounded by \{110\} surfaces. Then the sample temperature was increased up to 1800 K. The crystalline and amorphous specimens were produced by slow cooling and rapid quenching of the samples, respectively. The surface morphologies and the radial distribution functions (RDF) for these samples are shown in Figure 1. Larger area of the crystalline sample is seen to be surrounded by \{111\} surfaces, which has lowest energy in fcc structures. The RDF shows sharp peaks for fcc structure. On the other hand, surface of amorphous sample is disordered and RDF peaks are not sharp. The split second peak is characteristic to the amorphous structures.

**Figure 1.** Surface morphology and radial distribution function for polycrystalline (a) and amorphous sample (b).
Figure 2. Time variation and power spectrum for polycrystalline (a) and amorphous sample (b). A and C are atoms near the center and B and D are atoms on the surface of samples.

3. Results and discussion

3.1. Damping of elastic vibration

An initial elastic strain was applied and released and motion of individual atom was monitored.

\[ u = A \cos \left( \frac{2 \pi x_i}{L} \right) \]  

where \( x_i \) is the x-coordinate of \( i \)-th atom, and \( L \) is the diameter of the nanoparticle. Two atoms are chosen to monitor the elastic vibration. One is located near the center and the other is on the surface of nanoparticles. An example for the vibration of atom in nanocrystalline sample is shown in Figure 2 (a), and in amorphous sample is shown (b). In the figures curves shown by A and C are data for atoms near the center, and B and D are for atoms on the surfaces. The power spectra for these vibrations are also calculated and shown in the right of each figure. The vibration of center atoms in polycrystalline and amorphous samples are compared. Oscillation is quite irregular in polycrystalline sample. Reflection of wave by grain boundary in the sample is anticipated. On the other hand the oscillation is periodic and gradually damping away in the amorphous sample. A sharp peak is seen around 0.6 THz in the power spectrum of amorphous sample. The peak is broad and continues to higher frequency in the data of polycrystalline sample.

3.2. Propagation of atomic vibration

As a next step of the simulation initial velocity is given to atom A and C, and the propagation of ‘hot atom’ is monitored. Here, ‘hot atom’ is defined as that the magnitude of vibrational velocity is larger than the environmental atom. Cross sectional views for the distribution of hot atoms in polycrystalline
Sample are shown in Figure 3. By a rough estimation the size of the region occupied by hot atoms seems to be proportional to $t^{1/2}$. The mean velocity of each atom consisting nanoparticle is plotted as a function of distance from the center. The spatial distribution of mean velocity shows exponential character. The results for amorphous sample are also shown by symbol, x, in the same figure, and results for both sample are mostly piled up. These facts suggest the propagation of heat in the present model sample is diffusive. This may be due to the phonon scattering by the crystalline defects and the atomistic disorder.

Figure 3. Development of ‘hot atoms’ and distribution of mean velocity at (a) 50 MD steps, (b) 100 MD steps and (c) 200 MD steps.

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