Inelastic–neutron-scattering study of (111) LA phonons in Nb_3Sn

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(Received 25 May 1983)

The phonon dispersion of (ζ, ζ, ζ) LA phonons is determined for $\zeta \leq 0.24$. The pronounced anomaly predicted by a recent first-principles treatment of electron-phonon interactions is not observed.

Recently Weber[1] has calculated the phonon dispersion relations of Nb_3Sn using a method in which the electron-phonon interaction is calculated from nearly first principles. Specifically, electron-phonon screening effects are calculated using the nonorthogonal tight-binding energy bands of Mattheiss and Weber[2] and are combined with phenomenological short-range force constants obtained from an analysis of neutron scattering measurements on Nb_3Sb by Pintschovius *et al.*[3] This method of treating electron-phonon coupling has proven useful for other *d*-electron metals.[4]

This treatment reproduces fairly accurately the softening of the (110) TA modes (C_{11}-C_{12}) responsible for the elastic phase transformation in Nb_3Sn which has been previously studied by us.[5,6] In addition, the paper predicts anomalous behavior of several other modes which have not been studied. The most dramatic of these is a pronounced dip in the (111) LA branch at about $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ (see Fig. 1). This paper reports on measurements designed to explore the correctness of this predicted feature.

The sample is the same 0.05-cm^3 single crystal used in our previous studies,[5,6] which is much too small for a complete study. However, it was possible to measure (111) LA phonons about halfway to the Brillouin-zone boundary at several temperatures, as summarized in Table I and Fig. 1. Representative phonon groups, showing the general quality of the data, are shown in Fig. 2. The data were taken at the high flux beam reactor with a triple-axis spectrometer using pyrolytic graphite monochromators.

Several conclusions can be drawn from the data:

(1) In general, Weber's calculations substantially underestimate the $(\zeta\zeta\zeta)$ LA phonon frequencies for $\zeta \gtrsim 0.1$.

(2) There is a small, but anomalous, softening of the $(\zeta\zeta\zeta)$ LA phonon frequencies with decreasing temperature, in the range $300 > T > T_M = 45$ K.

(3) $(\zeta\zeta\zeta)$ LA phonons become difficult to detect beyond $\zeta \approx 0.25$, either due to rapid changes in the inelastic structure factor (i.e., the phonon eigenvector), the phonon width, or both. Unfortunately, larger sample specimens would be necessary to further explore this effect.

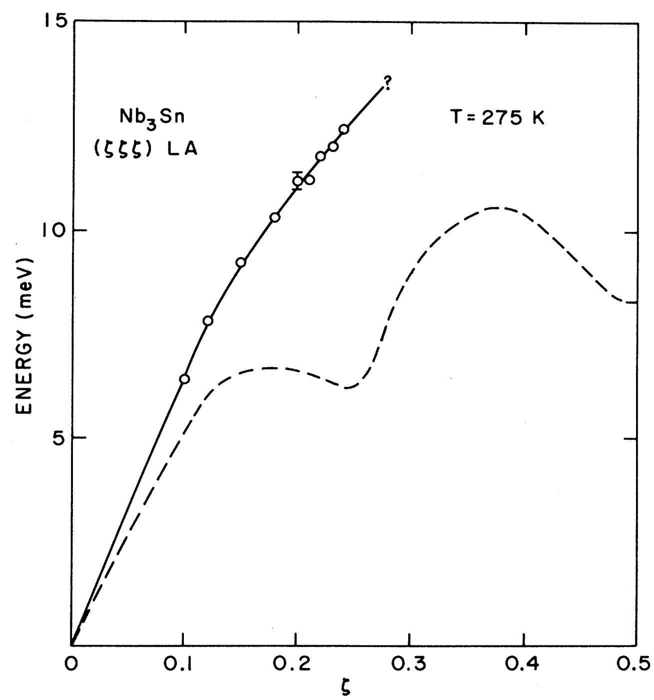

FIG. 1. Solid line (——), measured phonon dispersion at $T = 275$ K. Dashed line (– – –), dispersion curve calculated in Ref. 1.

ACKNOWLEDGMENTS

We acknowledge a useful discussion with W. Weber and the cooperation of M. L. A. MacVicar in facilitating the loan of the Nb_3Sn sample. The work at Brookhaven National Laboratory was supported by the Division of Materials Sciences, U. S. Department of Energy, under Contract No. DE-AC02-76CH00016.

TABLE I. $(\zeta\zeta\zeta)$ LA phonon energies (meV).

ζ	$T = 275$ K	$T = 107$ K	$T = 51$ K
0.1	6.4(0.2)	6.5	6.3
0.12	7.8	7.5	7.3
0.15	9.2	8.7	8.6
0.18	10.3		
0.20	11.2		
0.21	11.2		
0.22	11.8		
0.23	12.0		
0.24	12.2		
0.25	?		

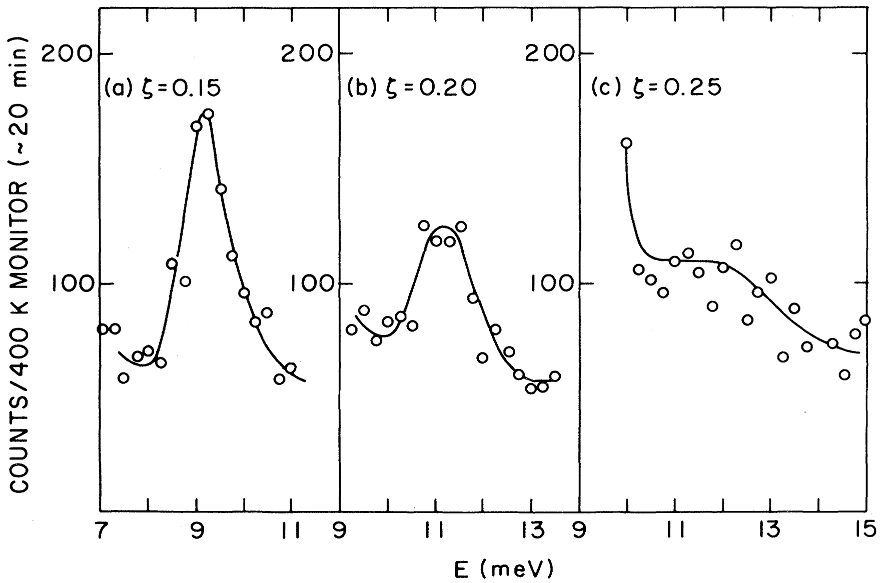

FIG. 2. Examples of (ζζζ) LA phonon groups showing the gradual loss of definition with increasing ζ. All data were taken with 30.5-meV fixed final energy and either (a) 40′-20′-40′-40′ or (b) and (c) 40′-40′-20′-20′ collimation.

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