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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-TaSe₂, 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 (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/cm². Estimates of Gruneisen parameters, the Debye temperature, and strain dependences of the ICDW transition temperature will also be discussed.

D. E. Moncton, J. D. Axe, and F. J. Di Salvo, Phys. Rev. B **16**, 801 (1977).

CC 9 Magnetoresistance of 1T-TaSe₂, P. D. HAMBOURGER, Cleveland State U., and F. J. Di SALVO, Bell Laboratories. --The transverse magnetoresistance of single-crystal 1T-TaSe₂ has been measured at $T=4.2$ K in magnetic fields up to 23 kG with $H \parallel [0001]$. 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 $H \parallel [0001]$ than for $H \parallel [1001]$. The anisotropy is therefore the reverse of that observed in 2H-TaSe₂ (ref. 1) and 2H-NbSe₂ (ref. 2) and suggests that in the presence of the charge density wave the Fermi surface of 1T-TaSe₂ may not be dominated by cylinders parallel to $[0001]$ as is the case in 2H-TaSe₂ (refs. 1,3) and probably also in 2H-NbSe₂ (ref. 2).

1P. D. Hambourger, Phys. Rev. B **15**, 1640 (1977).

2P. D. Hambourger and N. E. Lewis, (abstract submitted for the Charge Density Wave Symposium, University of Warwick, January, 1978).

3J. E. Graebner, Solid State Commun. **21**, 353 (1977).

CC 10 Electronic Structure and Lattice Instabilities in 1T-TaS₂ and 1T-VSe₂, * A.J. FREEMAN, Northwestern U. and Argonne, and A. ZUNGER**, Northwestern U.--A first principles self-consistent band structure calculation on 1T-TaS₂ 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 VSe₂ 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 q and consequently the transition temperature.

*Supported by NSF, AFOSR, and USDOE

CC 11 Phonon Spectra in 1-T TiSe₂, N. WAKABAYASHI and H.G. SMITH, Oak Ridge National Lab.,* and K.C. WOO and F.C. BROWN, Univ. of Illinois.--Phonon frequencies of several branches for the layered compound 1-T TiSe₂ 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.

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

CC 12 Superlattice Formation in 4Hb-TaSe₂, J.R. DUFFEY, R.D. Kirby,* U. of Nebraska-Lincoln, R.V. Coleman, U. of Virginia, --- The 4Hb-polytype of TaSe₂ 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 TaSe₂, 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-TaSe₂.²

* 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-TaS₂, * S. J. HILLENIUS and R. V. COLEMAN, Univ. of Virginia.--Quantum oscillations have been studied in 2H-TaS₂ 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 $\omega_c/\sin \theta$ while others show an angular dependence more characteristic of three dimensional Fermi surface sections. Comparison to results on 4Hb-TaS₂ 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-TaS₂ 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 TaS₂·NH₃, * 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 intercalated compound TaS₂·NH₃ as a function of temperature ($77 \leq T \leq 300$ K) 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 ($T = 190$ K) and T_1 is minimum are within experimental