absorption derivatives observed were often quite asymmetrical and the tabulated shifts refer to the intersection of base line with the most strongly sloping segment of the recorder trace. θ is calculated by fitting $\Delta H = C/(T+\theta)$ to shifts in P^{31} resonance at 195°K and 77°K. These values of θ are usually not very different from those obtained using shifts at 298°K and 77°K.

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Detection of Optical Lattice Vibrations in Ge and ZrH by Scattering of Cold Neutrons*

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LATTICE vibrations in solids can be studied by measuring the energy distribution of scattered slow neutrons that have exchanged energy with the lattice vibrations. In experiments now under way at the Brookhaven reactor, an incident cold neutron beam is produced by filtering thermal neutrons in Be, and the velocity of the scattered neutrons is measured by the slow chopper, time-of-flight method. The filtered beam, which contains only the low-energy end of the Maxwellian distribution, has a sharp cutoff at 0.005 ev, and an effective energy of 0.004 ev. The cold neutron flux at the position of the scatterer is a factor of 25 greater than used previously;[1] this increase results from the use of a large beam port, with a full angular divergence of 9°, constructed in the top shield of the BNL reactor.[2] The resolution has been improved by using a chopper with much narrower slits, with a resolution of 3 μsec/m. The present equipment is well adapted to detecting sharp neutron peaks in the spectrum of scattered neutrons in the 0.1-ev range, and it has now been successfully used to measure optical modes of vibration in Ge and ZrH.

The spectrum of neutrons inelastically scattered from crystalline materials is markedly different for coherent and incoherent nuclear scattering. In most elements, including germanium, the nuclear scattering is mainly co-

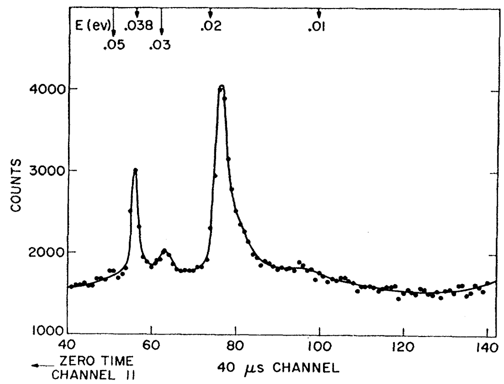

FIG. 1. Spectrum of neutrons inelastically scattered by a single crystal of Ge; the peak at 0.038 ev results from gain of energy from an optical lattice vibration.

herent, and the scattered neutrons must satisfy a coherence condition as well as energy conservation. In this case discrete energy peaks are observed in any given scattering direction. In hydrogen and vanadium, however, the nuclear scattering is incoherent and only energy conservation must be satisfied. The spectrum of neutrons inelastically scattered by acoustic vibrations is then continuous and is directly related to the lattice vibration spectrum of the scatterer.[3]

Among the peaks observed in the scattered neutron spectrum from a single crystal of germanium[4] is one at the relatively high neutron energy of 0.038 ev. The neutron peak is shown at channel 56 in Fig. 1. Subtraction of the incident energy yields an energy of 0.034 ev for these vibrations. Whereas the energies of the other peaks, corresponding to acoustic vibrations, vary with different orientations of the crystal, the energy of this peak remains constant to within $\pm 5\%$. Since a difference in orientation causes interaction with lattice vibrations of different wave numbers, the small energy variation reveals the presence of lattice vibrations with energy relatively independent of wave number. This behavior, as well as the high energy

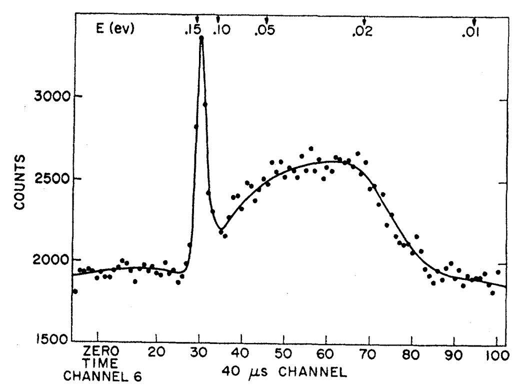

FIG. 2. Spectrum of neutrons inelastically scattered by polycrystalline ZrH; the peak at 0.134 ev corresponds to an optical lattice vibration.

relative to acoustic vibrations, shows that the peak is associated with an optical mode of vibration, in which the atoms of a unit cell vibrate "against" each other, relatively independently of other atoms.

Since the scattering from zirconium hydride is primarily the result of the hydrogen, the inelastically scattered neutrons that have gained energy from acoustic vibrations form a continuous spectrum typical of incoherent scattering. In this case, a gain of energy from an optical vibration can be easily identified if present, for only an optical mode can produce a sharp peak. Such a peak is observed with a sample of polycrystalline ZrH at 0.134 ev (Fig. 2) with an energy of ±0.015 ev, of which ±0.005 results from resolution and incident energy spread. The corresponding energy of the lattice vibration is $E=0.130$ ev. It is interesting to note that this transition, which is so prominent in the present measurements, does not appear in infrared absorption measurements. Further discussion of the ZrH results is contained in the accompanying Letter by Andresen, McReynolds, Nelkin, Rosenbluth, and Whittemore.

Thus the cold neutron energy gain technique appears to be a useful method of detecting optical lattice vibrations up to energies of about 0.25 ev, this limit being set by the characteristics of the present chopper. Experiments with other materials are planned to investigate the value of these measurements to solid state investigations.

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† On leave from Weizmann Institute, Rehovoth, Israel and the Israel Atomic Energy Commission.

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[4] We wish to thank H. P. R. Frederikse of the National Bureau of Standards and S. M. Christian of RCA laboratories for supplying single crystals of Ge for this measurement. A detailed analysis of the Ge data in cooperation with F. Herman of RCA is now under way.

Neutron Investigation of Optical Vibration Levels in Zirconium Hydride*

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We have investigated certain properties of zirconium hydride by studying the spectrum of neutrons scattered elastically and inelastically from polycrystalline samples. A consideration of the zirconium hydride lattice shows that its thermal vibration spectrum should include in addition to the usual band

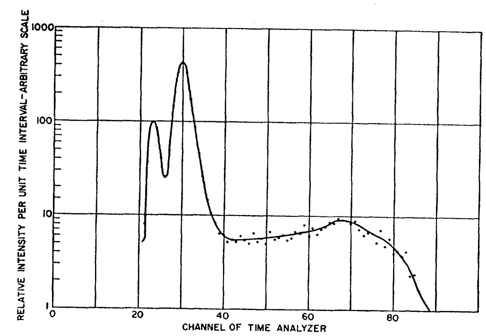

Fig. 1. Distribution of flight time for neutrons scattered by $ZrH_{1.5}$. Channel number 6 is zero time, each channel is 40 μsec, and flight path is 487 cm.

of acoustical frequencies also a sharp "optical" frequency, ν, corresponding approximately to vibrations of the individual hydrogen atoms in an isotropic harmonic well. This implies a set of optical energy levels for the lattice, $E_n=nh\nu$. Peaks corresponding to transitions between these optical energy levels are seen in Fig. 1, which shows the spectrum of neutrons scattered at 90° from zirconium hydride. The average incident energy was 0.004 ev. Measurements were made in collaboration with Pelah, Eisenhauer, Hughes, and Palevsky on the Brookhaven Laboratory slow chopper, which they described in the preceding Letter. The $ZrH_{1.5}$ sample for Fig. 1 was heated to 393°C to make evident the second level (Channel No. 23), as well as the first level (Channel No. 30). Still higher levels should exist but the equipment discriminates so severely against neutrons of these higher energies that the levels do not appear.

By transforming the coordinate from time of flight to energy, we obtain Fig. 2. From this figure, we can see the shape of the optical levels and their location as well as the acoustical Debye cutoff which occurs at about 0.02 ev. For comparison, we have shown the results obtained at $T=24$°C and 393°C. At 393°C the width of the first level at half its maximum value is about 0.037 ev. The Doppler broadening of the level due to simultaneous acoustical and optical transitions has been estimated to be 0.031 ev, a value about three

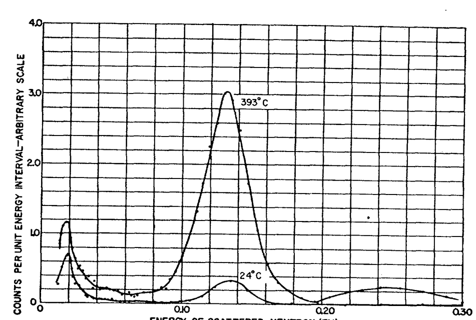

Fig. 2. Energy distribution of neutrons scattered by $ZrH_{1.5}$ at 90° angle. The average incident neutron energy is 0.004 ev.