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Neutron Scattering Investigation of Impurity Phonon Modes in Ge(9.2% Si)†

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The frequencies of the local modes in a Ge single crystal containing 9.2 at.% Si have been measured. A $\vec{Q}$ dependence of the local-mode frequencies has been observed, contrary to the prediction of the isolated mass-defect theory. The theory of Elliott and Taylor gives values for the local-mode frequencies that are in good agreement with the present results. The changes of the in-band mode frequencies of the longitudinal branch along the [001] direction were also measured and the results were in reasonable agreement with the theory.

The frequencies of the local modes and of some in-band modes in a Ge single crystal containing 9.2 at.% Si have been measured by coherent inelastic neutron scattering. The experiments were performed using a triple-axis spectrometer at the HFIR. The sample crystal[1] is a 25-mm-long cylinder having a loaf-shape cross section with maximum and minimum diameters of 15 and 10 mm, respectively. The lattice constant determined from the neutron Bragg reflections is 5.630 Å, which is in good agreement with the result of Dismukes *et al.*[2] Constant-$\vec{Q}$ measurements were made with the scattered neutron energy E' fixed usually at a value corresponding to a frequency of 6.0 THz, although in order to check certain results some measurements were carried out with an E' of 7.0 THz. All of the measurements described here were obtained with the neutron momentum transfer $\hbar\vec{Q}$ along the [001] direction. The scattered neutron groups that were obtained in measurements of the local-mode frequency for two different points in the reciprocal space are shown in Fig. 1.

The similarity of the phonon dispersion curves for Ge[3] and Si[4] suggests that a theory of the lattice dynamics of this alloy which includes only the mass change might be a good approximation. The theory for an isolated mass defect[5] gives a unique value of 11.25 THz for the local-mode frequency ν_l, which is independent of $\vec{Q}$. However, Fig. 1 clearly shows a substantial difference in the local-mode peak positions for two different values of $\vec{Q}$, and the frequencies measured are larger than those given by the isolated mass-defect theory.

Several recent theoretical treatments of the mass-defect problem attempt to take into account the effects of a finite impurity concentration.[6-8] In the present paper we shall compare our results with the theory of Elliott and Taylor.[6] Although this theory is considered to be inadequate in many respects,[7,8] the computations required in making a comparison with experiment are more easily carried out and it does provide a surprisingly good description of the present results.

In this theory, the local-mode frequency is determined by the equation

$$\epsilon\nu_l^2\int \frac{g(\nu)}{\nu_l^2-\nu^2}\,d\nu=\left(1-\frac{c\epsilon\nu_l^2}{\nu_l^2-\nu_j^2(\vec{q})}\right)\frac{1}{1-c}\,, \quad (1)$$

where c is the impurity concentration, $\nu_j(\vec{q})$ is the in-band mode frequency of the unperturbed lattice with wave vector $\vec{q}$ and branch index j, $g(\nu)$ is the frequency distribution function, and $\epsilon=1-(M_i/M_h)$, where M_i is the impurity mass and M_h is the host mass. Since in the present work the measurements

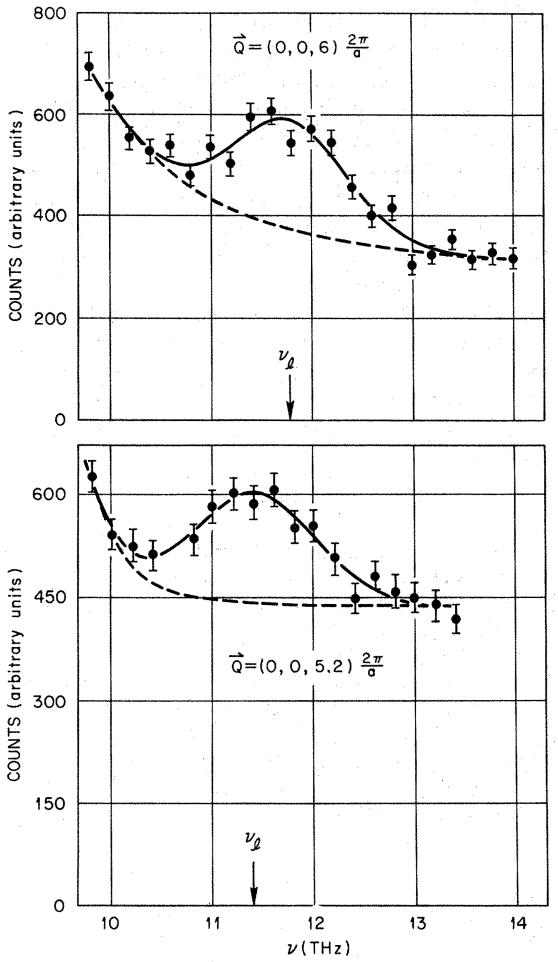

FIG. 1. Neutron groups obtained in constant-$\vec{Q}$ measurements of the local-mode frequencies. The solid lines represent computer fits to the experimental points.

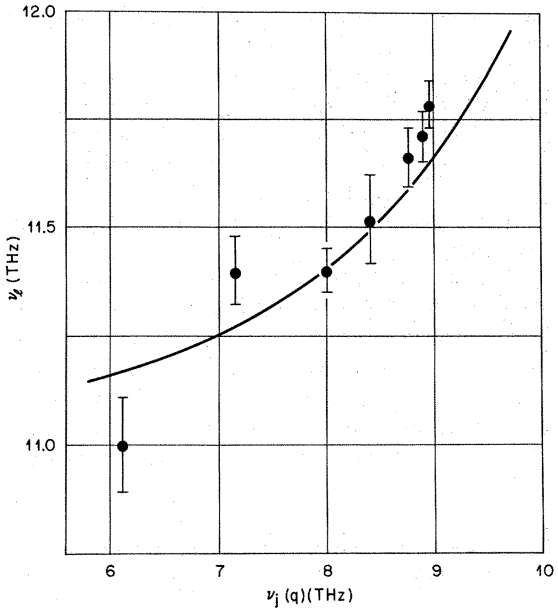

FIG. 2. The local-mode frequencies plotted against the corresponding in-band mode frequencies. The solid line represents the relation given by Eq. (1).

were performed with a purely longitudinal configuration ($\vec{Q} \parallel \vec{q}$), the observed ν_l's correspond to $\nu_j(\vec{q})$ of the longitudinal acoustic and optic modes along the [001] direction. In this direction the longitudinal acoustic and optic branches are degenerate at the Brillouin zone boundary owing to the crystal symmetry, and the structure factors for these branches vary from zero to finite values in alternate zones, so that in each zone only one of the branches can be observed. Thus one observes experimentally one continuous branch with a periodicity twice as large as that of the usual Brillouin zone. Identical structure factor considerations apply for the local-mode scattering as well. Therefore for each Q at which measurements were made, the local-mode frequency corresponding only to the $\nu_j(\vec{q})$ branch having a finite structure factor will be observed.

The local-mode frequencies were measured for $\vec{Q}=(0, 0, Q)$ with $Q=6.0$, 5.8, 5.6, 5.4, 5.2, 5.0, and 4.8 (in units of $2\pi/a$). In Fig. 2, the measured local-mode frequencies are plotted against the corresponding in-band mode frequencies $\nu_j(\vec{q})$. The solid line represents a calculation based on the relation given by Eq. (1) with $g(\nu)$ for pure Ge. The good agreement between the measured and calculated values for ν_l seems to support some of the approximations made by Elliott and Taylor.[6] Additional measurements for $\vec{Q}=(2, 2, 6)$, (4, 4, 2), and (2, 2, 2), all of which correspond to $\vec{q}=0$, were consistent with $\nu_l = 11.78 \pm 0.06$ THz, which was obtained for $\vec{Q}=(0, 0, 6)$. This value is in very good agreement with 11.81 THz deduced from the results of

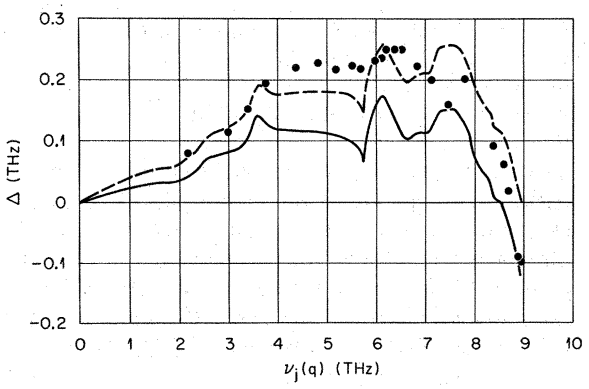

FIG. 3. The changes of the band mode frequencies of the longitudinal branch along the [001] direction compared with theoretical predictions. The dotted curve includes a correction for the lattice contraction.

the Raman scattering experiment performed by Feldmann *et al.*[9]

The changes of the in-band mode frequencies of the longitudinal branch along the [001] direction were also measured and the results are shown in Fig. 3 together with the theoretical prediction (solid line). As the addition of 9.2% Si to Ge decreases the lattice constant by about 0.5%, the in-band mode frequencies should be expected to have a relative increase which is given approximately by $\gamma(\Delta V/V)$, where γ is the Grüneisen constant for the longitudinal branch and $(\Delta V/V)$ is the relative change of the crystal volume. Using $\gamma = 1$, an average value of the Grüneisen parameter as calculated by Dolling and Cowley,[10] the increase in the frequency due to the lattice contraction was estimated and added to that calculated from the mass-defect theory. The resultant change is shown by the dotted line in the same figure. The over-all variation of the change as a function of the corresponding in-band mode frequency is qualitatively in good agreement with the experimental results, though the theory predicts a finer structure than that observed. This discrepancy may be due to the effects of the finite concentration that are not included in the theory. A change in the force constants may also have significant effects on the in-band mode frequencies. In order to examine this point further, an experiment on a Ge crystal with 5% Si will be performed in the near future.

We are grateful to G. Dolling for supplying the $g(\nu)$ for pure Ge.

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†Research sponsored by the U. S. Atomic Energy Commission under contract with Union Carbide Corporation.

[1]The crystal was kindly loaned by E. F. Hockings of RCA Laboratories to whom we are very grateful.

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PHYSICAL REVIEW B VOLUME 4, NUMBER 8 15 OCTOBER 1971

Transverse Negative Resistance in *n*-Type Germanium

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(Received 15 March 1971)

For *n*-type germanium the mobility in the [001] direction in the presence of a strong electric field in the [110] direction has been calculated using a detailed model of the material including higher ⟨100⟩ minima. The method of calculation is a Monte Carlo approach capable of giving differential quantities. At room temperature no instability is found, while at 77 °K an instability is obtained if the scattering rate between ⟨111⟩ and ⟨100⟩ minima is sufficiently strong.

I. INTRODUCTION

It was first noted by Erlbach[1] that in *n*-type germanium a negative resistance might exist in a direction transverse to a strong electric field. The origin of this effect will be discussed in Sec. II. Erlbach found that this effect could be present in germanium only in a uniaxially stressed material. Shyam and Kroemer[2] measured a transverse polarization in *n*-type germanium at room temperature and interpreted this as an indication of the presence of the Erlbach effect. They explained this as a consequence of a strong repopulation induced by higher ⟨100⟩ valleys.

A calculation of the resistance in the [001] direction in the presence of a strong electric field in the [110] direction is presented in this paper. The model of the material includes the effect of the ⟨100⟩ valleys and is similar to the one used by Paige[3] in a study of the bulk negative conductivity in this material. This model was later used by the author[4] to calculate the anisotropy of the high-field conductivity with the Monte Carlo method. In Sec. III this method is generalized to give the differential conductivity. The numerical results are presented in Sec. IV. At room temperature no instability is found, while at 77 °K the transverse resistance can be negative if the intervalley scattering rate be-