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Electron Transport in Se-Doped LT-TaS2

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unambiguous symmetry assignment for the two-photon transition ($A_g \leftarrow A_g$), and absolute oscillator strengths for both the one-photon and two-photon transitions (0.8 and 1.5 respectively). Cross sections for two-photon absorption in polydiacetylene are by far the largest ever reported for an organic molecule ($\sim 10^{-46}$ cm^4-sec/photon-repeat unit). These remarkably large values are quantitatively explained theoretically.

[1]G. N. Patel, R. R. Chance, and J. D. Witt, J. Polym. Sci., Polym. Lett. Ed. 16, 607 (1978).

SESSION JP: LAYERED COMPOUNDS I, TRANSPORT AND MAGNETIC PROPERTIES

Thursday morning, 22 March 1979
Great America Room II at 9:00 A.M.
S.A. Jackson, presiding

JP 1 "Direct" Observation of Charge Density Waves by Molecular Beam Diffraction. G. BOATO, P. CANTINI and R. COLELLA*, University of Genoa, Italy -- A diffraction pattern of neutral helium atoms (λ = 0.57 Å) has been obtained from the surface of a TaS_2 single crystal at 80°K. Cleaning of the surface was accomplished by heating up to 350-400°K, and by cryopumping with liquid helium in proximity of the crystal. Satellite peaks are also observed in addition to the ordinary Bragg reflections, consistent with the $\sqrt{13}a \times \sqrt{13}a$ superstructure of the $1T_3$ phase, expected at 80°K. What is surprising is that, while in electron, neutron and x-ray diffraction the intensities of the satellite peaks are 20-50 times weaker than ordinary Bragg reflections, in this experiment they have about the same intensity. Since a molecular beam has no penetration whatsoever in the crystal our results are interpretable in terms of diffraction effects from a corrugated surface. What is observed, then, is most likely the direct effect of charge modulation in the electron sea, rather than the reaction of the positive ion lattice to the charge modulation.

*On sabbatical leave from Purdue University, Physics Department, West Lafayette, IN 47907, U.S.A.

JP 2 Does β-$MoTe_2$ Have a CDW Instability? ROY CLARKE*, P. WONG, and P.M. HORN, University of Chicago,** and E. MARSEGLIA, Cavendish Laboratory, Cambridge. -- The recently reported [1] monoclinic-orthorhombic structural transition in β-$MoTe_2$ (quenched from the metallic, paramagnetic β phase) is unusual in that the lower temperature phase has the higher symmetry. We present magnetic susceptibility (χ) measurements which show that β-$MoTe_2$ is diamagnetic at 300K and that χ exhibits a gradual downward step going into the orthorhombic phase with thermal hysteresis over a wide temperature range. Although there is as yet no direct evidence of charge density wave (CDW) formation in β-$MoTe_2$ the results suggest a possible explanation [2] for the transition in which a competition between Coulomb and elastic interactions drives a first-order lock-in transition to the orthorhombic phase below 250 K.

*IBM-James Franck Fellow.
**Supported by NSF Mats. Res. Lab., University of Chicago.
1) R. Clarke, E. Marseglia, and H.P. Hughes, Phil. Mag. B 38 , 121 (1978)
2) G.A. Thomas, D.E. Moncton, F. Wudl, M. Kaplan, and P.A. Lee, Phys. Rev. Lett. 41, 486 (1978)

JP 3 Angle-Resolved Photoemission Studies of the Band Structure of $TiSe_2$ and TiS_2. C.H.CHEN*, W.FABIAN†, F.C. BROWN, K.C.WOO#, and A.H.THOMPSON‡, U. of Illinois at Urbana-Champaign†--The electronic structure of high quality $TiSe_2$ and TiS_2 crystals has been investigated using angle-resolved photoemission with HeI and HeII resonance radiation. Results compare favorably with recent energy band calculations although differences occur which may be due to the three rather than two dimensional nature of specific bands. Occupied d states at the zone edge are observed in both materials. A small overlap with the s/p valence band at Γ is observed in the case of $TiSe_2$ in approximate agreement with other workers. Our results of TiS_2 show very interesting behavior of valence band near Γ. Specifically a band near Fermi energy was observed near Γ. The size of the band gaps depend crucially upon the nature of this band. Various implications will be discussed.

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†Work at U. of Illinois supported in part by the National Science Foundation under grant no. DMR 76-01058.

JP 4 Composition-Dependent Binding Energies in GaS_xSe_{1-x} Compounds. G. MARGARITONDO, A.D. KATNANI and T.E. MILLIMAN, Dept. of Physics, Univ. of Wisconsin-Madison, F. LEVY, Institut de Physique Appliquee, EPF, Lausanne, Switzerland, and I. ABBATI, Istituto di Fisica del Politecnico, Milano, Italy. -- We have carried out a systematic study of GaS_xSe_{1-x} compounds in the range x = 0-1 employing photoemission spectroscopy with synchrotron radiation. The atomic orbital character of each valence band peak is reflected in the dependence on x of its binding energy (measured with respect to the top of the valence band). For example the p_z-like states near the top of the valence band are shifted downwards by $\sim$ .25 eV when x is changed from 1 to 0. On the contrary the p_{xy} states are shifted upwards by .15-.25 eV. For large values of x the photon polarization dependence of these peaks reveals a rehybridization of the p_z and p_{xy} states. The Ga 3d binding energy also decreases linearly with x, an effect not clearly revealed by previous measurements on GaS and GaSe. The above composition effects and the dependence on x of other valence band peaks will be discussed in terms of the chemical bonding properties of these materials.

JP 5 Resistivity of $Zr_xTi_{1-x}Se_2$.* W.R. NIEVEEN+ and R.D. KIRBY, U. of Nebraska.--Pure $TiSe_2$ shows a large resistivity peak near 200 K arising from a second-order transition to a charge-density-wave (CDW) state. Our resistivity measurements on $Zr_xTi_{1-x}Se_2$ show that the CDW transition temperature shifts downward with increasing x. By x = 0.3, the CDW transition is suppressed, and the resistivity can be characterized by a simple power law dependence: $(\rho-\rho(T=0)) = T^{1.7}$. This expression holds for temperatures betwee 20 K and 300 K. Wilson[1] has suggested that the unusual temperature-dependent resistivity of TiS_2 (where an $\sim T^2$ dependence was found[2]) is due to scattering of carriers by homopolar optic phonons. Our results on $Zr_xTi_{1-x}Se_2$ are consistent with this picture.

*Work supported by the NSF under grant DMR 77-10217.

+Present Address: Materials Science Center, Northwestern University.

[1]J.A. Wilson, Solid State Commun. 22, 551 (1977).

[2]A.H. Thompson, Phys. Rev. Letters 35, 1786 (1975).

JP 6 Electron Transport in Se-doped 1T-TaS_2. P. D. HAMBOURGER, Cleveland State U., and F. J. DI SALVO, Bell Laboratories. --The electrical conductivity and Hall coefficient of single-crystal 1T-$TaS_{2-x}Se_x$ ($0<x<0.05$) have been measured at temperatures of 1.3-250 K. The Hall mobility (calculated by assuming that one band of carriers is dominant) diminishes rapidly upon cooling below 45 K. Doping increases both the ratio $\mu(45\ K)/\mu(1.3\ K)$ and the maximum temperature at which the behavior $\rho=\rho_0 \exp(T_0/T)^{1/3}$ is observed.[1] These data are consistent with localization of conduction electrons at T<45 K.[1,2] Extrapolation of $\ell n\rho$ vs 1/T to T=∞ to estimate minimum metallic conductivity suggests that conduction at T<45 K is not 2-dimensional.[2,3]

[1]F. J. Di Salvo and J. E. Graebner, Solid State Commun. 23, 825 (1977).
[2]N. F. Mott, M. Pepper, S. Pollett, R. H. Wallis, and C. J. Adkins, Proc. Roy. Soc., London A345, 169 (1975).
[3]P. Fazekas and E. Tosatti (private communication).