1978

Magnetoresistance of 1T-TaSe2

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them decrease with increasing x. We attribute this behavior to strong coupling between these modes and the CDW.

* Work supported in part by the NSF.

[1] F.J. Di Salvo, D.E. Moncton, and J.V. Waszczak Phys. Rev. B 14, 4322 (1976).

[2] J.A. Holy, K.C. Woo, M.V. Klein, and F.C. Brown, Phys. Rev. B 16, 3628 (1977).

CC 8 Elastic Properties of 2H-$TaSe_2$, J. L. FELDMAN, C. L. VOLD, and E. F. SKELTON, Naval Research Laboratory, and Shu-Cheng YU and I. L. SPAIN, University of Maryland--The elastic constants, in particular c_{13}, of the layered TM-chalcogenide materials are of interest for the interpretation of stress dependent information. In order to obtain c_{13} it is useful to combine linear compressibility values with neutron-measured[1] (zero sound) elastic constants. In this paper both pressure and temperature dependences of the lattice parameters are determined from x-ray diffraction measurements. A force model would be required to estimate zero sound-isothermal elastic constant differences arising from anharmonicity. The fact that we find from our thermal expansivities that isothermal-adiabatic elastic constant differences are negligible suggests that it is reasonable to combine our linear compressibilities with the zero sound elastic constants. Thus we obtain $-1.5<c_{13}<3$, in 10^{11} dynes/cm^2. Estimates of Grueisen parameters, the Debye temperature, and strain dependences of the ICDW transition temperature will also be discussed.

[1] D. E. Moncton, J. D. Axe, and F. J. Di Salvo, Phys. Rev. B16, 801 (1977).

CC 9 Magnetoresistance of 1T-$TaSe_2$. P. D. HAMBOURGER, Cleveland State U., and F. J. DiSALVO, Bell Laboratories. --The transverse magnetoresistance of single-crystal 1T-$TaSe_2$ has been measured at T=4.2K in magnetic fields up to 23 kG with $J \perp [0001]$. Although the observed magnetoresistance was quite small ($\Delta\rho/\rho \sim 0.015$), substantial anisotropy was observed. At 22 kG, $\Delta\rho/\rho$ was $\sim$ 40% larger for $B \perp [0001]$ than for $B // [0001]$. The anisotropy is therefore the reverse of that observed in 2H-$TaSe_2$ (ref. 1) and 2H-$NbSe_2$ (ref. 2) and suggests that in the presence of the charge density wave the Fermi surface of 1T-$TaSe_2$ may not be dominated by cylinders parallel to [0001] as is the case in 2H-$TaSe_2$ (refs. 1,3) and probably also in 2H-$NbSe_2$ (ref. 2).

[1] P. D. Hambourger, Phys. Rev. B15, 1640 (1977).
[2] P. D. Hambourger and N. E. Lewis, (abstract submitted for the Charge Density Wave Symposium, University of Warwick, January, 1978).
[3] J. E. Graebner, Solid State Commun. 21, 353 (1977).

CC 10 Electronic Structure and Lattice Instabilities in 1T-$TiSe_2$ and 1T-VSe_2.* A.J. FREEMAN, Northwestern U. and Argonne, and A. ZUNGER**, Northwestern U.--A first principles self-consistent band structure calculation on 1T-$TiSe_2$ shows that a constant volume variation of the internal crystal parameter z (which determines the metal-nonmetal layer separation and the Ti-Se bond distance) produces an electronic phase transition from the normal semi-metal to a semi-conductor. Since a 2% reduction uncrosses the p-d band overlap at L, and since the observed bond shortening is 2.4%, such a phase transition may account for the observed decrease in conductivity and susceptibility in the CDW state. In VSe_2 we find that the p-d band overlap increases and the volume of the electron Fermi surface decreases rapidly as the (anomalously large) c/a ratio decreases. In a model in which the CDW instability is associated with d-band nesting, small changes in c/a would drastically affect the magnitude of the nesting $\vec{q}$ and consequently the transition temperature.

*Supported by NSF, AFOSR, and USDOE

CC 11 Phonon Spectra in 1-T $TiSe_2$. N. WAKABAYASHI and H.G. SMITH, Oak Ridge National Lab.,* and R.C. WOO and F.C. BROWN, Univ. of Illinois.--Phonon frequencies of several branches for the layered compound 1-T $TiSe_2$ have been measured along Γ-M and A-L directions by slow neutron scattering techniques. Mixing of acoustic and optic characters of modes seems to exist for various branches. Dispersion curves in the Γ-M direction measured at 50 K and room temperature have been found to show little difference. Special attention was paid to transverse modes having the polarization vectors parallel to the layer. At the L point where a super lattice reflection exists below 200 K, a phonon has been observed to exhibit a temperature dependence which may be expected for a soft mode. However, no diffuse scattering was observable near L possibly due to the small sample size. A lattice dynamical model has been constructed to interpret these results as well as the results obtained recently by Moncton et al.[1]

*Operated by Union Carbide Corporation for the Department of Energy.

[1] D. E. Moncton, F. J. DiSalvo, and J. D. Axe, private communication.

CC 12 Superlattice Formation in 4Hb-$TaSe_2$, J.R. Duffey, R.D. Kirby,* U. of Nebraska-Lincoln, R.V. Coleman, U. of Virginia, --- The 4Hb-polytype of $TaSe_2$ consists of alternating layers of octahedral and trigonal prismatic coordination. A charge density wave (CDW) commensurate state transition occurs in the octahedral layers at 410°K, while the trigonal prismatic layers undergo a transition to an incommensurate CDW state at 75°K.[1] Our Raman measurements above 75°K show a low frequency spectrum very similar to that observed in the 1T-polytype of $TaSe_2$, with many CDW induced lines. Below 75°K, a broad temperature dependent mode occurs near 40 cm^{-1}. We attribute this mode to an amplitude mode of the coupled CDW-lattice. Its behavior is very similar to the incommensurate state amplitude mode observed in 2H-$TaSe_2$.[2]

* Work supported in part by NSF

[1] F.J. Di Salvo, D.E. Moncton, J.A. Wilson, and S. Mahajan, Phys. Rev. B 14, 1543 (1976).
[2] E.F. Steigmeier, G. Harbeke, H.Auderset, and F.J. Di Salvo, Solid State Commun. 20,667(1976

CC 13 Quantum Oscillatory Effects in 2H-TaS_2.* S. J. HILLENIUS and R. V. COLEMAN, Univ. of Virginia.--Quantum oscillations have been studied in 2H-TaS_2 using both the Shubnikov de Haas and de Haas van Alphen effect. The observed frequencies are in the range .04 to 6 MG and correspond to Fermi surface sections in the charge density wave state of the crystal. Four of the strongest frequencies follow a two dimensional angular dependence described by $\omega_1/\sin\theta$ while others show an angular dependence more characteristic of three dimensional Fermi surface sections. Comparison to results on 4Hb-TaS_2 shows a comparable range of frequencies in both phases but different precise values and dimensional behavior are observed. The perfect 2H phase crystals were produced by thermally transforming 4Hb-TaS_2 crystals and the measurements have been made in the range 0-150 kG.

*Work supported by U.S. DOE contract EY-76-S-05-3105.

CC 14 Pressure Derivative Sign Reversal for Proton Spin-Lattice Relaxation Times in $TaS_2 \cdot NH_3$.* H.T. WEAVER, J.E. SCHIRBER, Sandia Labs., and B.G.SILBERNAGEL, Exxon Research.--Proton spin-lattice relaxation times (T_1) have been measured for the intercalculated compound $TaS_2 \cdot NH_3$ as a function of temperature ($77 \leq T \leq 300K$) and pressure to 6 kbar. Pressure effects on T_1 were sufficiently large that the sign reversal for dT_1/dP, which is predicted by simple diffusion models, is observed. The temperatures at which dT_1/dP changes sign ($T = 190K$) and T_1 is minimum are within experimental