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BRIEF COMMUNICATIONS

Modulus of Elasticity of Polycrystalline Simple Cubic Metals from Morse Potential Energy Function

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Investigation of the elastic properties of a solid from the viewpoint of interatomic potential energy functions is important in the sense that it leads one to a better understanding of the nature of interactions between atoms of the solid.

Recently (*1*) we developed a simple theoretical model for calculation of the modulus of elasticity of polycrystalline simple metals using the inverse power type potential energy function. This model, which incorporates only the nearest neighbor interactions, yields results that are in good agreement with the experimental data in most cases. In this work we repeat the calculations using the Morse potential energy function (*2*) in order to compare the results with the previous work and to discuss the applicability of each potential.

The Morse potential function is given by

$$\varphi(r) = D_0[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}], \quad (1)$$

in which D_0 and r_0 are the dissociation energy and the equilibrium interatomic distance, respectively. α is a constant with the dimension of reciprocal length. The values of D_0, r_0, and α have been determined by Girifalco and Weizer (*3*) for several cubic metals. According to this potential energy function, the force required to hold two atoms at a distance r from each other is given by

$$\begin{aligned} f &= -\left(-\frac{\partial\varphi}{\partial r}\right) \\ &= -2\alpha D_0[e^{-2\alpha(r-r_0)} - e^{-\alpha(r-r_0)}] \\ &= -2\alpha D_0[e^{-2\alpha r_0(\Delta r/r_0)} - e^{-\alpha r_0(\Delta r/r_0)}], \quad (2) \end{aligned}$$

where $\Delta r = r - r_0$. For an infinitesimal state of stress we have $\Delta r/r_0 \ll 1$. Since the quantity αr_0 is of the order of 3 to 5 for most simple metals (*3*), therefore, we may expand the exponential terms of Eq. (2) into power series and neglect terms higher than the first-order term. This gives

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TABLE I

THEORETICALLY CALCULATED AND THE EXPERIMENTAL VALUES OF THE MODULUS OF ELASTICITY OF POLYCRYSTALLINE SIMPLE CUBIC METALS IN UNITS OF 10^{10} Nm^{-2}

Metal	E(theory) Morse potential	E(theory) Inverse power type potential	E(expt)
Pb	3.49	3.66	1.57
Ag	8.23	8.31	8.06
Ni	15.31	17.15	19.33
Cu	10.84	12.65	12.36
Al	6.77	8.72	7.10
Ca	1.29	1.55	1.96
Sr	0.93	1.11	1.36
Mo	33.08	32.07	32.77
W	38.25	43.56	39.73
Cr	24.55	27.15	24.33
Fe	20.31	23.71	20.99
Ba	1.11	1.55	1.27
K	0.31	0.34	0.35
Na	0.64	0.78	0.89
Cs	0.16	0.19	0.18
Rb	0.20	0.26	0.27

$$f = 2\alpha^2 D_0 r_0 \left(\frac{\Delta r}{r_0}\right). \tag{3}$$

In a polycrystalline metal, the line of action of the force f is randomly oriented, making an angle between 0 and $\pi/2$ with the direction of stress. The mean component of f in this direction is, therefore, given by (*1*)

$$\bar{f}_s = f\overline{\cos\theta} = f\left(\frac{2}{\pi}\right) = \frac{4}{\pi}\alpha^2 D_0 r_0 \left(\frac{\Delta r}{r_0}\right), \tag{4}$$

where θ is the angle between the line of action of f and the direction of stress. Since the average number of atoms per unit cross-sectional area of the metal is $(d/M)^{2/3}$ where d is the density and M is the atomic mass, therefore, stress will be given by

$$s = \frac{4}{\pi}\alpha^2 D_0 r_0 \left(\frac{\Delta r}{r_0}\right)\left(\frac{d}{M}\right)^{2/3}. \tag{5}$$

Strain, e, on the other hand, is given by $\Delta r/r_0$ regardless of the direction of the line connecting the centers of the two atoms (*1*). Therefore, the modulus of elasticity, E, is given by

$$E = \frac{s}{e} = \frac{4}{\pi}\alpha^2 D_0 r_0 \left(\frac{d}{M}\right)^{2/3}. \tag{6}$$

The dissociation energy is related to the cohesive energy, ΔH_s°, the coordination number, W, and the Avogadro's number, N, according to (*4*)

$$D_0 = \frac{2\Delta H_s^\circ}{NW}. \tag{7}$$

Furthermore, we note that for fcc lattices

$$r_0(\text{fcc}) = 2^{1/6}\left(\frac{M}{d}\right)^{1/3} \tag{8}$$

and for bcc lattices

$$r_0(\text{bcc}) = 3^{1/6}\left(\tfrac{3}{4}\right)^{1/3}\left(\frac{M}{d}\right)^{1/3}. \tag{9}$$

Thus, we obtain

$$E = C\frac{\alpha^2 \Delta H_s^\circ}{NW}\left(\frac{d}{M}\right)^{1/3}, \tag{10}$$

where $C = 2.8583$ and 2.7785 for fcc and bcc lattices, respectively.

The moduli of elasticity of 16 simple cubic metals are calculated from Eq. (10) and listed in Table I along with the experimental values (*5*) and those obtained from the inverse power type potential energy function (*1*). The parameters needed for calculations have been taken from the following sources: ΔH_s° from Gschneidner (*5*), d and M from the American Institute of Physics Handbook (*6*), and α from Girifalco and Weizer (*3*). The results indicate that the moduli of elasticity obtained from the Morse potential energy function are also in

good agreement with the experimental data and the degree of agreement is the same for both potentials. Both, the inverse power type and the Morse potential energy functions, are equally well applicable in this theory.

Clearly, the above model is not the only one which leads to a theoretical calculation of an elastic modulus in terms of interatomic potential energy parameters. However, the significance of the present model lies in its simplicity.

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