A Molecular Dynamic Study on Nonlinear Vibration Behaviors of Fe Nanowires

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Abstract

In this paper, nonlinear behaviors in the vibration of Fe nanowires are investigated by using the large scale Molecular Dynamics (MD) simulations. It is observed that the vibration frequency of nanowires rises slightly and nonlinearly with the increase of initial actuation amplitude. Based on the atomic arrangement, a discrete spring-mass model is developed. Its geometric nonlinearity is used to explain this phenomenon. In addition, Fe nanowires with different sizes show different vibration properties in this work. The ratio between the length (L) and the height (h) of nanowires has a significant influence on vibration behaviors. The vibration frequency changes linearly with h/L^2 when the ratio is relatively large, while it changes nonlinearly when the ratio is relatively small.

Keywords: nonlinear vibrations, Fe nanowires, molecular dynamics, initial actuation, size, spring-mass model.

Introduction

Nanowires have been widely investigated with the rapid development of nano science and technology. Due to their unique electronic, thermal, mechanical and optical properties, nanowires have been widely applied 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]. These 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 [9]. Therefore, it is of great significance to study the nanowire's mechanical properties under vibration.

In the past few years, there have been lots of studies on the nanowire's vibrational behaviors and properties, including the experimental studies [10-13], theoretical modeling [14-18] and computational simulations [19-26]. Copper, silver, gold and silicon nanowires have been studied on their vibrational properties respectively by several researchers [19, 22-26]. Two-dimensional vibration has been studied by Conley et al. theoretically [14] and used for mass sensing and stiffness spectroscopy by Gil-Santos [6]. In the nanowire's two-dimensional vibration, beat phenomenon is a special physical characteristic, which is reported and investigated by Zhan [19, 20]. Unfortunately, little attention has been paid to nonlinear vibration behaviors of nanowires, especially the Fe nanowires. Additionally, initial actuation and nanowires' sizes are rarely considered in the study on nonlinear vibration behaviors of nanowires. Therefore, the mechanism behind nonlinear vibration behaviors is still not clear, which is quite important to study the properties of nanowire vibrations.

Therefore, a fundamental numerical and theoretical study of nonlinear vibration behaviors of Fe nanowires is presented in this work. We investigate the nonlinear vibration behaviors of Fe nanowires in two aspects: initial actuation amplitude and nanowires' size. Based on the atomic structure, a valid discrete spring-mass model has been proposed to study the vibrations of the nanowire. With the results of MD simulations and the spring-mass model, the vibration frequency of nanowires is found to increase slightly and nonlinearly with the rise of initial actuation amplitude. On the other hand, based on the MD simulations performed on a number of Fe nanowires with different sizes, it is found that the ratio between the length and the height of nanowires has a significant influence on vibration behaviors. We introduce the slender beam and thick beam depend on this ratio L/h. The results from MD simulations signify that the slender beams' vibration frequencies have a linear correlation with h/L^2. In contrast, thick beams have a nonlinear correlation between vibration frequency and h/L^2.

Models and Methods

Atomistic Simulation.

In this work, double clamped Fe nanowires are investigated for their vibration properties. We use the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [27] to perform these simulations. Fig. 1 shows the model of nanowires used in MD simulations, which is created with iron atoms in positions corresponding to a perfect BCC crystal lattice. The shape of cross-section is chosen to be rectangle. The Fe lattice constant a is chosen as 0.287 nm. For the Fe nanowires, the length L ranges from 20a to 100a, while the width b and height h ranges from 4a to 30a. Atoms at both ends of the nanowires are fixed in their positions, which are denoted by "A" in Fig. 1. The rest of the nanowires are free to move. We assume that the vibrations of these Fe nanowires occur in a vacuum. Thus no damping is applied in these simulations. The periodic boundary conditions are not imposed in any directions.

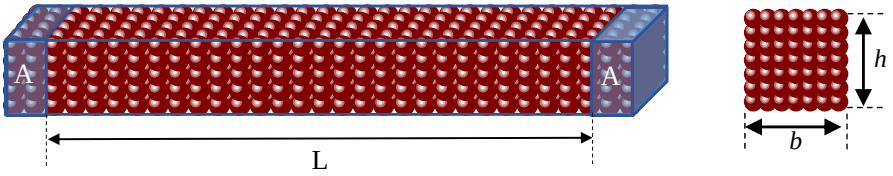

Figure 1. A schematic visualization of a fixed-fixed Fe nanowire used in simulation. The atoms in the areas 'A' are fixed in all directions and the residual atoms can move freely.

The embedded-atom-method (EAM) potential developed by Mendelev et al [28] is utilized to describe the atomic interactions between Fe atoms in these simulations, which is a semi-empirical function fitted to a group of parameters, including elastic constants, equilibrium lattice constant, cohesive energy, unrelaxed vacancy formation energy and others. In this model of atomic interaction, the total energy E_{tot} of a system of N atoms is a sum of two terms, which are classical pair potential and many-body embedding energy [29].

$$E_{tot} = \sum_{i=1}^{N} F_i(\rho_i) + \sum_{i=1}^{N}\sum_{j=1}^{N} \phi_{ij}(R_{ij}) \tag{1}$$

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

At the beginning of each simulation, the nanowires are relaxed to the initial equilibrium configuration using the conjugate [30]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.

$$\mathbf{v}(z) = \lambda \sin(\frac{\pi z}{L}) \tag{2}$$

Here, λ is actuation amplitude and L is the effective length of the nanowires that exclude

the two fixed edges.

Theoretical Models.

As mentioned before, nanowires are usually utilized as resonating beams in NEMS. According to the classical Euler-Bernoulli beam theory, the governing partial differential equation for the beam is

$$EI\frac{\partial^4 w}{\partial x^2}+\rho A\frac{\partial^2 w}{\partial t^2}=0 \tag{3}$$

where E is Young's modulus, I is moment of inertia, ρ is density and A is the cross-sectional area of the nanowire. $w(x,t)$ is the nanowire's transverse displacement. By using the clamped-clamped boundary conditions, the vibration frequency can be determined by

$$\omega=\pi^2\sqrt{\frac{EI}{\rho AL^4}} \tag{4}$$

where L is the length of the nanowire. With $I=bh^3/12$ and $A=bh$ (b and h are the width and the height of the nanowire's cross-section), the vibration frequency equals

$$\omega=\pi^2\sqrt{\frac{Eh^2}{12\rho L^4}}=\sqrt{\frac{E}{12\rho}}\times\frac{\pi^2 h}{L^2} \tag{5}$$

For the theoretical calculation of the vibration frequency for Fe nanowire, density ρ equals 7.87 g/cm^3.

To explore the relation of vibrations in different directions from the view of lattice structure, we develop a simplified discrete spring-mass model. According to the atomic arrangement of the 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, lattices along the *x*-axis and *y*-axis have the same influence on the internal lattice. Fig. 2a shows the structure.

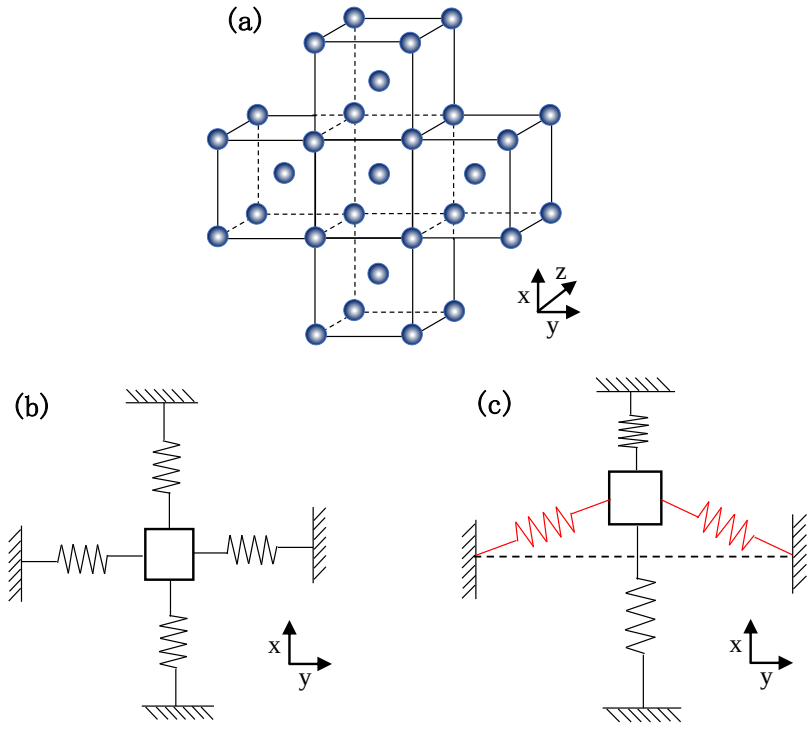

Figure 2. (a) The typical atomic arrangement of Fe nanowires with several lattices. (b)

A schematic of simplified discrete spring-mass model according to the atomic arrangement of Fe nanowires. (c) A schematic of this spring-mass model when the mass move along the *x*-axis. The red springs result in geometric nonlinearity of this model.

For simplicity, we interpret this structure as a spring-mass system as illustrated in Fig. 2b. This spring-mass system consists of linear springs, which are defined as

$$m\ddot{\mathbf{x}} = -k\Delta\mathbf{x} \tag{6}$$

where m is mass of the object, k is elastic constant of the spring. Due to the symmetric cross-sectional plane and the same influence along the *x*-axis and *y*-axis, the springs are chosen to be the same. The dynamic equations of this spring-mass system are described as

$$\begin{cases} m\ddot{y} = -4ky - kl_0\left(\dfrac{l_0 - y}{\sqrt{x^2 + (y - l_0)^2}} + \dfrac{-l_0 - y}{\sqrt{x^2 + (y + l_0)^2}} + \dfrac{-y}{\sqrt{(x + l_0)^2 + y^2}} + \dfrac{-y}{\sqrt{(x - l_0)^2 + y^2}}\right) \\ m\ddot{x} = -4kx - kl_0\left(\dfrac{-x}{\sqrt{x^2 + (y - l_0)^2}} + \dfrac{-x}{\sqrt{x^2 + (y + l_0)^2}} + \dfrac{-l_0 - x}{\sqrt{(x + l_0)^2 + y^2}} + \dfrac{l_0 - x}{\sqrt{(x - l_0)^2 + y^2}}\right) \end{cases} \tag{7}$$

where m is mass of the object, k and l_0 are elastic constant and initial length of the spring.

In this work, we focus on the one-dimensional vibration. Thus, we can let *y*=0 for all the time. Then, we can get the simplified dynamic equation as

$$m\ddot{x} = -4kx + 2kx\frac{l_0}{\sqrt{x^2 + l_0^2}} \tag{8}$$

In Eq. 8, it is obvious that the second item on the right is a nonlinear item for this equation. As shown in Fig. 2c, when this system vibrate along the *x*-axis, because of the spring-mass model's structure, the red springs produce the nonlinear forces, which correspond to the nonlinear item in Eq. 8. This is what we call the geometric nonlinearity.

Results and Discussion

Nanowires in Vibration

We begin this paper with MD simulations and corresponding analysis on the vibrational Fe nanowires. External energy is defined as the difference of the potential energy before and after the transverse velocity actuation is applied to the nanowire [19]. We can obtain the energy data directly from the simulations. By analyzing the external energy time history with the Fast Fourier transform (FFT), the vibration frequency and modes of the nanowire can be obtained. In this section, MD simulations are carried out on the Fe nanowire with the size of $20a \times 10a \times 100a$. Fig. 3a depicts the time history of the external energy during the free vibration after the initial velocity actuation. Fig. 3b presents part of the periodogram regarding the power of the discrete Fourier transformation versus frequency. The whole simulation last about 4000 picoseconds at a time step of 1 femtoseconds. The amplitude frequency curve is depend on these data. As is seen in Fig. 3b, one main frequency component is identified, which is about 53.41 GHz. This result indicates that the Fe nanowire is under a vibration with the frequency of 26.70 GHz, because the frequency of the external energy is twice that of the actual vibration.

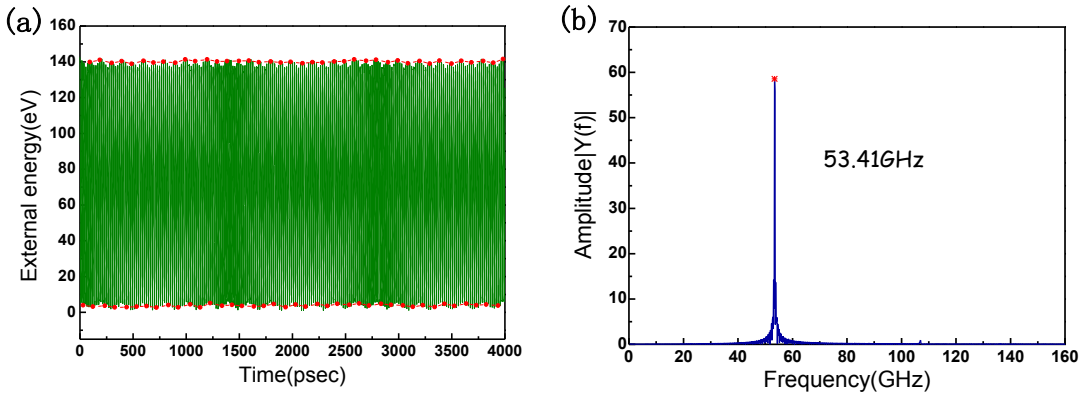

Figure 3. (a) External energy time history of the Fe nanowire with the size of $20a\times10a\times100a$ for a free vibration MD simulation at 0.2K. The simulation time is from 0 to 4000 picosecond. Circle markers highlight the maximum and minimum of external energy during each vibration circle. (b) The frequency spectrum from FFT analysis on the previous simulation (from 0 to 160 GHz). The star marker highlights the maximum of the main frequency component.

Initial Actuation Amplitude

Then, the relation between initial actuation amplitudes and vibration frequencies is studied. We perform MD simulations on the Fe nanowires with the size of $4a\times4a\times20a$, $10a\times10a\times50a$, $5a\times5a\times50a$ and $10a\times10a\times100a$. Initial velocity excitations as Eq. 2 are imposed on these nanowires. In Eq. 2, several different amplitudes λ ranging from 0.2 Angstrom/psec to 1.4 Angstrom/psec are chosen for tests. Figs. 4 describe the frequencies received from the free vibration MD simulations of Fe nanowires under different initial actuation amplitudes. As observed in Figs. 4, it is found that the vibration frequency from the MD simulations rises slightly and nonlinearly with the increase of initial actuation amplitude.

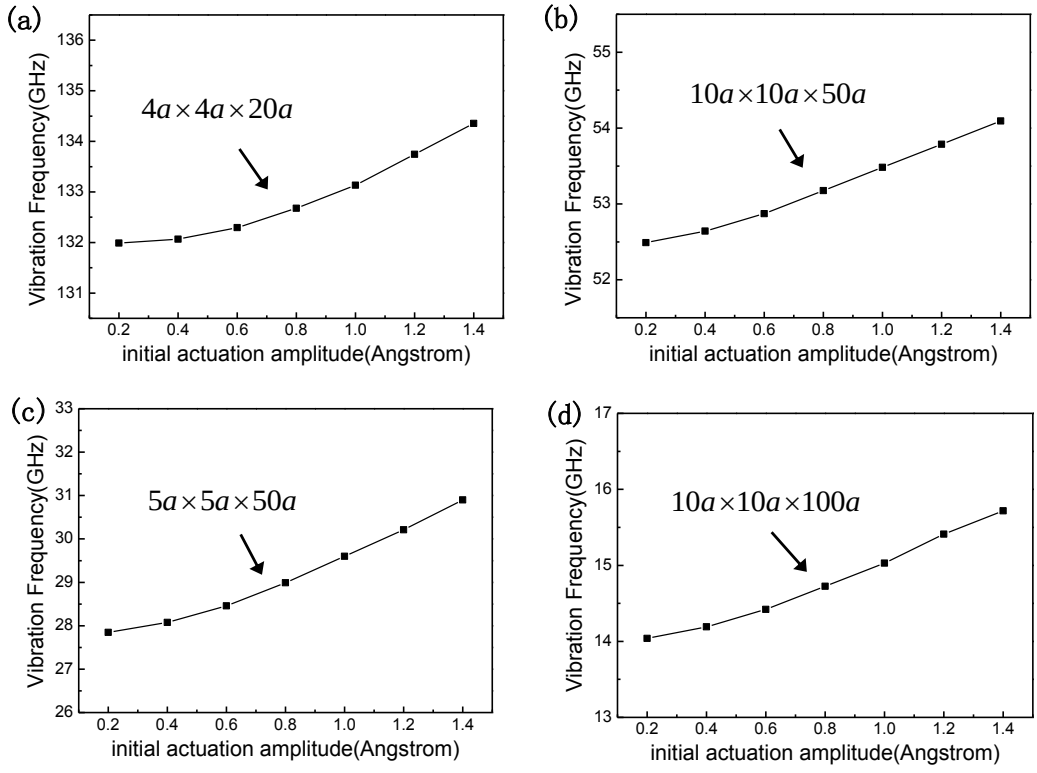

Figure 4. These lines represent the vibration frequencies vs initial actuation amplitude.

In this situation, we use the frequencies obtained from FFT analysis when we apply different initial actuation amplitude on different Fe nanowires. They are nanowires with (a) the size of $4a \times 4a \times 20a$. (b) the size of $10a \times 10a \times 50a$. (c) the size of $5a \times 5a \times 50a$. (d) the size of $10a \times 10a \times 100a$.

In addition, we test initial boundary conditions of different actuation amplitudes on the spring-mass model. The results in Fig. 5 show that with the increase of initial actuation amplitude, the vibration frequency rises slowly, which is similar to the results from the MD simulations.

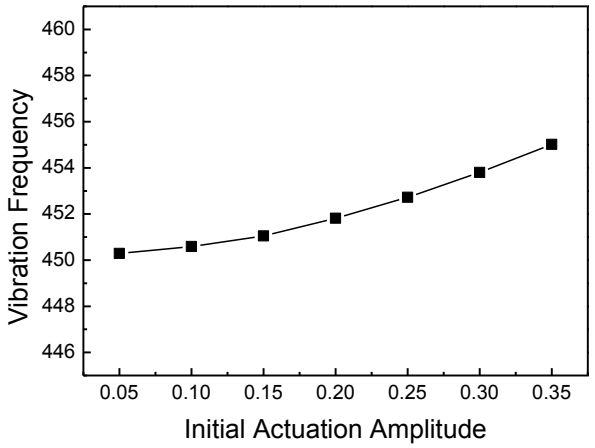

Figure 5. The vibration frequencies vs initial actuation amplitude. In this situation, we apply different initial conditions' value on the spring-mass model. Then, the frequencies can be obtained from FFT analysis on the numerical results.

According to the classical theory (Eq. 5), the Euler-Bernoulli beams have fixed natural frequencies, which is irrelevant to initial actuation amplitude. However, the results from MD simulations signify that the vibration frequency has a nonlinear correlation with initial actuation amplitude. We suggest that, in the nano scale, the lattice structure has a big influence on the properties of the nanowires' vibrations. As mentioned above, according to the atomic arrangement, the spring-mass model has geometric nonlinearity, which may result in the nonlinear correlation between vibration frequency and initial actuation amplitude. However, the classical Euler-Bernoulli model is a macro-continuity model, which may be not suitable for the nanowire in this scale. Therefore, in this case, it is found that the vibration frequency increase slightly with the growth of initial actuation amplitude.

Size Effect

Further interest is laid on the relation between nanowires size and vibration frequencies. During the simulations in this section, the initial actuation amplitude λ is fixed at 1.5 Angstrom/psec. Figs. 6a and 6b shows the vibration frequency height curve obtained from the simulations with the fixed *L* and *b*. As observed in Figs. 6a and 6b, it is obvious that the vibration frequency rises with the increase of height. According to the classical Euler-Bernoulli beam theory (Eq. 5), the vibration frequency has a linear correlation with the height of the nanowire. In the results from MD simulations, we can also find that when the value of height is relatively small, the correlation between vibration frequency and height is linear. However, the vibration frequency rises nonlinearly with the increase of height when the value of height becomes relatively large. Since *L* is a fixed value, the ratio between length and height (*L/h*) declines with the increase of height. We define the slender beams as the nanowires with relatively large value of *L/h* (usually larger than 5), while the thick beams are defined as the nanowires with relatively large value of *L/h* (usually smaller than 5). Thus, the observations signify that, in the nano size, the correlation between vibration frequency and height is linear for the slender beams, while the correlation is nonlinear for the thick beams.

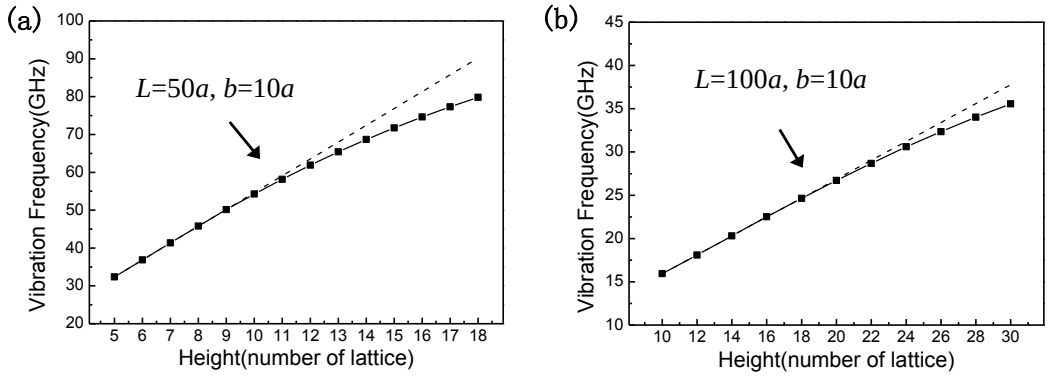

Figure 6. The solid lines in these figures represent the vibration frequencies in different heights. The dotted lines are the fitted straight lines based on vibration frequency values in the first five heights. In this situation, we use the frequencies obtained from FFT analysis on the MD simulations carried on different Fe nanowires. They are nanowires with the fixed *L* and *b* ((a) *L*=50*a*, *b*=10*a*.(b) *L*=100*a*, *b*=10*a*.).

We also perform MD simulations on the nanowires with the fixed *h* and *b*. Fig. 7a depicts vibration frequency length curve, which received from several MD simulations on Fe nanowires in different lengths. From Fig. 7a, it is found that, in the fixed *h* and *b*, the vibration frequency declines with the increase of the nanowires' length. According to the classical beam theory (Eq. 5), there is a linear correlation between vibration frequency and $1/L^2$. Thus, Fig. 7b describes the vibration frequency with $1/L^2$. It is found that the left half curve is almost linear, while the right half curve shows the nonlinear trend. Since *h* is fixed at 50a, it is suggested that the correlation between vibration frequency and $1/L^2$ is linear for the slender beams, while the correlation is nonlinear for the thick beams.

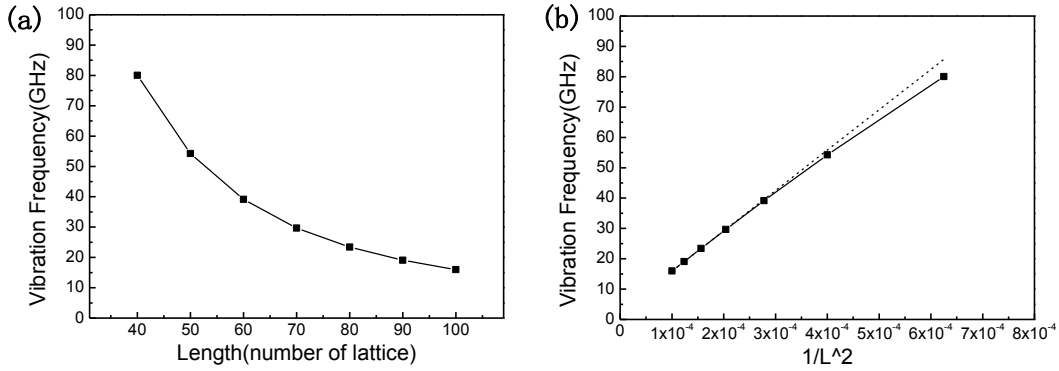

Figure 7. (a) The vibration frequencies vs nanowires' length. In this situation, we use the frequencies obtained from FFT analysis on the MD simulations carried on different Fe nanowires. They are nanowires with the fixed *h*=10*a* and *b*=10*a*. (b) The solid line shows the vibration frequencies vs $1/L^2$, while the dotted lines are the fitted straight lines based on vibration frequency values in the first three values of $1/L^2$.

Conclusion

In summary, based on large scale molecular dynamics simulations, we investigated nonlinear behaviors in the vibration of Fe nanowires. It is found that with the increase of initial actuation amplitude, the vibration frequency of nanowires grows slowly and nonlinearly. A discrete spring-mass model abstracted from the atomic arrangement is developed in this work. The geometric nonlinearity of this model is applied to explore this nonlinear correlation between initial actuation amplitude and vibration frequency, which cannot be explained by the classical Euler-Bernoulli model. Furthermore, simulations on Fe nanowires with different sizes are

performed to show the vibration properties. Fe nanowires with the change of L and h are considered respectively. Both the results shows that the vibration frequency has a linear correlation with h/L^2 for the slender beams, while the correlation becomes nonlinear for thick beams.

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