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[1]J. C. Slater, Phys. Rev. 81, 385 (1951).
[2]W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
[3]R. Gaspar, Acta Phys. Acad. Sci. Hung. 3, 263 (1954).
[4]R. D. Cowan *et al.*, Phys. Rev. 144, 5 (1966).
[5]B. Y. Tong and L. J. Sham, Phys. Rev. 144, 1 (1966).
[6]R. Latter, Phys. Rev. 99, 510 (1955).
[7]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N.J., 1963).
[8]L. I. Schiff, *Quantum Mechanics*, 1st ed. (McGraw-Hill, New York, 1949), p. 271.
[9]D. A. Liberman, in Proceedings of the International Colloquium on the Properties of Solids Under Pressure at Grenoble, 1969 (unpublished). The solid-state calculations were done in the same way as the atomic calculations. Both core and valence-band electrons were treated self-consistently. The eigenvalues and eigenfunctions in the bands were obtained from a Green's-function band-structure program. Pressures from which the quoted bulk moduli were obtained were calculated from the flux of momentum of the electrons on the boundaries of the Wigner-Seitz cell. A cohesive energy was obtained by taking the difference of two total energies, one from a solid-state calculation for a Wigner-Seitz cell and the other for an isolated atom (e.g., for iron the total energies were, respectively, $-2518.326$ and $-2517.814$ Ry). It was possible to subtract these large numbers and obtain a significant result because the solid-state calculation was designed to be virtually the same as the atomic one.
[10]F. Seitz, Phys. Rev. 47, 400 (1935); W. Kohn and N. Rostoker, *ibid.* 94, 1111 (1954).
[11]E. Wigner, Phys. Rev. 46, 1002 (1934); Trans. Faraday Soc. 34, 678 (1938).
[12]M. Gell-Mann and K. A. Brueckner, Phys. Rev. 106, 364 (1957).

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# Pseudopotential and the Phonon Dispersion in Aluminum

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The phonon-dispersion curves, binding energy, and compressibility of aluminum have been calculated using the pseudopotential approach involving two adjustable parameters in the model pseudopotential. An exponential term of the type $e^{-\rho q}$ is introduced in the repulsive part of the pseudopotential so that it vanishes rapidly outside the ion core. The exchange and the correlation effects in the Hartree dielectric function have been adequately considered. Comparison with the experimental data shows good agreement.

The phonon-dispersion relations for metals have been calculated from basic principles by several workers.[1–3] Recently, a method based on a pseudopotential concept was developed by Sham.[2] Using a local as well as a nonlocal pseudopotential, calculations were made for sodium. Harrison[3] used it in a slightly different way, with one adjustable parameter to compute the dispersion relations for aluminum, sodium, and magnesium, with very little success. He therefore adopted a model pseudopotential containing two adjustable parameters, which resulted in limited success in the case of aluminum and lead. The same method has been used by Wallace[4,5] for the calculation of phonon frequencies in sodium, potassium, and lithium.

In the present paper, we report calculations on phonon-dispersion relations for aluminum using a modified form of the model pseudopotential. The bare (unscreened) pseudopotential of Harrison[6] has been modified by introducing an exponential term $e^{-\rho q}$. The new form now becomes

$$\omega_b(q) = \frac{1}{\Omega_0}\left(-\frac{4\pi Ze^2}{q^2} + \frac{\beta e^{-\rho q}}{(1+q^2\gamma_c^2)^2}\right), \tag{1}$$

where $\beta$, $\rho$, and $\gamma_c$ are the adjustable parameters. $\beta$ is the strength of repulsion, and $\rho$ and $\gamma_c$ are constants of the order of the Bohr radius. Taking into account the effect of screening, we obtain the relation for the energy wave-number characteristic

$$E(q) = -\frac{\Omega_0 q^2}{8\pi Ze^2}\,\omega_b^2(q)\,\frac{\epsilon(q)-1}{\epsilon(q)}\,. \tag{2}$$

The symbols in these expressions carry the same meaning as those given by Harrison.[6] It is evident from Eq. (1) that for large $q$, the pseudopotential $\omega_b(q)$ drops to zero as demanded by theory. This condition was not fulfilled by the basic $E(q)$ of Harrison[3] where it approached a constant $\beta$ for large values of $q$. The computation of the

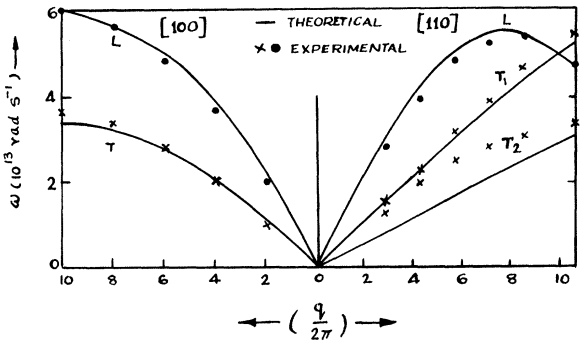


FIG. 1. Phonon dispersion in aluminum along the [100] and [110] directions, $q/2\pi$ is in units of $(1/10a)$.

phonon frequencies requires the knowledge of the numerical values of the parameters $\beta$, $\rho$, and $\gamma_c$. Since these are arbitrary parameters, we have taken $\rho = \gamma_c$ in our calculations. This amounts to having two parameters only in the pseudopotential. For the purposes of computation, we have selected two phonon frequencies from the experimental neutron-scattering results. Several numerical values for the parameters were tried until we were able to reproduce very nearly the two selected frequencies, as was done by Harrison.[6] It may be pointed out that the general nature of our $E(q)$ remains the same as reported by Harrison.[6]

The following values of the parameters were finally chosen to calculate the phonon frequencies: $\beta = 83.18$ Ry a.u.,[3] $\rho = \gamma_c = 0.305$ a.u. The results on aluminum are shown in Fig. 1, along with the experimental results of Yarnell, Warron, and Koenig.[7]

We have also calculated the binding energy and the compressibility of the metal, using the expressions given by Saxena *et al.*[8] with our own form of the pseudopotential and using the same values of the parameters mentioned above for the calculation of the phonon frequencies. For the purpose of comparison, we calculated these quantities with Harrison's model pseudopotential also. These are given in Table I along with the experimental values. Our binding-energy value is a distinct improvement over that of Harrison's and is in perfect agreement with the experiment. The percentage disagreement in the case of compressibility is the same for both the potentials, though in opposite directions.

Our new form of $E(q)$ is superior to the earlier ones in the sense that the electronic contribution to the dynamical matrix converges to a definite value by summing over about 60 reciprocal lattice points only. Harrison[6] had to sum over 500 points without really reaching a proper convergence. The inclusion of the exponential term, therefore, simplifies the calculations to a very great extent.

Our results are better than those of Harrison[3] with the basic $E(q)$ and also with the model $E(q)$.[6] The agreement between theory and experiment is found to be good except in the lower transverse branch of the [110] direction. Attempts have been made, with 4–6 adjustable parameters in the pseudopotential, to interpret phonon dispersion in metals[9] without much success. We expect this model potential to give consistently good results for other metals also.

TABLE I. Binding energy $E_b$(Ry/electron) and compressibility $(K/K_0)$ of aluminum.

| | Modified form of model pseudopotential | Harrison's form of model pseudopotential | Experimental value |
|---|---|---|---|
| Binding energy | 1.395 | 1.259 | 1.38 |
| Compressibility | 1.511 | 6.259 | 3.9 |

[1]T. Toya, J. Res. Inst. Catalysis, Hokkaido Univ. 9, 178 (1961).
[2]L. J. Sham, Proc. Roy. Soc. (London) A283, 33 (1965).
[3]W. A. Harrison, Phys. Rev. 136, A1107 (1964).
[4]D. C. Wallace, Phys. Rev. 176, 832 (1968).
[5]D. C. Wallace, Phys. Rev. 178, 900 (1969).
[6]W. A. Harrison, Phys. Rev. 139, A179 (1965).
[7]J. L. Yarnell, J. L. Warron, and S. M. Koenig, in *Lattice Dynamics*, edited by R. F. Wallis (Pergamon, New York, 1965), p. 57.
[8]V. K. Saxena, Q. S. Kapoor, and D. L. Bhattacharya, Phys. Status Solidi 34, 147 (1969).
[9]T. Schneider and E. Stoll, Phys. Kondensierten Materie 5, 331 (1966); 5, 364 (1966).