Temperature effect on elastic modulus of thin films and nanocrystals

Lihong Liang [a] , Meizhi Li [a] , Fuqi Qin [a] & Yueguang Wei [a]

[a] LNM, Institute of Mechanics, Chinese Academy of Sciences,
Beijing 100190, China
Version of record first published: 18 Sep 2012.

PLEASE SCROLL DOWN FOR ARTICLE

Taylor & Francis
Taylor & Francis Group

Temperature effect on elastic modulus of thin films and nanocrystals

Lihong Liang*, Meizhi Li, Fuqi Qin and Yueguang Wei

LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

The stability of nanoscale devices is directly related to elasticity and the effect of temperature on the elasticity of thin films and nanocrystals. The elastic instability induced by rising temperature will cause the failure of integrated circuits and other microelectronic devices in service. The temperature effect on the elastic modulus of thin films and nanocrystals is unclear although the temperature dependence of the modulus of bulk materials has been studied for over half a century. In this paper, a theoretical model of the temperature-dependent elastic modulus of thin films and nanocrystals is developed based on the physical definition of the modulus by considering the size effect of the related cohesive energy and the thermal expansion coefficient. Moreover, the temperature effect on the modulus of Cu thin films is simulated by the molecular dynamics method. The results indicate that the elastic modulus decreases with increasing temperature and the rate of the modulus decrease increases with reducing thickness of thin films. The theoretical predictions based on the model are consistent with the results of computational simulations, semi-continuum calculations and the experimental measurements for Cu, Si thin films and Pd nanocrystals.

1. Introduction

Thin films and nanocrystals have wide applications in microelectronics, optics, sensors, etc. The temperature increases in microelectronic integrated circuits and microelectronic package due to miniaturisation of the devices and weak heat dissipation. The elasticity and vibration behaviour becomes thermally softer with increasing temperature [1], which directly affects the stability and reliability of nanoscale devices. On the other hand, the reduced elastic modulus decreases the thermal stress produced in the thermal barrier coatings used in high temperature environments [2], which makes the components more durable. Therefore, an understanding of the temperature effect on the elastic modulus of thin films and nanocrystals is necessary in the fabrication and application of thin films and nanocrystalline materials.

The temperature effect on the elastic modulus of bulk materials has been studied since the 1960. Wachtman et al. [3] measured the Young's modulus of aluminium

---

*Corresponding author. Email: lianglh@lnm.imech.ac.cn

oxide over the temperature range 350–1123 K in 1961, and gave the phenomeno-logical model of the temperature (T) dependence of the modulus E as:

$$E(T) = E_0 - AT \exp\left(-\frac{T_0}{T}\right) \tag{1}$$

where E_0 is the modulus at 0 K; A and T_0 are constants [3]. Several years later, Anderson [4] derived an equation of the temperature-dependent bulk modulus based on the Grüneisen theory [4]:

$$E(T) = E_0 - \frac{\gamma\delta}{V} 3RT\mathrm{H}\left(\frac{\theta}{T}\right) = E_0 - \frac{\gamma\delta}{V}\int_0^T C_V \mathrm{d}T \tag{2}$$

where γ is the Grüneisen parameters, δ is the Anderson–Grüneisen parameter, V is the volume, R is the ideal gas constant, θ is the Debye temperature, C_V is the specific heat, and $\mathrm{H}(x) = \frac{3}{x^3}\int_0^x \frac{x^3}{e^x - 1}\mathrm{d}x$. Equation (2) indicates that the temperature effect on the modulus is related to the temperature integral of the specific heat, i.e. the cohesive energy. Following this idea, the temperature effects on the elasticity and vibration frequency of Si, Ge and diamond were also calculated based on the bond-order-length-strength model [5]. Molecular dynamics simulations and first principle calculations were also carried out to study the temperature effect on the elasticity of some metals and compounds [6–8].

However, the above models may not be suitable for thin films and nanocrystals. Studies have shown that nanomaterials possess different physical, chemical and mechanical properties compared to the corresponding bulk materials; especially for thin films and nanocrystals with a length-scale smaller than 10–20 nm, the effective elastic modulus is obviously size-dependent [9–12]. So what about the temperature effect of thin films and nanocrystals? Recently, molecular dynamics simulations [13] and semi-continuum method calculations [14] for Si thin films have been performed, and the temperature effect on the modulus of Pd nanocrystals was also measured [15]. A general theoretical model is desirable to describe the temperature effect on the elastic modulus of thin films and nanocrystals and to understand the underlying mechanism.

In this paper, an analytical equation for the temperature-dependent elastic modulus of thin films and nanocrystals is established based on the intrinsic relation between the modulus, the cohesive energy and bond length by considering the size effects of the cohesive energy and the thermal expansion coefficient of the thin films and nanocrystals. Furthermore, the elastic modulus of Cu thin films with different thickness at a series of temperatures was simulated by the molecular dynamics method. The theoretical predictions based on the model are in agreement with the results of the computational simulations, the semi-continuum calculations and the experimental measurements for Si, Cu thin films and Pd nanocrystals.

2. Theoretical model

It is known that the Young's modulus E is related to the force constant k [16]:

$$E = \frac{k}{h} \tag{3}$$

where h is the atomic distance in equilibrium or the bond length; the force constant $k = \left.\frac{d^2 u(r)}{dr^2}\right|_{r=h}$, where $u(r)$ denotes the interatomic potential, is a function of the atomic distance r. Therefore, the Young's modulus is inherently related to the atomic interaction energy and the atomic distance. Let the interatomic potential of an ideal crystal be $u(r) = \frac{pq}{p-q} e\left[\left(\frac{h}{r}\right)^p \frac{1}{p} - \left(\frac{h}{r}\right)^q \frac{1}{q}\right]$, where e is the atomic binding energy or the bond energy, the coefficients p and q are the parameters reflecting the shapes of the potential curves (when $p = 12$ and $q = 6$, the potential is the Lennard–Jones (L-J) potential) [17]. Therefore, $k = pqe/h^2$, combining with Equation (3), $E = c_1 e/h^3$, where $c_1 = pq$ is a constant for the crystal. The equation indicates that the elastic modulus is dependent on the bond length and the bond energy of crystals. Note that, for metals and ceramics, the EAM potential and the Morse potential is more appropriate, respectively, but the intrinsic relations between the force constant, the elastic modulus, and the bond energy and bond length are the same as in the simple L-J potential. The comparison between our model predictions for the size-dependent elastic modulus of some metals based on the ideal crystal potential [18] and the molecular dynamics simulations based on the EAM potential [9] also shows consistency, since the size effect is only related to the relative change in physical quantities compared to the corresponding bulk references.

The bond energy is related to the cohesive energy of crystals and the coordination number of atoms. Let the coordination number of an atom in the bulk crystals be Z, the corresponding cohesive energy of one molar single crystal $U = (ZN_0)e/2$ for the bulk materials, where N_0 is the Avogadro constant, i.e. $e = 2U/(ZN_0)$. Therefore,

$$E = c_2 \frac{U}{h^3} \tag{4}$$

where $c_2 = 2c_1/(ZN_0)$ is a constant independent of temperature. Equation (4) indicates that the temperature effect on the elastic modulus is related to the temperature effects of the cohesive energy and bond length, i.e. $E(T) = c_2 U(T)/h^3(T)$ with the temperature-dependent elastic modulus $E(T)$, the cohesive energy $U(T)$ and the bond length $h(T)$. Therefore:

$$\frac{E(T)}{E_0} = \frac{U(T)}{U_0}\left[\frac{h_0}{h(T)}\right]^3 \tag{5}$$

where E_0, U_0 and h_0 are the elastic modulus, the cohesive energy and the bond length at 0 K, respectively. Considering the thermal expansion effect and the binding energy weakening with increasing temperature T:

$$U(T) = U_0 - \int_0^T C_V dT \tag{6}$$

$$h(T) = h_0\left[1 + \int_0^T \alpha dT\right], \tag{7}$$

where α is the thermal expansion coefficient [5]. Therefore:

$$\frac{E(T)}{E_0} = \frac{1 - \frac{\int_0^T C_V dT}{U_0}}{\left[1 + \int_0^T \alpha dT\right]^3} = \frac{1 - \frac{C_V T}{U_0}}{(1 + \alpha T)^3}. \tag{8}$$

Equation (8) indicates that the temperature-dependent elastic modulus $E(T)$ can be obtained by the cohesive energy at 0 K, the specific heat and the thermal expansion coefficient. Note that the specific heat and the thermal expansion coefficient themselves are also functions of the temperature.; when $T > \Theta$, the specific heat is a constant approximately, and considering that the thermal expansion coefficient is normally in the range of 10^{-6}, the temperature effects of α and C_V is neglected at room or higher temperature.

For thin films and nanocrystals, assuming that Equation (8) is still valid, the cohesive energy U_0 and the thermal expansion coefficient α are size-dependent. The cohesive energy and the melting latent heat are both related to the thermal stability of the crystals. Recently, a physical model of the size-dependent melting latent heat (melting enthalpy) $H_m(D)$ has been established [19]:

$$\frac{H_m(D)}{H_m(B)} = \left(1 - \frac{1}{D/D_m - 1}\right) \exp\left(\frac{-2S_m}{3R} \frac{1}{D/D_m - 1}\right).$$

It is a product of the size-dependent melting temperature (the exponent term) and the melting entropy, where D denotes the thickness of thin films or the diameter of the nanoparticles, B represents the corresponding bulk, $H_m(B)$ is the bulk melting enthalpy, D_m is the critical size of the solid–liquid transition, and S_m is the bulk melting entropy. The $H_m(D)$ function as a general function for the size dependence of the phase transition heat is suitable for all kinds of the first-order phase transitions [20]. Therefore, the size-dependent cohesive energy (approximately equal to the sublimation heat) can be obtained as:

$$U_0(D) = U_0(B)\left(1 - \frac{1}{D/D_c - 1}\right) \exp\left(-\frac{2S_c}{3R} \frac{1}{D/D_c - 1}\right) \tag{9}$$

where $U_0(B)$ is the bulk cohesive energy, $D_c = h_0(B)/2$ is the critical size of the solid–vapour transition with the bulk atomic diameter $h_0(B)$, $S_c = U_0(B)/T_c$ is the bulk sublimation entropy of the solid–vapour transition with the boiling temperature T_c. When $D = 2D_c = h_0(B)$, $U_0(D) = 0$, which is reasonable since the structures of the solid and the vapour are indistinguishable for an atom. When $D \gg D_c$, $U_0(D) \to U_0(B)$.

According to the Lindemann model and the Grüneisen theory, the thermal expansion coefficient is related to the Debye temperature θ [21], $\alpha = \frac{c_3}{\theta^2 V^{2/3} M}$, where c_3 is a constant, V is the molar volume, M is the atomic weight compared to C^{12} [22], $\theta = c_4 \sqrt{\frac{T_m}{M' V^{2/3}}}$ with a constant c_4, the melting temperature T_m and the molecular mass M' [23], therefore, $\alpha \propto 1/T_m$. The size-dependent melting temperature function $T_m(D)$ is the exponent term in the $H_m(D)$ function as mentioned above,

i.e. $\frac{T_m(D)}{T_m(B)} = \exp\left(\frac{-2S_v}{3R}\frac{1}{D/D_m-1}\right)$ with the bulk melting temperature $T_m(B)$ and the vibration part of the melting entropy S_v [19]; therefore:

$$\alpha(D) = \alpha(B)\exp\left(\frac{2S_v}{3R}\frac{1}{D/D_m-1}\right), \tag{10}$$

where the critical size D_m is, respectively, $2h_0(B)$ and $6h_0(B)$ for thin films and nanoparticles [19]. For metals, $S_v = S_m = H_m(B)/T_m(B)$, for semiconductors, $S_v = S_m - R$ approximately [24]. Substituting Equations (9) and (10) into Equation (8), the temperature effect on the elastic modulus of thin films and nanocrystals can be predicted.

Note that the referred elastic modulus E_0 in Equation (8) is also size-dependent for thin films and nanocrystals, according to Equation (4):

$$\frac{E_0(D)}{E_0(B)} = \frac{Z(B)}{Z(D)}\frac{U_0(D)}{U_0(B)}\left[\frac{h_0(B)}{h_0(D)}\right]^3 \tag{11}$$

where the change in the coordinate number of atoms in nanosystems caused by the effect of surface broken bonding is considered since the surface–volume ratio is larger for thin films and nanocrystals, $Z(D) = n[Z(B) - m] + (1 - n)Z(B)$ denotes the coordinate number of atoms of thin films and nanocrystals, where $n = D_m/D$ represents the ratio of atomic number on the surface to that in the volume, m is the broken bonding number of atoms on the surface, $Z(B)$ denotes the coordinate number of atoms of the corresponding bulk crystals. The size-dependent cohesive energy can be obtained in terms of Equation (9). The size-dependent bond length can be obtained by the size-dependent intrinsic lattice strain ε of nanocrystals [25]. According to the Laplace–Young equation and the thermodynamic definition of the surface stress, $\varepsilon = \frac{h_0(D)-h_0(B)}{h_0(B)} = \pm\frac{f}{3D}\sqrt{D_mh_0(B)S_vH_m(B)/(KVR)}$, where the K is the bulk modulus of the crystals, f is 1 and 2 for nanocrystals with grain boundaries and single crystal thin films, respectively, the negative denotes the lattice contraction, the positive denotes the lattice expansion [25]. Therefore, the size-dependent bond length is:

$$\frac{h_0(B)}{h_0(D)} = \frac{1}{1 \pm \frac{f}{3D}\sqrt{D_mh_0(B)S_vH_m(B)/(KVR)}}. \tag{12}$$

Substituting Equations (9) and (12) into Equation (11), the size-dependent referred elastic modulus can be obtained.

3. Molecular dynamics simulations

The molecular dynamics (MD) simulations of the biaxial tension of Cu thin films at different temperatures were carried out to validate the temperature effect on the elastic modulus. The structures of Cu thin films with a thickness of 12 and 2.2 nm were established with x, y and z being the [100], [010] and [001] directions, respectively; the periodic boundary condition is set in the x and y directions, and the z direction is free. The embedded atom method (EAM) potential was used [26].
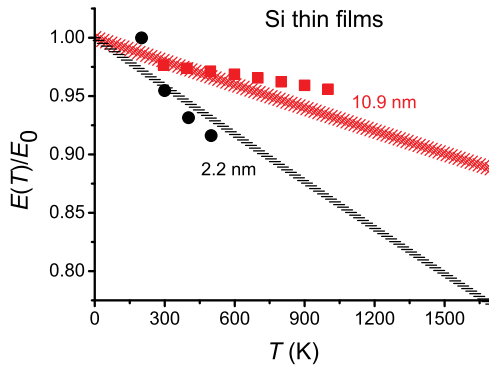
Figure 1. Temperature-dependent Young's modulus of Si thin films. The lines are predictions based on Equation (8). The symbols are the results of MD simulations (circles: 2.2 nm thickness [13]) and calculations based on the semi-continuum method (squares: 10.9 nm [14]).
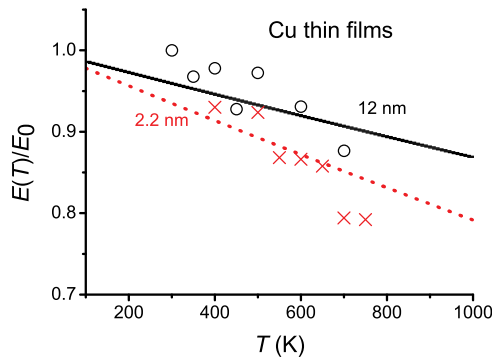

Figure 2. Temperature-dependent biaxial modulus of Cu thin films. The lines are predictions based on Equation (8). Circles (12 nm) and forks (2.2 nm) are the results of our MD simulations.

The displacement load was applied; equal strains were applied in the x and y directions. The Virial stress was taken in the stress calculation. The simulations were performed at the several temperatures in range 300–800 K; the stress–strain curves and thus the biaxial modulus were obtained at the different temperatures.

4. Results and discussion

The simulation results for Cu thin films, previous MD simulations [13] and the calculations based on the semi-continuum method [14] for Si thin films, plus the experimental measurements for Pd nanocrystals [15] were all compared to the theoretical predictions based on our model. Figures 1–3 show the temperature-dependent elastic modulus of Si and Cu thin films and Pd nanocrystals. It can be seen that the modulus decreases with increasing temperature, and the rate of the decrease increases with decreasing thickness of the thin films (Figures 1 and 2). The model's
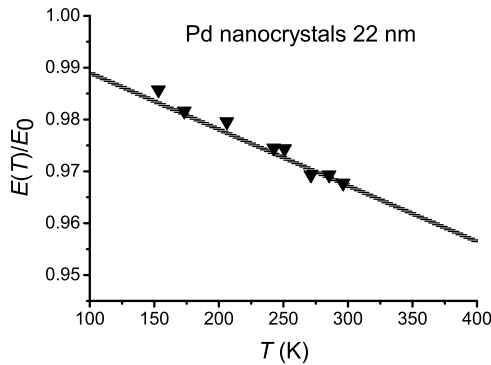
Figure 3. Temperature-dependent bulk modulus of Pd nanocrystals. The line is the prediction based on Equation (8). Triangles are the results of experimental observations ($>100 \, \mathrm{K}$) considering the effect of density and adulterant [15].

Table 1. Related parameters in Equations (8)–(12).

	Si	Cu	Pd
$h_0(B)$ (nm) [27]	0.3368	0.2826	0.304
$U_0(B)$ (kJ mol^{-1}) [28]	446	336	376
T_c (K) [29]	3540	2836	3237
S_c (J mol^{-1} K^{-1})	125.989	118.477	116.157
$H_m(B)$ (kJ mol^{-1}) [29]	50.55	13.05	17.6
$T_m(B)$ (K) [29]	1685	1357.6	1825
S_v (J mol^{-1} K^{-1})	21.686	9.613	9.644
$\alpha(B)$ (10^{-6} K^{-1}) [29]	4.2	16.5	11.2
C_V (J mol^{-1} K^{-1}) [29]	20	24.435	25.98
K (GPa) [30]	235.4	137.8	187
V (cm^3 mol) [29]	12.1	7.1	8.9

predictions based on Equation (8) with related parameters [27–30] in Table 1 are in agreement with the results of the MD simulations performed by ourselves and another group [13], the calculation based on the semi-continuum approach [14] and experimental observations [15]. Figures 4 and 5 show the thickness-dependent Young's modulus of Si and Cu thin films. The modulus changes nonlinearly with reducing thickness and the predictions based on Equation (11) are also consistent with the results of the MD simulations [13] and the calculation based on the continuum mechanics combined with consideration of the surface effect [31]. Figure 5 also shows that the modulus of nanocrystalline Cu decreases with reducing grain diameters; the model's prediction also agrees with the MD simulation results [10]. The size effect of the elastic modulus does not appear to follow the Hall–Petch relation, as with flow stress and the hardness of nanocrystals, which may be attributed to a different physical mechanism between elasticity and plasticity.

The model indicates that the temperature and size effects on the elastic modulus of thin films and nanocrystals are associated, since they are both intrinsically related
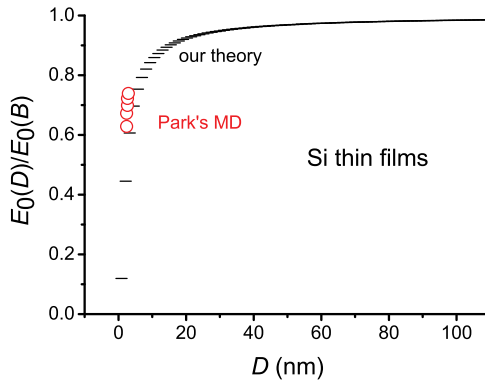
Figure 4. Thickness-dependent Young's modulus of Si thin films. The line is the prediction based on Equation (11) with $E_0(B) = 113$ GPa [30], $Z(B) = 16$, and $m = 6$, $f = 2$ in Equation (12) and the positive is taken considering the lattice expansion [13]. Circles are the results of MD simulations ($\langle 100 \rangle$ direction) [13].
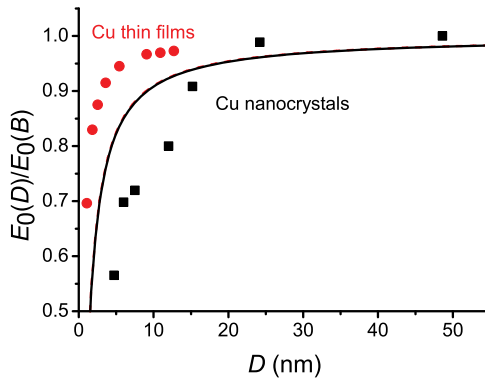

Figure 5. Thickness (diameter)-dependent Young's modulus of Cu thin films and nanocrystals. The lines are predictions based on Equation (11) with $E_0(B) = 137.8$ GPa [30], $Z(B) = 12$, and $m = 4$, $f = 1$ and 2, respectively, for nanocrystals and thin films in Equation (12) and the negative is taken considering the lattice contraction [31]. Circles and squares are the calculated results based on continuum mechanics for thin films ($\langle 100 \rangle$ direction) [31] and MD simulations for nanocrystals [10].

to the cohesive energy and bond length. The thermal expansion coefficient increases and the cohesive energy decreases with reducing thickness of the thin films in terms of Equations (10) and (9), respectively; therefore, according to Equation (8), the rate of decrease in the elastic modulus of thinner films increases as temperature increases, compared to that of thicker films (Figures 1 and 2). The trend is the same for nanocrystals. Experimental observations have also proved that the decrease in the modulus of the Al film with a grain size of 65 nm is clearly faster than that of bulk Al with a grain size of 300 μm with increasing temperature [32].

Note that the model is related to some thermodynamic material parameters, such as cohesive energy, specific heat, melting entropy, etc., which reflect the intrinsic

correlation of elasticity and those thermodynamic quantities, although the quantities may be difficult to obtain for some complex compounds. The model gives a general understanding of the intrinsic physical correlation between the elastic modulus, the cohesive energy and the bond length, despite the chemical bonding type and configuration of solids, since the model is established based on the corresponding reference state and predicts the relative change in the modulus compared to the corresponding bulk value at the referred temperature.

At the lower temperature, Equation (8) can be rearranged as $E(T) = E_0 - (E_0/U_0) \int_0^T C_V dT$, when the denominator is neglected considering the smaller value of the thermal expansion coefficient, which is consistent with the Anderson expression in Equation (2) and E_0/U_0 can give the value of the adjusting parameter $\gamma\delta/V$. At the higher temperature, the term $\exp(-T_0/T)$ equals $(1-T_0/T)$ approximately; thus the Wachtman expression in Equation (1) can be rearranged as $E(T) = (E_0 + AT_0) - AT$ approximately, which is also consistent with our expression, and the parameters $A = \frac{E_0}{U_0}\frac{C_V}{(1+\alpha T)^3}$ and $T_0 = (U_0/C_V)[1 - (1 + \alpha T)^3]$ can be obtained according to Equation (8). When the temperature is very low $(T < \Theta)$, $E(T) \rightarrow E_0$ and the $E-T$ curve shows a plateau, which agrees with previous results [3–5]. Note that the change in the elastic modulus at the low temperature is intrinsically non-linear owing to the Debye approximation nature and the T^3 approximation of the specific heat, although not shown in Figures 1–3. The slope of the linear part of the $E-T$ curve is inversely proportional to the atomic cohesive energy U_0. It is also reasonable, corresponding to the above discussion, that the slope of a smaller sample is greater than that of a larger one, because the cohesive energy drops with deceasing size and the effect of the thermal expansion coefficient is weak.

5. Conclusion

An analytical theoretical model, without any adjustable parameters, for the temperature-dependent elastic modulus of thin films and nanocrystals is developed based on the physical definition of the modulus considering the size effects of the cohesive energy and the thermal expansion coefficient. The temperature dependence of the elastic modulus of Cu thin films is further simulated by the MD method. The results show that the elastic modulus decreases with increasing temperature, and the rate of the decrease increases with reducing thickness of thin films. The model is a general formation of the Anderson equation and the Watchmen expression. The theoretical predictions are in agreement with the results of the MD simulations, calculations based on continuum mechanics and experimental observations for Cu, Si thin films and Pd nanocrystals. The theory reveals that the temperature and size effects of elasticity are closely related for thin films or nanocrystals. The model will be valuable guide to the design and applications of thin films and nanoscale devices in finite temperature environments.

References

[1] U. Gysin, S. Rast, P. Ruff, E. Meyer, D.W. Lee, P. Vettiger and C. Gerber, Phys. Rev. B 69 (2004) p.045403.

[2] A.G. Evans and J.W. Hutchinson, Surf. Coat. Technol. 201 (2007) p.7905.

[3] J.B. Wachtman, W.E. Tefft Jr, D.G. Lam Jr and C.S. Apstein, Phys. Rev. 122 (1961) p.1754.

[4] L. Anderson, Phys. Rev. 144 (1966) p.553.

[5] M.X. Gu, Y.C. Zhou, L.K. Pan, Z. Sun, S.Z. Wang and C.Q. Sun, J. Appl. Phys. 102 (2007) p.083 524.

[6] Z. Sun, J. Zhou, D. Music, R. Ahuja and J.M. Schneider, Scripta Mater. 54 (2006) p.105.

[7] Y. Wang, J.J. Wang, H. Zhang, V.R. Manga, S.L. Shang, L.Q. Chen and Z.K. Liu, J. Phys.: Condens. Matter 22 (2010) p.225 404.

[8] D. Music, J. Burghaus, T. Takahashi, R. Dronskowski and J.M. Schneider, Eur. Phys. J. B 77 (2010) p.401.

[9] F.H. Streitz, K. Sieradzki and R.C. Cammarata, Phys. Rev. B 41 (1990) p.12285.

[10] J. Schiøtz and K.W. Jacobsen, Science 301 (2003) p.1357.

[11] T.Y. Zhang, M. Luo and W.K. Chan, J. Appl. Phys. 103 (2008) p.104308.

[12] X.J. Liu, J.W. Li, L.W. Yang, Z.F. Zhou, Z.S. Ma, G.F. Xie, Y. Pan and C.Q. Sun, Appl. Phys. Lett. 94 (2009) p.131902.

[13] S.H. Park, J.S. Kim, J.H. Park, J.S. Lee, Y.K. Choi and O.M. Kwon, Thin Solid Films 492 (2005) p.285.

[14] J. Wang, Q.A. Huang and H. Yu, J. Phys. D: Appl. Phys. 41 (2008) p.165406.

[15] D.S. Agosta, R.G. Leisure, K. Foster, J. Markmann and J.J. Adams, Philos. Mag. 88 (2008) p.949.

[16] W.D. Nix and H.J. Gao, Acta Metall. 39 (1998) p.1653.

[17] J.G. Guo, L.J. Zhou and Y.P. Zhao, Surf. Rev. Lett. 15 (2008) p.599.

[18] L.H. Liang, H.S. Ma and Y.G. Wei, J. Nanomater. 2011 (2010) p.670857.

[19] Z. Zhang, X.X. Lu and Q. Jiang, Physica B 270 (1999) p.249.

[20] Q. Jiang, J.C. Li and B.Q. Chi, Chem. Phys. Lett. 366 (2002) p.551.

[21] C.C. Yang, M.X. Xiao, W. Li and Q. Jiang, Solid State Commun. 139 (2006) p.148.

[22] Y.H. Zhao and K. Lu, Phys. Rev. B 56 (1997) p.14330.

[23] J.G. Dash, Rev. Mod. Phys. 71 (1999) p.1737.

[24] Z. Zhang, M. Zhang and Q. Jiang, Semicond. Sci. Technol. 16 (2001) p.L33.

[25] Q. Jiang, L.H. Liang and D.S. Zhao, J. Phys. Chem. B 105 (2001) p.6275.

[26] S.M. Foiles, Phys. Rev. B 32 (1985) p.7685.

[27] H.W. King, *Structure of the pure metals*, in *Physical Metallurgy*, R.W. Cahn, ed., North-Holland, Amsterdam, 1970, p.60.

[28] C. Kittel, *Introduction to Solid State Physics*, 5th ed., Wiley, Chichester, 1976, p.74.

[29] *Table of Periodic Properties of the Elements*, Sargent-Welch Scientific, Skokie, IL, 1980, p.1.

[30] E.A. Brandes (Ed.), *Smithell's Metals Reference Book*, 6th ed., Butterworth, London, 1983, p.15-2.

[31] R. Dingrevillea, J.M. Qu and M. Cherkaoui, J. Mech. Phys. Solids 53 (2005) p.1827.

[32] M.A. Haque and M.T.A. Saif, Thin Solid Films 484 (2005) p.364.