

$$U_{[110]}^{[110]} = \left\{ \frac{1}{\rho_0} [\bar{Q}_{11}[110] + \bar{Q}_{12}[110]] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{\lambda^3}{2\rho_0} [\lambda(\bar{C}_{1111} + \bar{C}_{1122} + 2\bar{C}_{2323}) - 2\bar{p}] \right\}^{\frac{1}{2}} \quad (37)$$

$$U_{[110]}^{[1\bar{1}0]} = \left\{ \frac{1}{\rho_0} [\bar{Q}_{11}[110] - \bar{Q}_{12}[110]] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{\lambda^3}{2\rho_0} [\lambda(\bar{C}_{1111} - \bar{C}_{1122}) - 2\bar{p}] \right\}^{\frac{1}{2}} \quad (38)$$

$$U_{[001]}^{[110]} = U_{[001]}^{[100]} \quad (39)$$

which by virtue of (32) are such that

$$-U_{[110]}^{[110]} < U_{[001]}^{[110]} < U_{[110]}^{[110]}. \quad (40)$$

When  $v$  has the direction  $[111]$ ,  $v: (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ , then

$$U_{[111]}^{[111]} = \left\{ \frac{1}{\rho_0} [\bar{Q}_{11}[111] + 2\bar{Q}_{12}[111]] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{\lambda^3}{3\rho_0} [\lambda(\bar{C}_{1111} + 2\bar{C}_{1122} + 4\bar{C}_{2323}) - 3\bar{p}] \right\}^{\frac{1}{2}} \quad (41)$$

and

$$U_{[110]}^{[111]} = U_{[110]}^{[1\bar{1}1]} = U_{[011]}^{[111]}$$

$$= \left\{ \frac{1}{\rho_0} [\bar{Q}_{11}[111] - \bar{Q}_{12}[111]] \right\}^{\frac{1}{2}}$$

$$= \left\{ \frac{\lambda^3}{3\rho_0} [\lambda(\bar{C}_{1111} - \bar{C}_{1122} + \bar{C}_{2323}) - 3\bar{p}] \right\}^{\frac{1}{2}} \quad (42)$$

where

$$U_{[110]}^{[111]} < U_{[111]}^{[111]}. \quad (43)$$

Calculated values together with experimental data for sodium and potassium for the last-named two cases are shown in Figs. 3-6.

The agreement of the calculated and experimental pressure variation of the longitudinal wave speeds is good. For the shear wave speeds the agreement is not good at all. This is because the band structure

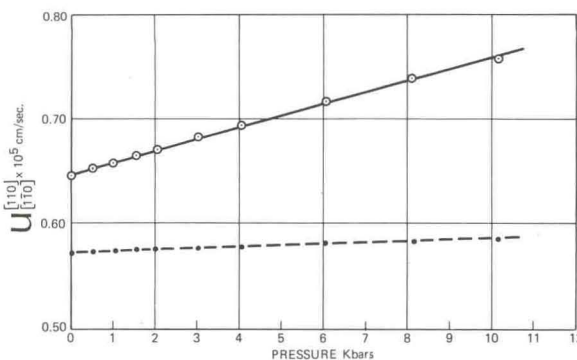
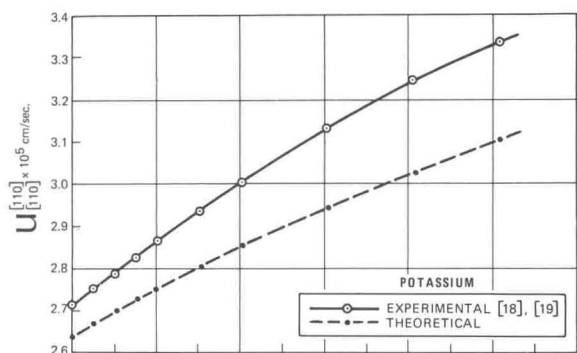


Fig. 4. Variation of  $U_{[110]}^{[110]}$  and  $U_{[110]}^{[1\bar{1}0]}$  with pressure for potassium.

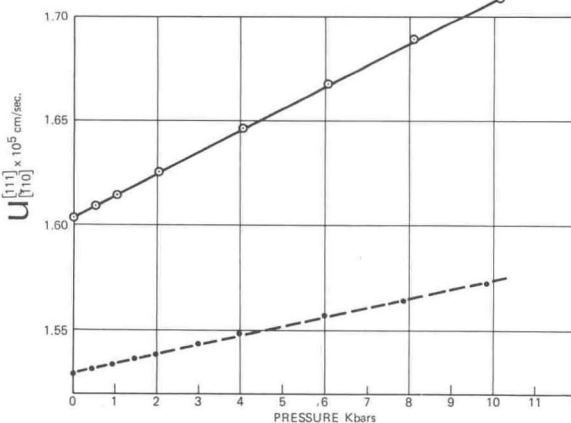
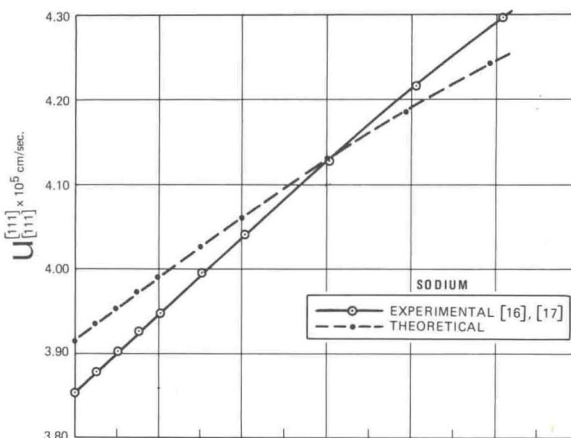


Fig. 5. Variation of  $U_{[111]}^{[111]}$  and  $U_{[110]}^{[111]}$  with pressure for sodium.

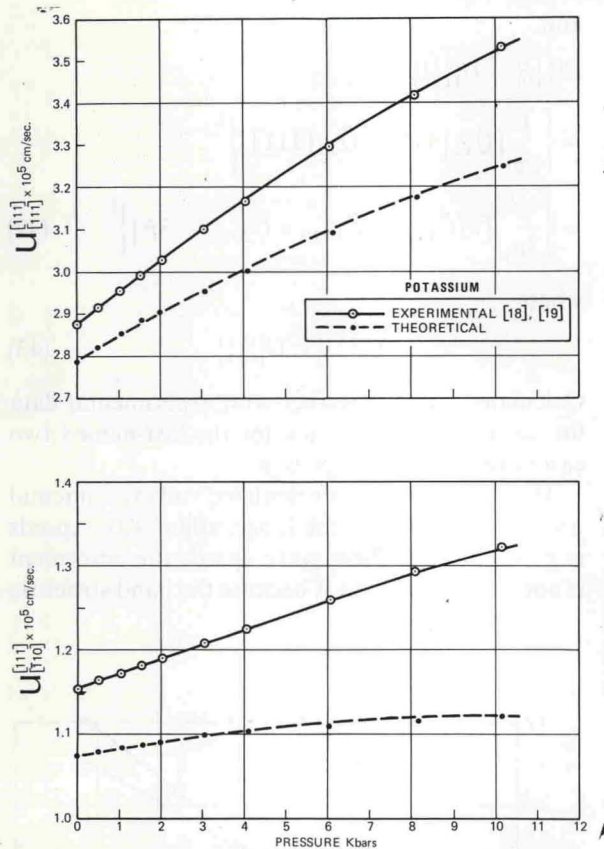


Fig. 6. Variation of  $U_{[111]}^{[111]}$  and  $U_{[110]}^{[110]}$  with pressure for potassium.

contribution (see Appendix) to the strain energy has been omitted<sup>2</sup>.

The formulation presented here suggests that the experimental data on the wave speeds and their variation with pressure can be compared directly with theoretical models for materials. This method would avoid the errors introduced into the experimental data when the wave speed data are reduced to values for the elastic coefficients.

#### ACKNOWLEDGEMENTS

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## APPENDIX

### THE BAND STRUCTURE ENERGY

The band structure energy is a second-order perturbation addition to the crystal energy, arising from a pseudopotential correction to the free electron crystal potential which can be shown to have the general form<sup>3</sup>

$$E_{p2} = \sum_m S^*(\mathbf{K}_m) \cdot S(\mathbf{K}_m) F(\mathbf{K}_m) = \sum_m F(\mathbf{K}_m) \quad (\text{A1})$$

where

$$S(\mathbf{K}_m) = 1$$

$$F(\mathbf{K}_m) = -\frac{\Omega K_m^2}{8\pi e^2} |\langle \mathbf{k} + \mathbf{K}_m | \hat{W} | \mathbf{k} \rangle|^2 \frac{\varepsilon - 1}{\varepsilon} \quad (\text{A2})$$

The structure factor  $S(\mathbf{K}_m)$  is unity for monovalent crystals.  $F(\mathbf{K}_m)$  is the energy wave number characteristic with  $e$  the electronic charge,  $\mathbf{k}$  the wave vector,  $\hat{W}$  the local electron-ion pseudopotential,  $\varepsilon$  the Hartree screening function,  $\Omega$  the atomic sphere volume and  $\mathbf{K}_m$  the reciprocal lattice vector.

The simplest local electron-ion pseudopotential suitable for the alkali metals is the Ashcroft form<sup>4</sup>, wherein

$$|\langle \mathbf{k} + \mathbf{K}_m | \hat{W} | \mathbf{k} \rangle|^2 = \frac{64\pi^2}{\Omega^2 K_m^4} \cos^2 \{r_c |\mathbf{K}_m|\} \quad (\text{A3})$$

Then in atomic units

$$E_{p2}^{\text{a.u.}} = \frac{8\pi}{\Omega_{\text{DL}}} \sum_m \frac{\cos^2 \{r_c |\mathbf{K}_m|\}}{K_m^2} \left( \frac{1}{\varepsilon} - 1 \right) \quad (\text{A4})$$

with

$$\varepsilon = 1 + \frac{4k_F - K_m^2}{2\pi K_m^3} \ln \left| \frac{2k_F/K_m + 1}{2k_F/K_m - 1} \right| + \frac{2k_F}{\pi K_m^2} \quad (\text{A5})$$

$$k_F = \left\{ \frac{6\pi^2}{\Omega_{\text{DL}}} \right\}^{\frac{1}{3}} \quad (\text{A6})$$

where  $\Omega_{\text{DL}}$  is the volume of a unit cell of the direct lattice. The significant contribution of the band structure energy to higher derivatives of the crystal energy comes from the derivatives of the logarithmic term in the screening function  $\varepsilon$ , which has a singularity at  $\mathbf{K}_m = 2\mathbf{k}_F$ .

The band structure contribution to the strain energy can be shown to be<sup>5</sup>

$$\frac{2}{\Delta^3 N} E'_{p2} = 4\beta_7 I_3^{-\frac{1}{2}} \sum_m \frac{\cos^2 \{ \beta_{13} (m_\alpha m_\beta C_{\alpha\beta}^{-1})^{\frac{1}{2}} \}}{m_\gamma m_\delta \bar{C}_{\gamma\delta}^{-1}}$$