

Anomalous phonon behaviour in V_3Si

M. Yethiraj*

Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6393, USA

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Abstract. In earlier studies of phonons in V_3Si , a gradual softening of the ($hh0$) branch was observed and attributed to the martensitic transition in this compound, which precedes the onset of superconductivity by a few degrees K. In this work, the temperature dependence of the transverse acoustic (TA) branch along the $hh0$ direction was studied in greater detail and it is shown that while the TA $hh0$ mode starts to soften at relatively high temperatures (> 200 K), an anomalous softening, which is rather localized in q , occurs just below T_c . The intensity of this soft-phonon peak correlates extremely well with the onset of the superconducting phase and appears to vary as the order parameter with temperature and applied field. The similarities in the phonon softening and Fermi-surface anisotropy between this compound and the rare-earth nickel borocarbides suggest the existence of a common mechanism for the superconducting transition.

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The A15 family of superconductors exhibited some of the highest critical temperatures prior to the discovery of the high- T_c cuprate (and related) compounds. The higher T_c A15 materials have martensitic distortions to their cubic crystal structures at temperatures somewhat higher than the superconducting transition temperature.

Unusual softening of the acoustic phonons in V_3Si have been reported [1]; the softening was seen to be direction dependent, even in this cubic material, and the temperature where the mode began to soften was near room temperature (or much higher than T_c). The changes in the phonon dispersion curve began to appear at relatively high temperatures (> 200 K) compared to the onset of superconductivity ($T_c \approx 17$ K in V_3Si), although it should be noted that the martensitic transition (at 21 K) precedes superconductivity by only a few Kelvin for V_3Si . Unfortunately, since the anomalous phonon behaviour was associated with the martensitic transition, only very few of the phonon measurements in A15 compounds in the published literature extend to below the superconducting transition temperature. For instance, in

Nb_3Sn , most of the data are for $T > 40$ K (in a system where $T_c = 18.3$ K and $T_M = 46$ K). However, ultrasound studies [2] performed in V_3Si has shown a strong anisotropy of the sound velocity in this material at low temperature.

Recent studies by two groups [3, 4] of the behaviour of the TA $h00$ phonon in the nonmagnetic borocarbide superconductors show a new peak which appeared at the superconducting transition temperature at a characteristic q of 0.505 rlu. This peak appeared to become more intense at the expense of the TA $h00$ phonon peak as the temperature was lowered. The new peak appeared to be rather localized in q and energy. In the second study, a complicated variation of structure factors of the acoustic and optic modes in different Brillouin zones as a function of temperature was observed [5] in $LuNi_2B_2C$. Systems with several atoms per unit cell often have complicated inelastic structure factors. Though it seems reasonable that two branches with the same symmetry that cross might show interaction in the form of the inelastic structure factor, the variation has not been fully explained.

It was suggested [6] that the new peak in the borocarbides was due to an incipient charge density wave instability in this compound which is never realized and that the peak was causally related to nesting features in the Fermi surface. The borocarbide system and the A15 system seemed to have several similar characteristics. Both have a T_c of about 15 K; both have a softening of a transverse acoustic mode, already evident at 200 K. Further parallels are found in the existence of the nesting features in the Fermi surface and flux lattice structure transitions (which are indicative of Fermi surface anisotropy) in both these compounds.

1 Experiment

The above phonon data on the borocarbides prompted this study of the phonons in V_3Si , of which a large high quality single crystal exists and on which previous flux line lattice measurements had been made. It was of interest to know whether the extra peak in YNi_2B_2C was a particular anomaly in the borocarbide family or whether this could possibly be involved in a more universal mechanism related to superconductivity, which results in the relatively high T_c 's of nearly

*Corresponding author. (E-mail: yethirajim@ornl.gov)

20 K. However, the studies of this compound are made difficult by the large incoherent cross-section of vanadium (giving rise to high background) together with its vanishingly small contribution to the coherent phonon scattering signal. Nearly all of the observed signal is due to the Si atoms in the lattice and measurements are fairly time-consuming. Hence, the measurements concentrated on establishing either the similarity or lack thereof with the phenomena in the borocarbide superconductors.

V_3Si has a cubic structure above 21 K, where it undergoes a small structural distortion (nominally referred to as 'martensitic' in the literature, the distortion lowers the symmetry to tetragonal). This distortion appears to persist into the superconducting phase, which occurs below 16.8 K. The material (indexed using a cubic unit cell, since the distortion is relatively small) has a lattice parameter of 4.72 Å at room temperature. The sample of V_3Si was a cylinder of diameter 8.3 mm and length 10.4 mm. The physical cylinder axis was determined to be the a -axis of the crystal to within an uncertainty of 2° . The mosaic was less than 0.4° , the resolution with which the measurement was made. The sample had a dH_{c2}/dT slope of -2 T/K and a critical temperature of 16.8 K (onset), as characterized by SQUID magnetization

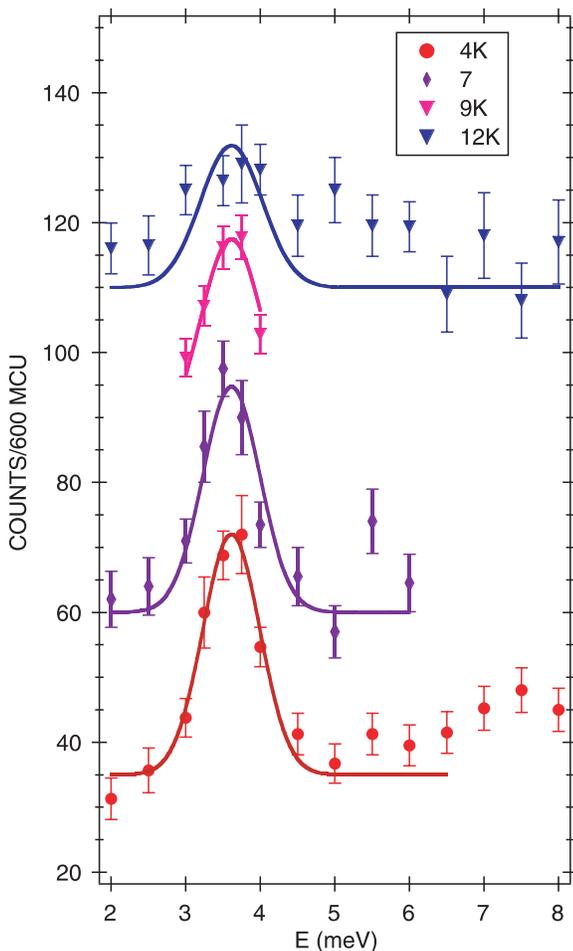


Fig. 1. Energy scan at $q = 0.15, 0.15, 0$ as a function of temperature shows a sharp peak at the lowest temperature at 3.75 meV which decreases in intensity as the temperature is raised. The Gaussians fit to the data were constrained in their width and position. Similar to the borocarbides, there appears to be a second peak gaining intensity as the temperature is raised

measurements on a small piece cut from the larger sample. Inelastic neutron scattering measurements were carried out on the HB3 triple axis spectrometer at the High Flux Isotope Reactor at Oak Ridge National Laboratory. The typical collimation used was $48'-40'-40'-120'$ with a fixed final energy of 14.8 meV with pyrolytic graphite filters in the scattered beam. Relatively good energy resolution had to be maintained as the elastic incoherent peak (due to the large contribution from vanadium) is relatively intense and because the energy transfers of interest were fairly low. The sample was oriented such that the $hk0$ zone of the crystal was in the scattering plane. Most measurements were made around the 220 Bragg peak. The intensity of this Bragg peak, discussed in more detail later, changes dramatically at 21 K. It has been previously reported that in Nb_3Sn [7] the onset of the martensitic transition causes a small distortion and, hence, strain in the sample, which causes an increase in Bragg intensity by reducing the effects of extinction. It is generally thought that the same phenomenon occurs in V_3Si also.

The transverse acoustic mode propagating along the $hh0$ direction has a dip reminiscent of a Kohn anomaly. And though some localization of the softening is noted already at 18 K, most of the effect occurs not only below T_M but also below T_c . It is clear that this softening is related to the superconducting transition. The minimum of the dip is at $q = (0.15, 0.15, 0)$. An energy scan at this q -vector (Fig. 1) shows a sharp peak at 3.75 meV which diminishes in intensity as the temperature is increased and extra intensity appears at a somewhat higher energy. The Bragg intensity of the 220 peak increases sharply at T_M , is higher by a factor of three just above T_c then the onset of superconductivity appears to reduce the intensity somewhat; the intensity is unchanged below T_c .

Finally, it was observed that the application of quite small (vertical) magnetic fields reduced the peak intensity of the excitation at $q = (0.15, 0.15, 0)$ and at 7 T (the highest field

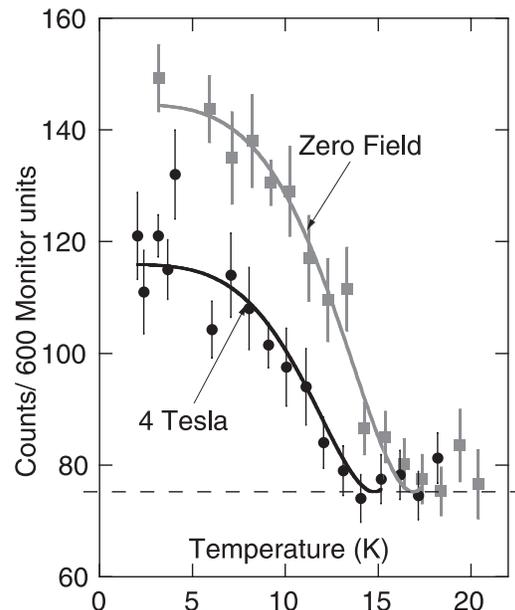


Fig. 2. The temperature dependence of the peak intensity at 3.75 meV and $q = 0.15, 0.15, 0$ is correlated with the superconducting fraction as described by a simple two-fluid model

achievable with the magnet used), the peak was reduced to 50% of its intensity at zero field. The temperature dependence of the peak intensity at zero field and 4 T is shown in Fig. 2. The solid lines in Fig. 2 are fits to the data with an extremely simple two-fluid model (and varying only a single variable per data set, namely T_c). The fit values obtained for $T_c(0)$ and dH_{c2}/dT_c are 16.8 K and 2 T/K respectively; these are all consistent with magnetization measurements done on a sample that was cut from the larger piece used in this study. It is clear that this model fits the data well and, hence, that the peak intensity is proportional to any scattering due to only the superconducting fraction in the sample.

2 Discussion and conclusion

Two theoretical explanations have been suggested; the first scenario suggests [8] an interaction of the phonons with the conduction electrons where the new mode is a mixed vibrational-superelectronic collective excitation. The theory predicts significant shift in the energy of the sharp resonance at a reduced temperature (T/T_c) > 0.5 . The energy of the peak shows no appreciable shift upto 12 K ($T/T_c = 0.7$) in V_3Si nor was this observed in the published data on the borocarbides. While this theory has been applied to Nb successfully, it is noted that two peaks are not observed in Nb. Further, the electron phonon coupling constant used to fit the Nb data is an order of magnitude smaller than that invoked to fit the data in the borocarbides, and the phonon widths changes in Nb are not direction dependent. The theory predicts that the sharp peak will have no dispersion; the observed resonance is rather localized. On the other hand, Kee and Varma [6] assume the existence of a nesting feature on the Fermi surface (which appears to exist from the Kohn anomaly seen in

the dispersion curve above the critical temperature) and that strong electron-phonon coupling interacts with this nesting to give rise to a charge-density wave transition. This theory predicts a shift in the energy of the sharp peak but only at relatively high T (where there was not sufficient signal for the measurement). One can speculate that the martensitic transition actually reflects a CDW which is arrested by the onset of superconductivity; the variation of the 220 Bragg intensity with temperature is not inconsistent with this picture. However, no CDW satellites have been observed to date.

In conclusion, it is clear there is a striking similarity between the measured properties in V_3Si and the borocarbides. It appears likely that the explanation for the properties in these two materials will be quite similar; a common mechanism for the superconducting transition is strongly suggested by the data.

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