Acta Mechanica Solida Sinica, Vol. 27, No. 2, April, 2014 ISSN 0894-9166
Published by AMSS Press, Wuhan, China

SIZE EFFECTS OF ELASTIC MODULUS OF FCC METALS BASED ON THE CAUCHY-BORN RULE AND NANOPLATE MODELS***

Jianyun Liu* **Jingru Song** **Yueguang Wei****
(*State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing* 100190*, China*)

Received 14 May 2012, revision received 3 April 2013

ABSTRACT In the present research, a simple quasi-continuum model, the Cauchy-Born rule model, is used to investigate the size effects of elastic modulus for fcc metals. By considering a nanoplate model and calculating the strain energy for the nano-sized plate under tension and bending, the relationship between the elastic modulus and the plate thickness is found. Size effects of the elastic modulus are displayed by the relative differences of the elastic modulus between the nano-sized plate sample and the bulk sample. By comparing the present results with those of others, the effectiveness of the Cauchy-Born rule model in studying the size effects of material properties are shown.

KEY WORDS quasi-continuum method, Cauchy-Born rule, size effect, elastic modulus, fcc-metal

I. INTRODUCTION

The micro-/nano-structured materials or materials at the micro-/nanoscale possess superior mechanical, physical and chemical properties, and have been widely investigated[1–3]. At the micro-/nanoscale, the size effects of mechanical properties of materials become prominent, and are usually considered to be partly from the surface effect, and partly from the interior micro-structured effect which usually is homogenized into the strain gradient effect displayed in the improved constitutive relations. The surface effect is usually associated with the surface energy and becomes significant when a geometrical parameter, called the specific surface area (ratio of surface area to volume for a sample), becomes relatively high[4]. The strain gradient effect is important for both cases: sample with small size and material with nano-scale structures, such as nanocrystalline materials[5].

A lot of researches have been performed to investigate the size-dependence of the Young's modulus and other mechanical properties. When measuring Young's modulus variation for material tungsten using the tensile test by considering a W/Cu multilayers, Villain et al.[6] found that the Young's modulus measured with the 3 nm-layer thick sample is obviously larger than that of bulk material, while the Young's modulus measured with the 24 nm-layer thick sample is smaller than that of the bulk one. Similarly, for material Gold, Renault et al.[7] found that the Young's modulus of a 260 nm-thick film is 23% larger than that of the corresponding bulk material by using the tensile test. On the

* Corresponding author. E-mail: liujianyun@lnm.imech.ac.cn
** Corresponding author. E-mail: ywei@lnm.imech.ac.cn
*** Project supported by the National Natural Science Foundation of China (Nos. 11021262, 10932011 and 91216108) and the National Basic Research Program of China (2012CB937500). The first author (J. Liu) would like to thank the helpful advice of Dr. Wei Xu from Institute of Mechanics, Chinese Academy of Sciences.

other hand, Miller and Shenoy[8] developed a simple theoretical model incorporating the surface stress effect to predict the size-dependence of the effective elastic modulus for nano materials. Duan et al. also took into account the surface/interface stress effect and showed the size-dependence of effective elastic constants for nano-inhomogeneity solid[9]. Sun and Zhang[10] applied a semi-continuum model to analysis of the size effect of plate-like nanostructured materials, and concluded that the predicted Young's modulus is dependent on the number of atom layers in the thickness direction. Furthermore, by employing a combination model of molecular static and *ab initio* calculation, Zhou and Huang[11] found that a solid surface may soften or stiffen elastically relative to its bulk counterpart, depending on the competition between electron redistribution and lower coordination of the surface atoms. Dingreville et al.[12] investigated the effect of surface energy on the elastic stiffness for nano-films, and their results showed that the overall elastic stiffness of a nano-film may be either reduced or increased by as much as 60% relative to that of the bulk case when film thickness varies in the nanometer ranges, depending on the material and surface orientations. They developed a semi-analytical method to compute the surface elastic properties of crystalline materials[13]. Wang et al.[14], and Zhu and Zheng addressed the strain gradient effect and modified the elastic properties of nanostructures[15].

The popularly used approaches for investigating the size effects mainly include the atomistic simulation[11,16], the continuum methods[8,9,17], as well as the multi-scale analysis[18]. In the present study, we intend to adopt a simple quasi-continuum model, the Cauchy-Born rule (CBR) model, to investigate the size effects of material properties. The CBR is usually used to develop the quasi-continuum model in simulating the overall mechanical behavior for discrete systems, which is based on the early work of Born and Huang[19] and then is further developed by Ericksen et al.[20], etc.. Based on the CBR, Park and Liu[21] presented a multiple-scale method to couple atomistic simulation to continuum simulation, which needed a much smaller computational cost than that of atomistic simulation. By proposing a temperature-related Cauchy-Born rule implemented in nanoscale continuum approximations, Xiao and Yang[22] studied temperature dependent physical phenomena of crystalline solids. Steinmann et al.[23] investigated the validity of the CBR by direct comparison of continuum with atomistic simulation. Recently, Park et al.[24–26] applied CBR to the lower-dimension surface problem and developed a surface Cauchy-Born model.

In current investigations, the size effects of elastic modulus due to the surface effect are studied for several typical fcc-metals by using the CBR model, and the relaxation process near the surface atom layers of the nano-sized plate sample is considered. The size effects of the elastic modulus are characterized by analyzing two basic mechanical issues, tension and bending of nano-sized plates. Moreover, in order to compare the results of the elastic modulus of nano-sized plate samples with those of the bulk material case, we also use the CBR model to analyze the bulk material case for three typical deformation states, i.e., volume expansion, uniaxial tension and pure shearing, and to obtain three independent elastic constants.

II. FUNDAMENTAL RELATIONS

2.1. The Cauchy-Born Rule

The Cauchy-Born rule is a quasi-continuum technique in describing the state of an atomic cluster, which can get information from the atom system across to the continuum system[23]. By the CBR, the distances between each atom and others before and after atom movement in an atomic cluster are assumed to satisfy the relation

$$\boldsymbol{r}_{ij} = \boldsymbol{F} \cdot \boldsymbol{R}_{ij} \tag{1}$$

where $\boldsymbol{R}_{ij}$ and $\boldsymbol{r}_{ij}$ are the vectors of distances between atom i and atom j in the initial state and current state, respectively, $\boldsymbol{F}$ is the deformation gradient tensor of the atomic cluster, providing that the atomic cluster can be homogenized as a continuum system. By means of both Eq.(1) and atomic potential (see below), the CBR can be used to simulate material mechanical properties.

2.2. Potential

In the present research, we intend to use the AEAM (analytical embedded-atom method) potential[27] to investigate the size effects of materials modulus. By the AEAM potential, the total energy $E_{\mathrm{t}}\left(r_{ij}\right)$

Table 1. Parameters of AEAM for fcc metals from Ref.[27].

Parameter	Au	Pt	Pd	Cu	Al
η	1.04	0.980	0.960	0.600	0.563
α/eV	0.0048	0.0051	0.00093	0.0032	0.00018
$E_{\rm c}$/eV	3.81	5.84	3.89	3.49	3.39
F_0/eV	2.91	4.64	2.59	2.32	2.75
k_0/eV	1.1566	−0.5866	1.7549	1.4995	−1.1175
k_1/eV	−0.4510	1.4604	−0.6746	−0.6502	1.2149
k_2/eV	0.0541	−0.5196	0.0767	0.0977	−0.3608
k_3/eV	0.00006	0.0020	0.0001	−0.00006	0.0012
k_4/eV	0.0803	0.134	0.118	0.0988	0.0502
k_5/eV	−0.9523	−0.7491	−1.443	−1.178	0.1116

of an atomic system can be expressed as[27]

$$E_{\rm t}\left(r_{ij}\right)=\sum_i F_i\left(\rho_i\right)+\frac{1}{2}\sum_i\sum_{j(\neq i)}\phi\left(r_{ij}\right)+\sum_i M_i\left(P_i\right) \tag{2}$$

in which

$$\begin{aligned}
&\phi\left(r_{ij}\right)=k_0+k_1\left(\frac{r_{ij}}{r_{1\rm e}}\right)+k_2\left(\frac{r_{ij}}{r_{1\rm e}}\right)^2+k_3\left(\frac{r_{ij}}{r_{1\rm e}}\right)^6+k_4\left(\frac{r_{ij}}{r_{1\rm e}}\right)^{-12}+k_5\left(\frac{r_{ij}}{r_{1\rm e}}\right)^{-1}\\
&F\left(\rho\right)=-F_0\left[1-\eta\ln\left(\frac{\rho}{\rho_{\rm e}}\right)\right]\left(\frac{\rho}{\rho_{\rm e}}\right)^{\eta},\qquad \rho_i=\sum f\left(r_{ij}\right)\\
&M\left(P\right)=\alpha\left\{1-\exp\left[-\left(\ln\left|\frac{P}{P_e}\right|\right)^2\right]\right\},\qquad P_i=\sum f^2\left(r_{ij}\right)\\
&f\left(r_{ij}\right)=f_{\rm e}\left(\frac{r_{1\rm e}}{r_{ij}}\right)^6,\qquad f_{\rm e}=\frac{E_{\rm c}}{\Omega}
\end{aligned} \tag{3}$$

where $F_i\left(\rho_i\right)$ is the embedding energy, $\phi\left(r_{ij}\right)$ is the pair potential, $M_i\left(P_i\right)$ is the modified term, r_{ij} is the distance between atom i and atom j in the current configuration, $r_{1\rm e}$ is the nearest distance from an atom to its nearest neighbors in equilibrium, Ω is the volume of one atom, $\rho_{\rm e}$ and $P_{\rm e}$ are the values of ρ and P in equilibrium, respectively. Other parameters are presented in Table 1. The cutoff radius of $\phi\left(r_{ij}\right)$ is $r_{{\rm c}\phi}=r_5+0.75\left(r_6-r_5\right)$, while for $f\left(r_{ij}\right)$ it is $r_{{\rm c}f}=r_6+0.75\left(r_7-r_6\right)$, r_i is the distance from one atom to its ith nearest neighbors. By employing the CBR and referring to Eq.(1), the total energy can be expressed as $E_{\rm t}\left(r_{ij}\right)=E_{\rm t}\left(\boldsymbol{F};\boldsymbol{R_{ij}}\right)$. At the initial state, $\boldsymbol{F}=\boldsymbol{I}$, where $\boldsymbol{I}$ is the identity matrix. The corresponding total energy can be expressed as $E_{\rm t}=E_{\rm t}\left(\boldsymbol{F}=\boldsymbol{I}\right)$, while after the deformation, given deformation gradient $\boldsymbol{F}$, the total energy can be expressed as $E_{\rm t}=E_{\rm t}\left(\boldsymbol{F}\right)$. Consequently, the material strain energy can be expressed as

$$W=E_{\rm t}(\boldsymbol{F})-E_{\rm t}(\boldsymbol{F}=\boldsymbol{I}) \tag{4}$$

III. DETERMINATION OF ELASTIC CONSTANTS

In order to verify the validity of the CBR model in determining the elastic constants and to pave a way for studying the size effects of elastic modulus in the next section, in this section we use the CBR model to calculate the elastic constants for a bulk material case.

The material stress-strain relation in matrix form is given by

$$\sigma_i=C_{ij}\varepsilon_j\qquad(i=1,6;j=1,6) \tag{5}$$

where C_{ij} is the elastic constant, σ_i and ε_i are stress and strain components, respectively. There are three independent non-zero elastic constants: C_{11}, C_{12}, C_{44}, for fcc metals. According to the elasticity theory, these constants can be determined by three independent equations corresponding to three deformation states, volume expansion, uniaxial tension and pure shearing.

In the case of volume expansion[28], the unit cell is expanded uniformly along the three coordinate directions, while bulk modulus K can be expressed as

$$K = V_0 \left(\frac{\partial^2 E_{\mathrm{t}}}{\partial V^2} \right)_{V_0} \tag{6}$$

where E_{t} is the potential function, V_0 and $V = V_0 (1 + \varepsilon_V)^3$ are the initial and current volumes of the cell, respectively, ε_V is the average strain.

In the case of uniaxial tension, the unit cell is only stretched along the direction of the lattice d, and C_{11} can be calculated by

$$C_{11} = \frac{1}{d_0} \left(\frac{\partial^2 E_{\mathrm{t}}}{\partial d^2} \right)_{d_0} \tag{7}$$

where d_0 and $d = d_0 (1 + \varepsilon_{\mathrm{T}})$ are the initial and current crystal constant, respectively, and ε_{T} is the tensile strain. According to the characteristics of the cubic crystal, C_{12} can be obtained by

$$C_{12} = \frac{1}{2} (3K - C_{11}) \tag{8}$$

In the case of pure shearing, C_{44} can be found via

$$C_{44} = \frac{1}{d^3} \left(\frac{\partial^2 E_{\mathrm{t}}}{\partial \theta^2} \right)_{\theta_0} \tag{9}$$

where θ is the shear angle.

In the present investigation, the corresponding deformation gradients $\boldsymbol{F}$ for three deformations states (volume expansion, uniaxial tension, and pure shearing) can be expressed respectively as follows:

$$\boldsymbol{F}_{\mathrm{expand}} = \begin{bmatrix} 1 + \varepsilon_V & & \\ & 1 + \varepsilon_V & \\ & & 1 + \varepsilon_V \end{bmatrix} \tag{10}$$

$$\boldsymbol{F}_{\mathrm{tension}} = \begin{bmatrix} 1 + \varepsilon_{\mathrm{T}} & & \\ & 1 & \\ & & 1 \end{bmatrix} \tag{11}$$

$$\boldsymbol{F}_{\mathrm{shear}} = \begin{bmatrix} 1 & \theta & \\ & 1 & \\ & & 1 \end{bmatrix} \tag{12}$$

where the applied external strain should be chosen to maintain elastic deformation of the system, (-0.6%∼0.6%) being taken in the present research.

In the present calculations based on the CBR model, the results of elastic constants for five fcc-metals, Au, Pt, Pd, Cu and Al, are presented in Table 2. Other scholars' theoretical and experimental results[29–32] are also given in Table 2 for comparison. The theoretical results by others[29,30] are based on an improved lattice mechanical model and embedded-atom-method, respectively. It can be seen from Table 2 that the present results agree well with those of others, especially with the theoretical results[30] and the experimental results[31]. The relative error between them is within 5%, while for Al the relative error is a little larger than other metals, which may be caused by the choice of the empirical atomistic potential, polynomial fitting accuracy and so on. From Table 2, through comparison of the present results based on the very simple CBR model with those based on theoretical models[30] and experiments by others, clearly the CBR model is an effective method of determining the elastic constants of materials.

IV. SIZE EFFECTS OF ELASTIC MODULUS

For micro-/nano-structured materials or materials at the micro-/nanoscale, such as nanowire, nanoplate, etc., the material properties are different from those of bulk material cases due to surface effects. In the present research, we use the CBR model to investigate the size effects of elastic

Table 2. Elastic constants for several typical fcc-metals (eVÅ^{-3})

Fcc-metals	Elastic constants	Present	Others' results	Experiments
Au	C_{11}	1.198	0.938[29], 1.163[30]	1.144[31], 1.260[32]
	C_{12}	1.015	0.804[29], 0.981[30]	0.994[31], 1.060[32]
	C_{44}	0.265	0.439[29], 0.263[30]	0.281[31], 0.284[32]
Pt	C_{11}	2.216	2.006[29], 2.169[30]	1.894[31], 2.169[32]
	C_{12}	1.671	1.525[29], 1.569[30]	1.706[31], 1.569[32]
	C_{44}	0.457	0.694[29], 0.478[30]	0.425[31], 0.478[32]
Pd	C_{11}	1.380	1.513[29], 1.463[30]	1.363[31], 1.446[32]
	C_{12}	1.099	1.088[29], 1.100[30]	1.150[31], 1.100[32]
	C_{44}	0.432	0.541[29], 0.445[30]	0.406[31], 0.445[32]
Cu	C_{11}	1.049	0.851[29], 1.063[30]	1.044[31], 1.101[32]
	C_{12}	0.763	0.749[29], 0.766[30]	0.775[31], 0.781[32]
	C_{44}	0.468	0.468[29], 0.474[30]	0.475[31], 0.511[32]
Al	C_{11}	0.633	0.737[8]	0.714[31]
	C_{12}	0.392	0.389[8]	0.387[31]
	C_{44}	0.160	0.229[8]	0.198[31]

modulus. The present results will be compared with other scholars' results based on the atomistic calculations and theoretical models.

Elastic modulus E can be calculated by analyzing the nano-sized plate under tension and bending, respectively. For a nanoplate model, the specific surface area is relatively high, so that the surface effects become important. The major difference between the surface atoms and bulk atoms is that the status of atoms for both cases differs from atom to atom; bulk atoms are fully coordinated, while surface atoms are under-coordinated. Therefore, surface relaxation must be considered for the nanoplate model. The strain gradient effect[33] is not considered in the present research. The nano-sized plate is assumed to be homogeneous and infinite length in-plane, compared with its small thickness, only several nanometers, as shown in Fig.1(a). It is also assumed that relaxation occurs only in the direction perpendicular to the plane[13]. The relaxation process is as usual one of considering an initial configuration of surface atom layer, and calculating the minimum energy of several atom layers near the surface, one can realize a relaxed surface. After relaxation and near a typical surface, atom layer spaces a_{0i} relative to bulk atom layer space a_0 are slightly changed, as shown in the sketch Fig.1(b) and in Table 3 for several typical fcc-metals. Because of the surface relaxation process, the initial distance between atom i and atom j near surface, R_{ij}, adopted in the calculation using the CBR model, varies slightly relative to the internal atoms.

4.1. Plate under Tension

For the nano-sized plate, the coordinate axes are located as follows, the directions 1, 2, 3 coincide with the [100], [010], [001] crystal orientations, respectively. The plate considered in the present research is subjected to the uniaxial tension along the direction 1, as shown in Fig.2(a). The deformation gradient corresponding to the tension is shown in Eq.(11). The strain energy density w is given by

Table 3. Atom layer spaces near surface after surface relaxation, a_{0i}, compared with the bulk atom layer space a_0 for several typical metals. Present results are compared with the results from Ref.[30]

Ratio	Au	Pt	Pd	Cu	Al
a_{01}/a_0	0.940 0.937[30]	0.941 0.931[30]	0.972 0.956[30]	0.998 0.986[30]	0.974
a_{02}/a_0	1.008 1.005[30]	1.002 1.006[30]	0.998 0.999[30]	0.998 0.997[30]	1.014

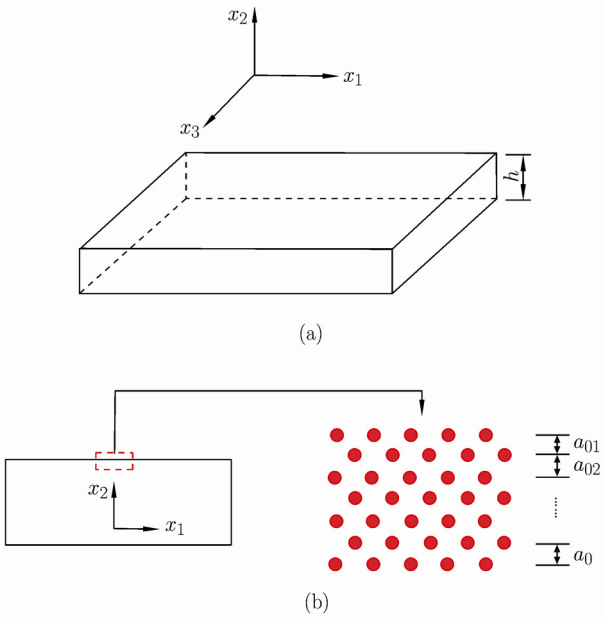

Fig. 1. (a) Schematic geometry of the nano-sized plate, and periodic boundary conditions are used in the 'x_1' and 'x_3' directions; (b) atom layer spaces near surface after surface relaxation, a_{0i}, is compared with the bulk atom layer space, a_0.

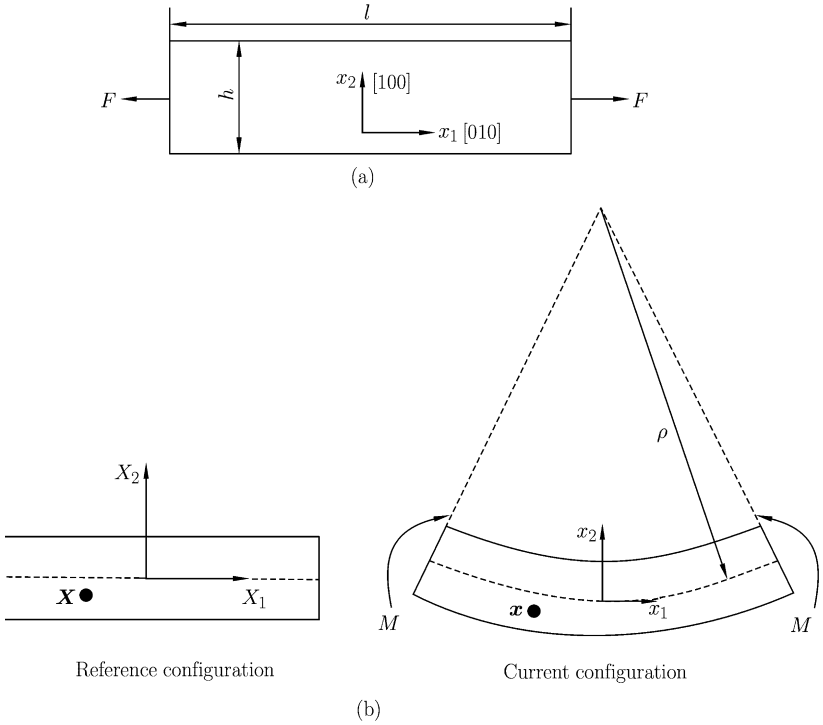

Fig. 2. (a) Schematic geometry of the plate in uniaxial tension (one dimensional deformation mode); (b) schematic geometry of the plate in bending.

$$w = \frac{1}{2}\lambda E \varepsilon_{\mathrm{T}}^2 \tag{13}$$

where E is the elastic modulus, $\lambda = (1-\upsilon)/[(1+\upsilon)(1-2\upsilon)]$, and $\upsilon = C_{12}/(C_{11}+C_{12})$ is the Poisson's ratio. E can be calculated by

$$E = \frac{1}{\lambda}\frac{\partial^2 w}{\partial \varepsilon_{\mathrm{T}}^2} \tag{14}$$

It is worth noting that w contains the surface effects. And E can be also calculated by $E_{\mathrm{c}} = C_{11} - 2C_{12}^2/(C_{11}+C_{12})$ in continuum mechanics without considering surface effects.

4.2. Plate under Bending

For the plate bending case, as shown in Fig.2(b), ρ is the radius of curvature of the deformed plate, M is an applied moment, and the relations between the coordinates $\boldsymbol{x}$ in the current configuration and $\boldsymbol{X}$ in the reference configuration can be expressed with the curvature κ_n ($\kappa_n = -1/\rho$) as

$$x_1 = \frac{\sqrt{1+2\kappa_n X_2}\sin(\kappa_n X_1)}{\kappa_n}, \qquad x_2 = \frac{\sqrt{1+2\kappa_n X_2}\cos(\kappa_n X_1) - 1}{\kappa_n}, \qquad x_3 = X_3 \tag{15}$$

The deformation gradient $\boldsymbol{F}$ is calculated by $\boldsymbol{F} = \partial \boldsymbol{x}/\partial \boldsymbol{X}$:

$$\boldsymbol{F} = \begin{bmatrix} \sqrt{1+2\kappa_n X_2}\cdot\cos(\kappa_n X_1) & \dfrac{\sin(\kappa_n X_1)}{\sqrt{1+2\kappa_n X_2}} & 0 \\ -\sqrt{1+2\kappa_n X_2}\cdot\sin(\kappa_n X_1) & \dfrac{\cos(\kappa_n X_1)}{\sqrt{1+2\kappa_n X_2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{16}$$

The strain energy can be expressed as $W = EIL\kappa_n^2/2$, where I is inertia moment of plate cross-section and L is the length of the plate in direction 1. Thus E can be calculated by

$$E = \frac{1}{IL}\frac{\partial^2 W}{\partial \kappa_n^2} \tag{17}$$

With the strain kept at zero in direction 3, the plane-strain case, E can also be calculated by $\overline{E}_{\mathrm{c}} = C_{11} - C_{12}^2/C_{11}$ in continuum mechanics without considering the surface effects.

The strain energy or strain energy density versus the applied strain can be fitted by a quadratic polynomial in elasticity, based on Eqs.(14) and (17), and E can be obtained for different thicknesses of nanoplates in tension and bending and compared with the conventional results based on the classical mechanics model.

In order to investigate the size effects of material properties at nanoscale, such as the size effect of elastic modulus, we applied the above Eqs.(1)-(4) to Eqs.(14)-(17), and obtained the elastic constants and variation relations of the elastic modulus.

V. RESULTS AND DISCUSSION

A series of elastic modulus values are obtained for different plate thicknesses. The relative difference of the elastic modulus, $(E-E_{\mathrm{c}})/E_{\mathrm{c}}$, between the nanoplate result E considering surface effect and the conventional bulk result E_{c} without surface effect is shown in Fig.3. Five types of fcc-metals, Al, Au, Pt, Pd and Cu, are investigated in the present research. To ensure the applicability of the CBR model, the plate thickness is taken greater than five layers of atoms. Thepresent results are also compared with those of others based on both the atomistic calculation and the surface stress theoretical model[8, 34], respectively.

The relative difference of elastic modulus based on the surface stress theoretical model[8] is expressed as follows:

For plate tension case,

$$\frac{D-D_{\mathrm{c}}}{D_{\mathrm{c}}} = \frac{E-E_{\mathrm{c}}}{E_{\mathrm{c}}} = 2\frac{S}{E_{\mathrm{c}}}\frac{1}{h} \tag{18}$$

where $D = Eh$ and $D_{\mathrm{c}} = E_{\mathrm{c}}h$.

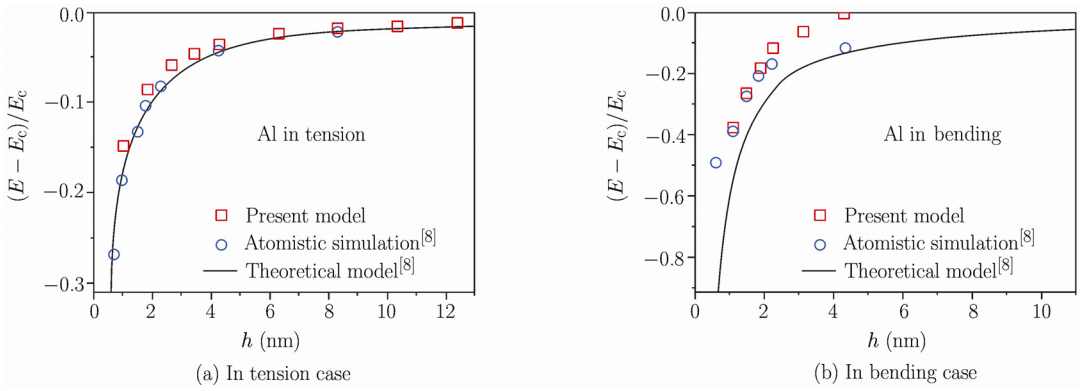

Fig. 3. The relative differences of elastic modulus with nano-plates thickness for Al: comparison between present model predictions with atomistic simulation[8] and the surface stress theoretical model[8].

For plane-strain plate bending case,

$$\frac{D-D_c}{D_c}=\frac{\overline{E}-\overline{E}_c}{\overline{E}_c}=6\frac{S}{\overline{E}_c}\frac{1}{h} \tag{19}$$

where $D=EI$ and $D_c=E_cI$, S is surface elastic modulus obtained from atomistic simulations[8,34], and the S values for the above five typical metals are shown in Table 4. Also the values of the coefficients, $2S/E_c$ and $6S/\overline{E}_c$, are presented in Table 5, while for Al are both in the plane-strain case.

Table 4. S Values for several fcc-metals along (001) crystal face (eVÅ^{-2})

S	Al	Au	Pt	Pd	Cu
Relaxed	−0.495[8]	−0.329[34]	−0.555[34]	−0.402[34]	−0.260[34]

Table 5. Values of coefficients in surface stress theoretical model[8] for fcc-metals (Å)

Coefficient	Al	Au	Pt	Pd	Cu
$2S/E_c$	−1.86	−2.47	−1.43	−1.97	−1.28
$6S/\overline{E}_c$	−5.58	−5.85	−3.49	−4.75	−3.15

In Figs.3(a) and (b), the relative differences of elastic modulus varying with the nanoplate thickness for single crystal Al are shown, which are based on the plate tension and bending analysis models, respectively. Obviously, the elastic modulus is size-dependent and decreases with a decrease in the thickness of nanoplates at the nanoscale, and when thickness of plate is less than 4 nm it drops sharply. For a very thin plate (about 1 nm), the relative difference of elastic modulus is about 20% in the tension case, while it is about 40% in the bending case. In the tension case, the relative difference of elastic modulus is about 5% when the thickness is at about 4 nm, then it gradually tends to zero with increasing thickness. In the bending case, the relative difference of elastic modulus approaches zero very quickly with an increase in the plate thickness.

The present results are compared with those of others based on the surface stress theoretical model (described in Eqs.(18) and (19)) and the atomistic calculations[8], respectively, as shown in Figs.3(a) and (b). By comparing Figs.3(a) with (b), we can find that the results based on the CBR model, a very simple model, are very consistent with those based on atomistic simulations. For the plate tension case, the results based on all three models are consistent with each other, while for the plate bending case the result based on the surface stress theoretical model[8] deviates from the predictions based on the other two models. However, the predictions of the relative difference of elastic modulus based on three models have the same trends. It has been found from a comparison with the atomistic simulation

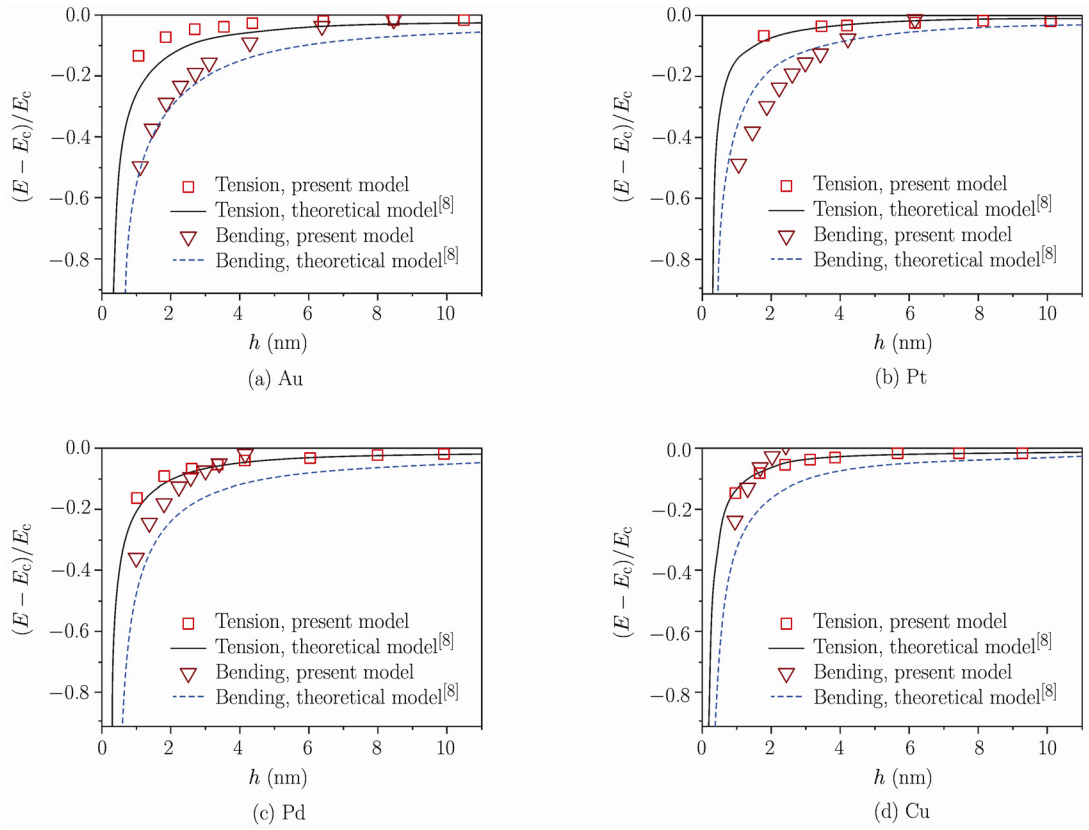

Fig. 4. The relative differences of elastic modulus with nano-plates thickness for other metals in both tension and bending cases: comparison between present model predictions with the surface stress theoretical model[8].

model that the CBR model, as a simple quasi-continuum model, is effective in describing the size effect of material properties.

In order to verify the reliability of the CBR model, further investigation is made on the size effects of elastic modulus for other single crystal metals, such as Au, Pt, Pd and Cu. For these materials, we also investigate the relations of the relative difference of elastic modulus with nanoplate thickness by considering the same typical mechanics problems as before, plate tension and bending.

The relative differences of elastic modulus between the present results based on the CBR model considering the surface effect and the conventional results without considering the surface effect are shown in Figs.4(a), (b), (c) and (d), for single crystal metals Au, Pt, Pd and Cu, respectively. Shown in the figures are the results for both the tension case and the bending case, respectively, as are comparisons of the present results based on the CBR model with those based on the surface stress theoretical model[8]. From Figs.4(a) and (b), the predicted relative differences of elastic modulus for Au and Pt based on both models are very consistent. Obviously, for both materials, two different results of relative difference of elastic modulus are obtained in the tension case and the bending case, respectively. However, from Figs.4(c) and (d), for materials Pd and Cu, similar results of relative difference of elastic modulus based on the CBR model are obtained for each material in the tension case and the bending case, respectively, and the result is consistent with the prediction of the surface stress theoretical model[8] in the tension case. The prediction result based on the surface stress theoretical model[8] in the bending case has a considerable deviation from the results based on the CBR model. This is because first, the CBR is a homogenization technique which assumes all atoms move in the same deformation gradient. For simple tensile deformation gradient, the CBR can well simulate the atomic motion; while the bending deformation gradient is relatively complex, the CBR could not be used to simulate the atomic motion very well as deviation of the results may occur. Second, the results may have something to do with the property of the metals. In addition, the results of Au and Pt in Figs.4(a) and (b) agree well with the

theoretical model, while the results for both Pd and Cu in Figs.4(c) and (d) do not agree well with those of the theoretical model.

VI. SUMMARY

A very simple quasi-continuum model, the CBR model, has been used to study the size effects of elastic modulus of nano-scale materials. Based on the CBR model and the analytical embedded-atom potential, the elastic constants for several typical fcc-metals, Au, Pt, Pd, Cu and Al, have been predicted by considering three deformation states. The size effects of the elastic modulus for the above metals have been also investigated using the CBR model with the surface effect taken into account to analyze the plate tension and plate bending of two simple problems. The results obtained from the relative modulus based on the present method agree well with those based on the atomistic simulation and the surface stress theoretical model.

In the present research, through the use of the CBR model to investigate the size effects of the elastic modulus for several typical fcc-metals considering the surface effect, the effectiveness of the CBR model is shown. One can expect to use the simple model to describe the size effects of other material properties in the future.

References

[1] Duan,X.F., Huang,Y., Cui,Y., Wang,J.F. and Lieber,C.M., Indium phosphide nanowires as building blocks for nanoscale electronic and optoelectronic devices. *Nature*, 2001, 409: 66-69.
[2] Friedman,R.S., McAlpine,M.C., Ricketts,D.S., Ham,D. and Lieber,C.M., High-speed integrated nanowire circuits. *Nature*, 2005, 434: 1085-1085.
[3] Lieber,C.M. and Wang,Z.L., Functional nanowires. *MRS Bulletin*, 2007, 32: 99-108.
[4] Chen,X.L., Ma,H.S., Liang,L.H. and Wei,Y.G., A surface energy model and application to mechanical behavior analysis of single crystals at sub-micron scale. *Computational Materials Science*, 2009, 46: 723-727.
[5] Wei,Y.G. and Hutchinson,J.W., Hardness trends in micron scale indentation. *Journal of the Mechanics and Physics of solids*, 2003, 51: 2037-2056.
[6] Villain,P., Goudeau,Ph., Renault,P.O. and Badawi,K.F., Size effect on intragranular elastic constants in thin tungsten films. *Applied Physics Letters*, 2002, 81: 4365-4367.
[7] Renault,P.O., Bourhis,E.L., Villain,P., Goudeau,Ph., Badawi,K.F. and Faurie,D., Measurement of the elastic constants of textured anisotropic thin films from x-ray diffraction data. *Applied Physics Letters*, 2003, 83: 473-475.
[8] Miller,R.E. and Shenoy,V.B., Size-dependent elastic properties of nanosized structural elements. *Nanotechnology*, 2000, 11: 139-147.
[9] Duan,H.L., Wang,J., Huang,Z.P. and Karihaloo,B.L., Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress. *Journal of the Mechanics and Physics of Solids*, 2005, 53: 1574-1596.
[10] Sun,C.T. and Zhang,H.T., Size-dependent elastic moduli of platelike nanomaterials. *Journal of Applied Physics*, 2003, 93: 1212-1218.
[11] Zhou,L.G. and Huang,H.C., Are surface elastically softer or stiffer? *Applied Physics Letters*, 2004, 84: 1940-1942.
[12] Digreville,R., Qu,J.M. and Cherkaoui,M., Surface free energy and its effect on the elastic behavior of nano-sized particles, wires and films. *Journal of the Mechanics and Physics of solids*, 2005, 53: 1827-1854.
[13] Dingreville,R., Kulkarni,A.J., Zhou,M. and Qu,J.M., A semi-analytical method for quantifying the size-dependent elasticity of nanostructures. *Modelling and Simulation in Materials Science and Engineering*, 2008, 16: 1-16.
[14] Wang,G.F., Feng,X.Q., Yu,S.W. and Nan,C.W., Interface effects on effective elastic moduli of nanocrystalline materials. *Materials Science and Engineering A*, 2003, 363: 1-8.
[15] Zhu,L. and Zheng,X.J., Modification of the elastic properties of nanostructures with surface charges in applied electric fields. *European Journal of Mechanics A/solids*, 2010, 29: 337-347.
[16] Horstemeyer,M.F., Baskes,M.I. and Plimpton,S.J., Computational nano scale plasticity using embedded atom potentials. *Theoretical and Applied Fracture Mechanics*, 2001, 37: 49-98.
[17] Huang,X. and Pelegri,A.A., Finite element analysis on nano indentation with friction contact at the film/substrate interface. *Composites Science and Technology*, 2007, 67: 1311-1319.
[18] Xiao,S.P. and Belytschko,T., A bridging domain method for coupling continua with molecular dynamics. *Computer Methods in Applied Mechanics and Engineering*, 2004, 193: 1645-1669.

[19] Born,M. and Huang,K., Dynamical Theory of Crystal Lattices, first ed. Oxford University Press, 1962.
[20] Ericksen,J.L., The Cauchy Born Hypotheses for Crystals, Phase Transformations and Material Instabilities in Solids. In: Gurtin,M.E. (Ed.). Academic Press, 1984, 61-77.
[21] Park,H.S. and Liu,W.K., An introduction and tutorial on multiple-scale analysis in solids. *Computer Methods in Applied Mechanics and Engineering*, 2004, 193: 1733-1772.
[22] Xiao,S. and Yang,W., Temperature-related Cauchy–Born rule for multi-scale modeling of crystalline solids. *Computational Material Science*, 2006, 37: 374-379.
[23] Steinmann,P., Elizondo,A. and Sunyk,R., Studies of validity of the Cauchy-Born rule by direct comparison of continuum and atomistic modeling. *Modelling and Simulation in Materials Science and Engineering*, 2007, 15: 271-281.
[24] Park,H.S., Klein,P.A. and Wagner,G.J., A surface Cauchy-Born model for nanoscale materials. *International Journal for Numerical Methods in Engineering*, 2006, 68: 1072-1095.
[25] Park,H.S. and Klein,P.A., Surface Cauchy-Born analysis of surface stress effects on metallic nanowires. *Physical Review B*, 2007, 75: 085408.
[26] Park,H.S. and Klein,P.A., A surface Cauchy-Born model for silicon nanostructures. *Computer methods in applied mechanics and engineering*, 2008, 2008: 3249-3260.
[27] Huang,Y.C., Shu,X.L., Kong,Y., Wang,L.L. and Hu,W.Y., Lattice dynamics of fcc transition metals by modified analytic embedded-atom method. *The Chinese Journal of Nonferrous Metals*, 2002, 12: 36-40. (in Chinese)
[28] Chen,L., Calculation and applicability analysis for elastic constants of fcc crystal. *Chinese Journal of Mechanical Engineering*, 2005, 41: 46-50. (in Chinese)
[29] Pandya,C.V., Vyas,P.R., Pandya,T.C., Rani,N. and Gohel,V.B., An improved lattice mechanical model for FCC transition metals. *Physica B*, 2001, 307: 138-149.
[30] Foiles,S.M., Baskes,M.I. and Daw,M.S., Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Physical Review B*, 1986, 33: 7983-7991.
[31] Simmons,G. and Wang,H., Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook. MIT Press, Cambridge, 1971.
[32] Kittel,C., Introduction to Solid State Physics. 7th edition. New York: Wiley, 1997.
[33] Wu,B., Liang,L.H., Ma,H.S. and Wei,Y.G., A trans-scale model for size effects and intergranular fracture in nanocrystalline and ultra-fine polycrystalline metals. *Computational Materials Science*, 2012, 57: 2-7.
[34] Shenoy,V.B., Atomistic calculations of elastic properties of metallic fcc crystal surfaces. *Physical Review B*, 2005, 71: 094104.