Research Article

Study on Vibration Behavior of Doubly Clamped Silicon Nanowires by Molecular Dynamics

H. Yu, W. W. Zhang, S. Y. Lei, L. B. Lu, C. Sun, and Q. A. Huang

Key Lab of MEMS of Ministry of Education, Southeast University, Nanjing 210096, China

Correspondence should be addressed to H. Yu, h_yu@seu.edu.cn

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The vibration behavior of doubly clamped silicon nanowires with square cross sections is studied by molecular dynamics method. Silicon nanowires have lengths ranging from 4.888 to 12.491 nm and cross sections ranging from $1.22\text{ nm} \times 1.22\text{ nm}$ to $3.39\text{ nm} \times 3.39\text{ nm}$. The size dependence of the resonant frequency is studied in detail. The results show that the vibration behavior of Si nanowire is quite different from the macroscopic beam, and the resonant frequency is much higher than the result based on the continuum theory, but close to the theoretical result based on the semicontinuum approach. Surface reconstruction can strongly affect on vibration behavior. These results demonstrate that the classic theory may not be suitable for analysis of performances of nanostructures, and the conclusion of the study has a certain practical significance on related fields.

1. Introduction

In last decade, resonant nanoelectromechanical systems (NEMSs) have been found in a variety of important applications, including ultrasensitive mass and force sensing [1, 2], ultralow-power radio frequency (RF) signal generation, timing [3–5], and switch [6]. Silicon-based nanowires and nanobeams with very small dimensions and high-performance form the basis of most experimental demonstrations in these applications, where the nanowires or the nanobeams appear either in cantilever or in doubly clamped beam resonators. Nanoscale cantilevers are preferred to be resonators in mass sensing and ultrahigh frequency applications. For example, the nanothick resonant cantilever is used to detect ppm level trace trimethylamine vapor via specific molecular adsorption by measuring the resonant frequency shift of the cantilever [7]. On the other hand, doubly clamped silicon nanowire or nanobeam is another type of resonators in nanomechanical systems. They are also very attractive to researchers. As early as the year 2007, the fundamental resonance of 215 MHz of the doubly clamped silicon nanowire was demonstrated by Feng et al. [3]. The demonstration of mass spectrometry based on single biological molecule detection by using a doubly clamped silicon resonant nanobeam was reported in 2009 [8]. Therefore, the

resonant or vibration behavior of the silicon nanowire is very important to the mass sensing and other applications and has been widely studied by researchers.

In the aspect of theoretical study, some of researches applied equations and software based on continuum assumption to nanowires when they studied the resonance of silicon nanowires and the relationship between resonant frequency and Young's modulus [3, 9, 10]. However, because of the low dimension of the nanowire, the mechanical properties and thus the vibration behavior may deviate from their microscopic and macroscopic counterparts. It means that classical theories based on continuum assumptions or computational design tools, which have been developed for microstructures and macrostructures, may not be directly applicable for the nanostructures. Some approaches have been proposed to extend classical continuum theories to nanostructured materials. By considering the discrete nature of nanomaterial, Sun and Zhang developed a semicontinuum model to calculate Young's modulus of the ultrathin film with a simple cubic lattice [11]. This approach was then developed to study Young's modulus of silicon nanoplate [12]. Based on this approach, a multiscale model was built to analyze the deflection and resonant frequency of silicon nanobeam [13, 14]. On the other hand, molecular dynamics method

FIGURE 1: Model of a doubly clamped silicon nanowire and one AFM probe: (a) before optimization and (b) after optimization.

is often used to study and simulate the mechanical and resonant properties of nanowires. Park et al. and Kim et al. [15, 16] simulated the flexural and longitudinal vibrations of silicon nanocantilevers by molecular dynamics method. They deduced the elastic modulus and Young's modulus for nanothick silicon cantilevers from the natural frequency equation based on the continuum theory.

In this paper, we study the resonant behavior of doubly clamped silicon nanowires by using a specific computer code, Forcite, which is based on molecular dynamics method. Our results are in well agreement with the results based on the multiscale model but much higher than those based on continuum theory.

2. Construction of Simulation Model

Simulation model of one doubly clamped silicon nanowire with a square cross section is built as shown in Figure 1(a) (yellow atoms). The red atoms at two ends of the silicon nanowire are clamped. The cross section and the orientation of the silicon nanowire are depicted in Figure 1, too. Periodic boundary condition is used in the longitudinal direction of Si nanowire, and lateral surfaces are under free boundary conditions in vacuum. The simulation has been carried out at the average temperature of 298 K with a time step of 1 fs. Compass (Condensed-phase Optimized Molecular Potential for Atomistic Simulation Studies) force-field is selected when simulation is performed.

To actuate the nanowire, an AFM probe is constructed above the nanowire, which is denoted by green atoms in Figure 1. After structure optimization, the nanowire begins to deflection as shown in Figure 1(b), because Van der Waals force exists between the AFM and the nanowire. Then the AFM is removed and the simulation starts. Because of the initial deflection, the nanowire will vibrate freely.

3. Simulation Results and Discussion

Figure 2 shows the kinetic and potential energy of the silicon nanowire when the nanowire is vibrating. It can be seen that after undergoing very short transient oscillations, the kinetic energy and potential energy start oscillating almost in one uniform period. At the maximum point of the kinetic

FIGURE 2: Energy of the nanowire while vibrating.

FIGURE 3: Vibration traces of the silicon nanowire in one oscillation period.

energy, the potential energy reaches to the minimum, and vice versa. Exchange between the kinetic energy and the potential energy occurs during one period.

Figure 3 shows the vibration traces of the nanowire in the successive time moment during one oscillation period. It is

FIGURE 4: Frequency response of a silicon nanowire.

FIGURE 5: Fundamental frequency as a function of nanowire thickness: simulation results by MD software (black), and calculation results based on (1) (green) while Young's modulus coming from [15, 16]. All nanowires keep the same length of 9.232 nm and the same width of 2.85 nm.

seen that the vibration mode is the first mode and the motion of the nanowire in one oscillation period is different from that of a macroscopic beam.

The frequency response of the silicon nanowire can be obtained by performing FFT of the kinetic energy or the potential energy. Figure 4 shows the frequency response of the nanowire with a length of 9.232 nm. The cross section is 1.22 nm × 1.22 nm. It can be seen that the fundamental frequency is about 179.4 GHz.

The vibrations of nanowires with different thicknesses are studied. The fundamental frequency as a function of thickness of the nanowire is shown in Figure 5 (black).

As we have known, the first mode frequency ω_0 and the j_{th} mode frequency ω_j for a doubly clamped Euler-Bernoulli beam can be written as [17]

$$\omega_0 = \sqrt{\frac{EI}{ml^4}}, \quad (1)$$

$$\omega_j = (j\pi)^2 \omega_0 \quad (j = 1, 2, \dots), \quad (2)$$

where E is Young's modulus, m is mass per unit length, $m = \rho A$, ρ is the density of the beam, A is the area of the cross section, and l and I are the beam length and the mass moment of inertia, respectively. Now we apply this model to calculate fundamental frequencies of doubly clamped silicon nanowires. Young's modulus in (1) takes the value obtained by Park et al. [15, 16] for silicon nanowire. The results calculated from (1) for nanowires with different thicknesses are also shown in Figure 5 (green).

It is noticed that there is a big deviation between simulation results and calculation results based on (1). The deviation is larger than 60%. This means that the classic theory may not be suitable for analysis of performance of nanostructures, since (1) is built based on continuum assumption, and the discrete nature must be considered in the model for nanostructures. By considering the discrete nature in thickness direction of nanobeam, a multiscale model is proposed to study the vibration frequency of silicon nanobeam [14]. In this model, the fundamental frequency of the doubly clamped silicon nanobeam is described as

$$f_0 = \frac{\omega_0}{2\pi} = \begin{cases} \frac{\pi}{3l^2t} \sqrt{\frac{2ka}{\rho} \times \frac{(N+1)(2N+1)}{2+t^2}}, & N \leq 3, \\ \frac{2\pi}{l^2} \sqrt{\frac{ka}{3\rho N} \left[\frac{1}{18} (N-3)(N-2)(2N-5) + \frac{3(N-3)^2 + 12(N-3)t + 14t^2}{t(2+t)^2} \right]}, & N > 3, \end{cases} \quad (3)$$

where l , ρ , and a are the length, the density, and the lattice constant of the silicon nanobeam, respectively. N is the number of lattices in thickness, k is the spring constant between two silicon atoms, 2.614×10^2 N/m, and t is the relaxation constant. For nonsurface relaxation, $t = 1$. Based on this multiscale approach, resonant frequencies for silicon nanowires are calculated and compared with our simulation results, as shown in Figure 6. It is clear that the discrepancy between them is smaller than the deviation in Figure 5. The deviation here is smaller than 20%. This figure shows that our results are in well agreement with the multiscale model results.

When the length of the nanowire is changed, the vibration behavior will change, too. The fundamental frequencies of doubly clamped silicon nanowires with different lengths are studied. Figure 7 shows the resonant frequency as a function of length of the silicon nanowire. The fundamental

FIGURE 6: Fundamental frequency as a function of nanowire thickness: simulation results by MD software (black), and calculation results based on multiscale model (red). The length of nanowire is 9.232 nm.

FIGURE 7: Fundamental frequency as a function of length of silicon nanowire. The width and thickness of nanowires are both of 1.22 nm.

frequency decreases monotonically with the length increasing.

When the width is changed, the frequency response of the nanowire does not change significantly, as shown in Figure 8. This concludes that the transverse vibration frequency is not related to the width of nanowire too much, which is similar with the result based on continuum theory.

Surface reconstruction can strongly impact on the elasticity of silicon nanoplate [18–20]. Therefore, the effect of surface reconstruction on vibration frequency of silicon nanowire is also studied in detail. The (2×1) dimer reconstruction is considered on four of lateral surfaces of the silicon nanowire. Figure 9 shows the vibration frequencies with and without reconstruction for nanowires with different cross sections. It can be seen that the frequency under surface

FIGURE 8: Frequency responses of doubly clamped nanowires with different widths.

FIGURE 9: Resonant frequency for nanowires with different cross sections with and without reconstructions on lateral surfaces.

reconstruction is much higher than that without reconstruction. The frequency is almost doubled by surface reconstruction for the nanowire with the cross section of 1.488 nm^2 . Because of the surface reconstruction, the nanowire becomes stiffer, and Young's modulus becomes larger, resulting in the resonant frequency increasing significantly. The size of cross section is smaller, the change of resonant frequency is greater, since the surface-to-volume ratio is higher for the nanowire with a smaller cross section.

4. Conclusions

Vibration behavior of doubly clamped silicon nanowires is studied by molecular dynamics software. The results are

different from those based on classic continuum theory but are close to the results obtained from semicontinuum approach. Resonant frequency of doubly clamped silicon nanowires strongly depends on the length and thickness of the nanowire. Surface reconstruction has strong impact on the vibration behavior of the silicon nanowire, especially on the nanowire with smaller size. The results show that the classic theory may not be suitable for analysis of the vibration of silicon nanowires.

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