one expects this model to produce reasonable results for their shear elastic constants. The results obtained by Fuchs for the Coulomb contribution to the shear stiffnesses of body-centered cubic metals with one valence electron per atom are:

$$C\equiv C_{44}=Ke^2/\Omega^{\frac{4}{3}},\quad C'\equiv\tfrac{1}{2}(C_{11}-C_{12})=K'e^2/\Omega^{\frac{4}{3}},\quad (1)$$

where e is the electronic charge, Ω is the atomic volume and K and K' are constants. In addition, Fuchs presents a modification to the above results to take into account the difference of the electron charge density at the surfaces of an atomic polyhedron, from the value e/Ω which would obtain if the electron charge were distributed uniformly over the volume Ω of the cell. The modification to C and C' consists of adding a multiplicative factor Z^2, where Z represents the ratio of the actual charge density at the cell boundary to the value e/Ω, yielding:

$$C=Z^2Ke^2/\Omega^{\frac{4}{3}},\quad C'=Z^2K'e^2/\Omega^{\frac{4}{3}}.\quad (2)$$

If one represents the valence electronic wave function in the crystal by

$$\psi_0(\bar{r})=[\mu_0(\bar{r})/\Omega^{\frac{1}{2}}]\exp i\bar{k}\cdot\bar{r},$$

where $\mu_0(\bar{r})$ is the wave function of the lowest electronic state, normalized over the volume of the atomic polyhedron, Z is given by: $Z=|\mu_0(\bar{r}_c)|^2$ where $\bar{r}_c$ is the position vector of any point on the cell boundary. If one examines the wave function in the approximation that the atomic polyhedron has been replaced by a sphere of equal volume, as has been done by Wigner and Seitz and others, the expression for Z becomes $Z=|\mu_0(r_s)|^2$ where r_s is the radius of the "S" sphere with volume Ω. That is, $\frac{4}{3}\pi r_s^3=\Omega$. This yields for C and C' the results:

$$C=|\mu_0(r_s)|^4Ke^2/\Omega^{\frac{4}{3}},\quad C'=|\mu_0(r_s)|^4K'e^2/\Omega^{\frac{4}{3}}.\quad (3)$$

Measurements of the elastic constants of the alkali metals lithium,[6] sodium,[11] and potassium[17] have been made over a range of temperatures. Results of these measurements are shown in reference (5), where the experimental values of C and C' are plotted as a^4C/e^2 and a^4C'/e^2 versus temperature in order to compare them with the corresponding Fuchs theoretical result which is indicated on the $T=0$°K ordinate. a is the lattice parameter and is proportional to $\Omega^{\frac{1}{3}}$. Bender's measurements on potassium were made only at 78°K and are marked by triangles. It may be seen that the agreement at 0°K is not perfect, but that it predicts the large anisotropy ratio C/C' which is observed in these materials. The results for the shear elastic constants are discussed in greater detail in reference (5).

It is possible to extend the theoretical results for the shear constants of the alkali metals to obtain a prediction of their pressure (or better, volume) variation. Using the unmodified equation (1),

$$d\ln C/d\ln\Omega=d\ln C'/d\ln\Omega=-\tfrac{4}{3}.$$

An experimentally determined value of each of $d\ln C/d\ln\Omega$ and $d\ln C'/d\ln\Omega$ can be found from the corresponding pressure derivatives, using the relation $d\ln G/d\ln\Omega=-B_T(dG/dP)$ where G may be any quantity. This with values of dC/dP and dC'/dP from Table II yields the results: $d\ln C/d\ln\Omega=-2.4$, $d\ln C'/d\ln\Omega=-2.4$, which are nearly a factor of two larger than the prediction. Possibly the most remarkable observation to be made about these experimental results is the indication they give that the elastic anisotropy is essentially independent of the compression of the crystal (at 299°K at least). *This observation rules out in the practical sense any interaction between neighboring ion cores of the crystal because the nearest neighbor ion core interactions in a low density bcc metal would be expected to increase C and decrease C′ from their respective values without ion core interaction, with rapidly increasing effect as the pressure was applied, contrary to the observations.* The indication is then that the electronic charge density at the boundary of the atomic polyhedron is changing with volume faster than $1/\Omega$, or in other words, $\mu_0(r_s)$ as defined earlier is increased as Ω is decreased. Using the equations (3) together with $d\ln C/d\ln\Omega$ and $d\ln C'/d\ln\Omega$, we obtain the result:

$$\left.\frac{d\ln C}{d\ln\Omega}\right|_{\Omega=\Omega_0}=-\tfrac{4}{3}+4\left(\frac{d\ln\mu_0(r_s)}{d\ln\Omega}\right)_{\Omega=\Omega_0}=-2.4,\quad (4)$$

where Ω_0 is the equilibrium zero pressure atomic volume. Whence:

$$\left(\frac{d\ln\mu_0(r_s)}{d\ln\Omega}\right)_{\Omega=\Omega_0}=-0.27.\quad (5)$$

The work of various theoretical investigations[18–20] indicates values of $[d\ln\mu_0(r_s)/d\ln\Omega]_{\Omega=\Omega_0}$ at $T=0$°K which lie between -0.08 and -0.13.

Interpretation of the pressure variation of the elastic constants of Aluminum[10] by Schmunk and Smith, required an assumption that the electrostatic contribution to the shear elastic constants varied as r^{-8} instead of r^{-4}.

Bulk Modulus

We consider now the more difficult question of interpretation of the value of the bulk modulus and its variation with volume. Interpretation of the elastic constants appropriate to strains which involve a volume change is, in general, more difficult and more susceptible to error than interpreting shear elastic constants and their volume variation. Since some of the contributions to the cohesive energy of the crystal may

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