

netic field, to stray electric fields, and to radial magnetic fields in the trapping region can be made negligibly small.

We would like to thank Dr. L. M. Lederman for a stimulating communication.

* This work is supported by the U. S. Atomic Energy Commission.

¹L. Landau, *Nuclear Phys.* **3**, 127 (1957).

²T. D. Lee and C. N. Yang, Brookhaven National Laboratory Report BNL-443, 1957 (unpublished).

³G. Feinberg, *Phys. Rev.* **112**, 1637 (1958).

⁴E. E. Salpeter, *Phys. Rev.* **112**, 1642 (1958).

⁵R. M. Sternheimer, *Phys. Rev.* **113**, 828 (1959).

⁶Smith, Purcell, and Ramsey, *Phys. Rev.* **108**, 120 (1957).

⁷Berley, Garwin, Gidal, and Lederman, *Phys. Rev. Letters* **1**, 144 (1958).

⁸R. L. Garwin and L. M. Lederman, *Nuovo cimento* (to be published).

⁹Schupp, Pidd, and Crane, *Bull. Am. Phys. Soc. Ser. II*, **4**, 250 (1959); and to be published.

¹⁰G. W. Ford (unpublished).

¹¹These equations refer to expectation values of the various operators over a wave packet whose dimensions are small compared with the lengths in which the fields vary appreciably.

THEORY OF THE LATTICE VIBRATIONS OF GERMANIUM

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(Received May 15, 1959)

The relation between frequency ω and wave vector \vec{q} (the dispersion relation) for the normal modes of germanium has been investigated experimentally by Brockhouse and Iyengar¹ (see also Brockhouse²) and by Ghose, Palevsky, Hughes, Pelah, and Eisenhauer.³ The results do not agree with prior calculations made by Hsieh,⁴ on the assumption that only nearest neighbor atoms interact and using the Born-von Kármán theory of lattice dynamics. Nor is it sufficient to introduce second neighbor interaction¹; indeed Herman⁵ has shown that force constants between atoms out to at least fifth neighbors are required to account for the experimental results. The theory then involves numerous parameters which have no clear physical significance. Lax⁶ proposes to fit the data to a force model involving one parameter to represent electrostatic interaction between quadrupoles generated by the lattice vibrations, and as many near neighbor parameters as proves necessary.

We have extended the Born-von Kármán theory to apply to a model of the germanium crystal in which each atom is treated as a charged core coupled isotropically to an oppositely charged shell of negligible mass. This atom model has had some success in accounting for the dielectric properties^{7,8} and lattice dynamics⁹ of alkali halide crystals. Its use introduces two long-range forces, firstly the electrostatic interaction between dipoles formed by the relative displacement of cores and shells, and secondly a force

which originates from the massless character of the shells. The shell model therefore simulates two effects which must occur in practice, electrostatic interaction and relatively widespread redistribution of valence electron density when the nuclei are displaced. The condition that the crystal as a whole can have no dipole moment⁶ is automatically satisfied, so that the electrostatic interaction need not be treated as quadrupole-quadrupole.

In the Born-von Kármán theory the dispersion relation is determined by the condition for solubility of the equations

$$\sum_{k'y} [M_{xy}(kk') - \omega^2 m_k \delta_{kk'}] U_y(k') = 0, \quad (1)$$

where $\vec{U}(k) \exp[i\vec{q} \cdot \vec{r}(lk) - \omega t]$ is the displacement from $\vec{r}(lk)$ of the k th atom in the l th cell. We define $M_{xy}(kk')$ by writing

$$M_{xy}(kk') = B_{xy}(kk') + C_{xy}(kk'),$$

where $B_{xy}(kk')$ is related to the bonding force constant $\Phi_{xy}(lk, l'k')$ between atoms (lk) and $(l'k')$ by the equation

$$B_{xy}(kk') = -\sum_{l'} \Phi_{xy}(lk, l'k') \times \exp i\vec{q} \cdot [\vec{r}(l'k') - \vec{r}(lk)], \quad (2)$$

and $C_{xy}(kk')$ is related to the electrostatic interaction between charged atoms by a similar expression.¹⁰ For a diamond-type crystal with \vec{q} along

[100] or [111] the set of Eqs. (1) can be reduced to three separate sets, each of which determines the dispersion relation for a single mode, and which can be written

$$\sum_k [M(kk') - \omega^2 m_k \delta_{kk'}] U(k') = 0 \quad (3)$$

where in general M is a linear combination of M_{xx} , M_{xy} , etc. For the shell model $k=1\dots 4$, indices 1 and 2 referring to the two cores per unit cell, indices 3 and 4 to the corresponding shells, and we take $m_1=m_2=m$, $m_3=m_4=0$. The number of independent $\Phi_{xy}(kk')$ when only near-est neighbor units interact is six. It is convenient

to define new coefficients

$$R = B(12) + B(32) + B(14) + B(34),$$

$$T = B(32) + B(34),$$

$$S = B(32).$$

Each is a function of \vec{q} and of two parameters. We introduce the abbreviations $\rho = R/R_0$, $\tau = T/T_0$, and $\sigma = S/S_0$, where $(R)_{q=0} = -R_0$, and similarly for T_0 and S_0 . We also abbreviate $\beta = \alpha/v$, where α is the atomic polarizability and v the volume of the (trigonal) unit cell. The dispersion relation derived from the set of Eqs. (3) is then

$$\begin{vmatrix} A_0 - m\omega^2 & A \\ A^* & A_0 - m\omega^2 \end{vmatrix} = 0, \quad (4)$$

where

$$A_0 = R_0 + B_1 \left\{ \frac{-(1+B_2+\beta C_1)(1+|\tau|^2) + \tau(\beta C_2^* + B_2\sigma^*) + \tau^*(\beta C_2 + B_2\sigma)}{(1+B_2+\beta C_1)^2 - |\beta C_2 + B_2\sigma|^2} \right\}, \quad (5)$$

$$A = R + B_1 \left\{ \frac{-2\tau(1+B_2+\beta C_1) + (\beta C_2 + B_2\sigma) + \tau^2(\beta C_2^* + B_2\sigma^*)}{(1+B_2+\beta C_1)^2 - |\beta C_2 + B_2\sigma|^2} \right\}. \quad (6)$$

Here B_1 and B_2 are constants, while C_1 and C_2 are dimensionless functions of \vec{q} depending only on the geometry of the crystal structure. For example,

$$(C_1)_{xy} = -v \lim_{\vec{r} \rightarrow 0} \left[\sum_l' \frac{\partial^2}{\partial x \partial y} \left(\frac{1}{|\vec{r} - \vec{r}_l|} \right) \exp i\vec{q} \cdot \vec{r}_l \right],$$

where \vec{r}_l is a lattice translation. These functions were evaluated by the Ewald method, as developed by Kellerman.¹⁰ The fact that the elastic constants of germanium satisfy Born's¹¹ identity now appears as a reflection of the fact that there are bonding interactions only between nearest neighbor units (cores or shells), and that $\rho = \tau$. Conversely, the fact that the elastic constants of silicon and diamond do not satisfy the identity may merely indicate $\rho \neq \tau$, and not that there are other than first neighbor bonding interactions. Three of the seven parameters involved in the dispersion relation are determined by the elastic constants. On physical grounds we also set $\rho = \sigma$, thereby eliminating a fourth parameter and making $\Phi_{xy}(kk')/\Phi_{xx}(kk')$ the same for $kk' = 12, 14$, and 34 . The value of β deduced from the dielectric constant of germanium¹² is 0.100, leaving only two free parameters, the constants B_1 and B_2 . In fact, we also treated β as a disposable

parameter in fitting the data of Brockhouse and Iyengar, and obtained $\beta = 0.105$, in satisfactory agreement with the value given by the dielectric constant. With the following numerical values,

$$R_0 = 2.923 \times 10^5 \text{ dyne cm}^{-1},$$

$$B_1 = 4.099 \times 10^5 \text{ dyne cm}^{-1},$$

$$B_2 = 3.200,$$

$$\beta = 0.105,$$

and

$$\Phi_{xy}/\Phi_{xx} = 0.6905 \text{ (in all three instances)}$$

we obtained a good fit to the experimental data, as is shown in Table I and Fig. 1. The chief de-

Table I. The elastic constants.

| | C_{11} | C_{12} | C_{44} |
|------------------------------|----------|----------|----------|
| Calculated | 1.292 | 0.492 | 0.676 |
| Measured, ^a 300°K | 1.288 | 0.483 | 0.671 |
| Measured, ^b 0°K | 1.310 | 0.490 | 0.687 |

^aH. J. McSkimin, J. Appl. Phys. 24, 988 (1953).

^bM. E. Fine, J. Appl. Phys. 26, 862 (1955).

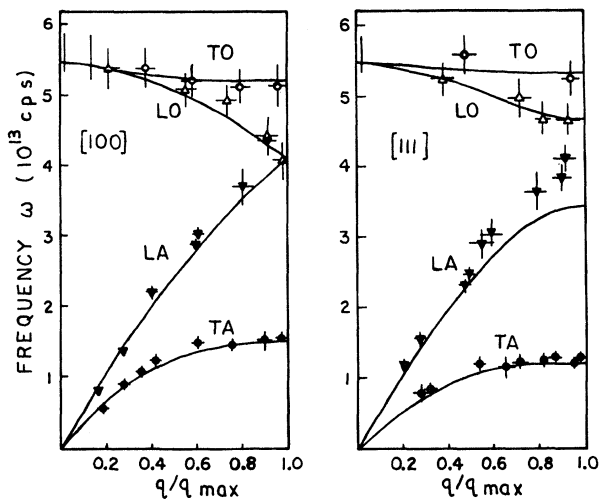


FIG. 1. A comparison of the theoretical dispersion curves with the experimental results of Brockhouse and Iyengar.

fect is that the calculated frequency of the LA mode is too low when \bar{q} is near the zone boundary in the [111] direction.

It is remarkable that such a simple model should fit the data as well as it does. Our procedure, however, finds theoretical backing in the work of Mashkevich and Tolpygo.¹³ Using the Hartree-Fock and adiabatic approximations, they have shown that the energy perturbation should be expressed as a quadratic function of the nuclear displacements and the atomic dipole moments. It

can be shown that the shell model represents the most general (and probably the simplest) way of accomplishing this.

I am greatly indebted to Dr. B. N. Brockhouse for many helpful discussions and suggestions.

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¹B. N. Brockhouse and P. K. Iyengar, *Phys. Rev.* **111**, 747 (1958).

²B. N. Brockhouse, *Phys. Rev. Letters* **2**, 256 (1959).

³Ghose, Palevsky, Hughes, Pelah, and Eisenhauer, *Phys. Rev.* **113**, 49 (1959).

⁴Y. C. Hsieh, *J. Chem. Phys.* **22**, 306 (1954).

⁵F. Herman, *J. Phys. Chem. Solids*, **8**, 405 (1959).

A similar calculation has been made by N. Pope (private communication).

⁶M. Lax, *Phys. Rev. Letters* **1**, 133 (1958).

⁷B. G. Dick and A. W. Overhauser, *Phys. Rev.* **112**, 90 (1958).

⁸J. E. Hanlon and A. W. Lawson, *Phys. Rev.* **113**, 472 (1959).

⁹Woods, Cochran, and Brockhouse, *Bull. Am. Phys. Soc. Ser. II*, **4**, 246 (1959).

¹⁰E. W. Kellerman, *Trans. Roy. Soc. (London)* **238**, 513 (1940).

¹¹M. Born, *Ann. Physik* **44**, 605 (1914).

¹²H. Y. Fan, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1955), Vol. 1, p. 281.

¹³V. S. Mashkevich and K. B. Tolpygo, *J. Exptl. Theoret. Phys. U.S.S.R.* **32**, 520 (1957) [translation: *Soviet Phys. JETP* **5**, 435 (1957)].

DETECTION OF COLLOIDAL CENTERS IN LITHIUM HYDRIDE BY ELECTRON RESONANCE

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(Received May 18, 1959)

This Letter reports electron resonance measurements on lithium hydride which has been irradiated with ultraviolet light and the results show that the lithium hydride contains colloidal centers of lithium metal, with diameters small compared with the microwave skin depth. The lithium hydride was irradiated for about fifteen minutes with 2537A radiation from a 250-watt mercury lamp and a fairly dark coloration was produced. These samples were then inserted in a 3-cm wavelength electron resonance spectrometer employing 100-kc/sec field modulation and phase-sensitive detection, and their electron

resonance spectra recorded. All the irradiated samples gave a single resonance line at $g=2.002 \pm 0.001$ with a half-width of 0.3 gauss—the latter being determined by the magnetic field inhomogeneity. In contrast to this, no signals at all were obtained from the unirradiated material.

This very narrow signal shows that the paramagnetic entity cannot be due to normal electron excess centers, which have wide inhomogeneously broadened lines.¹ It was therefore postulated that the absorption was in fact due to the conduction electrons in colloidal particles of lithium. In order to test this hypothesis a careful inves-