17

Abstract Submitted

for the Atlanta Meeting of the

American Physical Society

29 March 1976

Physics and Astronomy
Classification Scheme
Numbers 72.10.Ej, 78.40.Kc

Bulletin Subject Heading
in which paper should be placed
TTF-TCNQ or Organic Metals

Pressure Dependence of the Optical Reflectance of TTF-TCNQ and TSeF-TCNQ. B. WELBER, E. M. ENGLER, P. M. GRANT, and P. E. SEIDEN, IBM Corp.--We have measured the pressure dependence of the plasma reflectance edge of TTF-TCNQ and TSeF-TCNQ with the electric vector along the high conductivity axis. For these measurements a diamond anvil cell at room temperature was employed with pressures determined by the shift in the R-line fluorescence of a ruby chip incorporated in the sample space. Experimental conditions were hydrostatic over the range studied (up to 70 kbar). At the same time it was possible to determine the change in the lattice parameter by a direct optical observation of the sample size. The plasma frequency and the scattering time have been obtained for each pressure from a fit to the frequency dependence of the data using an appropriate Drude-Lorentz expression. The optical conductivity obtained from these data will be compared to the pressure dependence of the dc conductivity[1], and the implications of this comparison will be discussed.

[1]Chu, C. W., Harper, J. M. E., Geballe, T. H. and Greene, R. L., Phys. Rev. Lett. 31, 1491 (1973).

Submitted by

B. Welber

IBM T. J. Watson Research Center
P. O. Box 218
Yorktown Heights, N.Y. 10598

Dear Paul: I'm sorry the abstract was so hastily written — but we had to meet the deadline. BW

APS News – p. 210

bulletin

OF THE AMERICAN PHYSICAL SOCIETY

MARCH 1976

INCLUDING THE PROGRAM OF THE
1976 MARCH MEETING IN ATLANTA, GA.
29 MARCH – 1 APRIL 1976

Series II, Vol. 21, No. 3 (1976)
pp. 209-488

PUBLISHED FOR THE AMERICAN PHYSICAL SOCIETY
BY THE AMERICAN INSTITUTE OF PHYSICS

Award of the American Physical Society Prize for New Materials sponsored by the International Business Machines Corporation to William G. Pfann and Henry Theuerer.

DA 3. Response of the Prize Winner. "New Materials and Solid State Devices."
W.G. PFANN, *Bell Laboratories.*

Invention of the transistor, made possible by prior advances in the purification of Si and Ge, created even more stringent demands on the purity and control of composition of these semiconductors. The demands were met, at the time needed, by strenuous effort and inspiration. Ultra-pure Ge was produced by zone refining.[1] Uniform composition (± 10% at the level of 10^{-8} atom fraction) was produced by zone leveling, a by-product of which was a proof of the existence of dislocations. Ultra-pure Si was produced by invention of float zoning,[2] and allied techniques. Ultra-purification of $SiCl_4$ by a new adsorption technique[3] made possible the first successful epitaxial mesa transistor -- which led to the broad use of epitaxy in integrated circuits. Today, zone refining has been extended to other semiconductors, metals, chemicals (more or less in that time-order). About one-third of the elements, and hundreds of compounds have been raised to their highest purity by this simple technique -- and many fundamental studies have become possible. Today, this same highly pure $SiCl_4$ is being used to develop low-loss optical fibers, of radially variable index of refraction, which fibers have major potential for communication at optical frequencies.

[1]W. G. Pfann, Trans. AIME, 194, 747 (1952); Zone Melting, John Wiley and Sons, 2nd edition, 1966.
[2]H. C. Theuerer, J. Metals, 8, 1316 (1956).
[3]H. C. Theuerer, J. Electrochem. Soc., 108, 649 (1961).

TUESDAY AFTERNOON, 30 MARCH 1976
ESSEX ROOM AT 2:00 P.M.
A.J. Epstein, presiding

ORGANIC CONDUCTORS. OPTICAL AND TRANSPORT PROPERTIES

DB 1 Core Excitons and Charge Transfer in TTF-TCNQ. J.J. RITSKO, N.O. LIPARI, Xerox Webster Research Center and P.C. GIBBONS, S.E. SCHNATTERLY, Princeton University.--Energy loss spectra of fast electrons transmitted through 1000Å thick films of TTF-TCNQ have been measured for the excitations of nitrogen, sulfur, and carbon core electrons with an energy resolution of 0.1eV. In all cases the spectra consist of sharp excitonic transitions to molecular orbitals localized on separate TTF^+ or $TCNQ^-$ ions followed at higher energies by a continuum of transitions to free electron states above the ionization threshold of TTF-TCNQ. These measurements are in excellent agreement with new synchrotron radiation absorption results. Based on published ESCA data, transitions from sulfur 2P core states occur to the Fermi level (E_F) providing a limit to the conduction band width on the TTF stack of <0.8eV. Transitions from the nitrogen 1S core state to unoccupied molecular orbitals result in a single sharp peak 0.7eV wide 1.5eV above E_F. This single peak implies a single nitrogen state in bulk TTF-TCNQ and confirms an interpretation of the two observed ESCA peaks as being surface and bulk effects rather than different TCNQ charge states in the bulk material.

DB 2 Pressure Dependence of the Optical Reflectance of TTF-TCNQ and TSeF-TCNQ. B. WELBER, E. M. ENGLER, P. M. GRANT, and P. E. SEIDEN, IBM Corp.--We have measured the pressure dependence of the plasma reflectance edge of TTF-TCNQ and TSeF-TCNQ with the electric vector along the high conductivity axis. For these measurements a diamond anvil cell at room temperature was employed with pressures determined by the shift in the R-line fluorescence of a ruby chip incorporated in the sample space. Experimental conditions were hydrostatic over the range studied (up to 70 kbar). At the same time it was possible to determine the change in the lattice parameter by a direct optical observation of the sample size. The plasma frequency and the scattering time have been obtained for each pressure from a fit to the frequency dependence of the data using an appropriate Drude-Lorentz expression. The optical conductivity obtained from these data will be compared to the pressure dependence of the dc conductivity[1], and the implications of this comparison will be discussed.

[1]Chu, C. W., Harper, J. M. E., Geballe, T. H. and Greene, R. L., Phys. Rev. Lett. 31, 1491 (1973).

DB 3 The Effects of Polarizable Side Groups on the Elec Crystal Spectra of a Linear Triatomic Chromophore. C. J. ECKHARDT, G. A. GALLUP, J. TYLICKI, University of Nebraska Lincoln. -- The two molecules, $C_4H_8OTeI_2$ and $C_4H_8STeI_2$ hav trigonal bipyramidal coordination around the Te with I occ pying the axial positions. However, the crystals are not isomorphous and linear polymeric type chains are found in crystal of the thia-compound. Specular reflection spectra have been measured from two different faces of each of the crystals over the range 1.24 - 5.70 ev. The thia-compound shows a quasi-metallic peak near 50% reflectivity at 3.1 e for the "b" - axis polarized spectrum. Spectra polarized to this axis show crystal effects. Much weaker reflectivi peaks occur at 4.3 ev in all measured polarizations. In c trast, the oxa-compound possesses reflection spectra showi no significant solid state interactions. A system of four is observed which can be related to the electronic structu the molecule. Real and imaginary parts of the optical die constant are obtained by Kramers-Kronig transforms of refl spectra. These are related to the complex polarizability ferences between the two compounds. Theoretical calculati transition energies and dipole strengths are compared with mental results, and show that the observed and calculated differences are related to differences in atomic polarizab in the side groups.