

From the Current Literature*DIRECT OBSERVATION OF OPTICAL VIBRATIONS OF A CRYSTAL LATTICE OF A SOLID BY MEANS OF NEUTRON SCATTERING*

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THE modern view<sup>1</sup> is that the vibrations of a crystal lattice can be represented in the form of a set of "normal vibrations," each corresponding to an elastic wave propagating in the direction of the wave vector  $\mathbf{k}$  (the absolute value of which is  $2\pi/\lambda$ , where  $\lambda$  is the wavelength) at a frequency  $\nu = \omega/2\pi$ . An important characteristic of any particular lattice is its vibration spectrum, or the dependence of  $\omega$  on  $k$ . This dependence, even in the case of the simplest crystals, is given by several curves of two distinct types, the so-called acoustic and optical modes. Physically, the difference between these two types is that in the former case the near atoms vibrate "in phase," like neighboring volume elements of a continuous elastic medium, while in optical oscillations the neighboring atoms vibrate "in anti-phase" and move "opposite" each other. The  $\omega(k)$  curves of the optical mode lie above the acoustic curves (i.e., they are characterized by a higher frequency). They differ also in that  $\omega$  depends less on  $k$ , that  $\omega$  is finite when  $k = 0$  (in the case of acoustic vibrations  $\omega = 0$  when  $k = 0$ ), and that  $\omega$  is not greatly influenced by the direction of  $\mathbf{k}$  in the crystal.

Experiments on scattering of slow neutrons offer a powerful means of investigating the vibration spectrum of solids. The theory of scattering of neutrons by crystals, developed in its day by I. Ya. Pomeranchuk<sup>2</sup> and Wiek,<sup>3</sup> has received further development in recent years<sup>4</sup> and has served as the basis for numerous experimental investigations.<sup>5</sup> In particular, these investigations have clearly confirmed the character predicted for the spectrum by the modern theory of lattice dynamics, namely the absence of a sharp discontinuity in the  $\omega(k)$  curve (the Debye theory of specific heat is known to call for such a discontinuity existed at certain values of  $\omega$  and  $k$ ), and the presence of a double maximum on the  $\omega(k)$  curve for certain lattices such as vanadium (in the acoustic mode). Two recent papers<sup>6,7</sup> report that by scattering of cold neutrons it is possible to observe directly, for the first time, optical lattice vibrations in two substances, single-crystal germanium and poly-

crystalline zirconium hydride. The same experimental procedure was reported in both papers. A broad neutron beam from a nuclear reactor was passed through a filter made of polycrystalline beryllium. Neutrons with a de Broglie wavelength less than 3.96 Å experienced Bragg reflection from the corresponding beryllium lattice planes and were scattered, while the slower neutrons passed through the filter without great attenuation. This produced intense beams of slow neutrons with little divergence and with an average energy of approximately 0.004 eV. This beam was incident on the investigated target. A mechanical selector with rotating slits was used to sort neutrons scattered at given angles by their time of flight. The selector used in these experiments had a sufficiently high resolving power to permit observation of sharp peaks in the energy distribution of the scattered neutrons.

It was found that the scattered neutrons have considerable energies (compared with the energies of the incident neutrons), amounting to hundredths and tenths of an electron volt. This indicates that the scattered neutron acquires some energy from the vibrating lattice (the experiments were performed at room temperature and at higher temperatures). In the case of zirconium hydride, for example, this leads<sup>6</sup> to a continuous energy distribution (Fig. 1) with a broad maximum near 0.25 eV. This corresponds to energy transferred to the neutrons by lattice vibrations of the acoustic type. However, as can be seen from an examination of Fig. 1, a sharp peak is clearly pronounced against the background of this distribution near 0.134 eV

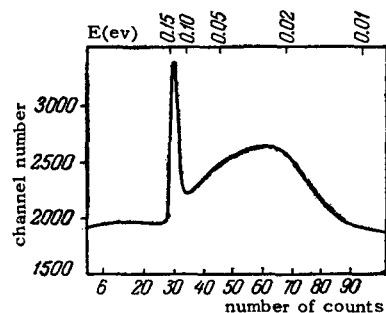


FIG. 1

( $\pm 0.015$  eV). This peak corresponds to optical lattice vibrations with energy 0.130 eV. A similar energy peak, corresponding to optical vibrations, is observed<sup>6</sup> also in neutron scattering by a single crystal of germanium. True, the optical peak is accompanied in this case by several other peaks, corresponding to coherent scattering of neutrons by acoustic vibrations. This optical peak can nevertheless be readily separated. It is located at a higher energy (0.038 eV). Furthermore, the energy of this peak (unlike those of other peaks) remains constant as the germanium crystal orientation is varied in the instrument. Since the scattered neutrons interact at various orientations with lattice vibrations corresponding to different values of  $k$ , the fact that the peak energy is independent of the orientation indicates that the energy and frequency of the corresponding lattice vibration are independent of  $k$ , which is precisely the characteristic feature of optical vibrations.

In the case of zirconium hydride, it was possible to investigate the observed optical vibrations in greater detail.<sup>7</sup> It can be assumed that in this case we deal with vibrations of the hydrogen atom in an isotropic potential well of parabolic shape. If this is so, there should exist a whole series of optical levels with energies  $E_n = nh\nu$  (where  $n = 1, 2, 3, \dots$ ). Indeed, the raising of the temperature of a zirconium-hydride target to 393°C resulted in a weaker (and more diffused) peak,  $E_2 \approx 2h\nu$ , in the spectrum of the scattered neutrons along with the above-mentioned principal peak ( $E_1 = h\nu$ ). It has been found that the population of the first optical level (a measure of which is obviously the intensity of the principal peak in the spectrum of the scattered neutrons) varies with temperature in

accordance with the Boltzmann law  $\exp(-E_1/kT)$ , with  $E_1 = -0.130 \pm 0.005$  eV. This value coincides with the directly-determined value of the energy of the optical vibrations.<sup>6</sup>

A recent report<sup>8</sup> states that scattering of slow neutrons has made it possible to determine directly, for the first time, the energy spectrum of elementary excitations in liquid helium II. The reviewed papers demonstrate the new opportunities which this progressive method offers to researchers in the field of solid state physics.

<sup>1</sup>See, for example, M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Russ. Transl.) IL, Moscow, 1958 (Oxford, 1954).

<sup>2</sup>I. Ia. Pomeranchuk, Phys. Z. Sowjetunion **13**, 65 (1938).

<sup>3</sup>G. C. Wick, Physik. Z. **38**, 403, 689 (1937).

<sup>4</sup>G. Placzek and L. van Hove, Phys. Rev. **93**, 1207 (1954) et al.

<sup>5</sup>B. N. Brockhouse, Trans. Roy. Soc. Can. III, 49 (1955), paper 118. B. Jacrot, Compt. rend. **240**, 745 (1955). Carter, Hughes, and Palevsky, Phys. Rev. **104**, 271 (1956). B. N. Brookhouse and A. T. Stewart, Revs. Modern Phys. **30**, 236 (1958). A. T. Stewart and B. N. Brookhouse, Revs. Modern Phys. **30**, 250 (1958). Eisenhouer, Pelah, Hughes, and Palevsky, Phys. Rev. **109**, 1046 (1958), et al.

<sup>6</sup>Pelah, Eisenhouer, Hughes, and Palevsky, Phys. Rev. **108**, 1091 (1957).

<sup>7</sup>Anderson, McReynolds, Nelkin, Rosenbluth, and Whittimore, Phys. Rev. **108**, 1092 (1957).

<sup>8</sup>See Usp. Fiz. Nauk **65**, 545 (1958).

Translated by J. G. Adashko