V. NUMERICAL RESULTS

In order to establish Φ as a function of x, using Eq. (26), c, s, γ and $U_{\text{vib}}(v_0,T_0)$ must be determined, for each metal. In columns 1 and 2 of Table I are listed the values of c and s determined directly from the intercept and slope of a line drawn through the experimental values[3] of U_s *vs* U_p. The metals chosen, Be, 24*ST* Al, Co. Ni, Cu, and Ag, are those for which the experimental measurements are most extensive. The values of c and s listed here are slightly different from those listed in Table X, reference 4. In column 3, Table I are listed values of γ determined by using Grüneisen's relation [Eq. (7)], along with literature references.

The vibrational energy at 20°C and 1 atmosphere, $U_{\text{vib}}(v_0,T_0)$, consists of the zero-point vibrational energy of the normal modes at $T=0$°K plus the energy required to heat the lattice at the constant volume v_0 from 0°K to 293°K. Thus we can write

$$U_{\text{vib}}(v_0,T_0)=U_{\text{vib}}(v_0,0)+\int_0^{T_0} C_{v_0}dT. \tag{28}$$

The zero-point energy is given by

$$U_{\text{vib}}(v_0,0)=\int_0^{\nu_m} \tfrac{1}{2}h\nu g(\nu)d\nu, \tag{29}$$

where $g(\nu)$ is the density of normal modes at frequency ν, and ν_m is the maximum vibration frequency. Since there are $3N$ modes of vibration of a lattice with N atoms, there is a normalization condition on $g(\nu)$, *viz.*:

$$\int_0^{\nu_m} g(\nu)d\nu=3N. \tag{30}$$

From Eqs. (29) and (30) it follows that the vibrational energy at 0°K is $3Nh\langle\nu\rangle/2$, where $\langle\nu\rangle$ is the average vibration frequency weighted over the density of modes. In order to determine $\langle\nu\rangle$ accurately, the detailed form of the density of modes is needed. Since there is no direct experimental information on the detailed form on the density of modes, we shall use the Debye approximation, i.e., that

$$g(\nu)=3N(3\nu^2/\nu_m{}^3). \tag{31}$$

The average frequency for this distribution is $\frac{3}{4}\nu_m$. Thus the zero point energy can be written as

$$U_{\text{vib}}(v_0,0)=(9/8)Nh\nu_m=(9/8)Nk\Theta_0; \tag{32}$$

where Θ_0 is defined by $k\Theta_0=h\nu_m$. The value of Θ_0 used in calculating $U_{\text{vib}}(v,0)$ from Eq. (32) will be obtained from measurements of the specific heat at low temperature. With this choice of Θ_0 the density of modes $g(\nu)$ will have the same curvature in the low-frequency region as the actual density of modes in the solid. If the Debye model is also used to estimate the integral of the specific heat from 0°K to 293°K, then Eq. (28) can be written as

$$U_{\text{vib}}(v_0,T_0)=3NkT\left[\frac{3}{8}\frac{\Theta_0}{T}+B(y_m)\right], \tag{33}$$

where

$$B(y_m)=3\left(\frac{T}{\Theta}\right)^3\int_0^{\Theta/T}\frac{z^3dz}{(e^z-1)}, \quad \text{(a)}$$

$$y_m=\Theta/T. \quad \text{(b)}$$

The function $B(y_m)$ has been calculated by Beattie.[19] The value of Θ used in calculating U_{vib} from Eq. (33) is the value appropriate to the high-temperature region $T\sim\Theta$. In this way we get the best fit of the Debye function to the specific heat data in the region of temperature which makes the largest contribution to U_{vib}. The values of Θ_0 and Θ required for the determination of $U_{\text{vib}}(v_0,T_0)$ are listed in columns 5 and 6 of Table I, along with literature references. It should be

TABLE II. Values of C^2, $U_{\text{vib}}(v_0,T_0)$ and $\Phi(v_0)$ used in the determination of $\Phi(v)$.

Metal	c^2 (ev/atom)	$U_{\text{vib}}(v_0,T_0)$ (ev/atom)	$\Phi(v_0)$ (ev/atom)
Be	6.20±2.4%	0.1303	3.33
Al	8.00[a]	0.0849	3.23
Co	13.7 ±1.2%	0.0883	4.56
Ni	13.8 ±1.2%	0.0846	4.40
Cu	10.0 ±5%	0.0829	3.52
Ag	11.8 ±2%	0.0787	3.00

[a] No error is listed for the 24*ST* Al data because the published results represent smoothed values of U_s and U_p obtained from a very large number of measurements.

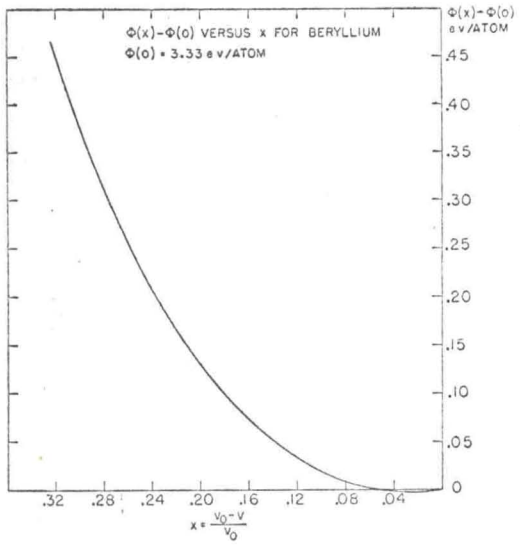


FIG. 1. The change in the cohesive energy $[\Phi(x)-\Phi(0)]$ of beryllium as a function of the volume decrement $x=(v_0-v)/v_0$. v_0 is the volume/unit mass at 20°C and $P=1$ atmos. $\Phi(0)$ is the cohesive energy at $v=v_0$.

[19] J. A. Beattie, J. Math and Phys. 6, 1 (1926).