

ions. Therefore, such calculations do not stringently test the various bare potentials and dielectric functions which have been obtained. In Al and Pb, however, conduction electron screening is much greater (on average, the actual phonon frequencies at the zone boundary are about 35% of the unscreened ionic lattice frequencies in Al, compared with 80% in Na), and the tests of modifications of the potentials are correspondingly more sensitive.

In most of this work we have used a local Heine–Abarenkov (1964, to be referred to as HA) model potential. Before dielectric screening this potential consists of a series of square wells of depth A_l for each angular momentum l , inside a radius R_M , and a Coulomb potential $-Z/r$ outside this radius. The values of $A_l(E)$ at several values of energy E are obtained from spectroscopic data for the free atom and then extrapolated to the energy of the solid (which involves R_M). They set $A_1 = A_2$ for $l > 2$. Shaw (1968) modified this by using a model potential only for those values of l for which there is an ionic core state, and by allowing R_M to vary with l and with energy. The potential was then variationally optimized according to the prescription of Cohen and Heine (1961). The full non-locality and energy dependence of the potential were included at all stages.

Using the local HA potential, we have calculated the dispersion curves for Na, Al and Pb, at variable volume, for a number of dielectric functions. These are discussed and compared with experimental zero pressure dispersion curves and pressure derivatives of the elastic constants in § 3. Where possible we have also performed calculations with Shaw's potential and with the 'semi-nonlocal'† version of the HA potential calculated by Animalu (1966). This gives an estimate of the differences in the bare model potentials. Shaw and Pynn (1969) have investigated the effects of the non-locality of the potential, and of exchange and correlation corrections to the dielectric function, on calculated phonon frequencies in hexagonal close-packed Mg. Our calculations for these cubic metals therefore supplement theirs, although we have studied the dielectric function more extensively. We have also estimated the effective mass corrections (Shaw 1969 b) to the dispersion curves in Al.

In § 4 we have tested our calculated pressure derivatives of the maximum phonon frequencies by calculating the pressure derivatives of the superconducting transition temperatures of Al and Pb using Hodder's (1969) technique.

We conclude, in § 5, that, when screened by a suitable dielectric function, the local HA potential is quite reliable in predicting these properties of simple metals, while the Shaw potential is even better where we have used it at zero pressure.

2. Theory and calculation details

In the harmonic approximation, the phonon frequencies $\omega^2(\mathbf{q}, \mu)$ where \mathbf{q} is the phonon wave vector and μ the polarization index, are the eigenvalues of the dynamical matrix $\mathbf{D}_{\omega p}(\mathbf{q})$. Along the principal directions of a cubic crystal they are given simply by

$$\omega^2(\mathbf{q}, \mu) = \omega_c^2(\mathbf{q}, \mu) + \omega_R^2(\mathbf{q}, \mu) - \omega_E^2(\mathbf{q}, \mu).$$

The $\omega_c^2(\mathbf{q}, \mu)$ arise from the direct Coulomb interaction between the (point) ions, and are treated by Ewald's method (Sham 1965). The contribution from the exchange overlap between cores, $\omega_R^2(\mathbf{q}, \mu)$, is negligible in Na (Vosko 1964) and is expected to be small in Al and Pb also. It may be treated in the Born–Mayer approximation (Sham 1965) when necessary. The final term, $\omega_E^2(\mathbf{q}, \mu)$, arises from the screening of the ions' vibration by the conduction electrons and is given by (Vosko *et al.* 1965)

$$\omega_E^2(\mathbf{q}, \mu) = \omega_p^2 \sum_{\mathbf{H}} \frac{(\mathbf{q} + \mathbf{H})_\mu^2}{(\mathbf{q} + \mathbf{H})^2} F(|\mathbf{q} + \mathbf{H}|) - \omega_p^2 \sum_{\mathbf{H} \neq \mathbf{0}} \frac{H_\mu^2}{H^2} F(|\mathbf{H}|) \quad (1)$$

where the sums are over all reciprocal lattice vectors \mathbf{H} of the crystal lattice, and ω_p is the plasma frequency. The dependence upon the electron–ion potential is contained in this term.

† This includes some features of the non-local potential, but omits others; see Shaw (1969a).