Letters to the Editor

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Normal Vibrations of Germanium by Neutron Spectrometry

B. N. BROCKHOUSE AND P. K. IYENGAR*

General Physics Branch, Atomic Energy of Canada Limited, Chalk River, Ontario, Canada

(Received September 9, 1957)

AS is now well known, energy distributions of neutrons scattered from a single crystal yield the frequency-wave number relation of the normal modes of the crystal.[1] The neutron groups observed satisfy the relations,

$$\mathbf{k}-\mathbf{k}'=2\pi\boldsymbol{\tau}-\mathbf{q}, \tag{1a}$$

$$E-E'=h\nu, \tag{1b}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the ingoing and outgoing neutron propagation vectors, E and E' are the ingoing and outgoing neutron energies, $\boldsymbol{\tau}$ is a reciprocal lattice vector, and ν and $\mathbf{q}$ are, respectively, the frequency and propagation vector of the normal mode with which the neutron interacted. Equations (1) enable ν and $\mathbf{q}$ for the phonons to be determined from the measured energy distributions.

We have made such measurements on a single crystal of germanium. The elastic constants of germanium[2] satisfy (to within $1\frac{1}{2}\%$) an identity due to Born[3] which is a necessary, though not sufficient, condition that only first-neighbor interactions are important. If only first-neighbor interactions exist in the crystal, then the entire vibration spectrum would be calculable from the elastic constants. Neutron spectrometry measurements done early this year showed deviations from the first-neighbor calculations of Hsieh[4] which seemed to indicate that the first-neighbor interaction model is probably not valid. In the meantime it was brought to our notice[5] that very detailed measurements of the long-wavelength infrared absorption in germanium by MacFarlane, McLean, Quarrington, and Roberts[6] indicated that the longitudinal and especially the transverse acoustic modes in the [111] direction at the zone boundary are markedly different from the values calculated by Hsieh. The interpretation of the infrared experiments also indicated the existence of excitons in germanium,[7] and gave important information about the structure of the electron energy bands. It therefore seemed important to check in detail the acoustic branches of the normal modes in the [111] directions.

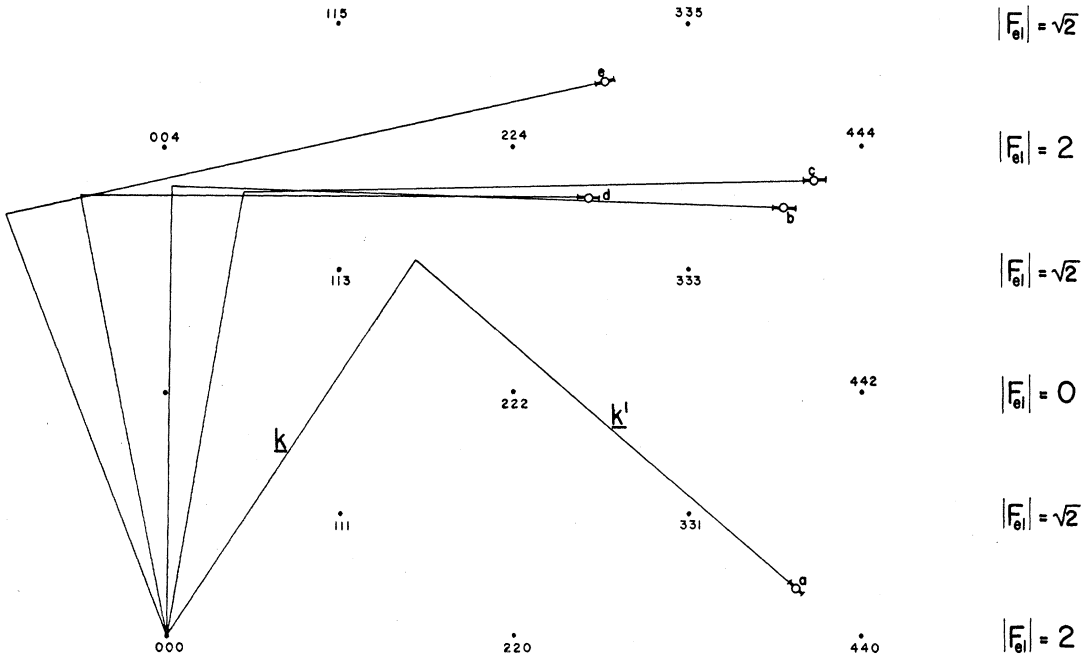

FIG. 1. Reciprocal lattice of germanium ($1\bar{1}0$ plane). Vector diagrams [Eq. 1(a)] for incoming neutrons of wavelength 1.525 A are shown. Open circles indicate positions of neutron groups with error bars indicating their full width at half-maximum. The structure factors for Bragg reflection (which also apply approximately to the acoustic modes) are indicated on the figure in units of the bound scattering amplitude.

In the experiments the monoenergetic incident neutrons were obtained from a crystal spectrometer and the energy distributions of the neutrons scattered at some particular angle (ϕ) were measured by means of another crystal spectrometer.[8] In the first instance the angle of scattering and the incoming wave vector $\mathbf{k}$ were arranged so that the direction of the outgoing wave vector $\mathbf{k}'$ passed close to a reciprocal lattice point and lay along a [111] direction with respect to that lattice point. Any neutron groups observed then represent phonons whose propagation vectors lie near [111] directions. Once an approximate $\nu(\mathbf{q})$ relation had been obtained it was improved by arranging conditions so that a desired phonon should appear. Then, utilizing the perhaps slightly different phonon which did appear, the $\nu(\mathbf{q})$ relation was improved. Conditions with respect to structure-factor, polarization, etc., were always arranged so that the intensity and resolution were especially favorable. Some of the results are shown in Fig. 1 on a reciprocal lattice diagram.

Neutron groups which represent $\mathbf{q}$'s within $\pm 5°$ of a [111] direction on the reciprocal lattice diagram were selected from the complete experimental results. The frequencies ν of the phonons corresponding to these neutron groups are plotted against their wave numbers $q/2\pi$ in Fig. 2. The first-neighbor calculations of Hsieh are shown as dashed lines. The experimental points for the transverse modes are seen to diverge widely from the calculated curve. The values of MacFarlane *et al.*, shown as crosses, are in good agreement with our measurements for both the longitudinal and transverse branches. This agreement must be taken to add substantially to the certainty of the above-mentioned deductions from the infrared measurements.

The results for other directions and branches will be published on completion of the work.

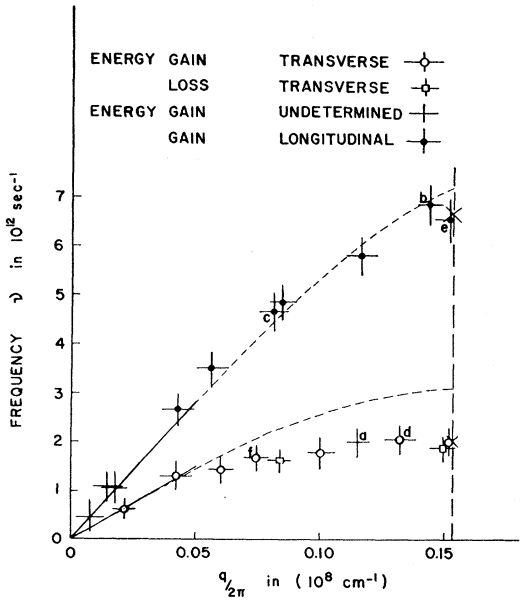

FIG. 2. The frequency (ν) plotted as a function of the wave number $q/2\pi$ for the acoustic modes in the [111] direction. The dashed curves show Hsieh's calculations using first-neighbors interactions only. The crosses at the zone boundary are the results of MacFarlane *et al.* The solid lines have the slope of the velocities of sound as determined by McSkimmin. The phonons shown in Fig. 1 are identified by lower case letters.

* On deputation from Atomic Energy Establishment, India.

[1] R. Weinstock, Phys Rev. **65**, 1 (1944); G. Placzek and L. Van Hove, Phys. Rev. **93**, 1207 (1954); B. N. Brockhouse and A. T. Stewart, Phys. Rev. **100**, 756 (1955) and Revs. Modern Phys. (to be published); Carter, Hughes, and Palevsky, Phys. Rev. **106**, 1168 (1957).

[2] H. J. McSkimmin, J. Appl. Phys. **24**, 988 (1953).

[3] See H. M. J. Smith, Trans. Roy. Soc. (London) **241**, 105 (1948).

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

[5] We wish to thank Dr. R. A. Smith for bringing these results to our attention and Dr. R. J. Elliott for some helpful discussions.

[6] MacFarlane, McLean, Quarrington, and Roberts, Phys. Rev. (to be published).

[7] R. J. Elliott, Phys. Rev. (to be published).

[8] For details see B. N. Brockhouse, Phys. Rev. **99**, 601 (1955); **106**, 859 (1957).

Dispersion of Elastic Waves in Sodium Chloride*

ANDREW GRANATO, JOHN DEKLERK, AND ROHN TRUELL

Metals Research Laboratory, Division of Applied Mathematics, Brown University, Providence, Rhode Island

(Received September 11, 1957)

IT is well known that dislocations decrease the apparent elastic moduli of crystalline materials because the motion of dislocations under an applied stress decreases the rigidity of the specimen. It has been predicted[1] that, at megacycle frequencies, the dislocation motion would be sufficiently damped so that the dislocations would no longer be able to follow in phase with the applied stress and that a dispersion would appear. This effect has been found in the case of NaCl. The problem under discussion arose in connection with the examination of nuclear irradiation effects in alkali halides where it has been found that the radiation effects depend strongly on previous deformation.

The apparatus necessary for the measurement of velocities to two parts in 10^4 is described elsewhere.[2] In these measurements, compressional waves were propagated along the [100] direction of an NaCl single crystal (obtained from Harshaw). The specimen was subsequently deformed in compression by 0.06% and remeasured. (The actual deformation may be slightly more since some pressure was applied in attaching the transducer.) The time of transit of the leading edge of the sound echoes is measured, and the velocities are computed from the measured thickness of the specimen. Before deformation, the velocities found at 20, 60, and 100 Mc/sec are 0.4763, 0.4771, and 0.4777 cm/μsec,