

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<sub>1</sub> and T<sub>2</sub>. The elastic constants and their pressure derivatives are treated similarly in table 3.

Table 1. Physical data and exchange-correlation parameters  $\beta$  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 <sup>-3</sup>	1.01	2.73	11.50
Pressure to produce 1% compression	10 <sup>8</sup> N m <sup>-2</sup>	0.70 <sup>a</sup>	7.50 <sup>b</sup>	4.04 <sup>b</sup>
$\beta_H$ (equation (5))	—	0.902	0.593	0.631
$\beta_{AS}$ (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<sup>13</sup> rad s<sup>-1</sup>

Experiment <sup>a</sup>	Calculations:	potential	$f(q)$	$\beta$ (author and number of relevant equation in text)	100L	100T	111L	111T
					6.08	3.65	6.06	2.63
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	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<sup>11</sup> N m<sup>-2</sup>) and pressure derivatives

	$C_{11}$	$dC_{11}/dP$	$C_{44}$	$dC_{44}/dP$	$C'$	$dC'/dP$
Experiment <sup>a,b</sup>	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 <sup>c</sup>	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  $\beta$  used for each set.