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Size-dependent Young′s modulus of the FCC metallic films

M. Li[1,a], G. H. Su[2,b]*

[1]School of Physics and Electric Information, Huaibei Normal University, Huaibei, 235000, China

[2]Department of Material Engineering, Yancheng Institute of Technology, Yancheng 224003, China
[a]liming2010@chnu.edu.cn, [b]su_guihua@163.com

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Abstract. Young′s modulus is one of the most fundamental parameter to depict the elasticity of a given material. It determines the basic elastic deformation capacity of a structure under a bear load. When the diameter of nanocrystals is in the scale of several nanometers, the Young′s modulus is quite different from that of bulk. In order to determine elastic deformation capacity of nanocrystals, it is necessary to study the size dependent Young′s modulus. Based on above consideration, a simple thermodynamic model is developed for size dependent Young′s modulus of nanocrystals according to the "universal" binding energy curve and Laplace-Young equation. According to this model, the Young′s modulus of several FCC metallic films is predicted and the Young′s modulus increases with the size reduction. The prediction is agreed with computer simulation results.

Introduction

When the dimensions of crystals reduce to nanometer scale, their physical properties are usually different from those of bulk crystals. Size dependent physical properties of nanocrystals, such as melting point [1], glass transition temperature [2], and cohesive energy [3], have been confirmed by experimental observations. These dependences are mainly due to the large surface volume ratio of nanocrystals and have been validated by theoretical models [4-7].

Besides the above properties, it is also demonstrated experimentally that the Young′s modulus of nanocrystals is size dependent. Several experimental and simulation results have shown that when the diameter of nanocrystals is in several nanometers, the Young′s modulus is quite different from that of bulk [8-14]. The main reason is considered to be the surface stress. For the bulk crystals, the surface volume ratio is so small that the surface stress has no effect on the crystals. When the crystal is in nanoscale, the ratio of surface and volume is significant, the lattice contraction in the surface region changes Young′s modulus of the whole nanocrystals.

In this contribution, a thermodynamic model for the size dependent Young′s modulus of nanocrystals is developed considering the surface effect. The model result shows a good agreement with the reported simulation results.

Model

The binding energy of metallic crystals could be expressed as the so-called "universal" binding energy curve [15],

$$E(\varepsilon)=(E_0-F_0eh\varepsilon)\exp\left[\frac{F_0eh}{E_0}\varepsilon\right] \tag{1}$$

where $E(\varepsilon)$ is the binding energy for the atoms with strain ε, E_0, F_0, and h are the equilibrium binding energy, the break force, and the equilibrium bond distance, respectively. Since the Young′s modulus is defined as $Y(\varepsilon)=\frac{1}{V(\varepsilon)}\frac{d^2E(\varepsilon)}{d\varepsilon^2}$ where $V(\varepsilon)$ is the volume of crystals with strain ε [10], it could be deduced as,

$$Y(\varepsilon)=-\frac{1}{V(\varepsilon)}\frac{F_0eh}{E_0}\left(1+\frac{F_0eh}{E_0}\varepsilon\right)\exp\left[\frac{F_0eh}{E_0}\varepsilon\right] \tag{2}$$

In the above equation, when the crystals is at the equilibrium state where $\varepsilon = 0$, the Young′s modulus is deduced as,

$$Y_0=-\frac{1}{V_0}\frac{F_0eh}{E_0} \tag{3}$$

where Y_0 and V_0 are separately the Young′s modulus and volume of the crystals at equilibrium state. For the isotropic crystals, there is a relationship as $V(\varepsilon)=V_0(1+\varepsilon)^3$. Thus, the Eq. (2) can be rewritten as,

$$Y(\varepsilon)=\frac{Y_0}{(1+\varepsilon)^3}\left(1+\frac{F_0eh}{E_0}\varepsilon\right)\exp\left[\frac{F_0eh}{E_0}\varepsilon\right] \tag{4}$$

For the isotropic nanocrystals, there is high interior pressure induced by surface stress which is deduced according to Laplace-Young equation [16],

$$P=\frac{4f}{D} \tag{5}$$

where P is the interior pressure, f is the surface stress and D is the dimension for nanocrystals. D represents diameter for nanoparticles or nanowires and thickness for thin films. This high pressure can induce lattice contraction when the size of nanocrystals is rather small [17]. There is a relationship for the pressure-volume change as $\kappa=-\frac{\Delta V}{V_0P}$ where κ is the compressibility coefficient and ΔV is the volume change. According to the above expression, $\frac{\Delta V}{V_0}=\frac{V(\varepsilon)-V_0}{V_0}\approx 3\varepsilon$. Thus, the lattice contraction for the nanocrystals is deduced as,

$$\varepsilon=-\frac{4\kappa f}{3D} \tag{6}$$

Based on the above analysis, the Young′s modulus of nanocrystals is different from that of bulk due to the surface stress. Inserting Eq. (6) into Eq. (4), the Young′s modulus of nanocrystals is deduced as,

$$Y(D)=\frac{Y_0\left(1-\frac{4\kappa fF_0eh}{3DE_0}\right)\exp\left[-\frac{4\kappa fF_0eh}{3DE_0}\right]}{\left(1-\frac{4\kappa f}{3D}\right)^3} \tag{7}$$

where $Y(D)$ is the Young′s modulus of nanocrystals.

Table 1: The relevant data used in the calculations of Eq. (7).

	κ (10^{-12}Pa^{-1}) [18]	f (J/m^2)	F_0 (eV/ Å) [13]	h (Å) [13]	E_0(eV) [13]
Cu	7.042	1.106 [9]	0.44	2.59	-0.59
Au	5.556	1.714 [9]	0.44	2.96	-0.51
Ni	5.524	1.67 [19]	0.64	2.49	-0.86
Ag	9.2	1.041 [9]	0.34	2.93	-0.44

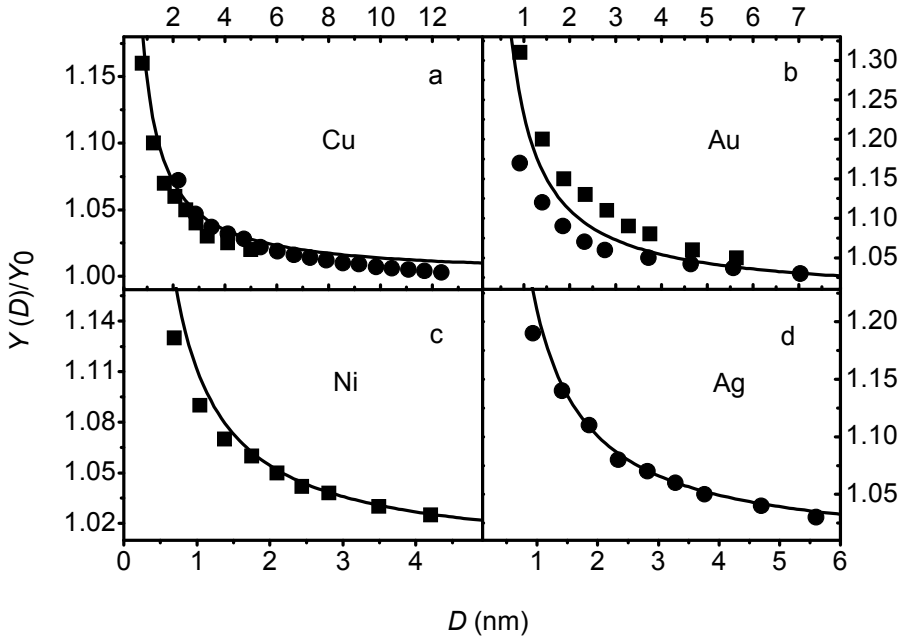

Figure 1. Curves representing $Y(D)/Y_0$ values as a function of D for (a) Cu (111) thin films; (b) Au (111) thin films; (c) Ni (111) thin films; (d) Ag (111) thin films separately. The symbols are computer simulation results. (a) Cu (111) thin films : ■ [9] and ● [10]; (b) Au (111) thin films: ● [8] and ■ [9]; (c) Ni (111) thin films: ■ [9]; (d) Ag (111) thin films ● [9].

Results and discussion

Figure 1 shows the comparison between the $Y(D)/Y_0$ values figured out by Eq. (7) and the simulation results of several metallic thin films such as Cu, Au, Ni, Ag. From the model, it is found that the Young′s modulus increases with the size reduction, which is well agreed with the simulation results. However, it has been found experimentally and theoretically that Young′s modulus of nanocrystals decreases with decreasing size [8,10-11]. As inferred above, the nanocrystals is considered isotropic in our model. While for thin films or nanowires, the size reduction is only in one or two directions. This anisotropy of nanocrystals may lead to the different change tendency of Young′s modulus. The simulation results adopted in this article are all for (111) FCC metallic thin films. Unlike the thin films in other directions, in the (111) plane, the Young′s modulus and elastic strain are both independent of direction [20]. For the thin films with several nanometer thicknesses, high pressure is induced in plane by surface stress, but not out of plane [9]. Thus, the (111) FCC thin films have a perfect two-dimension in-plane isotropy. This two-dimension isotropy could be approximately equivalent to three-dimension isotropy. This may be the reason why the calculated results by our model agree with the simulation results. For as (100) thin FCC metallic films, although the elastic strain is isotropic under isotropic hydrostatic pressure, the Young′s modulus is in-plane anisotropic [16]. For example, based on the simulation results, when the thickness of (100) thin films is reductive, on the (100) plane, the Young′s modulus increases in [110] direction but decreases in [100] direction [10]. This Young′s modulus reduction in [100] direction may be associated with the well-known Bain transformation, which has been widely viewed as a mechanism for FCC↔BCC transition [21]. This Young′s modulus reduction is also found for (110) thin films [8] and [111] and [100] direction nanowires [11]. Another explanation is that the Young′s modulus reduction may be due to the binding energy change [22]. It has been demonstrated that the binding energy of nanocrystals is size dependent [6]. According to the definition of Young′s modulus, it may be decreasing with the reduction of the binding energy. Since there are still many problems as considered above, the anisotropic Young′s modulus of nanocrystals needs to be further considered.

Conclusion

In summary, the size dependent Young′s modulus of nanocrystals is evaluated by considering the effect of surface stress and the Young′s modulus increases with the size reduction. The calculated results are agreed with the previous simulation ones. The anisotropic Young′s modulus of nanocrystals is also analyzed.

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