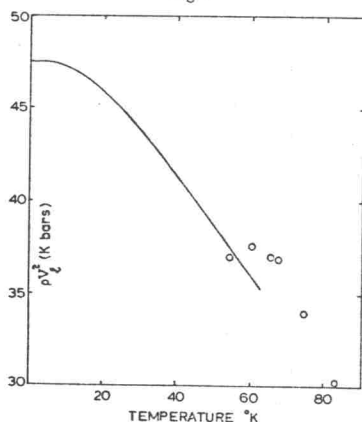


For an isotropic stress p , the constants S_{iso} are related to the more usual elastic constants c_{iso} by the equations (with the usual Voigt contractions):

$$c_{11} = S_{11}, \quad c_{12} = S_{12} + p, \quad c_{44} = S_{44}.$$

Full details of the calculation will be presented elsewhere (see also C. Feldman, Ph.D. Thesis, Rutgers University, 1967). From c_{11} , c_{12} and c_{44} the polycrystalline constants are then obtained by the method indicated in the previous section. Some results for argon are shown in figs. 1, 2 and 3 for the special case of a Mie-Lennard-Jones (12-6) nearest-neighbour model. The potential parameters of Horton and Leech (1963) which

Fig. 2



Temperature dependence of the polycrystalline longitudinal wave velocity plotted as ρV_L^2 versus temperature, where ρ is the crystal density. The circles are taken from Lawrence and Neale (1965). The smooth curve is calculated for a Mie-Lennard-Jones (12-6) nearest-neighbour model.

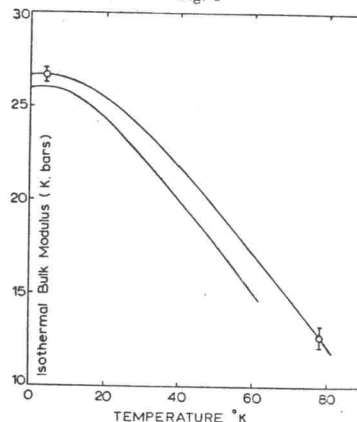
were fitted to the experimental latent heat and the 0°K molar volume were used. Our calculations were carried out at the observed experimental molar volumes, no attempt being made to solve the equation of state for the equilibrium molar volume of the model.

§ 4. COMPARISON WITH EXPERIMENT

Unfortunately our theoretical calculations are restricted to the range $0 < T \leq 60^\circ\text{K}$ but comparisons with experiment can still be made. Figure 1

shows a comparison of our model calculations with the data of Jones and Sparkes (1964). The theoretical curve, corresponding to $G = (G_V + G_R)/2$ is uncertain due to the averaging procedure (the difference between G_V and G_R is approximately 10%) but the temperature dependence is well defined (the difference between G_V and G_R is approximately temperature independent). Jones and Sparkes (1964) claimed a relative accuracy of 2%

Fig. 3



Temperature dependence of the isothermal bulk modulus for solid argon. The upper curve and the point at 4.25°K are taken from Peterson *et al.* (1966), the point at 77.7°K is taken from Urvas, *et al.* (1967). The lower curve is calculated for a Mie-Lennard-Jones (12-6) nearest-neighbour model.

and an absolute accuracy of about 4%, consequently there is considerable latitude for adjustment to the figure. Even so, the agreement of the model with the experimental temperature dependence is quite reasonable. Figure 2 compares the results of Lawrence and Neale (1965), plotted as ρV_L^2 versus temperature, with our (12-6) nearest-neighbour model. The agreement here is again quite reasonable. Figure 3 compares the isothermal bulk modulus of Simmons and his co-workers with our model calculations. At the highest temperatures there is beginning to be a significant difference between the theoretical and experimental temperature dependence. This discrepancy is probably due to the neglect of the higher order anharmonic terms in our model. In fact, the work of Wallace (1965) already indicates that these higher-order terms would tend to increase the bulk modulus.