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PHONON DENSITY OF STATES IN V_3Si

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PHONON DENSITY OF STATES IN V_3Si

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The A-15 superconductors are among the most interesting and widely studied of the high-T_c superconducting materials, but, there are very few coherent inelastic neutron scattering data available, (Axe and Shirane, 1972; Shirane, Axe, and

[1]Operated by Union Carbide Corporation with the U. S. Department of Energy.

Birgeneau, 1971; Cox and Tarvin, 1978) primarily because of small sample sizes (Nb_3Sn) or poor coherent neutron scattering properties (V_3Si). Although the A-15 compounds are cubic, the symmetry is sufficiently low that even in the principal directions in the crystal, there are from 16 to 24 branches to the dispersion curves, and the sparse neutron data are insufficient to derive a set of force constants as is customarily done from single crystal data. Schweiss et al. (1976) have exploited the incoherent neutron scattering properties of V and have extracted the weighted phonon density of states of several polycrystalline A-15 compounds containing V, namely, V_3Si, V_3Ge, and V_3Ga. The maximum frequencies observed occured in V_3Si and they attributed a strong peak in V_3Si of 10 THz to modes containing the lighter Si atoms, since this peak appeared to shift downward in frequency in V_3Ge and V_3Ga. Achar and Barsch (1976a, 1976b, 1979) made a theoretical lattice dynamics study of V_3Si based on a psuedopotential approach and two of their models predicted frequencies of the Γ_2 and Γ_{12} modes between 15 and 21 THz. These modes are of particular interest since they involve out-of-phase motions of neighboring V atoms and should play a major role in understanding the electron-phonon interaction in this and other high-T_c A-15 compounds.

We report here the observation by inelastic neutron scattering techniques of a high energy peak in the phonon spectrum ($\approx$14 THz) shown in Fig. 1 which we attribute to a peak in the phonon density of states due to vanadium motions by the incoherent inelastic neutron scattering process. The miniscule coherent scattering amplitude (-0.5 fm) of V precludes the observation of modes containing only V motion by the one-phonon coherent scattering process; nevertheless, a search for such modes was made, but was unsuccessful. In fact, even the optic modes consisting mainly of Si motions were not observed, presumably because of the large incoherent background of V. This is part of a larger study (to be reported elsewhere) of the tetragonal transformation of single crystal V_3Si at 20.5 K and the determination of the acoustic and if possible, low lying optic modes and their temperature dependence. Recently, Wipf et al. (1978) succeeded in measuring the $_{12}$ modes in single crystal V_3Si by Raman scattering techniques; however, they obtained a value of 8.5 THz. This measurement has been confirmed by Schicktanz et al. (1979) from Raman studies of stoichiometric and nonstoichiometric V_3Si. The latter authors also report broad scattering centered about 14 THz which they attribute to peaks in the phonon density of states. This was not observed in the numerous neutron scattering studies of the A-15 compounds, but this may be due to the fact that the investigators did not extend their measurements to high enough energies.

In bcc V the mode frequencies corresponding to near neighbors vibrating out-of-phase are of the order of 9 THz. In V_3Si the V-V near neighbor distance is 2.6 A vs 2.8 A in bcc V, therefore, it does not seem unreasonable to expect optic modes in V_3Si, which involve V out-of-phase motions, to be appreciably higher than 9 THz. This is not necessarily in conflict with the Raman scattering results for it is quite possible to have high frequency phonon branches which are soft in selected regions of the Brillouin zone, in this case at Γ, particularly in systems with large electron-phonon interactions. Additional work to confirm these preliminary results is scheduled for the near future.

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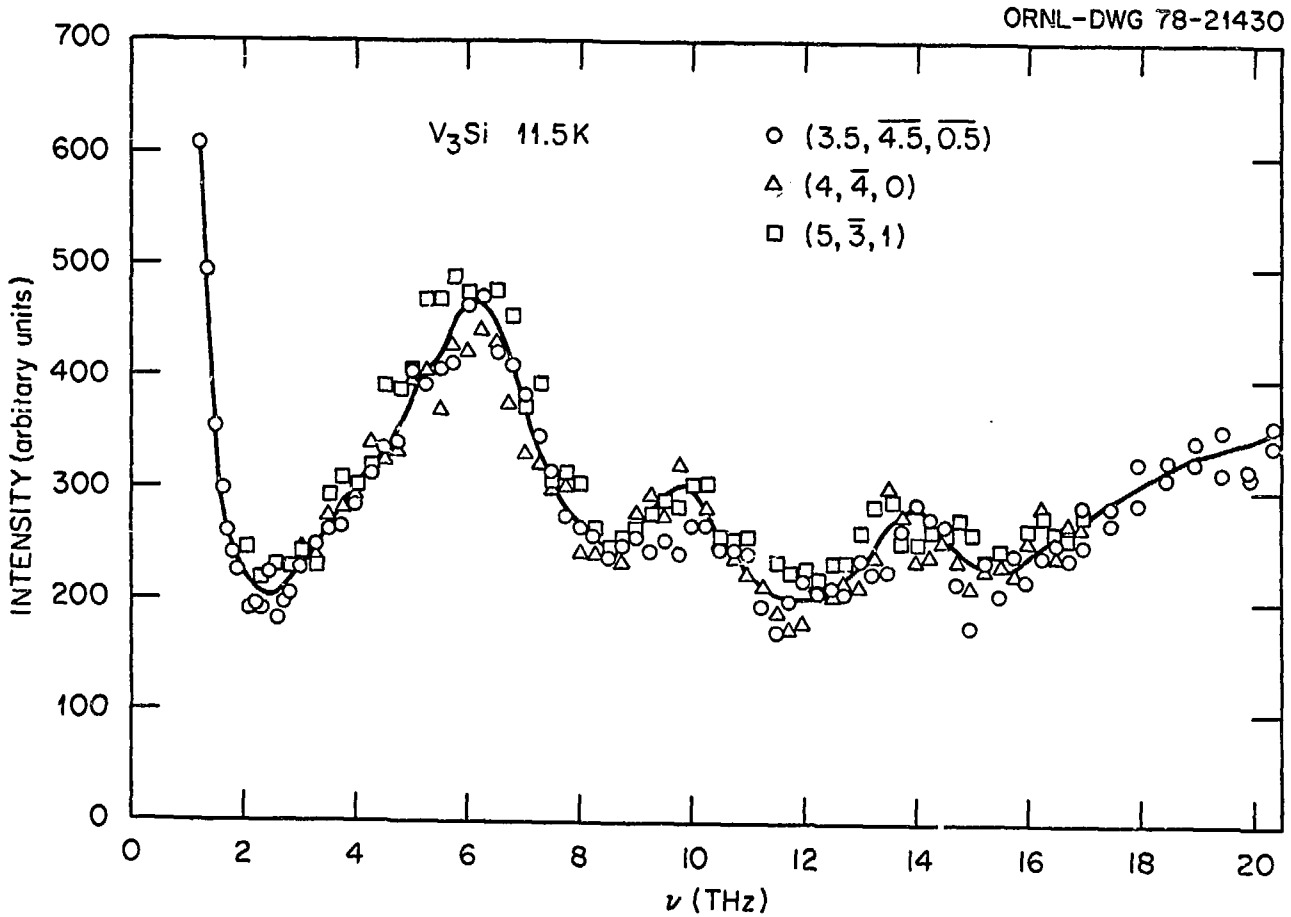
FIGURE 1. Incoherent inelastic neutron scattering in single crystal V_3Si.


ORNL-DWG 78-21430
V_3Si 11.5K
○ (3.5, $\overline{4.5}$, $\overline{0.5}$)
△ (4, $\overline{4}$, 0)
□ (5, $\overline{3}$, 1)
INTENSITY (arbitary units)
700
600
500
400
300
200
100
0
0
2
4
6
8
10
12
14
16
18
20
ν (THz)