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Phonon Dispersion in Lithium

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The phonon dispersion relations for lattice waves propagating along the three major symmetry directions of lithium are computed on the basis of the lattice dynamical model of Sharma and Joshi. The calculations are in reasonable agreement with the experimental results of Smith *et al.* obtained from slow-neutron scattering.

The study of lattice vibrations is of fundamental importance in the theory of metals. The past few years have seen the application of powerful new techniques, both theoretical and experimental, to the study of lattice dynamical properties of metals. Because of the complicated nature of the interatomic forces, it is still difficult to work out the lattice dynamics of crystals in an exact way. Thus for a calculation of the properties of solids, it is imperative to resort to various approximate lattice dynamical models—see, for instance, reviews by de Launay,[1] Cochran,[2] and Joshi and Rajagopal.[3] Because of the difficulties involved in developing a theory from first principles, in most of these studies the electronic term in the dynamical matrix is calculated from phenomenological considerations. Essentially, in all these previous studies, attempts have been made to include the effect of conduction electrons in the Born–von Kármán theory of lattice vibrations of solids. Sharma and Joshi[4] have proposed a semiphenomenological model for the lattice dynamics of cubic metals by considering a central interaction between the nearest and the next nearest ions, and an electron-ion interaction due to the presence of the electron gas. The model has been found to give a plausible explanation of the lattice dynamical behavior of a number of alkali,[5] noble,[6] and transition[7] metals.

Since lithium is, in principle, the simplest of all metals, a knowledge of its lattice dynamics is of importance to any theory of metals. Smith *et al.*[8] have recently reported the phonon dispersion curves for the lattice waves propagating along the symmetry directions in lithium at 98°K from their experiments on coherent inelastic neutron scattering. The theoretical phonon dispersion curves for lithium have been calculated by the method of pseudopotential.[9–11] However, in all these calculations the agreement with experiment for most branches is poor.

Krebs's[12] calculations on the basis of the screened Coulomb interaction between the ions embedded in a sea of Bloch electrons are also in poor agreement with the experimental results. In view of the success of the Sharma-Joshi model in cubic metals, it was thought worthwhile to reconsider the theoretical side of lattice vibrations in lithium on the basis of this model.

The phonon dispersion curves for lithium for the lattice waves propagating along the symmetry directions [ζ00], [$\zeta\zeta$0], and [$\zeta\zeta\zeta$] are computed from the dispersion relations for a bcc metal.[4] The calculated dispersion curves are shown in Fig. 1, where for comparison the experimental points of Smith *et al.* have also been plotted. The force constants have been estimated from the experimental values of the elastic

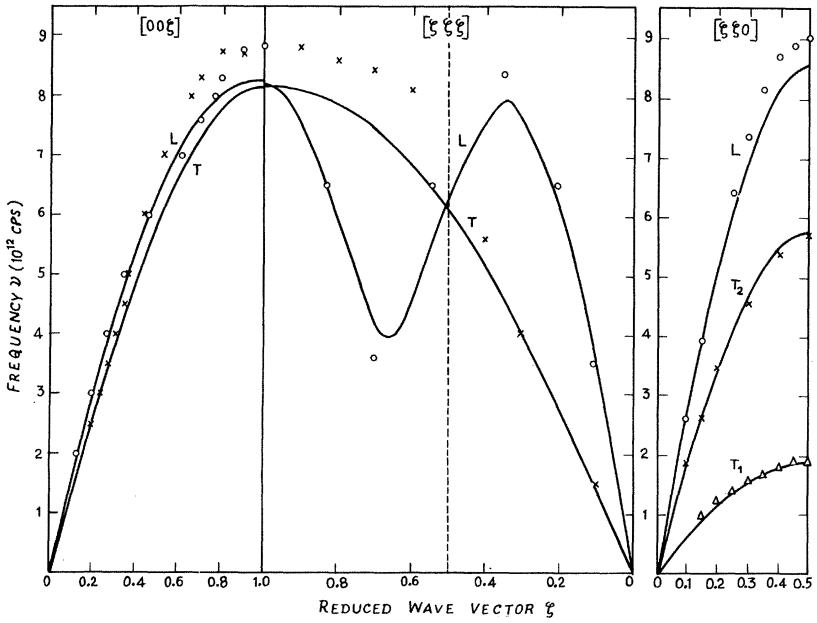

FIG. 1. Dispersion curves along the symmetry directions for lithium. The experimental points are due to the measurements of Smith *et al.*

constants at 78°K taken from the recent measurements of Slotwinski and Trivisonno.[13] The numerical values of these elastic constants and the other relevant parameters used in the calculations are

$$C_{11}=14.44\times10^{10}\text{ dyn cm}^{-2},$$

$$C_{12}=12.11\times10^{10}\text{ dyn cm}^{-2},$$

$$C_{44}=10.94\times10^{10}\text{ dyn cm}^{-2},$$

density $\rho=0.5454$ g cm^{-3} and lattice parameter $2a=3.4826$ Å.

The over-all agreement of the calculated phonon dispersion curves on the basis of Sharma and Joshi's electron gas model with the experimental data is quite satisfactory except for the fact that the model could not predict the crossing over of the longitudinal and transverse branches in the [ζ00] direction. The computed frequencies slightly violate the symmetry requirements at the zone boundary in the [ζ00] and [ζζζ] directions.

The discrepancy between theory and experiment may be attributed to the anisotropy of the Fermi surface of lithium and to the fact that the interatomic forces in lithium are of a fairly long-range nature.

The special feature of the Sharma-Joshi model in the present form is that while using only two force constants, it provides agreement between the theoretical dispersion curves and the experimental data which is much better than that obtained by other authors,[9–12] and is as good as that furnished by the curves computed by Smith *et al.* with the help of the six force constants.

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