Pressure dependence of phonon dispersion curves in simple metals

Table 6. Parameters for pressure dependence of transition temperatures

	Al		Pb		
	L	Т	L	Т	
$I_{\mu} (\text{mev}^2)$	120	27	14	6	
ω_1^{μ} (mev)	37	21.5	8.5	4.3	
α_{μ}^{2} (meV)	3.25	1.25	1.6	1.4	
λ_{μ}	0.175	0.116	0.38	0.65	
$d \ln I_{u}/dP (10^{-6} \text{ bar}^{-1})$	1.20	1.60	2.0	0.1	
$d \ln \omega_1^{\mu} / dP (10^{-6} \text{ bar}^{-1})$	2.9	2.75	5.0	4.0	
λ	0.41 ± 0.01		1.7 ± 0.1		
$d \ln T_{\rm c}/dP (10^{-6} {\rm bar}^{-1})$	-($-(20 \pm 3)$		$-(1 \pm 4)$	

More detailed calculations of λ by Pytte (1967) and Trofimenkoff *et al.* (1968) both yielded values of 0.46 for Al, while Trofimenkoff *et al.* obtained 1.69 for Pb. From tunnelling measurements, McMillan and Rowell (1965) and Franck *et al.* (1969) deduced values of 1.34 and 1.53 respectively for Pb. Values of α_{μ}^2 for Pb have been obtained by Carbotte and Dynes (1968) from calculations— $\alpha_{L}^2 = 1.6$ and $\alpha_{T}^2 = 1.2$ —and by Rowell *et al.* (1969) from experiment— $\alpha_{L}^2 = 1.6$ and $\alpha_{T}^2 = 1.5$. For Al, Carbotte and Dynes' calculations yield $\alpha_{L}^2 = 2.8$ and $\alpha_{T}^2 = 1.1$. Considering the approximations involved, our results agree adequately with all previous work.

The peaks in the phonon density of states correspond to maxima in the phonon dispersion curves, so we can immediately calculate d ln ω_1^{μ}/dP for the different branches. We have performed calculations for 1% compression of the metals and obtained pressure derivatives via the data in table 1. The average values, with likely errors for the local HA potential of $\pm 5\%$ for Al and 20% for Pb, are also included in table 6. The experimental values of Franck and Keeler (1967) for Pb are d ln $\omega_1^{L}/dP = 7.0 \pm 0.7$ and d ln $\omega_1^{T}/dP =$ 5.3 ± 0.7 in the same units. Our values agree poorly with these.

Taking d ln $\omega_c/dP = d \ln \omega_1^L/dP$, since $\omega_c \simeq \omega_1^L$, equation (9) then yields, for Al,

$$\frac{d \ln T_{\rm c}}{dP} = -(20 \pm 3) \times 10^{-6} \, {\rm bar}^{-1}$$

and for Pb,

$$\frac{d \ln T_c}{dP} = -(1 \pm 4) \times 10^{-6} \text{ bar}^{-1}$$

where the errors arise from estimates of the reliability, within the HA local approximation for the electron-ion model potential, of our results. In Al the d ln I_{μ}/dP contribute 30% of the final value, compared with 10% in Pb, while errors in each are dominated by the uncertainties in the d ln ω_1^{μ}/dP .

From the experimental data summarized by Smith and Chu (1967) we find d ln $T_c/dP = -22$ and -5.3×10^{-6} bar⁻¹ in Al and Pb respectively, with uncertainties of about 5%. Our result for Al therefore agrees quite well with experiment, and suggests that the pressure derivatives of the phonon frequencies near the zone boundary are also predicted satisfactorily by the local HA potential. For Pb, uncertainties in our calculated phonons are sufficiently great for our results not to be meaningful.

Hodder (1969) obtained d ln $T_c/dP = -5.0 \times 10^{-6} \text{ bar}^{-1}$ for Pb, by using the Scalapino et al. (1965) fit for $F(\omega)$, McMillan and Rowell's (1965) estimates of α_{μ}^2 , Harrison's (1966) point ion pseudopotential, and Franck and Keeler's (1969) measured d ln ω_1^{μ}/dP ; this is in very good agreement with experiment, but uncertainties and errors in these quantities amount to an uncertainty of about $\pm 30\%$ in the final result.

In another recent calculation of d ln T_c/dP , Trofimenkoff and Carbotte (1969) calculated