

A THESIS SUBMITTED FOR THE DEGREE OF MASTER OF SCIENCE

Molecular Dynamics Simulation on Mechanical behavior of Si Nano Cantilever under Ar Bombarding

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Abstract

In nano world, it is cheap and repeatable to make 2-dimensional structures, such as nanoholes and thin nanofilms. However, it is expensive to build 3-dimensional structure in a repeatable manner. Ion bombardment is a technique which is widely applied in engineering areas, such as thin film deposition, etching, and analysis. In this thesis work, classical molecular dynamics is used to study the mechanical behavior of silicon cantilever under neutral Ar bombardment. Initially, a single crystal silicon cantilever is set in a simulation box using molecular dynamics simulation. Thermal vibration of the cantilever without any bombardment is studied using Euler-Bernoulli model. Then the cantilever is bombarded under neutral Ar atoms, with different bombarding energy and bombarding angle. The results shown that Ar bombardment can make significant plastic deformation (around 6 nm) comparing with the thickness of the cantilever (1.5 nm). The low energy bombardment, with its high efficiency and quite low sputtering, is potentially to be applied for 3D nano architecture of Si.

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1 Introduction

Modern development of nanotechnology enables scientists and engineers to produce two-dimensional (2D) nano structures, such as nano-holes and nano-cantilevers, in a repeatable manner. When considering their applications in Microelectromechanical systems (MEMS), the 2D nano structures have limited performance.[1] If the 2D nano materials could be manufactured into three-dimensional (3D) structures, such as nano-rings or nano-tube, the performance will be enhanced. 3D nanostructures have unique properties that can be potentially applied in mechanical, optical and electrical areas. Recent developments in nanotechnology have heightened the needs to produce the 3D nano structures in a quick, cheap and repeatable way.

Several attempts have been made to build 3D nano structures from 2D nano cantilevers. [2][3][4] The process that fabricates 3D nano structures from 2D nano materials is named as nanomechanical architecture. Different classes of 3D nanostructures are formed in the same design principle, which is the tendency of strained films to bend (or to fold)[2]. The nano beam can be strained in a variety of ways, such as mechanical stress, surface tension, magnetic or electric field, or chemical modification of the surface. The bending or folding of the 2D cantilever releases build-in strain, which minimizes total strain energy within the elastic regime. The final shape of the 3D products is influenced by three key parameters, which are geometry, elastic property of cantilever, and magnitude of the gradient of built-in strain [2][3][4]. With the control of those three parameters, complex structures can be made by nanomechanical architecture. Specific examples of 3D structures are shown in figure 1.

However, nanomechanical architecture is imperfect because of two main reasons. First, nanomechanical architecture uses bi-layer thin films and they can be made from limited kinds of materials. Moreover, the control of the final shape of 3D structure is difficult to perform. It asks for precise design of geometry

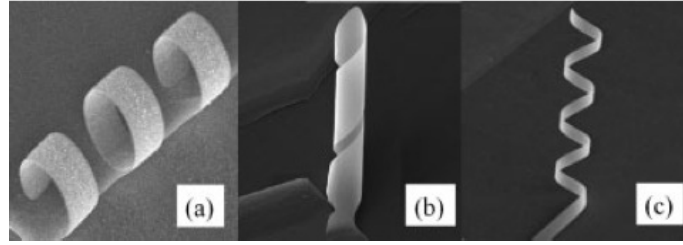


Figure 1: Scanning electron microscopy images of nanoarchitectures fabricated from strained Si/SiGe bi-layer films. Adopted from reference [2]

and accurate magnitude of the gradient of build-in strain. Both of these two limitations result from the mechanism of nanomechanical architecture, which is the release of build-in intrinsic strain. Therefore, introducing extrinsic strain, instead of building in intrinsic strain, offers more options for material choice and less needs for parameters control. Ion bombardment can bring extrinsic strain to make the 2D cantilever deform. This paper focused on one possible method to produce 3D nano structure through Ar bombardment on silicon cantilever. In the process of bombardment, energetic particles with high kinetic energy collide with a target. Because of the collision, those energetic particles have momentum exchanges with the target (cantilever). So the extrinsic strain is brought and the cantilever is deformed. If the deformation is plastic, 3D nanoshape can be manufactured irreversibly. Conclusively, this study examines the possibility to produce 3D nano structure with Ar bombardment on silicon cantilever.

Molecular dynamics (MD) simulation is used in this work. A one-end clamped silicon nano cantilever beam model is simulated according to the aspect ratio in real engineering. The cantilever is 65 nm long, 11 nm wide and 1.5 nm thick. A simulation is first made to measure the effective Youngs modulus of the cantilever at room temperature (300K). It turns out that the effective Youngs modulus of the beam is 80 GPa. Comparing with macro silicon materials at the same crystallographic direction (130 GPa), the cantilever beam is softened because of size effect.

After measuring the amount of effective elastic modulus, the simulation is performed without Ar bombardment at room temperature. The cantilever is observed to have thermal vibration during the simulation. Shape of the cantilever profile is close to the Euler-Bernoulli modes shape and the frequency of different vibration modes obtained from simulation is close to the theoretical one. Comparing the root mean square amplitude of the vibration of simulation with the theoretically calculated ones, it shows that the data of the simulated results and calculated ones has a big difference. Possible reasons can be mainly attributed to the change of the cantilever geometry at the start of vibration and the change of mechanical properties during vibration.

Next the beam is bombarded with Ar atoms. A model, with bombarding energy of 200 eV and bombarding angle at 45° is set as standard. The cantilever bends with a deformation of 6 nanometers at the free end after 396 Ar atoms bombarded. 429 Si free atoms are created after the bombardment. The sputtering yield is 1.15. Then simulation is continued without Ar atoms bombarded on the cantilever. The deformation of the cantilever does not change. Meanwhile, the average potential energy of the atoms of the cantilever does not change as well. It can be concluded that the cantilever beam is plastically deformed after the bombardment.

In the final step of the work, 2 bombarding parameters, kinetic energy of Ar atoms and the bombarding angle of Ar atoms, are investigated to examine whether they can influence the magnitude of deformation. The effects of the two parameters are tested by comparing the results of the sputtering and the magnitude of deformation of the cantilever. First, when considering different bombarding angles, similar Ar fluence leads to the approximately identical bending deformation and sputtering results. It can be inferred that the change of bombarding angle does not influence the bending deformation and the sputtering results much. Second, for Ar with different kinetic energy, it turns out that, the higher of the kinetic energy, the more free Si atoms created and the more Ar atoms pierced inside the cantilever. Furthermore, to achieve the same deformation state at the free end (6 nm), more bombarding Ar atoms with the higher kinetic energy are needed.

Conclusively, compared with the thickness of the cantilever (1.5 nm), the Ar bombardment can make significant plastic deformation (6 nm). The Ar bombardment with lower kinetic energy, is potentially to be applied for 3D nano architecture of Si because of the high efficiency to deform and small damage on the cantilever, .

2 Literature Review

2.1 3D architecture of Strained Thin Film

As discussed in the previous section, the 3D nanostructures are created by self-assembly based on the principle of stress-driven actuation. [2][3][4] The material system to build 3D nano structure is 2D nano cantilever. Intrinsic strains are stored via standard deposition and patterning techniques when the cantilever is fabricated. The intrinsic strain initiates the bending and rolling process of the cantilever. With different design principles, 2D cantilevers were built into the intended 3D nano structure. In this section, prior studies reviewed are about the generic design principles relevant to the nanomechanical architecture of strained nanomembranes. Specifically, two aspects are discussed: 1) the method to store intrinsic strain; 2) the control of 3D geometry.

The physical principle of storing intrinsic strain is similar to bimetallic strip thermostat. [2] Because of different thermal expansion, two metal layers in a bimetallic strip have different thermal stress at same temperature. The stress difference makes the bimetallic strip bend. The cantilevers to build 3D nano structure are fabricated with two different material layers. There is lattice-misfit strain between the interface of the two different material layers. Because the bi-layer nano cantilever is at nano scale, the effects of lattice-misfit strain become significant. The strain creates a large bending magnitude so that the nano beam can fold into tubular shapes with multiple turns as shown in figure 1. Different shapes are formed through controlling geometric properties of membranes and the magnitude of the built-in strain gradient in the cantilever.

There are several important variables to control the final shape of the 3D nanostructure. As indicated in previous studies [2][4][5][6], first variable is isotropic and anisotropic mechanical properties of materials.

Isotropic elastic properties mean that mechanical properties of materials are uniformity in all directions, while anisotropic elastic properties are direction dependent. For instance, single crystal silicon is one kind of elastically anisotropic material. The Young's modulus of Si has the smallest value along $\langle 100 \rangle$ direction. So the $\langle 100 \rangle$ is the mechanically most compliant direction. Intuitively, the silicon nano cantilever will curl along the softest $\langle 100 \rangle$ direction. An example is shown in figure 2 [2].

According to Huang [2], Si-Ge bilayer nano cantilever was used to build 3D nano structure. Energetically, Si/Ge strained membrane is favored to curl only along the $\langle 100 \rangle$ compliant direction. [2] The final shape of 3D nano structure depends critically on the alignment between the intended rolling direction and the most compliant $\langle 100 \rangle$ direction. In the upper panel of figure 2, the strained cantilever beams are patterned with different directions and the final rolled up shapes are shown in the lower panel of figure 2. When the desired rolling direction is along $\langle 100 \rangle$, the strained beam curls along $\langle 100 \rangle$ to form a tube or ring; if the desired curling direction is aligned off the $\langle 100 \rangle$ direction, the strained cantilever still rolls along $\langle 100 \rangle$. Instead of forming rings or tubes, the final rolled up shape is coil.

The second key variable is the relative thicknesses of the two layers making up a bilayer strained membrane. The strain in a bilayer membrane can be released by both bending and stretching of the whole film. Whether it bends or stretches depends on the relative thickness of the two layers. [5] The influence of the membrane thickness on bending or stretching of a bilayer can be explained with Fig 3. The mechanical interaction between the two layers of a bilayer structure includes stress and torque. The stress is responsible for stretch while the torque is responsible for bend. The magnitude of the stretch is proportional to the strain and the film thickness ($F \propto \epsilon d$); the magnitude of torque equals the force (F) times the distance (l) from the mean position of the applied force (middle of the film) to the line of the center of the whole system [middle of the (film + substrate)].

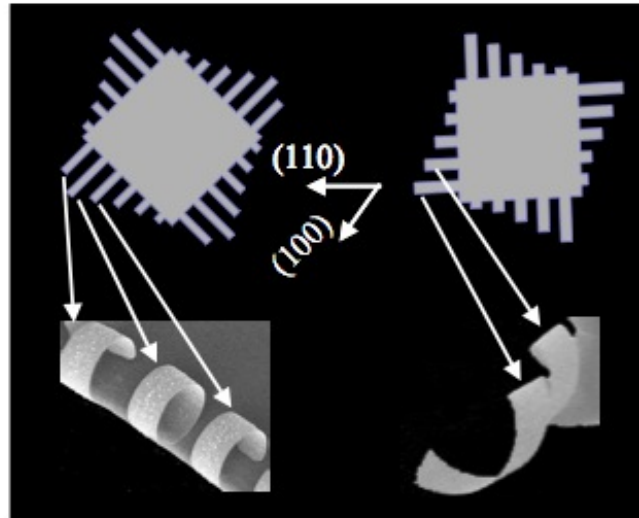


Figure 2: Experimental demonstration of strained Si/SiGe bi-layer cantilevers folding into nanorings (downside of left panel in the figure) when they are patterned along $\langle 100 \rangle$ direction, but into nanocoils when they are patterned along $\langle 110 \rangle$ direction, as they prefer to fold along the most compliant $\langle 100 \rangle$ direction. The nanorings have a thickness of 60 nm, radius of $3.2 \mu\text{m}$, and width of $3 \mu\text{m}$; the nanocoils have a thickness of 76 nm, radius of $2.8 \mu\text{m}$, and width of $4 \mu\text{m}$. Adopted from reference [2]

The geometry of the cantilever is the third variable to affect the cantilever morphology. The characteristic curvature of the bending beam can be calculated using Timoshenko formular. [6] Figure 4 indicates the geometric effects.

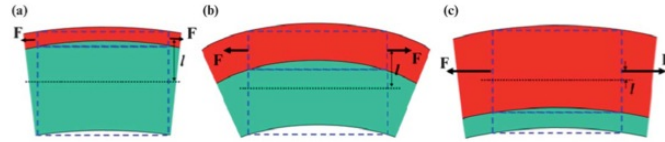


Figure 3: 2D schematic illustration of the force (F) and torque ($F \times l$) applied by a compressively strained film (red) grown on a substrate (green) for different film-to-substrate thickness ratios. Adopted from reference [5]

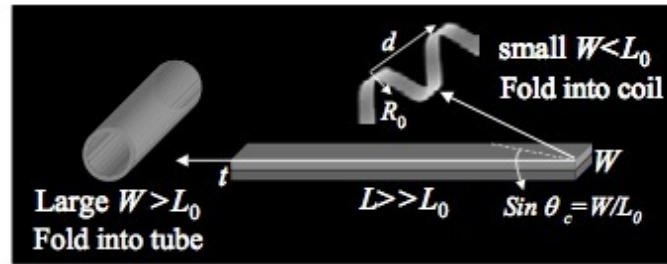


Figure 4: Schematic diagram of rolling or curling a strained bilayer membrane illustrating the geometric parameters. Adopted from reference [2]

2.2 Summary

Previous studies have shown that 3D nano structures can be made from 2D nano cantilevers. Bi-layer cantilever structure is used to store intrinsic energy, which is the driving force for bending, rolling and curling. However, there are some problems for bi-layer cantilever structure. Firstly, limited kinds of materials can be build into bi-layer system to store intrinsic energy. The material selection problem limits the application. Secondly, when considering the shape control, bi-layer system asks for strict control of initial cantilever shape, crystalline direction alignment and layer thickness. Because ion bombardment introduces external

strains, a wide range of materials could be chosen. The final shape of the 3D product can be created by controlling the parameters, such as bombarding angle, fluence and bombarding energy. Ion bombardment has its potential for 3D nano structure production.

3 Methods

This research investigates the mechanical behavior of the silicon nano cantilever under neutral Argon bombardment utilizing classical molecular dynamics. In order to examine thermal noise of the cantilever at room temperature without bombardment, one of the continuum elasticity models (Euler-Bernoulli model) is applied. In this section, molecular dynamics, Euler-Bernoulli model and silicon properties are reviewed and discussed.

3.1 Molecular Dynamics

Molecular dynamics simulation is a kind of N-body simulation that the physical movement of the atoms or molecules is calculated. The atoms' trajectories is calculated through solving the Newton's Equation of motion, which is shown in equation 1. In equation 1, $i=1,2,3,4...N$ and N is the total number of atoms, F_i is the force, r_i is the distance between atoms, t is time.

$$F_i = m_i a_i = m_i \frac{d^2 r_i}{dt^2} \quad (1)$$

The force in equation 1 is determined by the total energy of the system. According to the Newton's law, the total energy of the system U is a function of all N atomic positions shown in equation 2.

$$F_i = -\nabla_{r_i} U(r_1, r_2, r_3, ..., r_n) = -\left(\frac{\partial U}{\partial x_i}, \frac{\partial U}{\partial y_i}, \frac{\partial U}{\partial z_i}\right) \quad (2)$$

The second order differential equation with a given time step for MD could be solved by several algorithms, for instance, Runge-Kutta and Verlet. In this work, the time interaction is calculated by Velocity-Verlet

algorithm. A schematic figure for the algorithm is shown in figure 5.

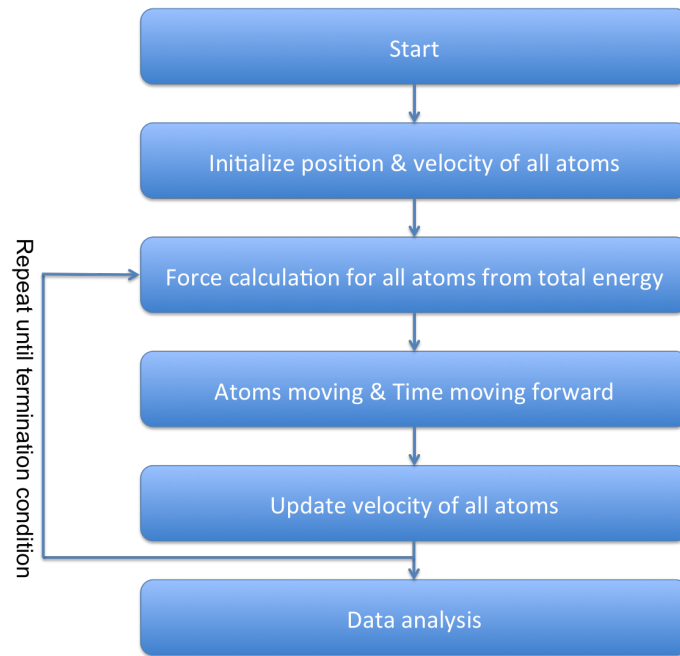


Figure 5: Velocity-Verlet algorithm for velocity, position and acceleration calculations in each time interaction.

In the scheme shown in figure 5, the only element to elaborate on is the total energy, which is the factor to calculate the force field of atoms. The total energy is obtained from the potential. So the quality of the MD simulation is determined by the potential applied. In previous studies, there are several approaches for the silicon potential that tries to simulate true properties of silicon via MD simulation. Modified embedded atomic method (MEAM) is a specific one. MEAM formalism, first introduced by Bakes [7], represents a better framework to explain the silicon behavior. In MEAM formalism, the total energy of the system is expressed as a sum of pair and single atom contributions [8], which is shown in equation 3. In equation 3, ϕ_{ij} , S_{ij} , $h(r_{ij})$ are pair potential, angular screening factor and radial cut-off function between atoms at distance r_{ij} respectively. The Angular screening factor indicates the weakening of pair interactions as a

result of screening caused by the atoms in between those pairs. The Radial cut-off function shows the limits of the interaction range for potential. In this study, MEAM-L potential is applied. Detailed performance of MEAM-L potential on modeling of silicon is given later.

$$U = \sum_{i=1}^N \sum_{j=1, j \neq i}^N \frac{1}{2} S_{ij} \phi_{ij}(r_{ij}) + \sum_{i=1}^N F_i(\rho_i) \quad (3)$$

3.2 Properties of Silicon: Experimental and Simulation

Experimental Results The melting point of silicon is 1687 K and the boiling point is 3538 K [9]. The outer electron orbital of silicon has four valence electrons. The 1s, 2s, 2p and 3s subshells are completely filled while the 3p subshell contains two electrons out of a possible six. Silicon has a diamond cubic crystal structure (shown in figure 6). The lattice constant is 5.43 Å. The silicon atoms are sp³ hybridized and bonded to four nearest neighbors. The length of the covalent bonds are 2.35 Å and the strength of the bond is 226 kJ/mol [10]. In the work of Hopcroft and Nix [11], the Young's Modulus of silicon is measured and calculated for different crystallographic direction. Some of the results is obtained and shown in figure 7.

At the surface of the silicon crystal, the covalent bonds are broken and there exist dangling bonds (shown in figure 8). Those dangling bonds increase the surface energy of the material. So thermodynamically, the silicon atoms at the surface adjust themselves at new positions to reduce the number of dangling bonds. When the number of the dangling bonds decreases, the surface energy of the silicon is reduced. The reduction of the dangling bonds leads to a variety of surface reconstructions on silicon surfaces.

In this study, the surface reconstructions of Si {100} planes are of great importance due to the simulation

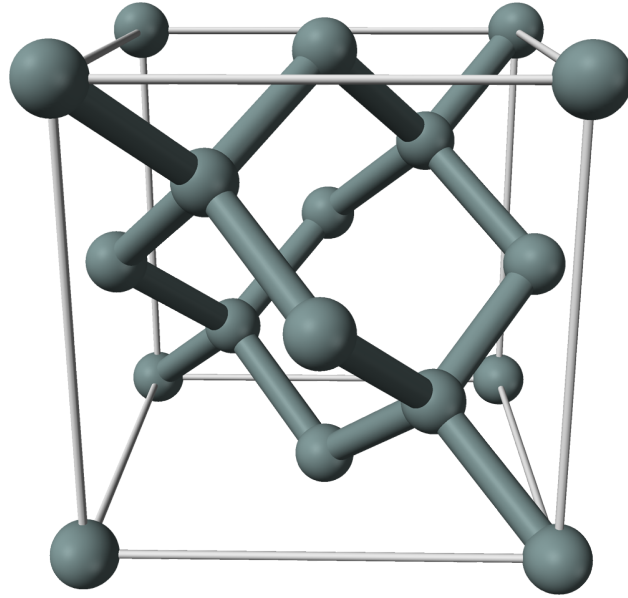


Figure 6: Crystalline structure of silicon. Obtained from [12]

Load Case	Symbol	Appropriate E value
Axial stress/strain, incl. beam bending <110> directions ("X" or "Y axis") <100> directions ("45° off-axis")	E	169 GPa 130 GPa
Plate bending, $\nu = 0.064$ for <110> in (100)	E'_{110}	170 GPa
Thin film biaxial stress/strain, (100) plane	B_{100}	180 GPa
Shear load, twisting a <110> ("X" or "Y") beam	G	50.9 GPa
Stress Concentrations	E_V	166 GPa
Hydrostatic loads (Bulk modulus)	B	97.8 GPa
Temperature Coefficient of E	TCE	- 60 ppm/°C

Figure 7: Common Values of E for Silicon, adapted from [11]

model. The $\{100\}$ planes have a square unit cell. Each silicon atom below the surface is bonded with two atoms in the plane below and two atoms in the plane above. The reconstruction of $\{100\}$ surface can be described by the dimer model. In figure 9, the solid circles represent the silicon with 2 dangling bonds and the open circles represent the bulk silicon. Two silicon atoms with dangling bonds form a silicon dimer at the surface and the dangling bonds is decreased by 50%. For bulk silicon crystal, surface reconstruction does not affect the mechanical properties much. However, when considering the nanoscale material, which has a higher surface to volume ratio, the surface reconstruction can affect the mechanical properties significantly. A work done by Dr. Sadeghian shows that because of the surface reconstruction, the effective elastic modulus of a silicon nanoplate containing 20 layers of silicon atoms is reduced by 39% [13].

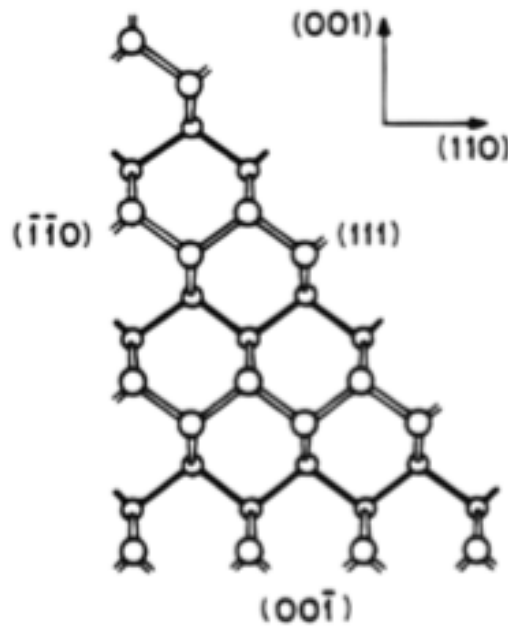


Figure 8: Dangling bonds of silicon which without reconstructions. Circles stands for silicon atoms while the lines among circles represents the covalent bonds between silicon atoms. Three low index planes are represented as example. The sizes of the Si atoms are shown to decrease away from the page. Adapted from [14]

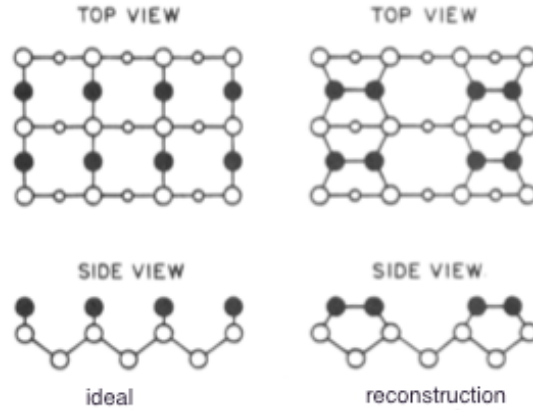


Figure 9: Top and side view of silicon (100) surface. Adapted from [14]

Si Properties Simulation In the molecular dynamics simulation, the molecules or atoms are simplified as small spheres. The spheres are allowed to interact with each other for a short period of time. As indicated in previous section, the definition of a potential function, which is the description of how the particles in the simulation will interact, is of great importance. There are a lot of famous potentials to describe the particle-particle interactions, for instance, Lennard-Jones potential[15], Tersoff potential [16] and Tight-Binding Second Moment Approximation (TBSMA) potentials [17]. The more appropriate the potential used during the simulation, the more accurate results can be obtained. In this study, the Modified Embedded-Atom Method (MEAM) developed by Virtual Materials and Mechanics group in TU Delft is applied as the potential. In this section, silicon is modeled using MEAM potential and the properties of generated from the simulation are compared with the experimental ones.

In the work of Timonova and Thijsse, the extensive test of MEAM-L potential was done by calculating crystal, liquid, and amorphous phase properties. [18] Comparison was made with other potentials modeling silicon: Stillinger-Weber (SW), Tersoff (T3), Modified Tersoff (MOD), and the Environment-Dependent Interatomic Potential (EDIP). The potentials calculated from density-functional theory (DFT) are utilized

as the potentials in reality. The simulation in this study is carried out at room temperature (300 K). At 300 K, the crystal structure of silicon is diamond cubic. The potential energy of cubic-diamond crystalline structure at 0 K with different Si-Si distance is shown in figure 10. It can be seen from figure 10 that the MEAM-L potential with $\zeta = 0$ is much more close to the reality. Additionally, the potentials for other silicon crystalline structures and silicon molecules are also calculated. Figure 11 obtained from [18] shows a table containing the results of energy for different crystals and molecules. Figure 11 shows the energy differences among the equilibrium cubic diamond structure, face centered cubic (fcc), simple cubic (sc), body-centered cubic (bcc), and β -tin structures. It can be seen that the MEAM-L potential has a good performance which well matches the results calculated from density-functional theory. Therefore, it can be concluded that when considering the potentials with different structures, MEAM-L potential has a better performance and is reliable for modeling silicon.

A correct description of the elastic properties of diamond silicon is another important benchmark of the potential. Figure 12 shows a table containing the elastic properties, which are calculated using homogeneous deformation method. The simulation results of MEAM-L potential are much closer to reality than that of other potentials. So it can be inferred that when modeling the mechanical behavior of the silicon, the simulation with MEAM-L potential will give reliable results.

3.3 Continuum Elasticity Theory

At room temperature, cantilever at nano scale vibrates because of the thermal noise. In this study, the cantilever is one end fixed and one end free. The schematic model of the cantilever is shown in figure 13. In order to test the influence of thermal noise, Euler-Bernoulli model is applied to interpret the vibration of

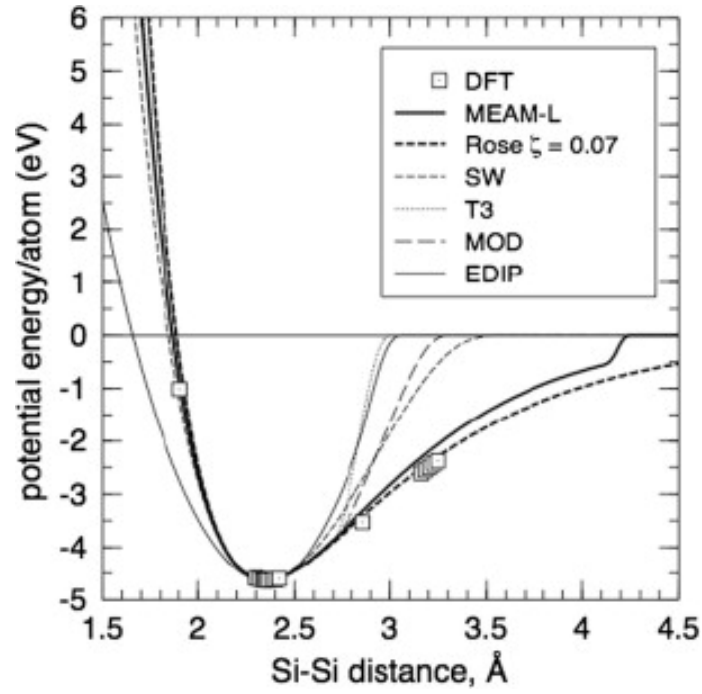


Figure 10: Potential energy minima in diamond structure as a function of the nearest neighbour R_e . The SW, T3, MOD, and EDIP potentials are plotted, compared with DFT energy calculations. The solid line of MEAM-L potential is calculated from Rose pair potential[19], with the parameter $\zeta = 0$. The dashed line, which with the parameter $\zeta = 0.07$ is also plotted.

Property	DFT	MEAM-L	SW	T3	MOD	EDIP
$\Delta E_{sc-diam}$, eV/atom	0.38	0.40	0.29	0.32	0.31	0.53
R_e , Å	2.53	2.64	2.61	2.54	2.50	2.50
$\Delta E_{\beta tin-diam}$, eV/atom	0.32	0.39	0.21	0.33	—	—
a , Å	4.84	4.99	4.97	4.91		
c/a	0.532	0.524	0.561	0.524		
$\Delta E_{bcc-diam}$, eV/atom	0.58	0.50	0.30	0.43	0.44	1.59
R_e , Å	2.68	2.71	2.81	2.67	2.63	2.81
$\Delta E_{fcc-diam}$, eV/atom	0.60	0.40	0.42	0.76	0.45	1.84
R_e , Å	2.75	2.64	2.93	2.76	2.72	2.89
$\Delta E_{dimer-diam}$, eV/atom	2.82	2.83	3.47	3.30	3.21	3.08
R_e , Å	2.29	2.52	2.35	2.30	2.22	2.28
r_c , Å	—	4.30	3.77	3.00	3.20	3.12

Figure 11: Potential energy minima and the nearest neighbour R_e of different silicon structures, compared with diamond cubic crystals ($E_{ref} = -4.63\text{eV}$, $R_{ref,e} = 2.35\text{\AA}$). Results of different potentials were compared with MEAM-L together with the density-functional theory (DFT) results, which was considered as experimental value. The radial cutoff distances for different potential were also presented. It can be seen that MEAM-L potential had a better performance.

Property	Exp	MEAM-L	SW	T3	MOD	EDIP
C_{11} , GPa	166	167	162	143	166	175
C_{12} , GPa	64	65	82	75	65	62
C_{44} relaxed, GPa	80	80	60	69	77	71
B , GPa	99	99	108	98	99	100

Figure 12: Elastic constants C_{11} , C_{12} , and C_{44} , and bulk modulus B from MEAM-L and other four potentials. Experimental results are also presented.

cantilever without bombardment. Under equipartition theorem, the root mean square amplitude at the end of the beam can be calculated considering all different vibration modes. According to the Euler-Bernoulli beam theory, the vibrations of a bar in the z direction could be described by the partial differential equation:

$$\frac{\partial^2 z(x, t)}{\partial t^2} + \frac{EI}{\rho A} \frac{\partial^4 z(x, t)}{\partial x^4} = 0 \quad (4)$$

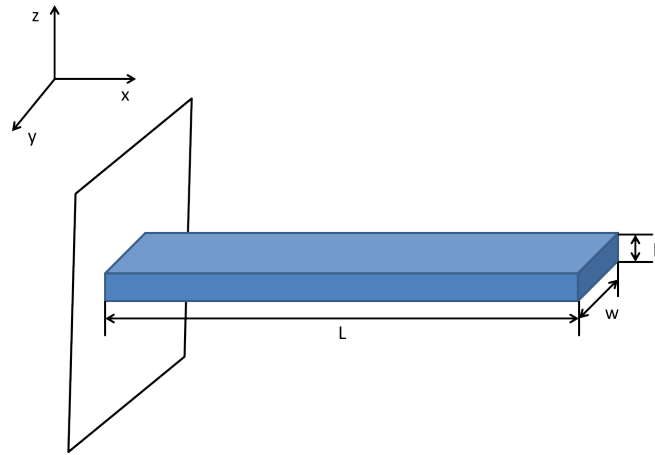


Figure 13: Schematic view of the cantilever model.

The curve $z(x, t)$ describe the beam vibration in z direction at some position x ($0 \leq x \leq L$, L is the length of the cantilever) at certain time. E is the Young's modulus, I is the area moment of inertia of the cantilever, ρ is the density of the cantilever material, A is the cross-sectional area of the cantilever. In order to solve equation 4, which is fourth order differential equation, four conditions are needed. The fourth order differential equation can be solved as [20]

$$z(x, t) = \sum_{i=1}^{\infty} C_i \sin(2\pi f_i t + \delta_i) h_i(x) \quad (5)$$

where t is time, i is the vibration mode index, f_i is the vibration frequency. C_i is the amplitude of the vibration. C_i depends on initial conditions and differs from time to time, but its mean square value can be

calculated. Detailed derivation of C_i is shown later. δ_i depends on the initial state of the cantilever and may differ from time to time. For instance, when $t=0$, the cantilever is at initial state and $z(x,0)$ is zero, then δ_i is 0. $h_i(x)$ is the mode shape, which is a function of x . Expression of $h_i(x)$ is shown in equation 6.

$$h_i(x) = (\sin \alpha_i + \sinh \alpha_i) \left(\cos \frac{\alpha_i}{L} x - \cosh \frac{\alpha_i}{L} x \right) - (\cos \alpha_i + \cosh \alpha_i) \left(\sin \frac{\alpha_i}{L} x - \sinh \frac{\alpha_i}{L} x \right) \quad (6)$$

With

$$\alpha_i^4 = \frac{12\rho\omega_i^2 L^4}{Eh^2} \quad (7)$$

where h is the thickness of the cantilever, ω_i is the angular vibration frequency, $\omega_i = 2\pi f_i$.

According to the boundary conditions, only some discrete values of α_i is allowed. When referring the boundary conditions for this study, which is a cantilever with one end fixed and a free end, the α_i can be determined by:

$$\cos \alpha_i \cosh \alpha_i = -1 \quad (8)$$

By applying the equation 8, the for a cantilever with a free end, the first four modes of vibration are $\alpha_1 = 1.88$, $\alpha_2 = 4.96$, $\alpha_3 = 7.85$, $\alpha_4 = 11.00$. When the $i \geq 5$, $\alpha_i = (i - 0.5)\pi$. By plotting the equation 8, the shape of first four mode vibration is shown in figure 14

In this research, the temperature of the system is set at room temperature (300K). To study the thermal vibration of a cantilever, equipartition theorem is applied. In this report, the vibration at z direction (see figure 14) is studied. So the mean value of the kinetic and potential thermal energy of the system at z direction are both $\frac{1}{2}kT$, where k is the Boltzman constant and T is the thermodynamic temperature. When bending a cantilever by a small amount of ς at the end, (at z direction) its potential energy is $\frac{1}{2}K\varsigma^2$ (neglecting the

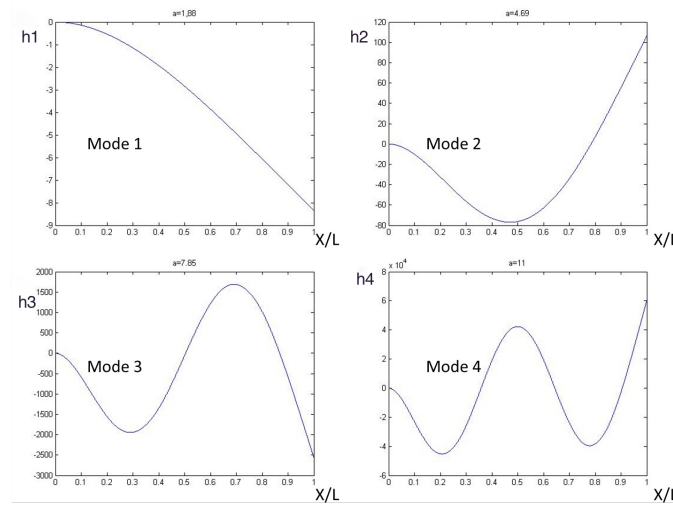


Figure 14: First four bending mode shape.

momentum, rotation, etc.), where K is the spring constant, which could be calculated as $K = \frac{Ewh^3}{4L^3}$. Hence, the equipartition theorem demands $\frac{1}{2}kT = \frac{1}{2}K\hat{z}^2$, where $\hat{z}^2$ represents the mean square deflection at the end of the cantilever caused by the thermal energy. So the amplitude of thermal deflection in the z direction for a cantilever with a free end and a clamped end is

$$\sqrt{\hat{z}^2} = \sqrt{\frac{kT}{K}} \quad (9)$$

The equation 9 does not show the distribution of different vibration modes. In order to study the distribution of different vibration modes, the total vibration energy W of the bar is given by [20]:

$$W = \frac{Ewh^3}{24} \int_0^L \left(\frac{d^2z}{dx^2} \right)^2 dx + \frac{\rho wh}{2} \int_0^L \left(\frac{dz}{dt} \right)^2 dx \quad (10)$$

In the equation 10, the first term accounts for the potential energy, while the second term accounts for the

kinetic energy. By inserting the equation 5, referring to the calculation in literature [20], the equation is simplified as:

$$W = \frac{K}{2} \sum_{i=1}^{\infty} q_i^2 \alpha_i^4 \frac{I_i}{3} + \frac{1}{2M} \sum_{i=1}^{\infty} p_i^2 I_i \quad (11)$$

where $q_i = C_i \sin(2\pi f_i t + \delta_i)$, $p_i = 2\pi M f_i C_i \cos(2\pi f_i t + \delta_i)$, $I_i = (\sin \alpha_i + \sinh \alpha_i)^2$, M is the total mass of the cantilever which is $M = \rho w h L$.

To study the thermal deflection due to the mode i at the end of the cantilever, equating the $\frac{1}{2}kT$ to $\hat{W}_{i,pot} = \frac{K}{2} \hat{q}_i^2 \alpha_i^4 \left(\frac{I_i}{3}\right)$, then

$$\hat{q}_i^2 = \frac{3kT}{\alpha_i^4 K I_i} = \frac{1}{2} \hat{C}_i^2 \quad (12)$$

Then it can be concluded that, the mean square amplitude of each vibration mode C_i is calculated as:

$$\hat{C}_i^2 = \frac{6kT}{\alpha_i^4 K I_i} \quad (13)$$

Knowing $\hat{q}_i^2$, the mean square deflection at the end of the cantilever can be calculated since

$$\hat{z}_i^2 = \hat{q}_i^2 h_i(L)^2 \quad (14)$$

The detailed deviation of the equations can be found in literature [20]. In conclusion, it can be obtained that

for each different vibration mode, the mean deflection at the end of the cantilever could be calculated as:

$$\hat{z}_i^2 = \frac{12kT}{K\alpha_i^4} \quad (15)$$

In the study, the simulation results together with the theoretical free end deflection shown in equation 15 will be calculated. Meanwhile, the vibration modes of the cantilever are also fitted. The results are shown in section 4.

3.4 Argon Silicon Interactions: Experimental and Simulation

In this study, neutral Ar bombardment was applied on the silicon cantilever. So the literatures representing the interaction between the Ar and silicon during bombardment are reviewed in this section. Initially, sputtering yield data, which contains a lot of predictions such as surface cleaning, sputter etching, draws numerous interests. The definition of sputtering yield is the average number of atoms ejected from the target per incident atom. It has been shown in the reference [21] [22] and [23] that the sputtering yield of silicon is highly dependent on the bombardment energy of the incoming particles, the mass of the bombardment particles, the bombardment angle, and the temperature which influence the binding energy of the surface. In this study, molecular dynamic simulation of Ar bombarding on silicon with a 200 eV energy, which is quite low compared to the etching process in practical, is applied. There are many previous researches including [24], [25], and [26] studying the low energy sputtering. Experimentally, the sputtering yield of single crystal silicon (Si/Ar) at 200 eV is 1.33 with a bombarding angle of 45° according to the reference [22].

The performance for MEAM-L potential when doing the bombardment simulation is also of great importance. Simulations to study the formation and crystallization of amorphous Si by neutral Ar bombarding have been carried out by Virtual Materials Laboratory of Delft University of Technology. In the references [27][28], MEAM-L potential is utilized to do the bombardment simulation. The Si-Si interactions in reference [27] and [28] are described by either the MEAM potential. The Firsov-Moliere pair-potential is utilized to describe the interactions of Ar-Ar and Si-Ar at all distance and Si-Si at short distance. Although the potential used is different with this study, because the crystal structure and bombarding conditions used in those studies are similar, results from those studies can be a reference for this work.

In the simulation of reference [28], Si single crystal was performed 500 eV Ar bombardment at room temper-

ature. The target contains 27,000 atoms with 60 monolayers (ML). The surface area of the Si (0 0 1) surface is $81 \text{ \AA} \times 81 \text{ \AA}$. The lowest 2 ML were harmonically fixed to their crystal locations. Periodic boundary conditions were applied in the two directions parallel to the surface. The overall temperature of the system was controlled by Berendsen damped velocity scaling, which enable the system to interact at a constant temperature. Every 7 ps a Ar atom was introduced. The location of the Ar atom to come into is a randomly chosen location above the surface area. The energy of the Ar atoms is 500 eV, with a polar angle of 45° and an azimuthal angle of 0° with respect to the $[1\ 1\ 0]$ direction.

The product of Ar sputtering are the ejection of Si atoms and Si_2 dimer molecules. Besides, an amorphous Si phase formed at the top of the eroding surface of the crystal. Meanwhile, some Ar atoms were injected under the surface. Side snapshot of the system is shown in figure 15. The MEAM potential, after 7.2 ns of bombardment, with a Ar fluence $1.53 \times 10^{15} \text{ cm}^{-2}$ has a sputter yield of 1.78, which is close to the experimental value 1.63 [22]. According to the reference [22], comparing with the results of other potentials, MEAM has one of the best performances in modelling silicon bombarded by Ar.

Considering the results at 500 eV, the sputtering results are closed to the reality and better than other potentials. Conclusively, the MEAM-L potential can be used to study the Si properties under bombardment.

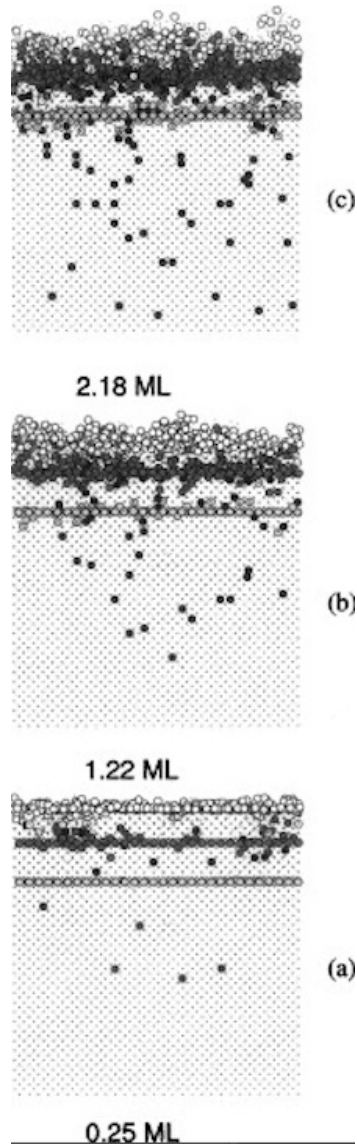


Figure 15: A snap shot of side view Si(0 0 1) after bombardment (for illustration only). The white, dark gray, and light gray circles represent the atoms from 1, 8, 17 (counted from top) planes initially respectively. The black circles are implanted Ar atoms. Under the snap shots the number of MLs sputtered is shown. Left column represents the MEAM results, while right column represents the SW results. Adapted from [24].

4 Results and Discussion

4.1 Model and Effective Young's Modulus

A simulation box for the silicon cantilever is set up. Silicon nano cantilevers are created with the atomic positions corresponding to the cubic diamond crystal, which is shown in figure 16. The cantilever is 120 unit cells long, 20 unit cells wide, and 3 unit cells in thickness, and contains 57600 Si atoms in total. The directions x, y, z are corresponding to the crystallographic direction $[100], [010], [001]$ respectively in this case. The cantilever is positioned in the middle of the simulation box. Some space between the cantilever and wall of the box (shown in figure 17) is left in order to create vacuum regions for the shape changing. Periodic boundary conditions are not applied. Therefore, once the atoms leave the box, they cannot come back again. The temperature during the simulation process is set to be at room temperature (300 K) by scaling the velocities in all MD time steps. Anchor point, at which the atom is fixed during the simulation, is made from $x=0$ along the x axis. Three atomic layers with 360 atoms are made as anchor points. Therefore, the silicon cantilever is one end clamped and another end free. Euler-Bernoulli equation can be used to model the vibration of the beam.

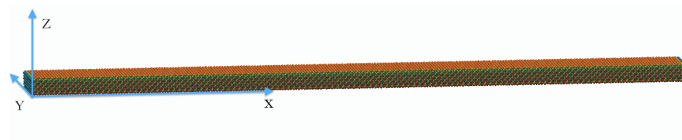


Figure 16: Initial state of the silicon cantilever. Different colour stands for different principle stress tensor at x direction (σ_{xx})

According to previous study [11], the elastic modulus of bulk silicon along $[100]$ direction could be calcu-

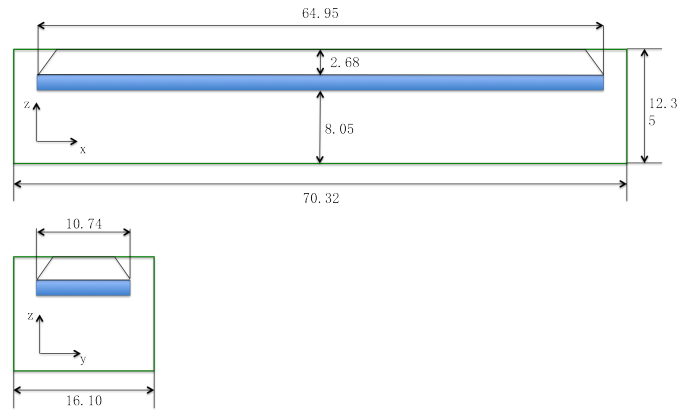


Figure 17: Schematic side view of the simulation box. The unit of the length is nano meter.

lated with the equation 16:

$$E[100] = C_{11} - 2 \frac{C_{12}^2}{C_{11} + C_{12}} \quad (16)$$

The calculation result reveals that the value of $E[100]$ is 130 GPa. When the size of the cantilever is at nanoscale, the mechanical properties are quite different with that of the bulk. It is concluded that the elastic modulus of the nanocantilever is dependent on the size.[29] [30] At nanoscale, there are many size effects that can influence mechanical properties, for instance, surface effects. So the $E[100]$ value for bulk silicon cannot be used in this study and it is necessary to calculate it by simulation.

A similar simulation model is used to calculate the effective Young's Modulus. The cantilever is 120 unit cells long, 20 unit cells wide, and 3 unit cells in thickness, which contains 57600 Si atoms in total. The directions x, y, z are corresponding to crystallographic direction $[100], [010], [001]$ respectively. Periodic boundary conditions are applied along x direction and there is no boundary conditions applied along y and z direction. The cantilever fills the x directions completely, but does not fill the y and z direction completely. The vacuum regions between the cantilever and the walls of the box avoid the interaction resulting from

the periodic images. Therefore the cantilever has four free surfaces. The temperature is set at 300 K. The cantilever is fully relaxed for 91 ps to a minimum energy and there is no pressure applied. Figure 18 shows a snapshot of the beam surface after relaxation. Surfaces display a (2×1) -type reconstruction along $[110]$ or $[1\bar{1}0]$ directions. Rows of dimers are formed imperfectly because of the finite sizes of the boundary planes.

After the cantilever is fully relaxed, tensile forces are applied on the two sides of the cantilever. To calculate the stress and strain, data from *camelion* is collected. The stress-strain curve is shown in figure 19. The elastic modulus is calculated as 80 GPa. Due to the size effects, such as surface reconstruction shown in figure 18, the stiffness of the cantilever decreases significantly. Then the theoretical resonance frequency of each vibration mode (from mode 1 to mode 6) for this cantilever beam is calculated with equation 19. Numerical results are listed in table 1.

4.2 Mechanical Behavior of Nano Cantilever in Simulation Box

In figure 20, the side views of cantilever at different time periods are exaggerated by $z \times 3$. The cantilever experiences a multiple-modes vibration. The vibration of the beam is fitted to Euler-Bernoulli equation. In Euler-Bernoulli equation, the vibration of the cantilever beam z is a function of time t and of position x . As shown in equation 17, the mathematical expression could be divided into two part: $T_i(t)$, where $T_i(t) = C_i \sin(2\pi f_i t + \delta_i)$; and $h_i(x)$, which is the mode shape function. Euler-Bernoulli vibration equation describes a 2D model. Because in the simulation, the cantilever is a 3D structure, which cannot be fitted into 2D Euler-Bernoulli model, the finite element method is applied to simplify the cantilever into a 2D model. The beam is 120 unit cells in length and it is divided into 120 parts. For each part of the beam, the average position value of both x and z direction is calculated. Then a series of position points containing x and z are

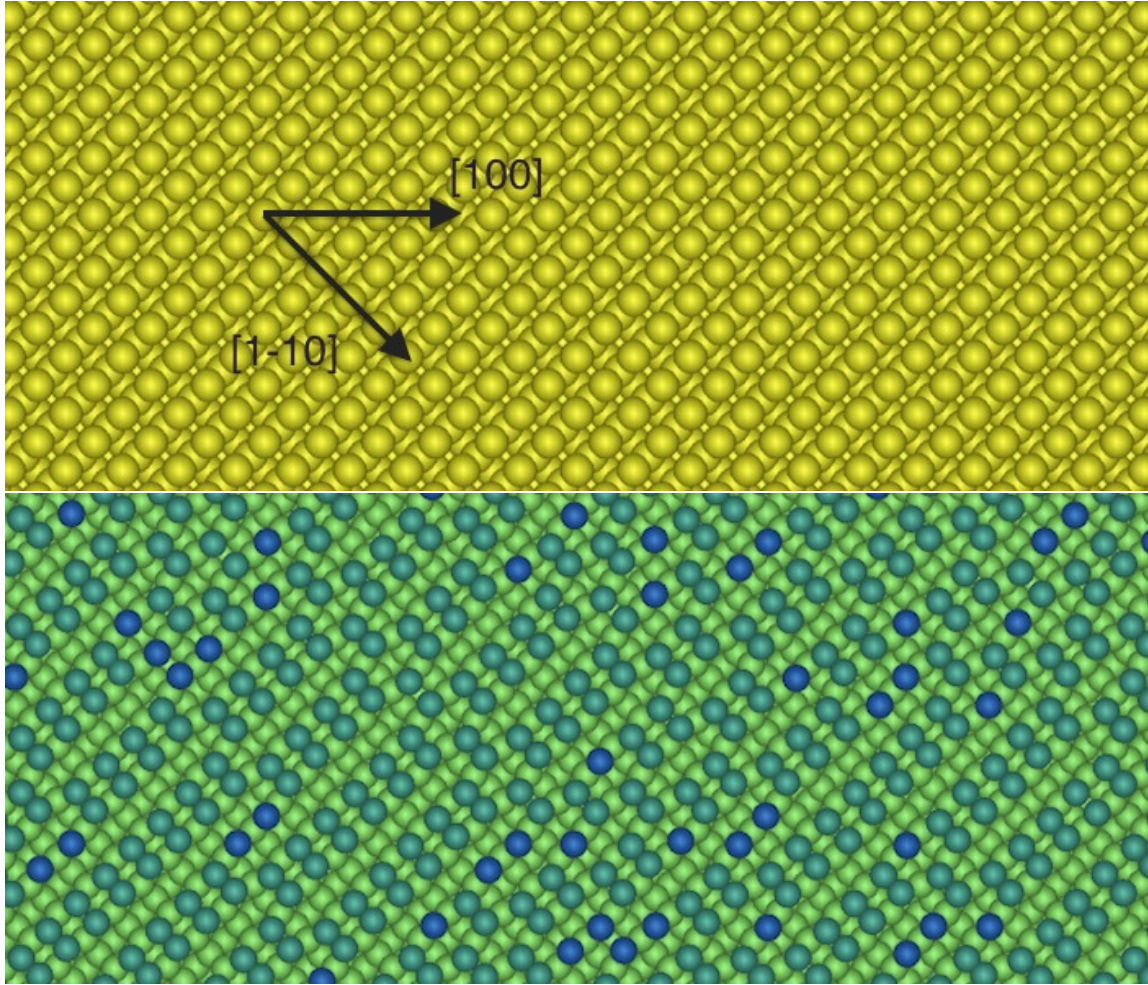


Figure 18: Snapshots of top view from the part of the cantilever. Top: the nanocantilever with initial atomic positions corresponding to the bulk diamond-cubic crystal, and below: fully relaxed nanocantilever at room temperature. The coloring method is the number of nearest neighbors.

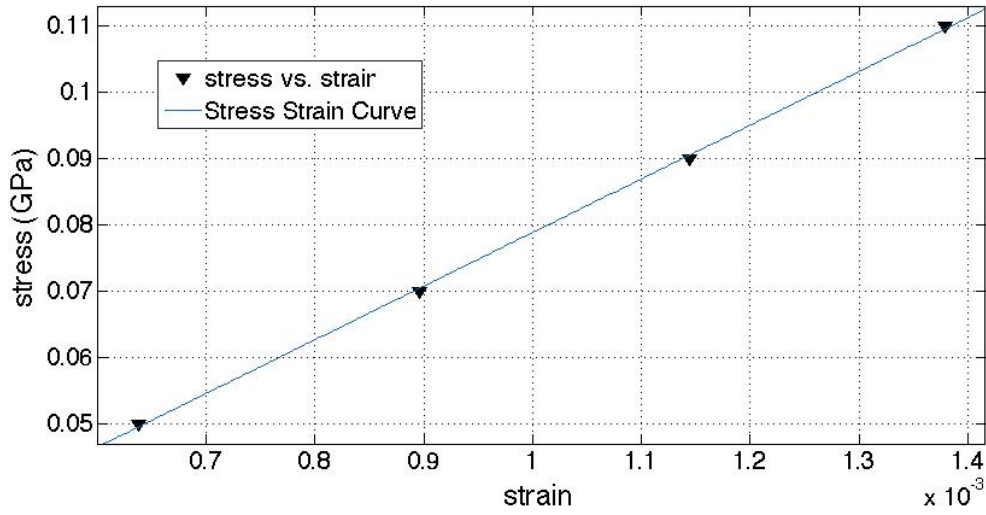


Figure 19: Stress-strain curve for calculation of elastic modulus.

obtained. By plotting those position points together, the cantilever profile is formed. The same work is done at different time. So various profiles are plotted. Some examples are shown in figure 21.

$$z(x, t) = \sum_{i=1}^{\infty} C_i \sin(2\pi f_i t + \delta_i) h_i(x) \quad (17)$$

At a certain time point, $T_i(t)$ ($T_i(t) = C_i \sin(2\pi f_i t + \delta_i)$) is a constant for different vibration modes. The vibration function can be considered as the sum value of different vibration modes, which is calculated to be a constant factor $T_i(t)$ at a certain time multiplying the corresponding cantilever mode shape function $h_i(x)$. Thus at a certain time, the cantilever profile could be linear fitted into equation 18. Six-mode fit describes the z profiles to a very good precision (shown in figure 22, the error is around 0.2 nm). The mean square deflection of the cantilever at the end is calculated as $\hat{z}_i^2 = \frac{12kT}{K\alpha_i^4}$ in thermal equilibrium. $\hat{z}_i^2$ decreases significantly with the value of mode index increasing. The higher the value of mode index is, the

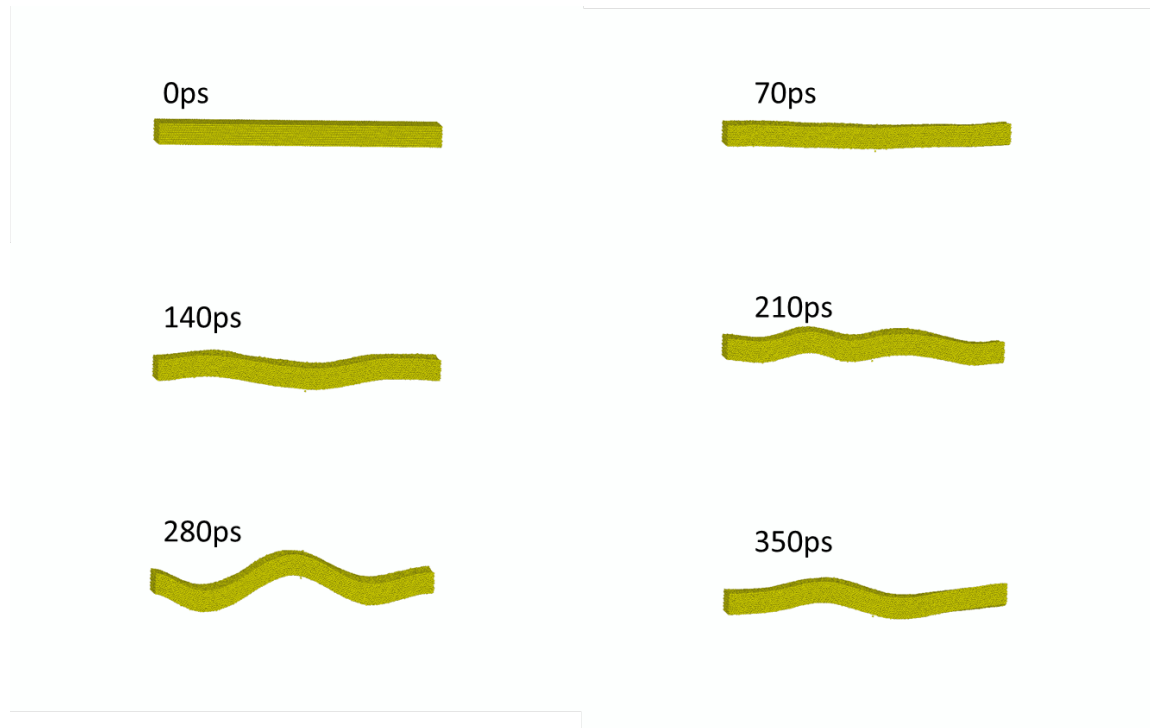


Figure 20: Snapshot of the cantilever during the vibration. Anchor points are at the left side of the cantilever. The signal is exaggerated by $\times 3$ in order to see the vibration clearly.

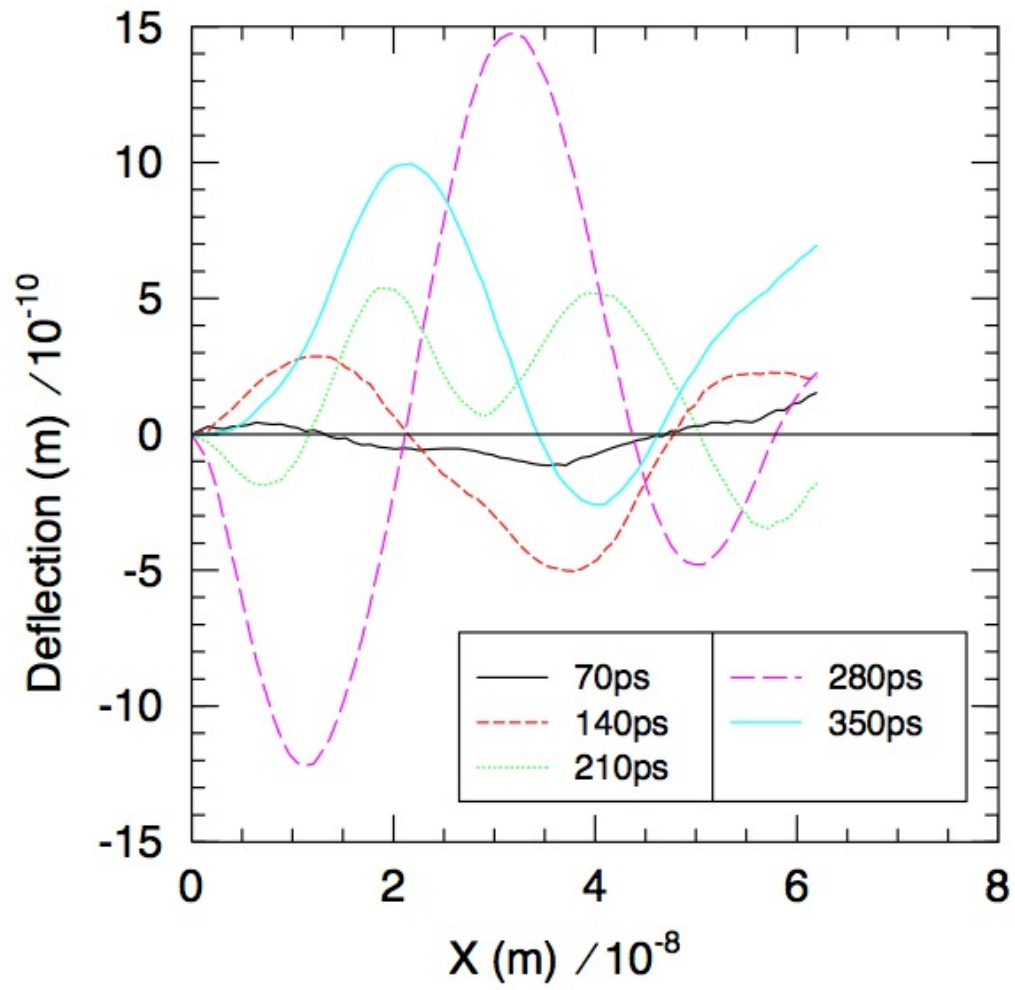


Figure 21: Cantilever beam profiles plotted with different time.

less distribution to the vibration the mode makes.

$$z(x, t) = T_1(t)h_1(x) + T_2(t)h_2(x) + T_3(t)h_3(x) + T_4(t)h_4(x) + T_5(t)h_5(x) + T_6(t)h_6(x) \quad (18)$$

If C_i and δ_i are constant in time, $T_i(t)$, where $T_i(t) = C_i \sin(2\pi f_i t + \delta_i)$, is a sine function of time, depending on the resonant frequency of each vibration mode. The resonant frequency of the cantilever of each oscillation mode could be calculated as:

$$f_i = \frac{1}{2\pi} \frac{\alpha_i^2}{\sqrt{12}} \sqrt{\frac{E}{\rho}} \frac{h}{L^2} \quad (19)$$

where α_i is the mode index ($\alpha_1 = 1.88, \alpha_2 = 4.96, \alpha_3 = 7.85, \alpha_4 = 11.00, \alpha_5 = 14.14, \alpha_6 = 17.28$), E is the elastic modulus along x direction ($E = 80$ GPa), ρ is the mass density ($\rho = 2.329 \text{ g} \times \text{cm}^{-3}$), h and L is the thickness and length of the cantilever respectively ($h = 1.62$ nm, $L = 64.95$ nm). The resonant frequency of each vibration mode is shown in table 1.

Table 1: Resonant Frequency Calculation

Mode Number	Resonant Frequency Theoretical (GHz)
1	0.463
2	3.172
3	7.954
4	15.601
5	25.772
6	38.493

The cantilever profiles at different time points are linear fitted into equation 18. Some examples are shown in figure 22. Numerical values are displayed later. The horizontal axis in the figures stands for the positions of the cantilever along x direction, while the vertical axis stands for the deflections at certain time. Black

dots are the simulation results, while the blue lines are the fitting function. The differences between the simulation results and the fitting function are less than 0.2 nm. Therefore the simulation results well match the model applied in this study.

Figure 23 shows the T_i versus time for all the six vibration modes used in the simulation. The simulation time is 371 pico-seconds. For mode 1 and mode 2 vibration, 371 ps cannot describe a whole vibration process, because the complete vibration period for mode 1 is 2160 ps, while that for mode 2 is 862 ps. However for modes from 3 to 6, 371 ps is enough for several vibration processes. It can be seen that, the amplitude shown in figure 23 is not constant and time difference between each peak is same. So the frequency of each mode could be calculated by determining the time difference between each peak in the plot. The results from the simulation and the theoretical calculations are listed in table 2. It can be seen that the theoretical calculations well match the frequencies calculated from the simulation.

Table 2: Resonant Frequency Calculation Comparison

Mode Number	Resonant Frequency Simulation (GHz)	Resonant Frequency Theoretical (GHz)
1	-	0.463
2	-	3.172
3	8.1 ± 0.8	7.954
4	16.8 ± 1.5	15.601
5	24.6 ± 0.9	25.772
6	37.7 ± 0.9	38.493

As shown in previous sections, if the vibration is thermally activated, according to the equilibrium theorem, the mean square value of amplitude in the vertical direction at the free end could be calculated as:

$$\hat{z}_i^2 = \frac{12kT}{K\alpha_i^4} \quad (20)$$

where the k is the Boltzmann constant, T is the temperature, K is the spring constant, where K could be

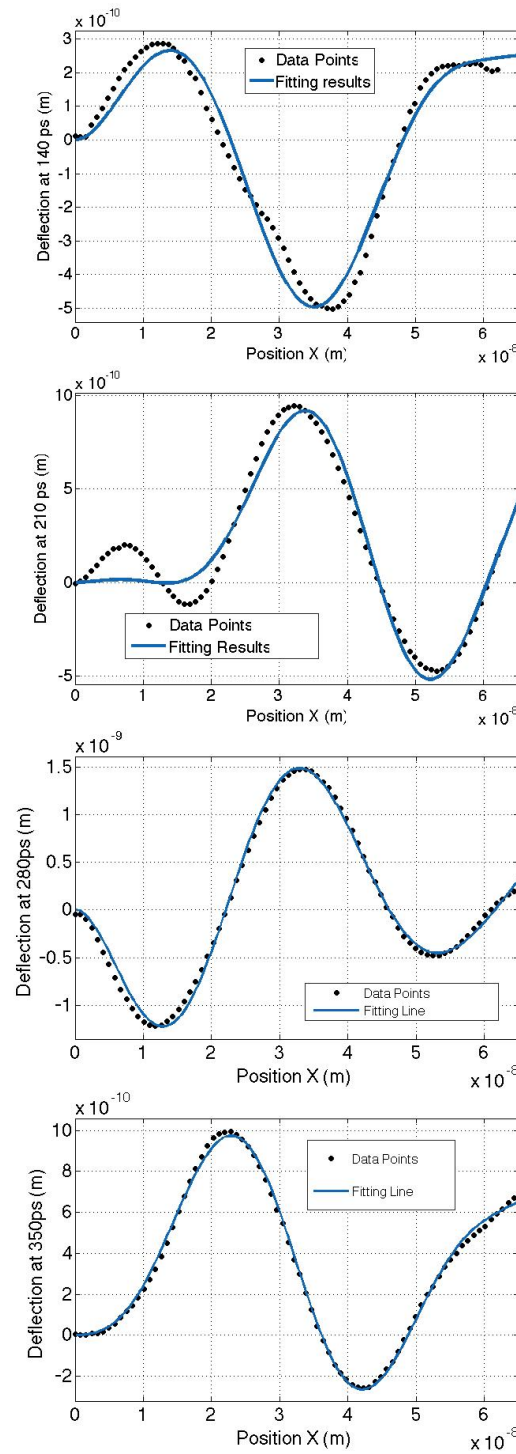


Figure 22: Fitting results examples.

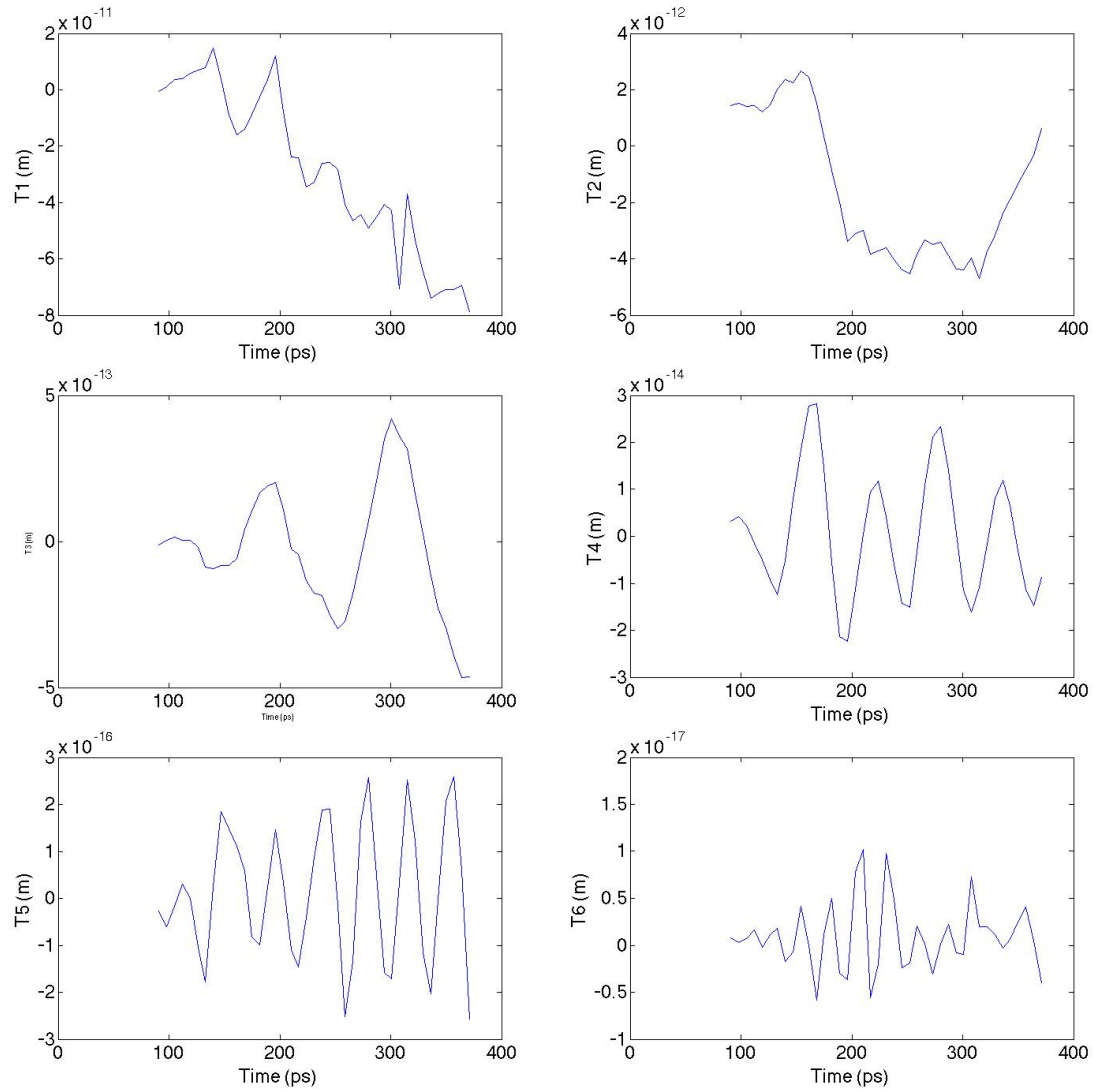


Figure 23: T_i plotted versus time (From 91ps to 371ps).

calculated as

$$K = \frac{0.25Ewh^3}{L^3} \quad (21)$$

At 300 K, the root mean square of deflection at the end of the cantilever beam could be simplified as

$$D_i = \frac{0.64\text{\AA}}{\sqrt{K}\alpha_i^2} \quad (22)$$

In principle, according to Euler-Bernoulli equation and equipartition theorem, the mean square of the amplitude factor C_i is calculated as $\hat{C}_i^2 = \frac{6kT}{\alpha_i^4 KI_i}$. The root mean square amplitude factor $\sqrt{\hat{C}_i^2}$ is proportional to a factor η_i , which can be calculated as

$$\eta_i = \frac{1}{\alpha_i^2 \times (\sin \alpha_i + \sinh \alpha_i)} \quad (23)$$

Meanwhile, as mentioned in previous paragraphs, $T_i(t)$, calculated as $T_i(t) = C_i \sin(2\pi f_i t + \delta_i)$, is a sine function. The root mean square (RMS) value of C_i can be estimated from the peaks shown in figure 23. Those values and the theoretical calculations are listed in table 3. It reveals that the RMS amplitudes of different vibration modes $|C_i|$ differ a lot from theoretical values. Meanwhile, the C_i values are not proportional to the factor η_i . The simulated thermal model does not match the theoretical one. There are two possible reasons. Firstly, due to the surface reconstruction, the geometry of the cantilever changes immediately from the beginning of the simulation. The surface reconstruction affects many factors such as spring constant K , which is a significant element in the amplitude calculation. Another reason is about the mechanical properties change during vibration. Because the continuous to thermal vibration, the microstructure may change during the mechanical process and the mechanical property changes due to the change of

microstructure.

Table 3: Absolute Value of Amplitude Factor C_i Calculation Comparison

Mode Number	$\sqrt{\hat{C}_i^2}$ Simulation	$\sqrt{\hat{C}_i^2}$ Theoretical Calculation from Equation 13 (nm)
1	0.15	0.187
2	4×10^{-3}	1.32×10^{-3}
3	3×10^{-4}	3.5×10^{-5}
4	2×10^{-5}	7.6×10^{-7}
5	2×10^{-7}	1.99×10^{-8}
6	6×10^{-9}	5.76×10^{-10}

In conclusion, the vibration of the cantilever match the six-mode Euler-Bernoulli vibration model. The RMS amplitude of the cantilever do not match the theoretical calculation for thermal noise only. The reason may be attributable to the initial conditions change and the mechanical properties change during vibration. Further research is needed to investigate how the initial conditions change and mechanical properties change influence the thermal vibration.

4.3 Bombardment with neutral Ar

4.3.1 General Model

Standard Model Description and Sputtering Results As the model shown in the previous section, the cantilever beam is bombarded with neutral Ar atoms coming from the top of the simulation box. In the standard model, the bombarding energy of Ar atoms is 200 eV. The polar bombarding angle is 45° and the azimuthal angle is set to be random. All of the Ar atoms are designated to bombard at the whole surface at the top of the cantilever. Figure 24 and figure 17 show a schematic view of the Ar bombardment. The blank rectangle outside stands for the simulation box, while the solid rectangle inside stands for the silicon

cantilever beam.

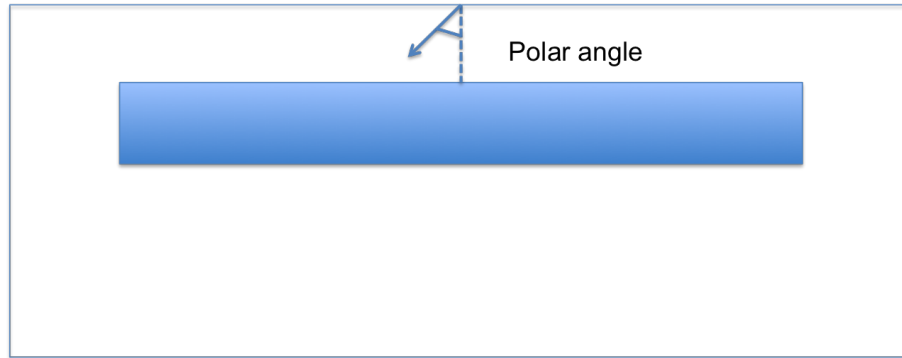


Figure 24: Schematic view of the Ar bombardment in this model.

The simulation of standard model runs for 420 ps. Through counting the number of atoms that leaves the simulation box, the results of sputtering can be obtained. The sputtering yield in this study is calculated as

$$Y = \frac{N_{Si}}{N_{Ar}} \quad (24)$$

where N_{Si} stands for the silicon atoms removing from the box, and N_{Ar} stands for Ar atoms bombarding on the cantilever.

In figure 26, the rectangle stands for the side view of the simulation box at a direction perpendicular to Y-Z surface. The sputtered atoms, Si and Ar, leave the box from the four surfaces at $y=0$, $y=w$, $z=0$, $z=h$, shown as four arrows in the figure 26. The sputtering results for Si and Ar are shown in figure 27 and figure 28 respectively. The total number of Ar atoms bombarded on the silicon cantilever beam is 396 with a fluence of $5.54 \times 10^{13}/cm^{-2}$ and the total number of Ar atoms left the simulation box is 286. Therefore, there are 110 Ar atoms piercing into the cantilever beam and being kept inside the beam. The number of Ar atoms injected inside the cantilever beam versus time is plotted in figure 25. Initially, the amount of Ar inside

the cantilever increases proportionally with time, then it becomes stable because the old Ar atoms inside the cantilever are bombarded out and are replaced by the new ones. The number of Ar atoms inside the cantilever is in equilibrium eventually. The final number of Ar atoms inside cantilever substrate is around 110.

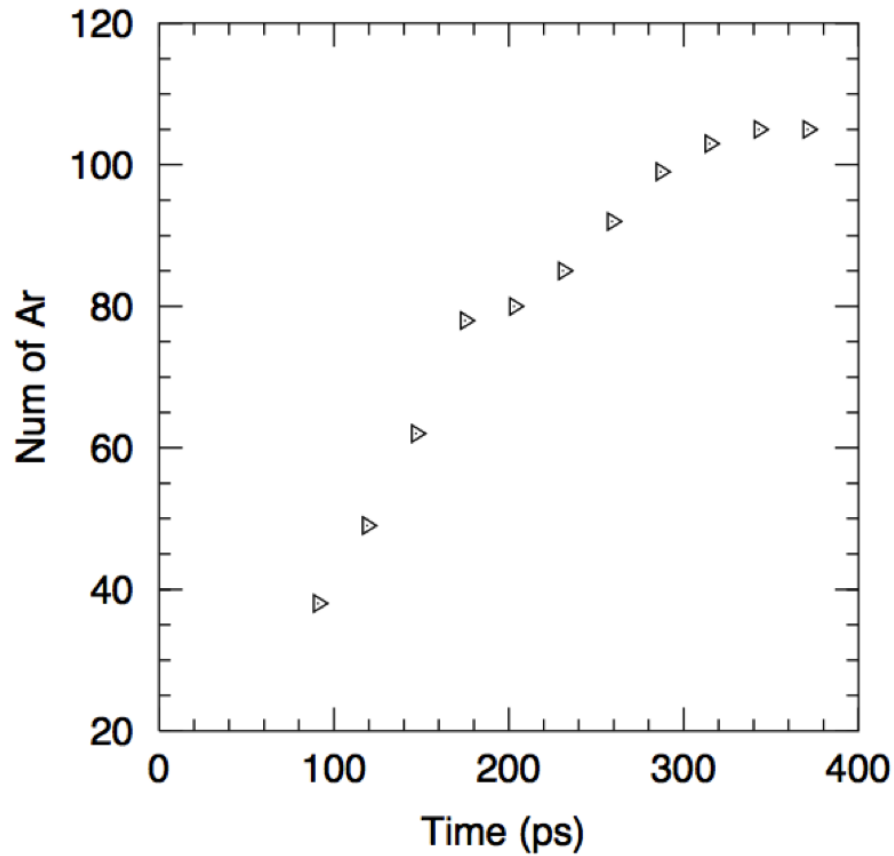


Figure 25: The Ar atoms inside the beam versus time

The sputtering yield is calculated according to equation 24. The total number of the ejected Si atoms is 429 and the total number of Ar atoms bombarded on the cantilever is 396. According to the equation 24, the sputtering yield is 1.08. Comparing to the experimental results in reference [22], this number is a bit lower

(experimental one 1.33) with the same bombarding condition. This is because thin film material is used in this study.

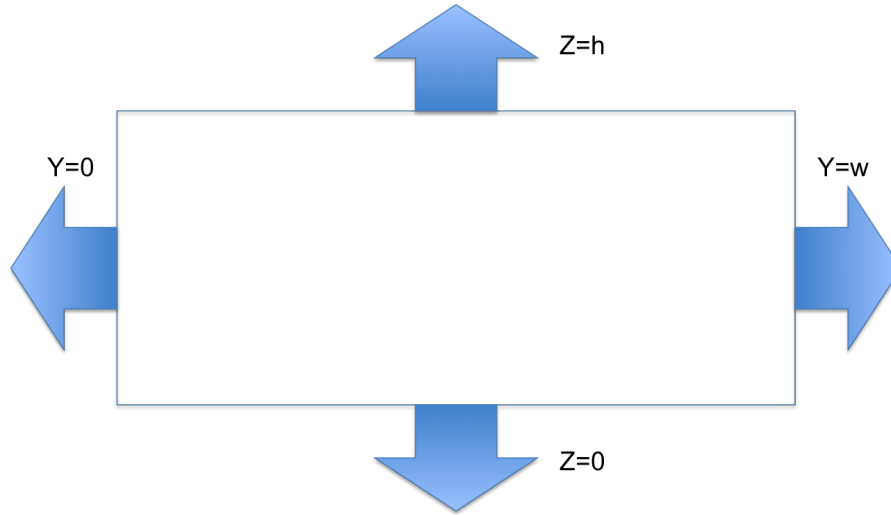


Figure 26: Schematic view of the simulation box from y-z view. The atoms sputtered can leave from $y=0$, $y=w$, $z=0$, $z=h$;

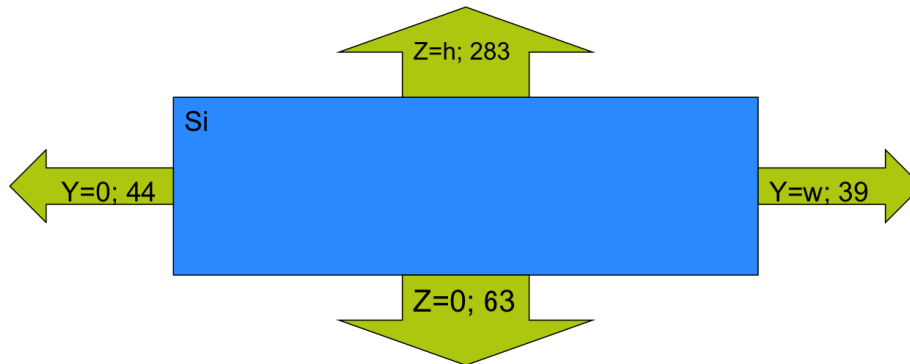


Figure 27: Schematic view of the sputtering results for Si atoms.

Bending The cantilever beam significantly bends after 371 ps bombardment. It can be seen from figure 29 that the average potential energy increases during the bombardment process. Then the bombardment of Ar stops and the simulation without bombardment lasts for 280 ps. Figure 30 shows that the average

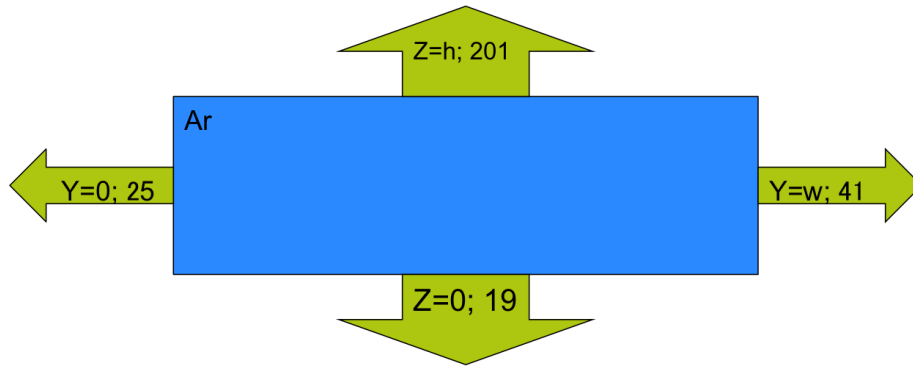


Figure 28: Schematic view of the sputtering results for Ar atoms.

potential energy remains after the bombardment stops. The cantilever profiles after bombardment are plotted versus time in figure 31. It can be seen that the cantilever beam still thermally vibrates. The position of the free ending is plotted versus time, which is shown in figure 32. Then the simulation continues with a cooling process in order to remove the thermal vibration. The temperature of the system decreases to 0 K with a cooling rate of 5 K per pico-second. The equilibrium position of the cantilever is shown in figure 33. In conclusion, because the average potential energy does not change after bombardment and the equilibrium state of the cantilever has a deformation around 6 nm, the cantilever is plastically deformed by Ar bombardment.

Energy Balance The energy is added to the system through bombarding Ar atoms. The energy leaves the simulation box in three ways. Firstly, the atoms leaving the simulation box bring energy out from the system. The energy includes the kinetic energy of Si and Ar atoms and the energy consumed to break Si-Si bonds. Secondly, as shown in figure 29, the average potential energy of the Si atoms in the cantilever increases during the process of the bombardment. Thirdly, the energy is also brought out from the system by thermostat. The thermostat keeps the temperature unchanged by controlling the kinetic energy of each

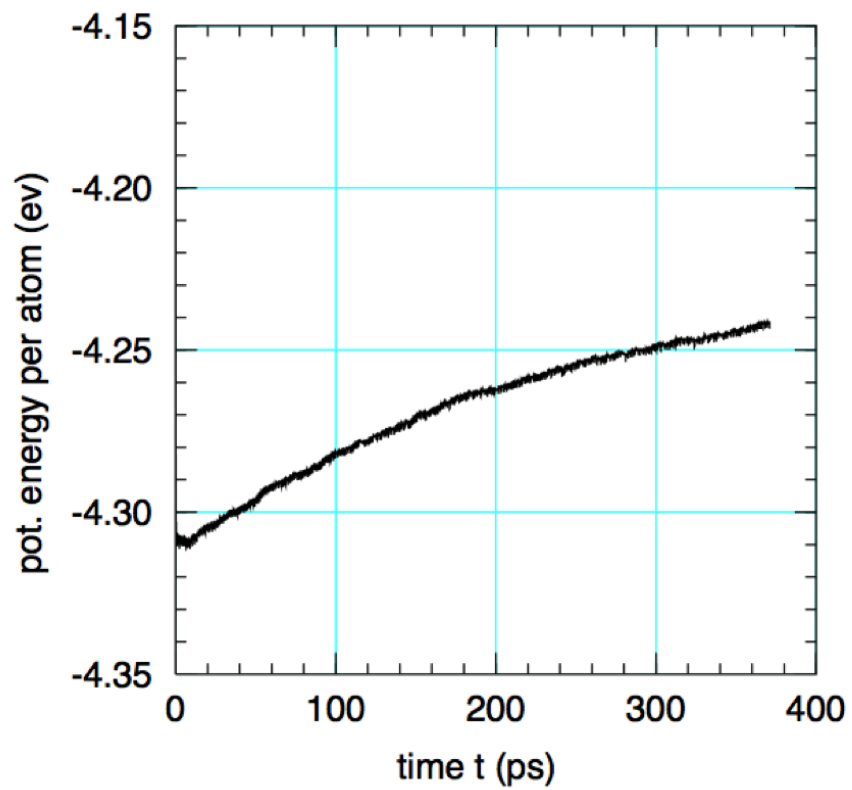


Figure 29: Average potential energy changes with time during bombardment.

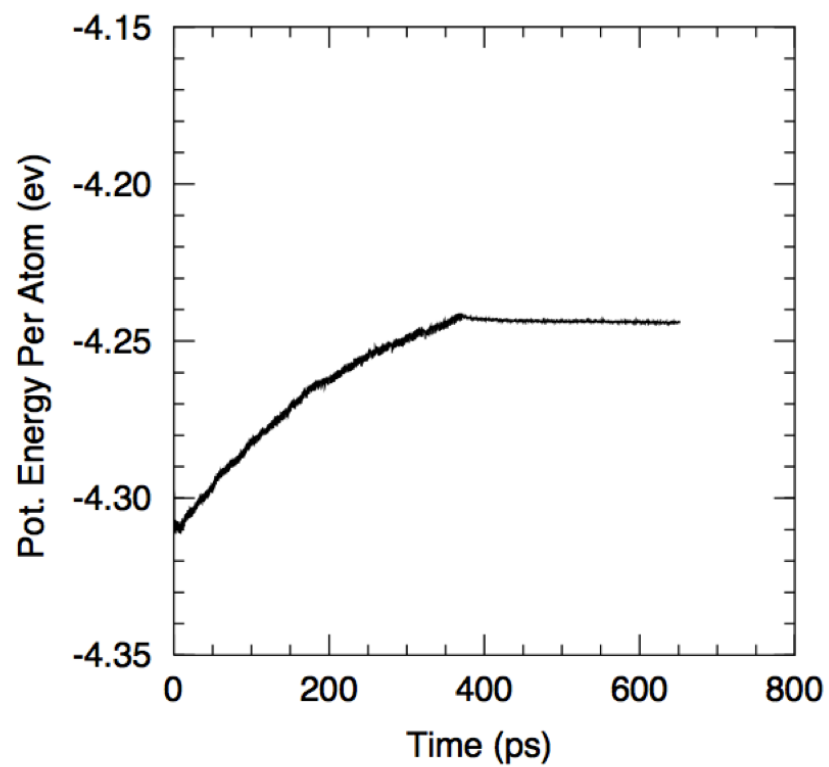


Figure 30: Beam potential energy versus time for the whole process.

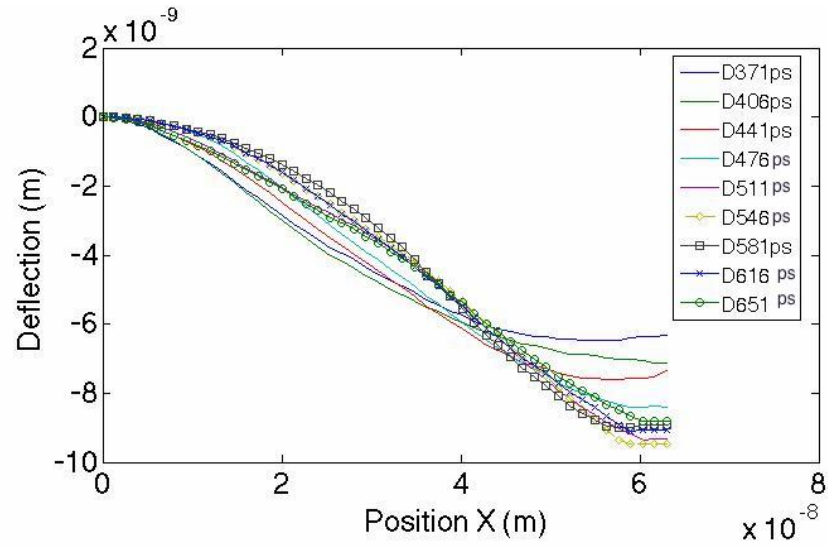


Figure 31: Beam profiles after 371 ps.

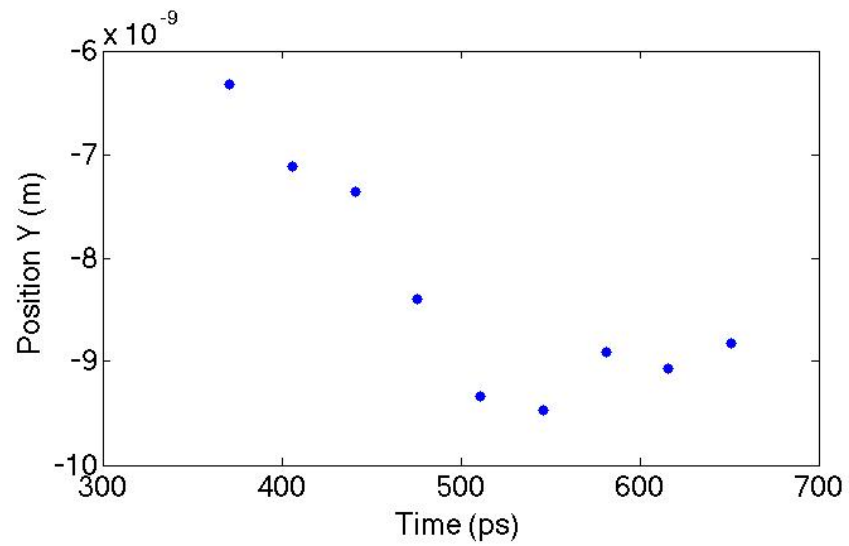


Figure 32: Ending point of the cantilever changing with time.

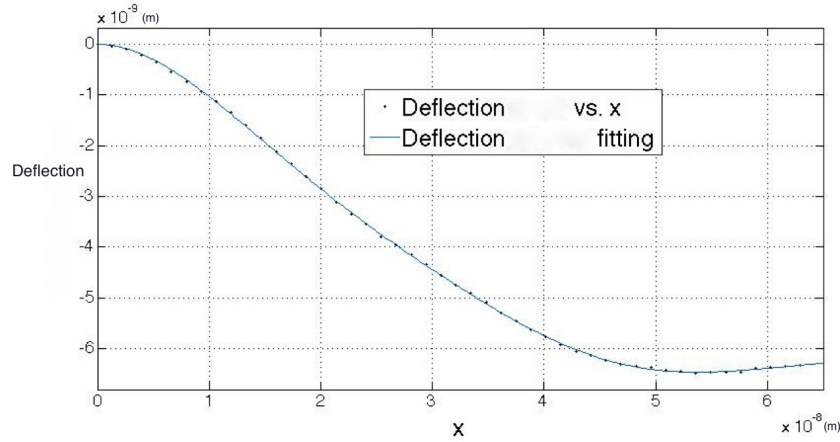


Figure 33: Beam profile after cool to 0 K at equilibrium position.

atom. When the Ar atoms bombarding on the beam, it is obvious that, the kinetic energy of the Si atoms that interact with Ar will increase and the temperature of the system is higher. To keep the system at a constant temperature, the thermostat decreases the kinetic energy of the atoms. The amount of energy brought out by thermostat is recorded by *camelion*. The results of the energy balance are listed in table 4. The total energy added to the system is 1.375 eV per silicon atom. The energy left the system is the sum of energy that atoms left simulation box take away, energy taken away by thermostat and potential energy increase of the cantilever. The numeri 1.373 eV per silicon atom.

However, there is a energy difference of 0.002 eV between the "income" and "cost". Two possible reasons can explain this phenomenon. First, when calculating the energy "income", the number of silicon atoms in cantilever beam is considered as a constant of 57600 during the bombardment. However, with the bombardment proceeding, some silicon atoms leave the box while some Ar atoms implant inside the cantilever. The amount of atoms in the system is no longer 57600 Si. Second, the temperature increase of the system is not taken into account when calculating the energy balance. Although the temperature is set to be 300 K during

the simulation, there is still a small increase of the average temperature due to the accuracy of thermostat. The temperature changes during simulation is plotted in figure 34. Average temperature is 318 K according to figure 34.

Table 4: Energy balance calculations

Type	eV/(Si atom)
Energy added from bombarding Ar	1.375
Energy that atoms left simulation box taken away	1.286
Energy taken away by thermostat	0.017
Potential energy increase	0.07
Energy left the system	1.373

Conclusion In conclusion, based on the results shown in this section, it is obvious that, the beam experiences a plastic bending under 200 eV Ar bombardment. The sputtering yield of the bombardment is 1.08. About one fourth (110/396) of the Ar atoms inject inside the cantilever and the implanted Ar atoms create defects. Most of the bombarding energy is used for sputtering and the rest contributes to the deformation, defects creation and temperature change.

4.3.2 Influences of Different Bombarding Energies

The Ar atoms with different kinetic energy are bombarded on the cantilever. Conditions of simulation are similar with that of the standard model shown in previous section. The polar angle is set to be 45° and temperature is 300 K. The whole cantilever top surface is bombarded. The Ar atoms come from the center at the top of the simulation box. Neither periodic boundary conditions nor stress are applied to the cantilever beam.

Temperature vs Time Thermoset along the Cantilever

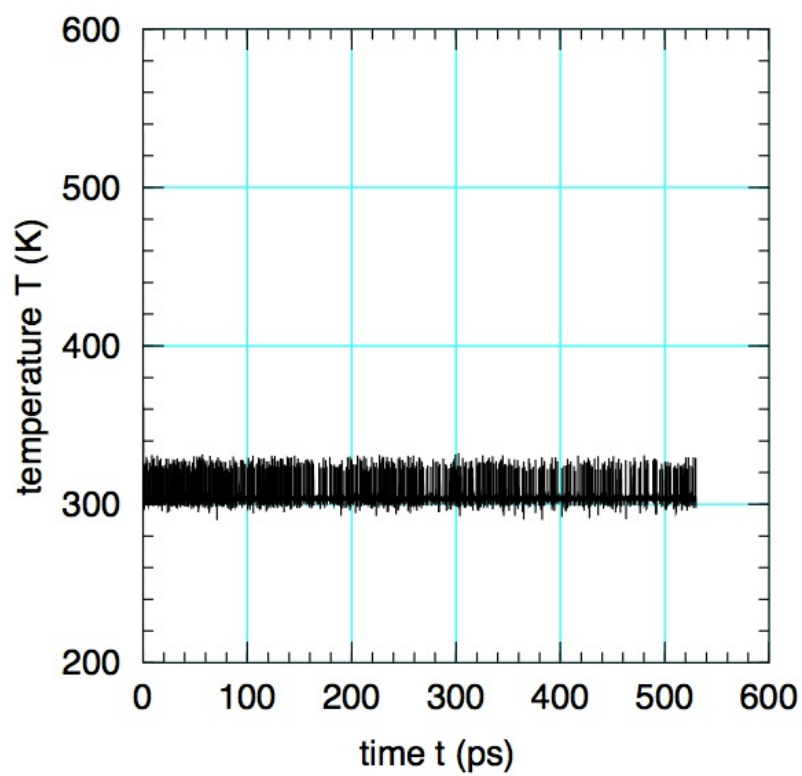


Figure 34: Temperature changes during bombardment.

Sputtering and Deformation Results In figure 35, cantilevers bombarding under different energy levels are bent resulting in similar deformation state at first time to reach it at the free end. The sputtering results are shown in the table 5, table 6, and table 7.

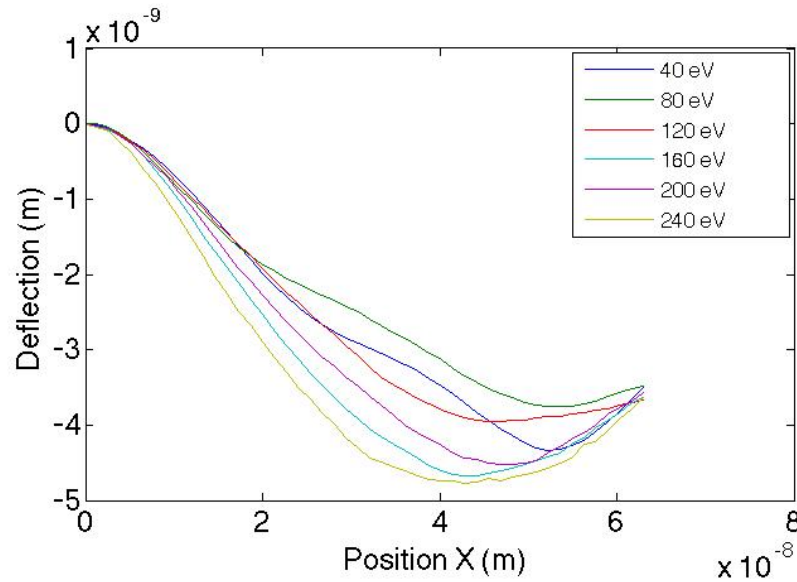


Figure 35: Cantilever bombarded with different energetic Ar atoms with similar deformation at the end.

In figure 37, the average increase of potential energy is plotted corresponding to different bombarding energy values. It can be seen that, with the similar level of deformation state at the free end, the higher value of bombarding energy is used, the more average potential energy increases. In figure 36, the number of trapped atoms corresponding to different values of bombarding energy is plotted. It reveals that the higher value of bombarding energy is, the more trapped atoms are made for the same deformation. In table 7, sputtering results are listed. It shows that, to achieve a similar level of deformation at the end of cantilever, the higher the bombarding energy used, the more Ar atoms needed. Considering the number of Ar atoms used and the deformation state, it can be concluded that lower bombarding energy has a higher efficiency to deform the cantilever. Possible reason could be that injected atoms in the beam create defects. Those defects increase

the strength of the cantilever. Therefore the cantilever is more difficult to deform. Another possible reason is should be the momentum transfer efficiency. The number of Ar atoms, which leave the system from the top of the simulation box, are shown in 6. It can be seen that when the bombarding energy increases, the number of Ar atoms being reflected by the cantilever decreases. The momentum exchange has a higher efficiency for low energy bombardment.

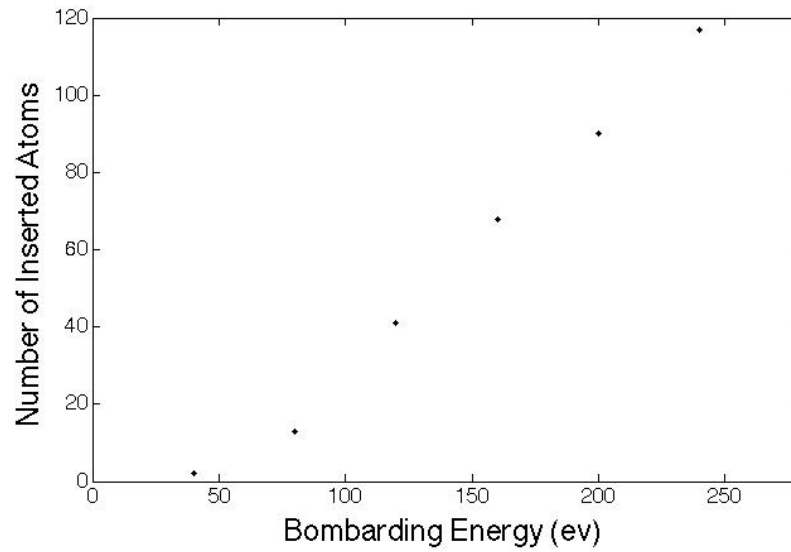


Figure 36: Number of Ar atoms implanted the cantilever plotted with different bombarding energy.

Table 5: Sputtering Results of Si (Different Energy)

Bombarding Energy (ev)	z=0	z=h	y=0	y=w	Total Removed
40	0	6	2	8	16
80	0	45	12	20	77
120	2	89	30	37	158
160	10	133	46	44	233
200	8	231	56	53	348
240	60	246	74	68	448

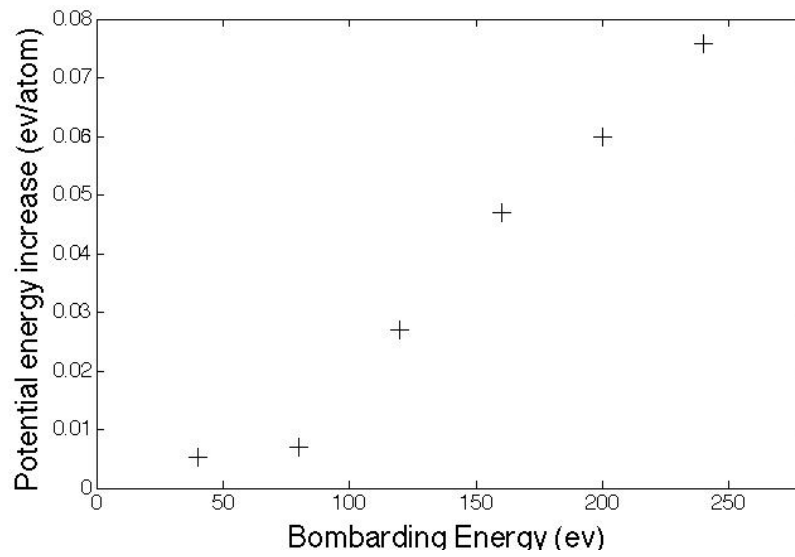


Figure 37: Average potential energy plotted with different bombarding energy.

Table 6: Sputtering Results of Ar (Part 1) (Different Energy)

Bombarding Energy (ev)	z=0	z=h	y=0	y=w
40	0	176	16	15
80	0	148	13	14
120	3	150	22	14
160	2	148	42	23
200	3	170	45	13
240	40	128	56	47

Table 7: Sputtering Results of Ar (Part 2) (Different Energy)

Bombarding Energy (ev)	Inside	Total Removed	Total Bombarded	Fluence $10^{13} \times cm^{-2}$	sputtering yield
40	2	207	209	2.92	0.0766
80	13	175	188	2.62	0.410
120	41	189	230	3.21	0.687
160	68	215	283	3.96	0.898
200	90	231	328	4.59	1.123
240	117	271	388	5.43	1.259

4.3.3 Influence of Bombarding Angle

In this section, models used are similar to the standard one. The bombarding energy of the Ar atoms is 200 eV. The polar angle varies, including 0°, 15°, 30° and 45°. The simulation time is 350 picoseconds. Fluence is $(4.98 \pm 0.35) \times 10^{13} \times \text{cm}^{-2}$.

The sputtering results are shown in table 8, table 9 and table 10. It reveals that, compared with results of the standard model (bombarding angle at 45°), the change of bombarding angle does not have a significant influence on the sputtering results. According to previous study [31], when the bombarding angle is in the interval of 0° and 45°, changing bombarding angle does not influence the sputtering results. The finding in this study match the previous one.

Table 8: Sputtering Results of Si (Different Angle)

Bombarding Angle (°)	z=0	z=h	y=0	y=w	Total Removed
0	21	191	64	73	349
15	41	231	65	54	391
30	78	139	70	60	347
45	52	236	42	38	368

Table 9: Sputtering Results of Ar (Part 1) (Different Angle)

Bombarding Energy (ev)	z=0	z=h	y=0	y=w
0	34	171	41	48
15	34	167	41	37
30	36	157	36	28
45	16	167	21	34

Table 10: Sputtering Results of Ar (Part 2) (Different Angle)

Bombarding Angle (°)	Inside	Total Removed	Total Bombarded	sputtering yield
0	78	294	372	1.07
15	97	279	376	1.08
30	89	257	346	1.00
45	92	238	330	1.12

The average potential energy increase for 0° , 15° , 30° , 45° is 0.063 eV, 0.068 eV, 0.096 eV, 0.069 eV respectively. The difference of average energy increase is due to the differences of bending state, which is shown in figure 38. The influence of the bombarding angle is not significant.

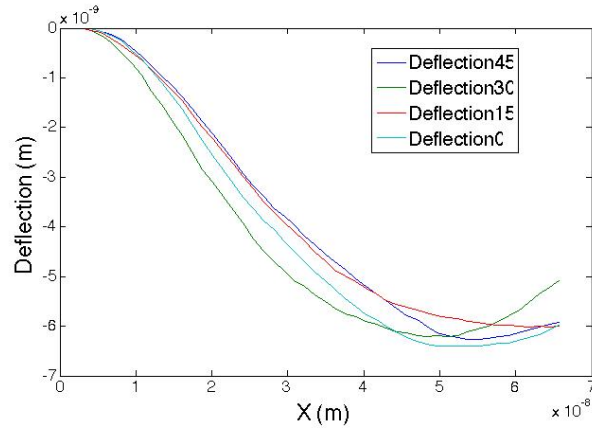


Figure 38: Number of Ar atoms pierced inside the cantilever plotted with different bombarding energy.

Conclusion In this section, the influence of polar angle of the bombardment is studied. According to the sputtering results, the energy results and the deformation results, it can be concluded that the influence of polar angle of the bombardment is not significant.

5 Conclusions and Future Work

The study was set out to explore the possibility to use Ar bombardment to build 3D nano structure from 2D nano cantilever. This paper conducts the thermal vibration of cantilever without bombardment and the mechanical deformation under Ar bombardment. It turns out that the beam thermally vibrates and the shape

profiles of cantilever matches the Euler-Bernoulli vibration model. The RMS amplitudes from simulations differ a lot from those of theoretical ones. First possible reason is the geometry change due to surface reconstruction and the second one is the mechanical properties change during vibration.

The cantilever bends plastically after Ar bombardment. The deformation is relatively large (6 nm) compared with the cantilever thickness (1.5 nm). Two parameters, bombarding angle and bombarding energy, are examined to study their influence on the magnitude of deformation of the cantilever. Because when changing the bombarding angle, the sputtering results and the level of deformation do not change significantly, it can be inferred that the bombarding angle does not influence the deformation of the cantilever. Meanwhile, with the increase of the bombarding energy, it takes more bombarding Ar atoms to achieve the same level of deformation state. So lower bombarding energy has a higher efficiency for deforming the cantilever.

In this work, the thermal vibration lasts for 420 ps. 420 ps is not enough for a complete vibration process. The frequency of mode 1 and mode 2 vibration cannot be obtained from 420 ps vibration. Future study should conduct a longer thermal vibration process. Moreover, two possible reasons has been defined to explain the difference between RMS amplitudes of thermal vibration from simulation and those from theoretical ones. Future research should focus on the quantitative analysis to find how the differences occur.

In this study, Ar bombardment plastically deforms the nano cantilever. It can be predicted that if the Ar bombardment continues, the nano cantilever can be manufactured into 3D nano structure. Only two parameters are examined to see the influence on deformation. In future studies, Ar bombardment should be extended to a longer period of time to deform the cantilever into 3D structures. Meanwhile, more parameters, such as aspect ratio of cantilever and bombarding position, could be examined.

Conclusively, this study gives a description of thermal vibration of nano cantilever and proves that Ar bom-

bardment can plastically deform the cantilever. Therefore, ion bombardment is a potential method that can be applied to build 3D nano structure.

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