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# Length and boundary effects on a nanorod

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We investigate length and boundary effects on the equilibrium strain of a ⟨100⟩ copper nanorod with {100} or {110} surfaces. Unlike a nanowire, a free-edged nanorod has finite length and has two more surfaces at both tip and root. Although the area of these two edge surfaces is generally much smaller than that of side surfaces, the effect of the edge surfaces should not be ignored in the equilibrium configuration of a nanorod. In this letter, an analytical model to estimate the equilibrium strain of the nanorod is proposed, and molecular statics simulations are performed to prove the proposed model. As the length of a nanorod increases, the equilibrium strain increases and converges to that of a nanowire. As for the boundary effect, we compare the equilibrium strain of a clamped nanorod with that of a free-edged nanorod.  [http://dx.doi.org/10.1063/1.4769881]

A nanowire as well as a nanofilm is a basic building block of a nano electromechanical system (NEMS), and its elastic and inelastic behaviors have been studied extensively. Especially, in order to investigate inelastic behaviors of nanowires, molecular dynamics (MD) simulation have been widely utilized. Inelastic deformations of face-centered cubic (FCC) nanowires by twinning and slip under tensile or compressive loading were showed by using molecular dynamics simulation.[1,2] Shape memory effect and pseudo-elasticity of a metal nanowire have been reported according to crystallographic orientation and loading condition.[3–7] The phase transform of a metal nanowire due to surface stress was demonstrated,[8] and that of a ZnO nanowire from wurtzite to hexagonal under tensile loading was reported.[9]

Besides these inelastic behaviors, size-dependent elastic characteristics due to surface effect have also been studied by a number of researchers. Effective tensile and bending rigidities of a nanowire were simply estimated along with the variation of its thickness by using atomistic calculation.[10] The thickness dependency of the Young's moduli and equilibrium strain of gold or copper nanowire according to crystallographic orientation were investigated.[11–13] As continuum approaches, an analytical model including surface effect and a semi-analytical method to quantify the size-dependent elasticity of nanostructures were proposed.[14,15]

However, these efforts on thickness-dependent elastic properties are limited only to the case in which the length of a nanowire is infinite. The length effect of a nanorod with finite length has not been studied yet. (Note that the authors distinguish a nanorod and a nanowire with their length. The former has finite length and the latter has infinite length.) Because a free-edged nanorod has two more surfaces than a nanowire at top and root edges, it may have different mechanical characteristics from those of a nanowire. Moreover, the mechanical behavior of a nanorod could be changed if one edge is clamped.

The equilibrium configuration of a nanorod is a very important characteristics in designing nano-structures because it is a starting point to analyze mechanical response of the structures. In this letter, we investigate the length effect on the equilibrium strain of a ⟨100⟩ copper nanorod with {100} or {110} surfaces. An analytic method to evaluate the equilibrium strain of a rectangular

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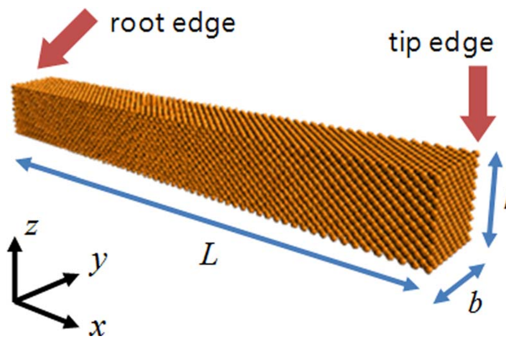


FIG. 1. An illustration of a ⟨100⟩ nanorod with rectangular cross-section.

cross-sectional nanorod is presented, and molecular statics (MS) simulation is undertaken to prove the proposed method. In addition to this length effect, we also report boundary effect on a nanorod, comparing a clamped nanorod with a free-edged nanorod.

Figure 1 shows an illustration of a free-edged nanorod with rectangular cross-section. The nanorod has two more surfaces at root and tip edges than a nanowire with same cross-section. To investigate the edge-surface effect on the equilibrium strain of a nanorod, we present the following analytic method.

The total internal energy of a nanorod consists of bulk energy and surface energy ($U_{total} = U_{bulk} + U_{surf}$). Under the assumption that the deformation of a nanorod is subject to the restriction of the uniform strain field, the internal bulk energy for a nanorod can be written in the following simple form:

$$U_{bulk} = \frac{1}{2} V_0 C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}, \tag{1}$$

where $V_0$ is the initial volume of a nanorod in the undeformed configuration, $C_{ijkl}$ is a fourth-order elastic constant, and $\varepsilon_{ij}$ is a Green-Lagrangian strain tensor component. The surface energy of a nanorod can be expressed in terms of surface stress ($\tau_{\alpha\beta}$) and surface strain ($\varepsilon^s_{\alpha\beta}$). If we use the linear elastic model in the surface constitutive relationship, $\tau_{\alpha\beta} = \tau^0_{\alpha\beta} + T_{\alpha\beta\kappa\lambda}\varepsilon^s_{\kappa\lambda}$, the surface energy can be written as

$$U_{surf} = \int_{S_0} \left( \tau^0_{\alpha\beta}\varepsilon^s_{\alpha\beta} + \frac{1}{2} T_{\alpha\beta\kappa\lambda}\varepsilon^s_{\alpha\beta}\varepsilon^s_{\kappa\lambda} \right) dS, \tag{2}$$

where $S_0$ is the initial surface area of a nanorod in the undeformed configuration, $\tau^0_{\alpha\beta}$ is an initial surface stress at zero strain, and $T_{\alpha\beta\kappa\lambda}$ is a surface elastic tensor. We can rewrite the surface energy equation in the following form:

$$U_{surf} = \frac{V_0}{h} \tilde{\tau}^0_{ij} \varepsilon_{ij} + \frac{V_0}{2h} \tilde{T}_{ijkl} \varepsilon_{ij} \varepsilon_{kl}, \tag{3}$$

$$\tilde{\tau}^0_{ij} = \frac{h}{V_0} \int_{S_0} \tau^0_{\alpha\beta} t_{\alpha i} t_{\beta j} dS, \tag{4}$$

$$\tilde{T}_{ijkl} = \frac{h}{V_0} \int_{S_0} T_{\alpha\beta\kappa\lambda} t_{\alpha i} t_{\beta j} t_{\kappa k} t_{\lambda l} dS, \tag{5}$$

where $t_{\alpha i}$ is a direction cosine between the surface direction $\alpha$ and the global coordinate $i$, and $\tilde{\tau}^0_{ij}$ and $\tilde{T}_{ijkl}$ are an effective initial surface stress tensor and an effective surface elastic tensor defined in three dimensional space, respectively. The equation to calculate equilibrium strain $\hat{\varepsilon}_{ij}$ can be obtained by

TABLE I. Surface properties of {100 and {110 copper surfaces (unit: N/m).

| | $T_{1111}$ | $T_{1122}$ | $T_{1212}$ | $\tau^0_{11}$ | $\tau^0_{22}$ |
|---|---|---|---|---|---|
| {100} | −0.7082 | 5.9148 | −0.2938 | 1.3950 | 1.3950 |
| {110} | −8.0679 | −3.7524 | −4.0636 | 1.1588 | 1.0105 |

minimizing the total internal energy with respect to a strain component, $\left(\partial U_{total}/\partial \varepsilon_{ij}\right)\big|_{\varepsilon_{ij}=\hat{\varepsilon}_{ij}} = 0$,

$$\hat{\varepsilon}_{ij} = -\frac{1}{h}\left(C_{ijkl} + \frac{1}{h}\tilde{T}_{ijkl}\right)^{-1}\tilde{\tau}^0_{kl} = -\frac{1}{h}X^{-1}_{ijkl}\tilde{\tau}^0_{kl}, \tag{6}$$

where $X_{ijkl}$ is an effective elastic tensor including surface effect. This analytical model was originally proposed by Dingreville *et al.*[14] for an ellipsoidal particle with an isotropic surface. Here, we extend this model to a nanorod with finite length and anisotropic surfaces. The vector form of the effective surface stress $\tilde{\tau}^0_{ij}$ of a nanorod with a rectangular cross-section is defined as $\tilde{\tau}^0_{ij} = \left\lfloor \tilde{\tau}^0_{11}\,\tilde{\tau}^0_{22}\,\tilde{\tau}^0_{33}\,\tilde{\tau}^0_{23}\,\tilde{\tau}^0_{31}\,\tilde{\tau}^0_{12}\right\rfloor^T$.

For example, if a free-edged nanorod has {100} surfaces, the components of the effective surface stress tensor are

$$\begin{aligned} \tilde{\tau}^0_{11} &= h\,(2/h + 2/b)\,\tau^{\{100\}}_{11} \\ \tilde{\tau}^0_{22} &= h\,(2/h + 2/L)\,\tau^{\{100\}}_{11} \\ \tilde{\tau}^0_{33} &= h\,(2/b + 2/L)\,\tau^{\{100\}}_{11}, \\ \tilde{\tau}^0_{23} &= \tilde{\tau}^0_{31} = \tilde{\tau}^0_{12} = 0 \end{aligned} \tag{7}$$

where $\tau^{\{100\}}_{11}$ is the initial surface stress of {100} surface. The effective elastic tensor yields

$$X_{ijkl} = C_{ijkl} + \frac{2}{h}T^{xy}_{ijkl} + \frac{2}{b}T^{xz}_{ijkl} + \frac{2}{L}T^{yz}_{ijkl}, \tag{8}$$

where $T^{mn}_{ijkl}$ is the three-dimensional surface elastic tensor, and superscript $mn$ represents the axes of the surface. If one edge of a nanorod is clamped, the $(2/L)$ terms in Eqs. (7) and (8) change to $(1/L)$. In a nanowire case, these $(2/L)$ terms are ignored because a nanowire has infinite length in axial direction.

As for material properties,$C_{1111} = 167.26$GPa, $C_{1122} = 124.15$GPa, and $C_{1212} = 76.44$GPa were used for bulk material, and surface properties of {100} and {110} surfaces are listed in Table I. The surface properties were calculated with the embedded atom method[16] (EAM) potential by using analytical method proposed by Dingreville and Qu.[17]

Figure 2 shows the equilibrium strain of a ⟨100⟩ copper nanowire with infinite length. The nanowire has square cross-section and four {100} surfaces. The red circles are the results obtained from MS simulation, and the blue solid line represent the analytic solution by using Eq. (6). As the thickness of the nanowire goes thinner, the equilibrium strain decreases due to surface effect. As shown in Fig. 2, the result of proposed method considerably has good agreement with that of MS simulation.

In addition to this thickness dependency, a nanorod has a length effect on the equilibrium strain due to additional edge surfaces. The normalized equilibrium strains of a free-edged and a clamped nanorod are illustrated in Fig. 3. They were normalized by results of the nanowire in Fig. 2. In both free-edged and clamped cases, the normalized equilibrium strain becomes larger as the length of a nanorod increases. This tendency occurs in all the test cases. In the case of analytic solution, only 3.1 nm case was plotted in Fig. 3 because all of the 1.6 nm, 3.1 nm, and 6.0 nm cases give very similar results.

As shown in Fig. 3, a clamped nanorod has different equilibrium strain from that of a free-edged nanorod even if their dimensions are same. The only different between the two is the number of edge surfaces; a free-edged nanorod has two edge surfaces, whereas a clamped nanorod has only one

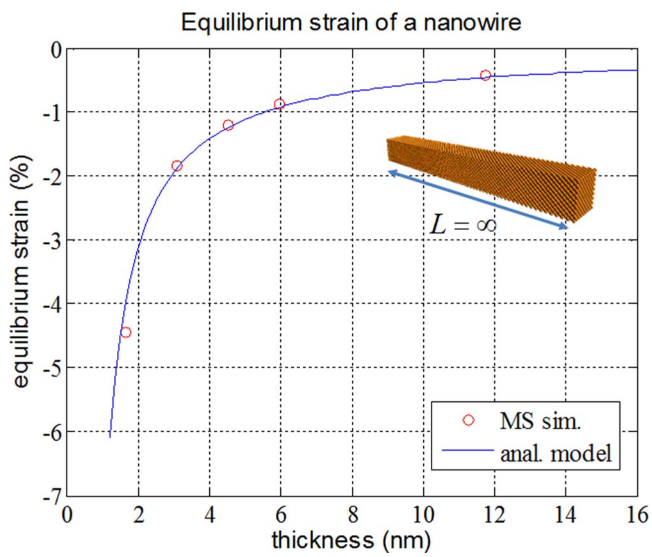


FIG. 2. Thickness dependent equilibrium strain of a ⟨100⟩/{100} copper nanowire with square cross-section.

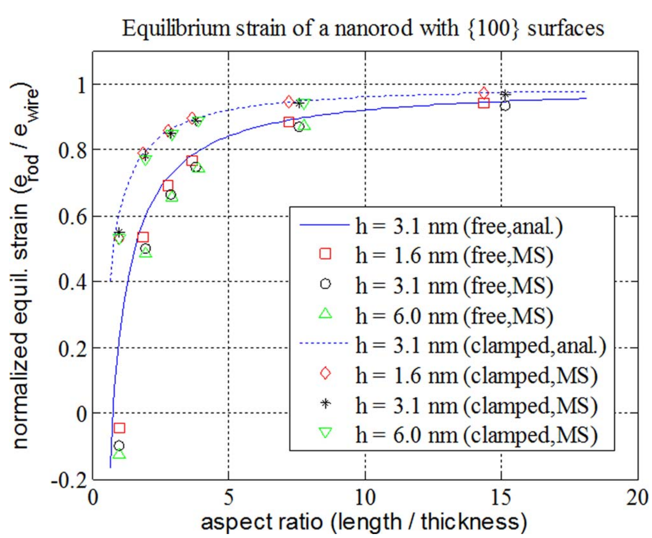


FIG. 3. Equilibrium strain of a ⟨100⟩ nanorod with {100} surfaces.

edge surface. The analytic solutions of equilibrium strains of a nanorod with 3.1 nm thickness are listed in Table II. The values in parentheses are the results of MS simulation. As shown in Table II, the magnitude of the equilibrium strain of a clamped nanorod is larger than that of a free-edged nanorod in the entire range of length. Remarkably, the magnitude of the equilibrium strain of a clamped nanorod with length $L$ is nearly the same as that of a free-edged nanorod with length $2L$.

As an another example, the equilibrium strains of a nanorod with {110} surfaces were investigated. Figure 4 shows analytical solution and MS results of the normalized equilibrium strains of the nanorod. In the normalization, the strain value of $-3.06\%$, $-1.28\%$, or $-0.61\%$ was, respectively, utilized as the value of a nanowire with 2.2 nm, 4.2 nm, or 8.3 nm thickness. Figure 4 indicates that the length effect and boundary effect on a ⟨100⟩/{110} nanorod are very analogous to those on a ⟨100⟩/{100} nanorod.

In this letter, we reported length and boundary effects on the equilibrium configuration of a ⟨100⟩ nanorod using an analytical model and MS simulation. The length as well as the thickness of a nanorod affects the equilibrium configuration of the nanorod due to edge surfaces. As the length of

TABLE II. Equilibrium strains of free-edged and clamped nanorods of 3.1 nm thickness.

| Length (nm) | 6.0 | 11.7 | 23.3 | 46.5 |
|---|---|---|---|---|
| free-edged nanorod (%) | −1.13 | −1.50 | −1.69 | −1.79 |
| | (−0.92) | (−1.37) | (−1.60) | (−1.71) |
| clamped nanorod (%) | −1.51 | −1.70 | −1.79 | −1.84 |
| | (−1.43) | (−1.63) | (−1.73) | (−1.78) |
| nanowire : −1.89 % (−1.84 %) | | | | |

() : results of molecular statics simulation.

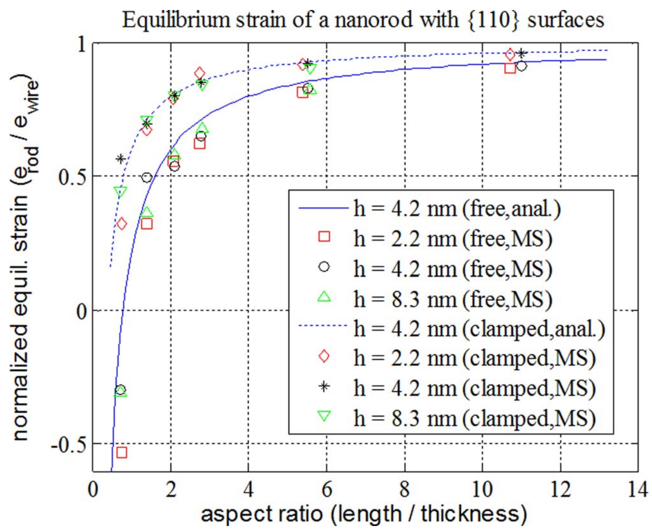


FIG. 4. Equilibrium strain of a ⟨100⟩ nanorod with {110} surfaces.

a nanorod increases, the equilibrium strain of the nanorod increases and gradually approaches that of the nanowire. To estimate the equilibrium strain of a nanorod, we proposed an analytical model consisting of elastic constants, surface elastic tensors, and initial surface stresses. The analytic solutions of this proposed model showed considerably good agreement with those of the MS simulations. Small discrepancy between the results of the analytical model and the MS simulation was due to the assumption of uniform strain field. In addition to the length effect, boundary condition also affected the equilibrium configuration. A clamped nanorod of length $L$ had nearly the same equilibrium strain value as a free-edged nanorod of length $2L$. The length and boundary effects should be considered in the equilibrium configuration of a nanorod, and the proposed analytic model will be very useful for the design of NEMS devices.

## ACKNOWLEDGMENTS

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