Crystal Dynamics of Metallic β-Sn at 110°K*

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The frequency/wave-vector phonon dispersion relation for all of the symmetry branches and some of the nonsymmetry branches with wave vectors along the [0,0,ζ], [1,0,ζ], [ζ,0,0], and [ζ,ζ,0] (Λ,*V*,Σ, and Δ) directions have been studied at 110°K using inelastic neutron scattering. In addition, selected portions of the [η,0,ζ] branches ($\eta=0.1$, 0.2, 0.3 *in units of* $2\pi/c$) which are parallel to the Λ and *V* directions have been studied. The experimentally determined dispersion relation shows much detailed structure, with several sharp kinks. This structure precludes a description of the crystal dynamics of β-Sn in terms of a Born–von Kármán model with forces extending to a limited number of shells of neighboring atoms. Although the structure in the dispersion relation is probably due to the strong electron-phonon interaction in β-Sn, straightforward analysis in terms of Kohn anomalies is impossible because of the complex Fermi surface of β-Sn. This suggests that the crystal dynamics of β-Sn can only be explained by a detailed calculation which takes the electronic band structure into account in a realistic manner.

I. INTRODUCTION

TIN lies between Ge and Pb in the fourth column of the periodic table and exists in two stable phases. One phase, α(grey) tin, which is stable below 286°K, has the same crystal structure as Ge and is a semiconductor with a very small band gap (~0.09 eV). The other phase, β(white) tin, which is stable above 286°K, has a body-centered tetragonal structure with basis atoms at (0,0,0) and ($a/2$,0,$c/4$) and is a metal. β-Sn is the only known example of this structure (which is shown in Fig. 1) at normal temperatures and pressures. The properties of α-Sn, and of the $\alpha \rightleftarrows \beta$ transition have been summarized by Busch and Kern[1] in a review article. It is possible to cool β-Sn through the transition temperature without significant transformation to the α phase, and hold it below 150°K for extended periods of time. Since the discovery[2] that Ge and Si transform to the β-Sn structure under high pressures, there has been renewed interest in this structure and in the $\alpha \rightleftarrows \beta$ transition. Several short-range-force models[3,4] derived from elastic data have been proposed for β-Sn, and one of these[4] was used to attempt to explain the $\beta \rightarrow \alpha$ transition in terms of a dynamic instability in β-Sn.

β-Sn is a superconductor with a reasonably high transition temperature ($T_c \approx 4.2$°K), indicating a strong electron-phonon coupling. It also has excellent neutron properties, with a coherent cross section of 4.6×10^{-24} cm^2, an incoherent cross section of $0.3\pm0.6\times10^{-24}$ cm^2, and an absorption cross section of 0.6×10^{-24} cm^2. In addition, large single crystals are readily available.

These considerations led several groups[5,6] independently to begin the study of the crystal dynamics of β-Sn by inelastic neutron scattering at approximately the same time. Most of the work[5] was carried out at room temperature, which is 60% of the melting temperature. At such a high temperature, anharmonic effects are expected to be important. The results of Ref. 6 showed that the structure in [0,0,ζ] branches was more pronounced at low temperatures, and that the neutron groups obtained were sharper. Therefore, the present work extended the measurements to other directions at 110°K. The results presented here include the earlier results of Ref. 6 for completeness. Many of these frequencies were remeasured during this experiment, and excellent agreement was obtained. The group-theoretical results[7] of Chen were used extensively in planning the experiments and analyzing the results.

The experimental methods and results are presented in Sec. II, while a brief discussion of the results comprises Sec. III.

II. EXPERIMENTAL METHODS AND RESULTS

Inelastic slow neutron scattering is a powerful tool for the study of the dynamical properties of solids. In particular, the phonon frequencies ν and wave vectors $\mathbf{q}$ which are connected by the dispersion relation $\nu=\nu_j(\mathbf{q})$ (j is a branch index) can be determined by a study of the peaks in the distribution of inelastically scattered neutrons. These peaks arise from one-phonon

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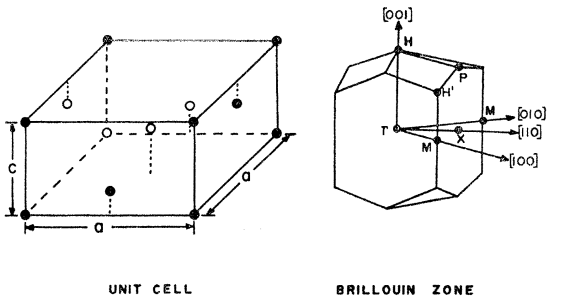

FIG. 1. The nonprimitive tetragonal unit cell of the β-Sn structure, and the first Brillouin zone of the reciprocal lattice showing the labeling of symmetry points.

coherent scattering processes which are governed by the conservation equations

$$\hbar\mathbf{Q}\equiv\hbar(\mathbf{k}_0-\mathbf{k}_1)=\mathbf{G}+\mathbf{q}, \quad (1a)$$

$$\pm h\nu=\pm\hbar\omega=E_0-E_1=(\hbar^2/2m)(k_0^2-k_1^2), \quad (1b)$$

where $\mathbf{k}_0(\mathbf{k}_1)$ is the incident (scattered) neutron wave vector; $E_0(E_1)$ is the incident (scattered) neutron energy; and $\mathbf{G}\equiv 2\pi\boldsymbol{\tau}$, where $\boldsymbol{\tau}$ is a reciprocal lattice vector. The plus (minus) sign in (1b) refers to creation (annihilation) of a phonon of frequency ν and wave vector $\mathbf{q}$.

In addition one must consider the dynamical structure factor,[7,8] which appears in the one-phonon cross section. As shown[7] in the preceding paper, one can define a "reduced structure factor" for the symmetry branches. Those which were used in the experiment are listed in Table I. For nonsymmetry branches some model must be used to estimate the structure factors. (For this experiment, the model of Musgrave was used.) Once the structure factors are known (or estimated), one can then proceed to use the standard methods[8] of "constant Q" and "constant E" to determine the dispersion relation.

The experiments were carried out using the Chalk River (C-5)[8] and the McMaster University[9] triple-axis crystal spectrometers. The two planes of the reciprocal lattice in which measurements were made are shown in Fig. 2. The cell dimensions of β-Sn at 110°K were interpolated from the results[10] of Rayne and Chandrasekhar. Two different specimens were used. One was approximately cylindrical ($1\frac{1}{2}$ in. D×4 in. long) with (1,0,0) planes oriented perpendicular to the cylinder axis. The other was tapered ($1\frac{1}{4}$ in. D at one end; $\frac{1}{2}$ in. D at the other end; and 4 in. long) with a (0,0,1) plane perpendicular to the cylinder axis. The [1,0,0] specimen was obtained from Metals Research Limited, Cambridge, England; the [0,0,1] specimen was obtained from Research Crystals Inc., Richmond, Virginia. Both crystals were tested for mosaic spread (<30 min of arc) and oriented in a liquid-nitrogen cryostat using a two-axis neutron diffractometer at the McMaster University Reactor. During the experiments, the sample temperature was continuously monitored by means of a copper-Constantan thermocouple attached directly to the crystal. During any particular run, the temperature never varied by more than 5°K; the mean temperature for individual runs varied from 95 to 125°K with 110°K the average value.

From Table I, it can be seen that Λ_1 is easily distinguished from Λ_3 and V_1 from V_3 although Fig. 3 shows that these branches are very close in frequency. Also, Fig. 2 shows that the V direction from H to M is a logical continuation of the Λ direction from Γ to H. In fact, Γ-Λ-H-V-M can be considered a single continuous branch $[0,0,\zeta]$ where $0\leqslant\zeta\leqslant 2\pi/c$. The structure factors are continuous over this branch, and as Chen[7] has noted, there is no change of symmetry at H. Also, for this direction, it is possible to classify the branches as longitudinal (L) or transverse (T), acoustic (A) or optic (O). Only the LA and LO branches are true symmetry branches with polarization vectors uniquely determined by symmetry. However, the doubly degenerate TA and TO branches are easily identified, and have been determined over their entire length. The TO, LA, and LO $[\Lambda_4(0), V_4(0), \Lambda_1, V_1, \Lambda_3, V_3]$ results presented here were taken from Ref. 6. The TA branch has been remeasured, at higher resolution, and the new results are given here.

For the $\Delta([\zeta,\zeta,0])$ direction, there are two symmetry branches Δ_1 and Δ_2 which may be classified as LA and LO, respectively. Of necessity, the other branches (Δ_3 and Δ_4) must be transverse. We have measured the Δ_3 (TA and TO) branches but none of the Δ_4 branches.

In the $\Sigma([\zeta,0,0])$ direction there are two symmetry branches Σ_3 and Σ_4 which may be classified as TA and TO, respectively. The other Σ branches are neither transverse nor longitudinal. We have measured only the Σ_3 and Σ_4 branches.

The results are collected in Table II, along with the 300°K results of Ref. 6. The errors shown in brackets were estimated from the shapes and widths of the observed neutron groups, and no simple interpretation is

TABLE I. Reduced inelastic structure factors[a] for β-Sn.

Branch (q)	$Q_x(2\pi/a)$	Q[b] $Q_y(2\pi/a)$	$Q_z(2\pi/c)$	Reduced structure factor Acoustic	Optic
$[\zeta 00]$T (Σ)	$2l+\zeta$	$2m$	0	4.0	0.0
$-1.0\leqslant\zeta\leqslant 1.0$	$2l+1+\zeta$	$2m$	0	0.0	4.0
$[\zeta\zeta 0]$L (Δ)	$2l+\zeta$	$2m+\zeta$	0	4.0	0.0
$-0.5\leqslant\zeta\leqslant 0.5$	$2l+1+\zeta$	$2m+1+\zeta$	0	0.0	4.0
$[0,0,\zeta]$L (Λ,V)	$2l$	$2m$	$4n+\zeta$	4.0	0.0
$-1.0\leqslant\zeta\leqslant 1.0$	$2l$	$2m$	$4n+2+\zeta$	0.0	4.0
	$2l+1$	$2m+1$	$2n+1+\zeta$	2.0	2.0

[a] See Ref. 7 for definitions. [b] $l, m, n=0, \pm 1, \pm 2, \cdots$.

[8] B. N. Brockhouse, in *Inelastic Scattering of Neutrons in Solids and Liquids* (International Atomic Energy Agency, Vienna, 1961); B. N. Brockhouse and P. K. Iyengar, Phys. Rev. **111**, 747 (1958).

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possible. However, from other work[11] we estimate that these errors correspond to about two standard deviations in the usual statistical sense. The 110°K results are presented graphically in Fig. 3. {Note that except where

TABLE II. Normal mode frequencies (in units of 10^{12} cps) for β-Sn.

ζ	ν 110°K	ν 296°K	ζ	ν 110°K	ν 296°K
$\Lambda_1[0,0,\zeta]$LA, $V_1[1,0,1-\zeta]$[a]			$\Lambda_3[0,0,\zeta]$LO, $V_1[1,0,1-\zeta]$[a]		
0.09	1.00[b]	1.00[b]	0.00		1.30±0.03
0.250		2.43±0.10	0.007	1.40±0.04	
0.263	2.67±0.06		0.075		1.51±0.03
0.333		2.75±0.10	0.081	1.70±0.04	
0.345	2.95±0.09		0.160	2.20±0.10	
0.400	3.06±0.06		0.167		2.00±0.10
0.425		2.80±0.10	0.200	2.37±0.04	2.25±0.08
0.450	3.00±0.08		0.250	2.69±0.04	2.55±0.05
0.500	2.87±0.09	2.68±0.10	0.300	2.93±0.04	2.80±0.05
0.550	2.81±0.07		0.350	3.09±0.04	2.97±0.07
0.575		2.64±0.10	0.400	3.08±0.04	2.98±0.06
0.600	2.78±0.07		0.425		2.89±0.08
0.625	2.78±0.07		0.450	2.91±0.06	2.78±0.09
0.650	2.92±0.07		0.475	2.77±0.06	
0.667		2.80±0.15	0.500	2.73±0.05	2.70±0.06
0.675	2.99±0.07		0.525	2.84±0.05	
0.700	3.03±0.08		0.550	2.98±0.05	2.90±0.08
0.750	2.89±0.08	2.60±0.10	0.575	3.02±0.05	2.94±0.06
0.833		2.20±0.10	0.600	3.03±0.06	2.94±0.06
0.844	2.38±0.09		0.625	2.96±0.05	2.85±0.08
0.850		2.18±0.05	0.650	2.91±0.05	2.81±0.07
0.900		1.80±0.04	0.700	2.70±0.04	2.66±0.06
0.903	1.99[b]		0.741	2.54±0.08	
0.907		1.74[b]	0.800		2.00±0.03
0.925	1.74[b]		0.830	1.90[b]	
0.950		1.47±0.03	0.839		1.74[b]
0.997	1.36±0.04		0.850	1.74[b]	
1.00		1.23±0.04	0.900	1.44±0.05	1.37±0.04
			0.925	1.35±0.03	
			0.950	1.30±0.03	1.24±0.04
			0.975	1.29±0.03	
			1.00		1.23±0.04
$\Lambda_5[0,0,\zeta]$TA, $V_5[1,0,1-\zeta]$			$\Lambda_5[0,0,\zeta]$TA, $V_5[1,0,1-\zeta]$		
0.100	0.53±0.03	0.52±0.03	0.00	4.00±0.07	3.85±0.10
0.150	0.69±0.03	0.68±0.03	0.100	3.99±0.06	
0.200	0.85±0.02	0.83±0.02	0.167		3.85±0.20
0.250	0.95±0.02	0.89±0.02	0.200	4.04±0.05	
0.300	1.00±0.02	0.92±0.04	0.300	4.00±0.06	
0.350	1.06±0.02	0.97±0.04	0.333		3.75±0.10
0.400	1.10±0.03	1.04±0.04	0.400	3.98±0.06	
0.450	1.14±0.02	1.07±0.04	0.500	4.03±0.07	3.80±0.20
0.500	1.14±0.02	1.07±0.04	0.600	4.09±0.07	
0.550	1.14±0.02	1.07±0.04	0.667		3.90±0.10
0.600	1.08±0.02	0.97±0.04	0.700	4.10±0.08	
0.650	1.01±0.03	0.92±0.04	0.800	4.12±0.09	
0.700	0.96±0.03	0.88±0.04	0.833		4.10±0.20
0.750	0.89±0.03	0.82±0.04	0.900	4.22±0.07	
0.800	0.86±0.03	0.79±0.03	1.00	4.23±0.06	4.07±0.08
0.850	0.85±0.03	0.77±0.03			
0.900	0.85±0.03	0.76±0.03			
0.950	0.84±0.03	0.76±0.03			
1.00	0.83±0.03	0.75±0.03			

ζ	ν 110°K	ζ	ν 110°K	ζ	ν 110°K
Δ_1, $[\zeta,\zeta,0]$LA		Δ_3, $[\zeta,\zeta,0]$TA		Σ_3, $[\zeta,0,0]$TA	
0.10	0.89±0.05	0.10	0.35±0.02	0.20	0.60±0.03
0.15	1.28±0.05	0.15	0.47±0.02	0.30	0.78±0.02
0.20	1.68±0.05	0.20	0.57±0.02	0.40	0.91±0.02
0.25	2.05±0.04	0.25	0.70±0.03	0.50	0.93±0.02
0.30	2.39±0.04	0.30	0.76±0.03	0.60	0.92±0.02
0.35	2.73±0.04	0.35	0.81±0.03	0.70	0.92±0.03
0.40	2.96±0.04			0.80	0.86±0.03
0.45	3.16±0.04	Δ_3, $[\zeta,\zeta,0]$TO		0.90	0.83±0.03
0.50	3.31±0.04			1.00	0.84±0.03
		0.0	3.97±0.04		
Δ_2, $[\zeta,\zeta,0]$LO		0.10	3.85±0.04	Σ_4, $[\zeta,0,0]$TO	
		0.125	3.80±0.04		
0.0	3.97±0.04	0.150	3.81±0.03	0.0	3.98±0.04
0.05	3.96±0.04	0.175	3.82±0.04	0.10	3.99±0.05
0.10	3.92±0.04	0.200	3.83±0.03	0.20	3.96±0.04
0.15	3.80±0.03	0.225	3.77±0.04	0.30	3.92±0.04
0.20	3.75±0.04	0.250	3.70±0.03	0.40	3.99±0.04
0.25	3.69±0.04	0.275	3.60±0.04	0.50	4.03±0.04
0.30	3.66±0.04	0.300	3.46±0.05	0.60	4.08±0.05
0.35	3.61±0.04	0.350	3.42±0.05	0.70	4.12±0.04
0.40	3.59±0.04	0.400	3.42±0.05	0.80	4.13±0.04
0.45	3.45±0.04	0.450	3.33±0.05	0.90	4.16±0.05
0.50	3.31±0.04	0.500	3.19±0.05	1.0	4.19±0.05

[a] Results taken from Ref. 6. [b] "Constant E" measurements.

[11] E. C. Svensson, B. N. Brockhouse, and J. M. Rowe, Phys. Rev. 155, 619 (1967).

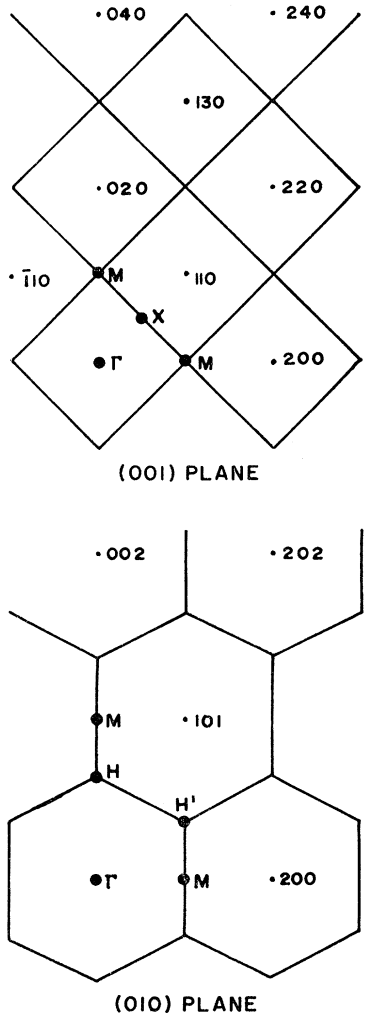

FIG. 2. The (001) and (010) plane of the reciprocal lattice of β-Sn, with symmetry points labeled as in Fig. 1. All measurements were done in these two planes. The dimensions $\Gamma-H=(1/2c)\times(1+p^2)$, $\Gamma-M=1/a$, $\Gamma-X=0.5\sqrt{2}/a$, and $H'-M=(1/2c)\times(1-p^2)$, where $p=c/a$. At 110°K, $a=5.815$ Å, and $c=3.162$ Å (see Ref. 10).

specifically mentioned (Fig. 4), the units of $\mathbf{q}$ are $[2\pi/a, 2\pi/a, 2\pi/c]$.}

Figure 3 has several features which should be noted: The first is the structure in the $[0,0,\zeta]L$ branches which was pointed out in Ref. 6. To study the nature of the dip at $\zeta=0.5$ in the LO (Λ_3) branch, results were obtained for the nonsymmetry branches $[\eta,0,\zeta]$. These results are presented in Fig. 4, and show that the dip is a local minimum, and that it is sharpest along the symmetry line, although it persists to $\eta=(0.3)2\pi/c$. The lack of points on the Λ_1 branch from $\zeta=0.09$ to $\zeta=0.263$ arises from experimental problems connected with the fact that this branch must be measured about the reciprocal lattice point (0,0,4). The point at $\zeta=0.09$ was measured by the "constant-E" technique along the line $[1,0,\zeta]$. Second, the Λ_5 and V_5 branches are both rather flat over their entire extent, with the acoustic

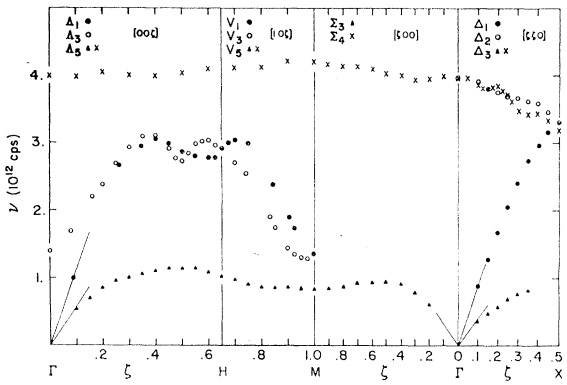

FIG. 3. The dispersion relation of β-Sn at 110°K. For actual values and errors see Table III. The straight lines give the initial slopes of the curves as calculated from the elastic constants.

branches being quite low in frequency while the optic branches are near the maximum frequency observed. This same behavior is apparent in the Σ_3 and Σ_4 branches, although there may be structure in the Σ_4 branch near $\zeta=0.2$. The third point to be noted is the behavior of the Δ branches. The Δ_1 (LA) branch is quite smooth, but the Δ_2 (LO) branch shows evidence of kinks near $\zeta=0.1$ and $\zeta=0.4$. The Δ_3 acoustic (TA) is smooth and low in frequency over its extent (this branch was not continued past $\zeta=0.35$ for experimental reasons). The Δ_3 optic branch is similar to the Δ_2 branch over most of its extent, but near $\zeta=0.15$ there is a pronounced kink so that it crosses the Δ_1 branch twice.

These results should be compared with the more extensive but less accurate symmetry direction results of Long-Price[5] which were obtained for 300°K. Such a comparison gives a detailed picture of the dispersion relation in β-Sn, and, for the symmetry branches, the data are adequate for a detailed comparison with model calculations.

III. DISCUSSION

The results of the previous section can be used to estimate the location of some of the critical points in the frequency distribution function. These estimates can then be compared to the location of structure in the second derivative of superconducting tunneling current measurements, which reflect the frequency distribution critical points. Such a comparison, using the tunneling-current results of Rowell and Kopf[12] is shown in Table III. In making this comparison, it must be noted that the tunneling measurements were done below ~4°K while the neutron results correspond to 110°K. The contents of Table III show that the results of the two experiments correlate well, although we are unable to explain the structure at 7.9 and 10.6 meV using only symmetry-direction results. However, recent calculations by Long-Price[5] using force models which approximate the general shape of the β-Sn dispersion relation show many peaks in the frequency distribution which do not arise from symmetry-direction critical points. This result is in accord with observations[13] on three hexagonal-close-packed metals, for which frequency distributions were calculated using the interpolation method[14] of Gilat and Raubenheimer. In all cases studied, peaks appear in the frequency spectrum which do not arise from symmetry-direction critical points.

The Born–von Kármán model[15] of crystal dynamics has been used extensively in the analysis of experimentally determined dispersion relations. In this model, the results are analyzed in terms of forces between all pairs of atoms less than a certain distance apart. Such models have been very useful as interpolation formulas for unmeasured regions of reciprocal space, and in "simple metals," probably have physical significance. The usefulness of the model is of course intimately connected with the range of interactions, and hence, the number of parameters. For metals with large electron-phonon interactions, the effective two-body potential[16] will have an appreciable long-range oscillatory behavior, leading to forces of effectively infinite range. If in addition, the Fermi surface of the metal is complex, the effective potential will be very complicated. β-Sn is a superconductor, with $T_c\approx4.2$°K, which suggests a strong electron-phonon interaction. The Fermi surface[17] is very complicated, and extends to at least the fifth Brillouin zone. Thus, one would expect that many

TABLE III. A comparison of 110°K neutron results with the superconducting tunneling measurements of Rowell and Kopf (Ref. 12).

Energy of structure in (d^2I/dV^2) (Rowell and Kopf) meV	10^{12} cps	Energy of assigned point on curves 10^{12} cps	Identification
3.5	0.85	0.84	M
3.9	0.92	0.92	[ζ,0,0]TA max
4.9	1.18	1.14	[0,0,ζ]TA max
5.8	1.4	1.40	Γ
7.9	1.91	...	
10.6	2.56	...	
11.2	2.71	2.73	[0,0,ζ]LO anomaly at $q/q_M=0.5$
13.1	3.17	3.12	[0,0,ζ]LO max
13.6	3.29	3.30	[ζ,ζ,0] at X
16.4	3.97	3.98	
17.1	4.13	4.10	[0,0,ζ]TO $q/q_M\approx0.8$
17.4	4.21		
17.7	4.28	4.20	[0,0,ζ]TO at M

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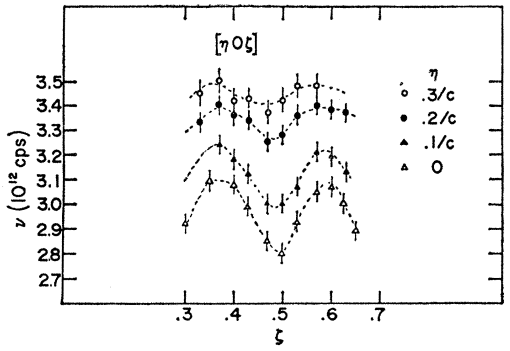

FIG. 4. Results for β-Sn at 110°K along the lines $[\eta,0,\zeta]$, showing the behavior of the anomaly seen in the Λ_3-V_3 branch away from the $[0,0,\zeta]$ direction. All results are plotted to the same scale.

parameters would be required to fit the dispersion relation to a Born–von Kármán model. The shape of the measured dispersion relation (Fig. 3) reinforces this conclusion. To test this point quantitatively, we have Fourier-analyzed the measured symmetry branches to interplanar force constants[18] of the type proposed by Foreman and Lomer. In particular, for this type of analysis, the branches Γ-Λ_1-H-V_1-M-V_3-Λ_3-Γ can be considered one continuous branch. Using linear least-squares analysis, it was found that at least twenty parameters were required to fit the "kinks" in this branch alone adequately. This shows that it is fruitless to analyze the dispersion relation in terms of a Born–von Kármán model.

We are thus led to consider whether these "kinks" can be explained by the Kohn[19] effect. This effect is a sudden change in phonon frequency at values of the wave vector for which $|\mathbf{G}+\mathbf{q}|$ exceeds an extremal dimension of the Fermi surface in a given direction, and is caused by corresponding changes in the screening ability of the conduction electrons. Unfortunately, with the complicated Fermi surface[17] of β-Sn, there are many extremal dimensions for any given direction. In addition, the non-Bravais crystal structure[20] imposes extra conditions on the electron-phonon interaction. The combined effect of these two facts is to virtually preclude assignment of the "kinks" in the dispersion relation to specific electronic transitions across the Fermi surface, as was done,[21] for example, for lead.

The above considerations show that no short-range-force model based upon elastic data can possibly explain the crystal dynamics of β-Sn, and the earlier models[3,4] bear little resemblance to the observed dispersion relation. Instead, a detailed calculation based upon a realistic band-structure model[17] appears to be required.

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