enhanced either by shining light or external injection. However, hot-electron experiments using these techniques are not yet reported. The conditions at room temperature may thus be considered marginal for a successful experiment as suggested in this paper.

At 77 °K, on the other hand, the collision frequency is increased about ten times. The condition $\omega\tau \gg 1$ may be satisfied by choosing the signal frequency one order lower. The wavelength for the signal is then required to be smaller than 370 μ. Since the Faraday rotation increases as λ^2, we find

that the rotation angle is increased by a factor of 10^2. Hence, experimental requirements will be more easily satisfied at 77 °K and the suggested experiment should be considered feasible at this temperature. It is also at this temperature that BNDC has been obtained in germanium, and the results of the experiment would be of particular interest.

*Present address: Department of Electronics and Telecommunication Engineering, Jadavpur University, Calcutta-32, India.

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Phonon Dispersion Relations in Ge at 80 °K

G. Nilsson and G. Nelin
AB *Atomenergi, Studsvik, Nyöping, Sweden*
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Phonon dispersion relations in Ge have been measured at 80 °K for all principal symmetry directions and on some lines at the boundary of the Brillouin zone. The measurements were performed by neutron inelastic scattering using a three-axis crystal spectrometer. In order to achieve maximum accuracy, care was taken to reduce resolution widths as far as possible. In general, the estimated uncertainties of the measured phonon frequencies range from 0.3% to 0.5% for optical and from 0.3% to 1% for acoustic phonons. Frequencies of 238 phonons are tabulated and phonon linewidths are given for the symmetry directions.

INTRODUCTION

Ge is an obvious material for phonon spectrometry with neutrons since it is a good representative for the covalent bond and diamond structure and is available in excellent large crystals with quite good coherent neutron scattering properties. Moreover, its technical importance lends it a special interest, particularly as regards thermodynamic properties

related to the phonon frequency distribution. In fact, it was among the first substances to be studied in the early days of neutron measurements. In 1958 Brockhouse and Iyengar[1] published phonon dispersion curves for the [100] and [110] directions obtained by crystal spectrometry, and in 1959 Ghose et al.[2] presented time-of-flight measurements for the [100] and [110] directions. The development of the neutron method now allows us to

achieve considerably greater accuracy and com-
pleteness. The present paper presents phonon
frequencies at 80 °K for all branches along most
of the symmetry lines in Ge, with an accuracy usu-
ally better than 0. 5%, as well as phonon widths.
The fact that the measurements are at 80 °K, while
the Debye temperature is about 360 °K and the
Grüneisen constant is as low as 0.4, should mean
that anharmonic effects on the mean phonon fre-
quencies are negligible.

The early measurements on Ge stimulated a con-
siderable amount of theoretical and experimental
work on the lattice dynamics of crystals possessing
the diamond structure. Phonon dispersion curves
have been determined experimentally in diamond,
Si and α-Sn. Dolling[3] reported Si dispersion rela-
tions whose qualitative features are in near agree-
ment with those obtained in the present experiment
on Ge and with those found by Price and Rowe for
α-Sn,[4] but the measurements on diamond by Warren
$et\ al.$,[5] reveal a large difference between the lattice
dynamics of this crystal and the other three. In
order to fit the experimental results of Brockhouse
and Iyengar, Herman[6] showed that a Born-von Kár-
mán model must include at least sixth-nearest-
neighbor interactions, and that the physical signifi-
cance of many of the 20 parameters of this model
is doubtful. Cochran[7] applied the shell model to
Ge (Dick and Overhauser[8]), and improved versions
of this have successfully described phonon disper-
sion relations in both diamond structures and alkali
halides. One of the purposes of our measurements
on Ge was to perform a detailed test of the accuracy
of these models, even off the symmetry directions.
This will be reported in a separate paper.

EXPERIMENT

The experiment was carried out at the 30-MW
research reactor in Studsvik. Our instrument, a
three-axis crystal spectrometer has been described
elsewhere.[9] In order to keep the reflectivity of
the analyzer crystal and the efficiency of the BF_3
counter constant, the setting of the analyzer was
kept fixed during the scan of a phonon resonance.
All phonons were measured with neutron energy loss
and using constant-κ programs.[10]

Much attention was paid to focusing and resolu-
tion.[11] The optimum conditions for a measurement
were obtained by consulting a computer (a PDP-8/I).
The associated wave vector, expected energy, and
energy surface gradient of the phonon to be mea-
sured were fed into the computer. For every re-
ciprocal lattice vector and collimator set chosen,
the following quantities were tabulated as functions
of the outgoing neutron wave vector: the monochro-
mator and analyzer reflections and beam path for
best focusing, the spectrometer angles, and the reso-
lution in energy and momentum space. The calcu-

lated resolutions also included their individual con-
tributions from different collimators and mosaic
widths. With this information it was easy to choose
the most favorable alternatives.

The monochromator used Cu (420) and (220) re-
flections, and the analyzer Cu (220) and (111).
Their mosaic widths were 0. 004 rad. The horizon-
tal collimation was before the sample usually 0. 0065
rad and after 0. 0033, 0. 0065, 0. 013, or 0. 019 rad.
Our instrumental energy resolution, measured by
the full width at half-maximum,[11] was in no case
larger than about 0. 20 THz and for acoustic phonons
always better than about 0. 10 THz. The radius
vector of the resolution ellipsoid in momentum space
was never longer than 0. 03 and often shorter than
0. 02 in units of $2\pi/l$, where l is the lattice constant.
The mosaic width of the sample is less than 0. 001
rad.

Phonon peaks often exhibit marked skewness due
to curvature of the dispersion in the region covered
by a measurement. The effect is especially pro-
nounced in the vicinity of reciprocal lattice points,
where the equienergy surfaces are strongly curved.
We almost entirely avoided this by minimizing mo-
mentum resolution widths.

No shifts in the phonon curves were observed for
different cells in reciprocal space or different scat-
tering planes. For example, we measured the Ra-
man frequency Γ'_{25} four times using different re-
ciprocal lattice vectors and scattering planes and
got the frequencies 9. 11, 9. 12, 9. 12, and 9. 13 THz
with the estimated statistical error 0. 02 THz. Fig-
ure 1 shows four examples of measured phonon reso-
nances.

RESULTS

Phonon-dispersion relations in Ge at 80 °K have
been measured for all branches in the principal
symmetry directions $\Delta = [100]$, $\Sigma = [110]$, and Λ
$= [111]$ and for most of the branches along the lines
U-W-K-L-W-X-U-L at the surface of the Brillouin
zone. Our data are presented in Fig. 2 and Table I.
Notations used for classification of points and di-
rections in reciprocal space are those introduced
by Boukaert $et\ al.$[12] and shown in Fig. 3 and of dif-
ferent branches those defined in Refs. 13–15.
The errors listed in Table I are based on considera-
tions of counting statistics only; systematic errors
are considered to be of no significance.

The branches of the dispersion curves are labeled
by the notations of the irreducible representations
of the symmetry group of the phonon wave vector.
The nature of polarization of a branch is given by
the transformation properties of the associated ir-
reducible representation. For example, the modes
Δ_1, Δ'_2, and Λ_1, are purely longitudinal; Δ_5, Λ_3,
Σ_2, and Σ_4 are purely transverse; and Σ_1 and Σ_3 non-
linearly polarized. For further information on this
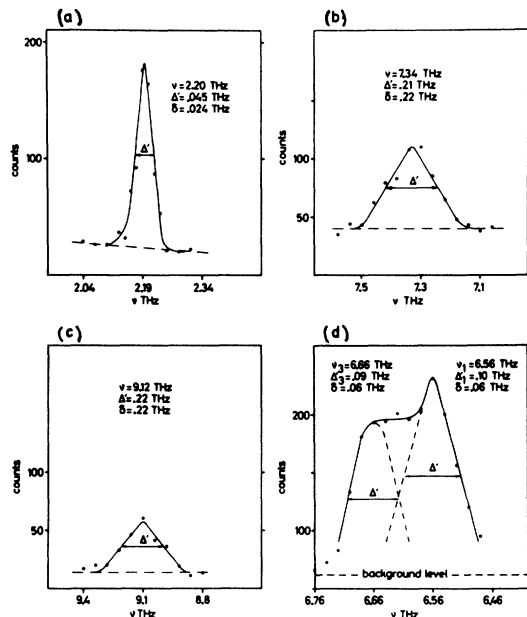subject we refer to Warren.[15] For the assignment

FIG. 1. Four examples of scanned resonances in order of increasing difficulty of measurement. Δ' is the observed width and δ the calculated energy resolution width (Ref. 11). (a) $\Delta_5(A)$ (0.5, 0, 0), (b)L_1, (c) Γ'_{25}, (d) $\Sigma_1(A)$ and $\Sigma_3(O)$ (1.0, 0.2, 0.2).

of the labels L_1 and L'_2 we have used the result of Johnson and Loudon.[14] No notations have been found in the literature for the branches on the lines L-U

$(L$-$K)$ and U-W $(K$-$W)$.

The full phonon linewidths at half-maximum together with their estimated errors are shown in Fig. 4 for the principal symmetry directions. The extraction of widths was performed in accordance with a method described by Stedman and Weymouth.[16]

DISCUSSION

In Fig. 2 the heavy lines indicate the slopes of the respective branches when approaching Γ_{15}, as calculated from the elastic constants of McSkimin.[17] These agree with our data within the accuracy of the two experiments. Our value of the lattice constant $(l = 5.651$ Å$)$ at 80 °K is a mean value of those given in Refs. 17–19.

The first neutron measurements on Ge were performed at room temperature. Many of these frequencies are higher than ours, contrary to expectations. There are, however, also other differences. Brockhouse and Iyengar,[1] who observed phonons on the Δ and Λ directions, did not resolve the optical modes Δ_5 and Δ'_2 and reported phonon curves where the transverse branch lies consistently above the longitudinal one. The results of the time-of-flight studies by Ghose et al.[2] in the Δ and Σ directions show little similarity with our data. In 1963 Brockhouse and Dasannacharya[20] published measurements of nine phonons at 100 °K and 700 °K, and these frequencies, in closer agreement with ours, are consistently lower. Brockhouse[21] mentioned observation of a phonon peak of 8.5 THz at $K = U$ and at room
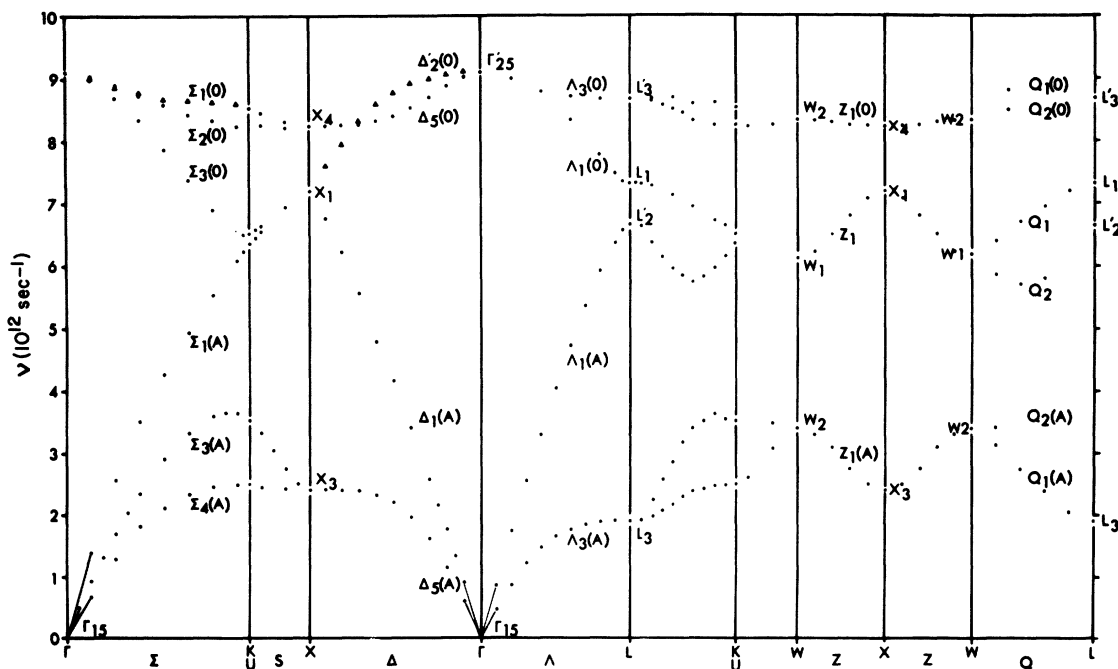

FIG. 2. Measured phonon-dispersion relations in Ge at 80 °K.

temperature, which was believed to be "an extreme-
ly close double." The present results show this to
be so. The $\Sigma_1(A)$ and $\Sigma_2(O)$ modes possess a simi-
lar polarization and inelastic structure factor in the
vicinity of $K = U$, where they come closer together
but have not been found to cross. The closest posi-
tioned phonons we could resolve were those at (1.0,
0.2, 0.2) shown in Fig. 1(d). Neither Dolling[3] nor
Price and Rowe[4] resolved the modes around $K = U$
in Si and α-Sn, respectively, but their shell-model
calculations show a behavior similar to our result
in the vicinity of this point.

    The lifetime of a phonon is a function of anhar-

monic effects and equal to the inverse of the half-
width of the phonon resonance expressed in angular
frequency ω. The anharmonicity of Ge is very
small, as evidenced, for example, by the low value
of its Grüneisen constant, which is about 0.4 at
80 °K.[22] Brockhouse and Dasannacharya[20] detected
no broadening of phonons even at 700 °K, in com-
parison with their peaks at 100 °K and did not try
to extract the intrinsic linewidths. The errors in
Fig. 4 reflect the difficulty in measuring the widths.
The limits of error are based on the statistical
uncertainties of recorded peaks and background,[16]
and also include a 10% uncertainty in the resolution

TABLE I. Measured phonon frequencies in Ge at 80 °K expressed in units of 10^{12} sec^{-1}.

A.

$(l/2\pi)\ (q_x,\ q_y,\ q_z)$	$\Delta_5(A)$	Δ_1	$\Delta_5(O)$	Δ_2'
0.00 0 0	$\cdots$	$\cdots$	9.12 ± 0.02	9.13 ± 0.02
0.10 0 0	0.60 ± 0.01	0.91 ± 0.01	9.05 ± 0.02	9.14 ± 0.02
0.15 0 0	$\cdots$	1.34 ± 0.02	$\cdots$	$\cdots$
0.20 0 0	1.15 ± 0.01	1.77 ± 0.02	8.91 ± 0.02	9.09 ± 0.02
0.25 0 0	$\cdots$	2.16 ± 0.02	$\cdots$	$\cdots$
0.30 0 0	1.62 ± 0.01	2.59 ± 0.02	8.73 ± 0.01	9.02 ± 0.03
0.40 0 0	1.96 ± 0.01	3.42 ± 0.01	8.56 ± 0.01	8.95 ± 0.03
0.50 0 0	2.20 ± 0.01	4.17 ± 0.01	8.42 ± 0.01	8.80 ± 0.02
0.60 0 0	2.32 ± 0.01	4.90 ± 0.01	8.35 ± 0.02	8.62 ± 0.02
0.70 0 0	2.39 ± 0.01	5.57 ± 0.01	8.29 ± 0.01	8.34 ± 0.03
0.80 0 0	2.40 ± 0.01	6.23 ± 0.01	8.28 ± 0.02	7.97 ± 0.02
0.90 0 0	2.41 ± 0.01	6.77 ± 0.01	8.27 ± 0.02	7.63 ± 0.02
1.00 0 0	2.40 ± 0.01	7.21 ± 0.01	8.26 ± 0.02	$\cdots$

B.

$(l/2\pi)\ (q_x,\ q_y,\ q_z)$	$\Lambda_3(A)$	$\Lambda_1(A)$	$\Lambda_3(O)$	$\Lambda_1(O)$
0.00 0.00 0.00	$\cdots$	$\cdots$	$\cdots$	9.12 ± 0.03
0.05 0.05 0.05	0.47 ± 0.01	0.86 ± 0.01	$\cdots$	$\cdots$
0.10 0.10 0.10	0.86 ± 0.02	1.74 ± 0.01	9.02 ± 0.02	9.03 ± 0.03
0.15 0.15 0.15	1.22 ± 0.01	2.56 ± 0.01	$\cdots$	$\cdots$
0.20 0.20 0.20	1.47 ± 0.01	3.30 ± 0.01	8.82 ± 0.02	8.81 ± 0.02
0.25 0.25 0.25	1.65 ± 0.01	4.05 ± 0.01	$\cdots$	$\cdots$
0.30 0.30 0.30	1.76 ± 0.01	4.73 ± 0.02	8.75 ± 0.03	8.36 ± 0.02
0.35 0.35 0.35	1.84 ± 0.01	5.37 ± 0.01	$\cdots$	$\cdots$
0.40 0.40 0.40	1.88 ± 0.02	5.93 ± 0.02	8.70 ± 0.03	7.80 ± 0.02
0.45 0.45 0.45	1.90 ± 0.02	6.37 ± 0.03	$\cdots$	7.50 ± 0.02
0.475 0.475 0.475	$\cdots$	6.57 ± 0.02	$\cdots$	7.36 ± 0.02
0.50 0.50 0.50	1.90 ± 0.02	6.66 ± 0.02	8.70 ± 0.03	7.34 ± 0.02

C.

$(l/2\pi)\ (q_x,\ q_y,\ q_z)$	K-L 1	K-L 2	K-L 3	K-L 4	K-L 5	K-L 6
0.750 0.750 0.00	$\cdots$	3.53 ± 0.03	6.37 ± 0.03	6.52 ± 0.04	8.27 ± 0.03	8.56 ± 0.03
0.725 0.725 0.05	2.48 ± 0.02	3.56 ± 0.02	6.17 ± 0.02	6.66 ± 0.01	$\cdots$	$\cdots$
0.700 0.700 0.10	2.47 ± 0.02	3.64 ± 0.02	5.98 ± 0.03	6.74 ± 0.02	8.28 ± 0.04	8.64 ± 0.03
0.675 0.675 0.15	2.42 ± 0.02	3.53 ± 0.02	5.84 ± 0.04	$\cdots$	$\cdots$	$\cdots$
0.650 0.650 0.20	2.38 ± 0.02	3.41 ± 0.01	5.76 ± 0.05	6.96 ± 0.02	8.35 ± 0.04	8.62 ± 0.04
0.625 0.625 0.25	2.29 ± 0.02	3.18 ± 0.03	5.86 ± 0.02	$\cdots$	8.54 ± 0.02	$\cdots$
0.600 0.600 0.30	2.16 ± 0.02	2.86 ± 0.04	5.97 ± 0.02	7.14 ± 0.03	8.54 ± 0.03	8.72 ± 0.04
0.575 0.575 0.35	2.06 ± 0.02	2.58 ± 0.04	6.15 ± 0.03	$\cdots$	8.60 ± 0.04	$\cdots$
0.550 0.550 0.40	1.97 ± 0.02	2.24 ± 0.02	6.38 ± 0.02	7.29 ± 0.02	8.67 ± 0.03	8.71 ± 0.03
0.525 0.525 0.45	1.91 ± 0.02	$\cdots$	6.64 ± 0.04	7.32 ± 0.02	$\cdots$	$\cdots$
0.5125 0.5125 0.475	$\cdots$	$\cdots$	$\cdots$	7.34 ± 0.02	$\cdots$	$\cdots$
0.500 0.500 0.50	1.89 ± 0.02	$\cdots$	$\cdots$	$\cdots$	8.70 ± 0.04	8.72 ± 0.03

TABLE I. (continued)

D.

$(l/2\pi)$ (q_x, q_y, q_z)	Σ_4	$\Sigma_3(A)$	$\Sigma_1(A)$	$\Sigma_3(O)$	$\Sigma_1(O)$	Σ_2
0.00 0.00 0.00	...	...	...	...	...	9.11±0.02
0.05 0.05 0.00	...	0.49±0.01	...	...	...	...
0.10 0.10 0.00	0.67±0.01	0.93±0.01	1.39±0.01	9.01±0.03	9.03±0.02	9.05±0.02
0.15 0.15 0.00	...	1.32±0.01	...	...	...	...
0.20 0.20 0.00	1.29±0.01	1.70±0.01	2.58±0.02	8.72±0.04	8.89±0.02	8.92±0.02
0.25 0.25 0.00	...	2.04±0.01	...	...	...	...
0.30 0.30 0.00	1.82±0.01	2.35±0.01	3.53±0.02	8.37±0.03	8.80±0.03	8.76±0.02
0.40 0.40 0.00	2.11±0.01	2.92±0.01	4.28±0.03	7.89±0.03	8.69±0.03	8.61±0.02
0.50 0.50 0.00	2.34±0.01	3.34±0.01	4.95±0.03	7.40±0.02	8.68±0.03	8.45±0.03
0.60 0.60 0.00	2.46±0.01	3.61±0.02	5.55±0.01	6.91±0.02	8.65±0.03	8.36±0.03
0.65 0.65 0.00	...	3.66±0.05	...	...	...	...
0.70 0.70 0.00	2.49±0.01	3.66±0.05	6.10±0.02	6.58±0.02	8.63±0.03	8.26±0.04
0.725 0.725 0.00	...	...	6.24±0.02	6.51±0.04	...	...
0.75 0.75 0.00	2.50±0.03	3.54±0.02	6.37±0.03	6.53±0.02	8.55±0.05	...
1.00 0.225 0.225	...	...	6.46±0.04	6.60±0.04	...	...
1.00 0.20 0.20	2.45±0.02	3.34±0.02	6.56±0.01	6.66±0.02	8.47±0.04	8.28±0.04
1.00 0.15 0.15	...	3.06±0.01	...	...	...	...
1.00 0.10 0.10	2.43±0.01	2.76±0.02	6.96±0.02	...	8.34±0.04	8.24±0.05
1.00 0.05 0.05	...	2.51±0.01	...	...	...	...
1.00 0.00 0.00	2.41±0.02	2.40±0.02	...	...	8.29±0.04	8.27±0.05

E.

$(l/2\pi)$ (q_x, q_y, q_z)	$Z_1(A)$	Z_1	$Z_1(O)$
1 0.0 0	2.40±0.02	7.21±0.01	8.26±0.02
1 0.1 0	2.50±0.04	7.10±0.02	8.27±0.03
1 0.2 0	2.76±0.05	6.82±0.02	8.28±0.03
1 0.3 0	3.10±0.04	6.52±0.02	8.33±0.02
1 0.4 0	3.31±0.04	6.24±0.04	8.35±0.02
1 0.5 0	3.41±0.04	6.20±0.05	8.36±0.03

F.

$(l/2\pi)$ (q_x, q_y, q_z)	$K\text{-}W\,1$	$K\text{-}W\,2$	$K\text{-}W\,5$
0.8 0.7 0.0	2.61±0.04	...	8.25±0.02
0.9 0.6 0.0	3.08±0.03	3.49±0.04	8.28±0.03

G.

$(l/2\pi)$ (q_x, q_y, q_z)	$Q_1(A)$	$Q_2(A)$	Q_1	Q_2	$Q_1(O)$	$Q_2(O)$
0.60 0.50 0.40	2.04±0.03	...	7.21±0.03	...	...	...
0.70 0.50 0.30	2.38±0.03	...	6.96±0.03	5.81±0.04	...	...
0.80 0.50 0.20	2.75±0.04	...	6.72±0.04	5.72±0.04	8.52±0.04	8.38±0.04
0.90 0.50 0.10	3.14±0.04	3.43±0.04	6.41±0.04	5.87±0.04	...	...

width. It is assumed that the natural phonon line is approximately Lorentzian in shape, and the errors are standard deviations. The width of the ob-
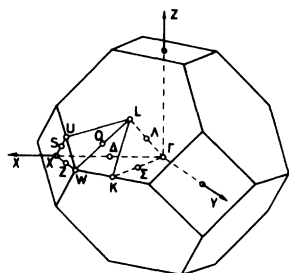

FIG. 3. Conventional notations of points and lines in the first Brillouin zone.

served peak was in most cases close to the resolution width, and the phonon widths in Ge at 80 °K are generally lower than 0.1 THz.

Parker et al.[23] observed first-order Raman scattering in Ge at room temperature and reported Γ'_{25} to have a frequency (9.01±0.02) THz and a full width of 0.16 THz, while we have found (9.02±0.02) THz at the same temperature and an extracted phonon width of (0.07±0.07) THz at both 80 °K and 300 °K. Cowley[24] used a method of Maradudin and Fine[25] to calculate the frequency shift of Γ'_{25} between the two temperatures mentioned and arrived at − 0.11 THz, while we observed − (0.10±0.03) THz. Using another theoretical approach, Klemens[26] ob-
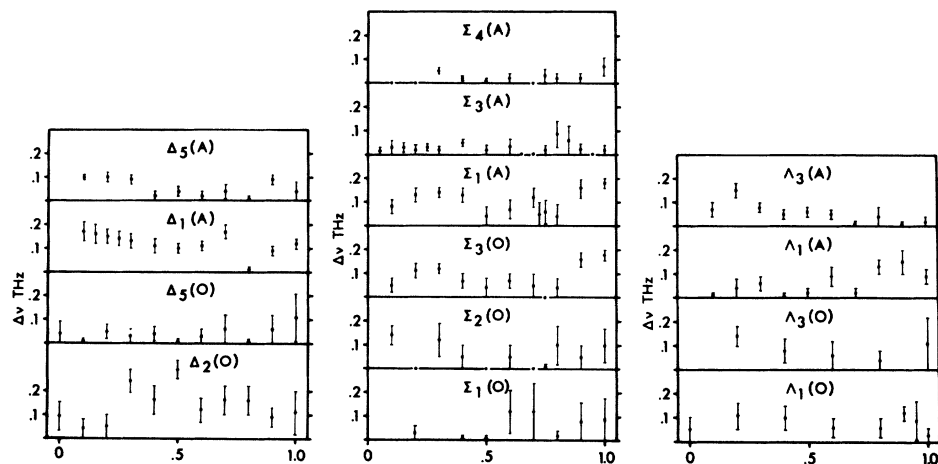
FIG. 4.   Full phonon linewidths for the symmetry directions as calculated from the present data in Ge at 80°K.

tained the phonon linewidth 0. 13 THz at 300 °K, where Cowley got 0. 50 THz. There is in the literature some confusion concerning the relation between lifetime and phonon width, which makes comparisons uncertain. The correct relationship[25] between lifetime τ, inverted lifetime Γ, phonon width in frequency $\Delta\nu$ and in angular frequency $\Delta\omega$ is $\tau^{-1} = \Gamma = \frac{1}{2}\Delta\omega = \pi \times \Delta\nu$, where Δ indicates the full width at half-maximum and the phonon energy $E = \hbar\omega = h\nu$. In many cases the (invalid) relation $\Gamma = \frac{1}{2}\Delta\nu$ is used.

Comparisons between neutron scattering and infrared absorption data on phonon frequencies are relatively common. Such comparisons are, however, of marginal value when only multiphonon processes are involved in the infrared absorption. The large number of closely positioned resonances affects their shapes and positions; to be able to make a correct assignment of the peaks one must

have a good knowledge of the phonon dispersion curves in advance, which for the present can only be obtained by means of neutron spectrometry. This subject will be analyzed later, when we are able to use more complete results.

Our measurements have been extended to other reciprocal lattice points within the irreducible $\frac{1}{48}$ part of the first Brillouin zone. Future papers will deal with the phonon frequency distribution and the thermodynamics of Ge together with anharmonic effects and with a theoretical interpretation of the data.

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