

limits for large and small q . The form of the correction factor for the intermediate range of q is still uncertain. We study the effects of these different forms for the dielectric function on the phonon dispersion curves in § 3.

For Shaw's non-local potential, the expression for the energy-wavenumber characteristic is much more complex (Shaw 1969 a), but reduces to (2) in the local approximation. Values for his $F(q)$ for Na and Al, including dielectric screening via equations (3) and (7), (but excluding the factor $(1 + \alpha_{\text{eff}})$, as discussed above), have been tabulated by Shaw and Pynn (1969).

Band effective mass corrections are difficult to include (Shaw 1969 b) and have been neglected throughout for simplicity. Although they are likely to have a significant effect on the calculated phonon frequencies, they should not affect our conclusions concerning the different dielectric functions. In §3.1, we have estimated their effects for Al, using an approximate calculation of Shaw (1969 b).

In all calculations with the HA potential we have included the damping factor suggested by Animalu and Heine (1965) to decrease the oscillations for large q . This greatly improves the convergence of the sums over reciprocal lattice vectors in $\omega_{\mathbf{q}}^2$ and increases the Al phonon frequencies by less than 5%. For face-centred cubic lattices, summation over the 282 vectors with $|\mathbf{H}| \leq (40)^{1/2} 2\pi/a$, where a is the lattice constant, gave convergence of $\omega(\mathbf{q}, \mu)$ to 1 part in 10^3 , and for body-centred cubic lattices summation to $|\mathbf{H}| = (20)^{1/2} 2\pi/a$, 200 vectors, gave similar convergence.

3. Dispersion curves and elastic constants

For each of Na, Al and Pb we have calculated the phonon dispersion curves at compressions of zero and one per cent, using the forms of dielectric function based on equations (4) to (8) to screen the local HA model potential. In all calculations we have used the model potential parameters given by Animalu and Heine (1965) unless specifically stated otherwise, and have set the band effective mass equal to 1.00, as discussed above. Shaw's non-local optimized model potential, screened via (3) and (7), has also been used at zero pressure for Na and Al. As this potential has been developed from the HA method and is based on firmer theoretical foundations, we expect it to be the more reliable. The results discussed below bear this out.

As mentioned by Animalu and Heine (1965), the variation of the HA potential with volume depends mainly on the explicit volume factor in the bare potential and the variation of the dielectric function with k_F . The remainder of the bare potential $u_b(q)$ contributes only about 5% of the pressure derivatives of the phonon frequencies. However, the local potential is readily recalculated exactly at variable volume, so we have done that here. The volume dependence of the A_l parameters was found to have a negligible effect on the pressure derivatives of the phonon frequencies and so was omitted.

The elastic constants have been calculated directly from the initial slopes of the dispersion curves. In several calculations for compressions of up to 4% the pressure derivatives of the elastic constants varied by only small amounts with volume, so our values from 1% compression should be reliable. Both Stedman and Nilsson (1966) and Cowley *et al.* (1966) have noted that the initial slopes of their measured dispersion curves in Al and K respectively may differ by up to 5% from the sound velocities determined in ultrasonic experiments. These variations in the slope for very small frequencies affect only slightly the comparison of our results with experiment.

Relevant physical data and values of the different exchange-correlation parameters β for each metal are given in table 1. All are for a temperature of about 80°K.

3.1. Aluminium

As Al is of the greatest interest for our calculations of superconducting transition temperatures, and its phonon frequencies depend sensitively upon the potential used to calculate them, it has been studied in more detail and will therefore be considered first. In table 2 we compare, with each other and with experiment, the frequencies of phonons

at the zone boundaries calculated using the different bare potentials and dielectric functions. We denote the longitudinal branches by L and the transverse branches by T_1 and T_2 . The elastic constants and their pressure derivatives are treated similarly in table 3.

Table 1. Physical data and exchange-correlation parameters β at 80°K

	Unit	Na	Al	Pb
Volume of unit cell	a_0^3	254.5	110.7	203.4
Fermi wave number	a_0^{-1}	0.4882	0.9293	0.8351
Density	g cm^{-3}	1.01	2.73	11.50
Pressure to produce 1% compression	10^8 N m^{-2}	0.70 ^a	7.50 ^b	4.04 ^b
β_H (equation (5))	—	0.902	0.593	0.631
β_{AS} (equation (6))	—	0.454	0.475	0.473

a_0 is the Bohr radius (= 0.5292 Å). a, Beecroft and Swenson (1961); b, Munson and Barker (1966).

Table 2. Al phonon frequencies at the zone boundaries in units of $10^{13} \text{ rad s}^{-1}$

			100 L	100T	111L	111T
Experiment ^a			6.08	3.65	6.06	2.63
Calculations: potential	$f(q)$ (author and number of relevant equation in text)	β				
1. HA local	none	—	7.78	4.68	8.04	3.27
2. HA local	Hubbard (4)	Hubbard (5)	6.76	4.40	6.73	3.25
3. HA local	Hubbard (4)	Ashcroft and Shaw (6)	6.55	4.36	6.44	3.25
4. HA local	Shaw (7)	Ashcroft and Shaw (6)	6.37	4.29	6.26	3.25
5. HA local	Kleinman (8)	Ashcroft and Shaw (6)	6.13	4.11	6.01	3.20
6. HA local	Shaw (7)	Ashcroft and Shaw (6)	6.09	3.67	6.13	2.89
7. Shaw non-local A_1 adjusted	Shaw (7)	Ashcroft and Shaw (6)	6.32	4.00	6.40	2.82

a, Stedman and Nilsson (1966), at 80°K.

Table 3. Al elastic constants (in units of 10^{11} N m^{-2}) and pressure derivatives

	C_{11}	dC_{11}/dP	C_{44}	dC_{44}/dP	C'	dC'/dP
Experiment ^{a, b}	1.14	6.9	0.31	2.3	0.26	1.7
	1. 1.92	8.5	0.57	2.8	0.32	1.6
	2. 1.20	7.3	0.50	3.0	0.36	1.7
	3. 1.02	7.2	0.49	3.0	0.37	1.7
Calculations ^c	4. 1.02	7.3	0.47	3.0	0.38	1.8
	5. 0.98	7.3	0.42	3.0	0.39	1.8
	6. 0.86	6.5	0.39	2.5	0.27	1.3
	7. 1.06	—	0.43	—	0.25	—

a, Kamm and Alers (1964), Vallin *et al.* (1964), at 80°K; b, Ho and Ruoff (1969), at 77°K; c, see table 2 for potential, $f(q)$ and β used for each set.