Beat phenomenon in metal nanowires: A molecular dynamics study

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ABSTRACT

In this paper, a special beat phenomenon of metal nanowires is investigated by using the large scale molecular dynamics simulations. It is observed that the beat phenomenon exists not only in the vibration of $\langle 1\,1\,0 \rangle$ orientated Face Center Cubic (FCC) nanowires of different materials, but also in the vibration of $\langle 1\,0\,0 \rangle$ orientated Body Center Cubic (BCC) nanowires. Based on the atomic arrangement, a discrete spring-mass model is developed to explain the displacement characteristics of nanowire's vibration. It is found that the vibration frequency of nanowires rises slightly with the increase of initial actuation amplitude. The displacements of a typical atom in the nanowire are used to show the dynamical characteristics of beat phenomenon in vibration experiments. In addition, the beat phenomenon driven by a single actuation along one of the elementary directions has also been observed and shown in this work. Furthermore, a theoretical analysis is given for the excitation mechanism of beat phenomenon by analyzing the relation of excitation frequency between the two elementary directions.

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1. Introduction

With the rapid progress of nano science and technology, theory and applications of the nanowires have been widely explored in many fields of science and engineering. Driven by their impressive electronic, thermal, mechanical and optical properties, nanowires have been widely used as active components of nanoelectromechanical systems (NEMS) such as force and pressure sensing [1,2], nanowire-nanopore sensors [3], field effect transistor [4], lithium battery anodes [5] and other devices [6–8]. Among various nanowires, BCC Fe nanowires are widely used in data storage and memory devices, spin electronics and smart sensors due to their excellent magnetic properties [9–13]. The NEMS utilize the nanowire as a resonating beam, in which the nanowire vibrates continuously at or near its resonant frequency. In addition, the changes in local environment including force, pressure or mass can be detected by the corresponding changes in the resonance frequency of the nanowire [14]. Therefore, it is of great significance to study the nanowire's mechanical properties under vibration.

In the past few years, there have been a large number of studies on the nanowire's vibrational properties, including the experimental studies [15–18], theoretical analysis [19–21] and computational modelling [22–24]. Olsson et al. studied the resonant properties of unstressed and prestressed gold nanowires and compared MD simulations' results with Euler Bernoulli beam theory and Timoshenko beam theory [25]. Two-dimensional vibration has been studied by Conley et al. theoretically. They explored the nonlinear dynamics of resonators and demonstrated that they can suddenly transit from a planar motion to a whirling, "jump rope" like motion [19]. Gil-Santos et al. proposed a new approach to mass sensing and stiffness spectroscopy based on the fact that the nanoresonator will enter a superposition state of two orthogonal vibrations with different frequencies when the symmetry is broken [6].

Beat phenomenon is a special physical characteristic in the vibration theory. A combination of two simple harmonic vibrations with almost same frequency can generate a periodic pulsation trend in energy and displacement amplitude of the vibration, namely the beat phenomenon [22]. Compared with the nanowires' mechanical properties, few studies have focused on the beat phenomenon because the continuum mechanics-based models do not capture the discrete lattice properties that are required to induce the beat phenomena. It is reported that for the beat phenomenon, there are two orthogonal elementary orientations in $\langle 1\,1\,0 \rangle$ orientated FCC metal nanowires [23]. However, the mechanism of beat phenomenon is still not clear. Additionally, in most papers, only energy time history has been used to show the properties of beat phenomenon. Are there any other characteristics that can be used to study the beat phenomenon? The displacement is such a characteristic. It is quite important for the study of the nanowires' vibrational properties. However, little attention has been paid to this characteristic.

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Therefore, a further numerical and theoretical study of beat phenomenon is presented in this work. We analyze the beat phenomenon on $\langle 1\,0\,0\rangle$ oriented BCC Fe nanowires, which remains valid for this phenomenon. Based on the atomic structure, a valid discrete spring-mass model has been proposed to show the lattice arrangement properties and study the vibrations of the nanowire. With the results of Molecular Dynamics (MD) simulations and the spring-mass model, the vibration frequency of nanowires is found to increase slightly with the rise of initial actuation amplitude. As the displacement characteristic is a significant property, we investigate it by studying the displacement time history of a typical atom, which is selected from the nanowire. The displacement time histories of the MD simulations reveal that the vibrations in the orthogonal elementary directions have an influence on each other. In addition, we find that there exists the beat phenomenon driven by a single actuation along one of the elementary directions, which is distinctly shown with the displacement characteristic by our method. By further study, we also give a reasonable excitation mechanism of the beat phenomenon.

2. Models and methods

2.1. Atomistic simulation

In this work, the vibration tests of double clamped Fe nanowires are performed by using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [26]. The Fe nanowires used in simulation are $\langle 1\,0\,0\rangle$ oriented and created with atoms in positions corresponding to a bulk perfect BCC crystal lattice. Fig. 1 shows the model of $\langle 1\,0\,0\rangle$ oriented Fe nanowires. In this model, the shape of cross-section is chosen to be square. Atoms at both ends of the nanowires are fixed, and are denoted by "A" in Fig. 1; while the rest of the nanowires are free to move. The periodic boundary conditions are not imposed in any directions.

The embedded-atom-method (EAM) potential developed by Mendelev et al. [27] is used to describe the atomic interactions between Fe atoms in these simulations. It is a semi-empirical function fitted to a group of parameters, including elastic constants, equilibrium lattice constant, cohesive energy, unrelaxed vacancy formation energy, et al. In this model of atomic interaction, the total energy E_{tot} of a system with N atoms is a sum of the classical pair potential and many-body embedding energy [28].
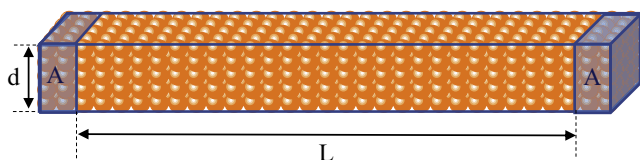
$$E_{tot} = \sum_{i=1}^{N} F_i(\rho_i) + \sum_{i=1}^{N} \sum_{j=1}^{N} \phi_{ij}(R_{ij}) \tag{1}$$

where F, ρ, ϕ, R_{ij} are the embedded energy, pair potential, electron cloud density and the distance between atom i and j, respectively.

The centro-symmetry parameter (CSP) is used to recognize the plastic deformation, which is defined by [29]

$$CSP = \sum_{i=1}^{4} |\mathbf{R}_i + \mathbf{R}_{i+4}|^2 \tag{2}$$

where $\mathbf{R}_i$ and $\mathbf{R}_{i+4}$ are vectors corresponding to the four pairs of opposite nearest neighbors in BCC lattice. The CSP value rises from zero for perfect BCC lattice to positive values for defects, and for atoms close to free surfaces.

At the beginning of each simulation, the nanowires are relaxed to the initial equilibrium configuration using the conjugate gradient energy minimization. Then, the Nose-Hoover thermostat [30,31] is employed to equilibrate the nanowires at 0.2 K. Finally, an initial velocity excitation $\mathbf{v}(z)$ is imposed on the nanowires along the z-axis as follows

$$\mathbf{v}(z) = \left[A_1 \sin\left(\frac{k_1 \pi z}{L}\right), A_2 \sin\left(\frac{k_2 \pi z}{L}\right) \right]^{\mathrm{T}}, \quad k_1, k_2 = 1, 2, \cdots \tag{3}$$

where the subscripts 1 and 2 refer to the x and y-axis. A is actuation amplitude and L is the effective length of the nanowires that exclude the two fixed edges.

2.2. Analysis methods

External energy is defined as the difference between the potential energy before and after the transverse velocity actuation is applied to the nanowire [22]. The energy data can be directly obtained from the simulations results, and the vibration frequency and vibration modes of the nanowire can be obtained by using the Fast Fourier transform (FFT).

The displacement of the nanowire is another important characteristic to show the mechanical properties of the nanowire, especially for the two-dimensional vibration. It is more intuitive to explore and show the properties of beat phenomenon by nanowire's displacement characteristic. However, there are few studies focused on the displacement characteristic of the two-dimensional vibrational nanowire due to the difficulties in collecting displacement data of the nanowire from the simulations. In this study, an atom of middle cross-sectional $(0\,0\,1)$ plane of the Fe nanowire is selected as a sample to study the time history of displacement. The process is shown in Fig. 2.

2.3. A discrete spring-mass model

From the view of lattice structure, a simplified discrete model is developed to explore the effects of nanowires' atomic structure on the vibrations. In the atomic arrangement of the $\langle 1\,0\,0\rangle$ oriented Fe nanowire, each internal lattice is surrounded by other six lattices. However, the two lattices along the z-axis have little effect on the displacements of atoms in the intermediate lattice because of the fixed end in the z-axis. Thus, we neglect the lattices along the z-axis. Besides, the lattices along the x-axis and y-axis have the
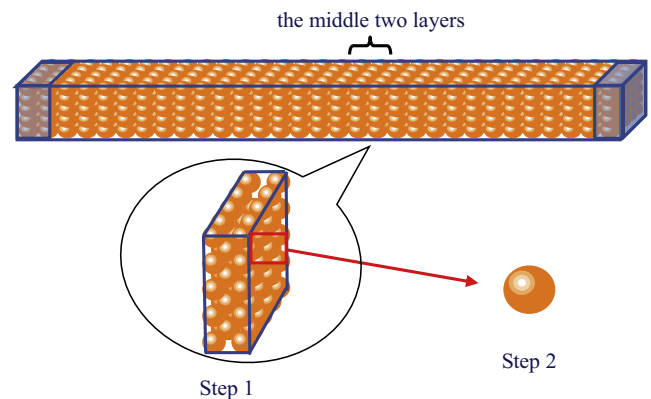
Fig. 2. Schematic visualization of the process of choosing a typical atom from $\langle 1\,0\,0\rangle$ oriented Fe nanowire. Firstly, we take out the middle cross-sectional plane from the $\langle 1\,0\,0\rangle$ oriented Fe nanowire. Then, we choose an atom from the plane randomly because atoms on the plane are similar to each other in displacement.

Fig. 1. Schematic visualization of a fixed-fixed $\langle 1\,0\,0\rangle$ oriented Fe nanowire. The atoms in the areas 'A' are fixed in all directions and the residual atoms can move freely.