several clusters in the same crystal. The results of the two methods will be compared with each other and to available experimental results.

[1]Boudeulle, Micheline, Ph.D. Thesis, "Contribution à l'étude crystallographique d'un composé moléculaire en chaine - Cas du polynitrure de soufre $(SN)_x$", L'universite Claude-Bernard de Lyon (1974)

CM 2 LCAO Band Structure for $(SN)_x$. W.I. FRIESEN, A.J. BERLINSKY, B. BERGERSEN, L. WEILER, University of British Columbia and T.M. RICE, Simon Fraser University--The band structure of the conducting polymer $(SN)_x$ has been calculated by a generalization of the extended Hückel method of Hoffman with use made of the crystal structure determination of Boudeulle[1]. The Fermi level is found to lie in a band made up of anti-bonding π-orbitals. Because of the presence of a screw axis there is a zone boundary degeneracy which gives rise to metallic behaviour. When interchain coupling is ignored the usual instabilities associated with one dimensional metals are expected. The role of interchain coupling in stabilizing the three dimensional structure is investigated.

1. M. Boudeulle, Thesis, University of Lyon 1974.

CM 3 Pressure Dependence of Conductivity in Polysulfur Nitride $(SN)_x$. W. D. GILL and G. B. STREET, IBM Research Laboratory, San Jose, Calif.--Crystals of $(SN)_x$ have been reported[1] to behave like a one-dimensional metal with room temperature conductivity along the fiber axis as high as 1730 $\Omega^{-1}cm^{-1}$. We report the effect of hydrostatic pressure on the 4-probe dc conductivity of $(SN)_x$ crystals over the temperature range from 4°K to 300°K. At high temperatures where the conductivity varies inversely with temperature[1] there is an initial very strong increase with pressure saturating at $\sigma(P)/\sigma(0) \approx 6$ for $P \approx 12$ kbar. The implications of the pressure dependence of conductivity on the electronic structure and on transport properties will be discussed.

[1]V. V. Walatka, Jr., M. M. Labes and J. H. Perlstein, Phys. Rev. Lett. 31, 1139 (1973).

CM 4 The Dimensionality of $(SN)_x$. MARSHALL J. COHEN, C. K. CHIANG, A. F. GARITO, A. J. HEEGER, A. G. MACDIARMID, and C. M. MIKULSKI, Univ. of Penna.--The thermopower and dc conductivity were measured as a function of temperature both parallel and perpendicular to the chain axis of $(SN)_x$. At room temperature, the parallel and perpendicular thermopowers are -1.5 and -3.5 $\mu V\text{-}K^{-1}$, respectively, while the parallel conductivity is approximately 2.5×10^3 $^{-1}\text{-}cm^{-1}$. The measured perpendicular conductivity is smaller and dominated by the polycrystalline nature of the samples in that direction. These data together with the polarized reflectance and low temperature specific heat data are used to discuss the dimensionality of the electrical properties of $(SN)_x$.

CM 5 Polarized Reflectance of $(SN)_x$. A. A. BRIGHT, M. J. COHEN, A. F. GARITO, A. J. HEEGER, A. G. MACDIARMID, and C. M. MIKULSKI, Univ. of Penna.--Polarized reflectance measurements have been made on single crystals and epitaxial films of polymeric sulfur nitride $[(SN)_x]$ from 500 cm^{-1} to 30,000 cm^{-1}. The spectra of the films and of the crystals agree well. The observed anisotropic reflectance is consistant with $(SN)_x$ being a highly anisotropic metal. For polarization parallel to the polymer axis, a Drude-like reflectivity is observed with a plasma edge at 22,000 cm^{-1} (2.85 eV), and a high reflectance throughout the infrared. The results for both parallel and perpendicular polarization will be discussed in relation to the electrical, thermal, and magnetic properties of this material.

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CM 6 Optical Properties of $(SN)_x$ Films. G. B. STREET, P. M. GRANT and R. L. GREENE, IBM San Jose.--The reflection and transmission spectra of thin polycrystalline films of polysulphur nitride $(SN)_x$ have been recorded in the wavelength range 2000Å - 40μ. A reflectance edge of medium steepness is observed near 2.5eV which is possibly associated with metallic behavior. Structure in the infrared occurs at 10.1, 13.2, 15.0, 16.2 and 21.0μ which is due to vibrational or vibronic states. The metallic-like reflectance edge is analyzed in terms of a tight-binding model for various band parameters and the results compared to findings from specific heat data.

CM 7 Low Temperature Specific Heat of Polysulfur Nitride, $(SN)_x$.* J.M.E. HARPER, Stanford Univ. and P.M. GRANT, G.B. STREET, and R.L. GREENE, IBM Res. Lab., San Jose--Specific heat measurements of crystalline $(SN)_x$ have been made over the range 1.5°K to 55°K. A fit of the data below 3.2°K to the relation $C = \gamma T + \beta T^3$ yields $\gamma = 18 \pm 2 \times 10^{-6}$ j/gm-K^2, and $\beta = 8.8 \pm 0.4 \times 10^{-6}$ j/gm-K^4. The linear temperature term is interpreted as arising from an electron state density of 0.18 states/eV-spin-molecule. Above 3.2°K the lattice heat capacity departs dramatically from T^3 behavior. The region from 4°K to 25°K follows a $T^{5/2}$ dependence with a gradual transition to lower temperature dependences above 25°K. This result is consistent with the chain-like structure of $(SN)_x$ and suggests the interchain coupling is weak. No evidence of a discrete phase transition was found between 1.5 and 55°K.

*Research at Stanford sponsored by the Air Force Office of Scientific Research, Air Force Systems Command, USAF, under Grant No. AFOSR-73-2435A.

CM 8 Conductivity of Polysulfur Nitride Below 4.2°K. R. L. GREENE and G. B. STREET, IBM San Jose, and L. J. SUTER*, Stanford University.--The d.c. conductivity (σ) of $(SN)_x$ has been measured between 0.07°K and 4.2°K. The conductivity remains metallic-like down to .07°K, i.e. no metal-insulator transition occurs as in other quasi one-dimensional conductors. The significance of this result for understanding the phase transition in other 1D conductors will be discussed.

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CM 9 Anomalous Pressure Dependence of the Metal-Nonmetal Transition of NiS.* R. E. Jones Jr. and W. J. Keeler, Lakehead U., Thunder Bay, Ont.--Electrical resistivity measurements were used to determine the pressure dependence of the metal-nonmetal transition temperature, T_t, in hexagonal NiS to 14 kbar. Below 4 kbar, pressure suppresses the transition with $dT_t/dP = -8.4$ K/kbar for a powdered sample with $T_t = 266$ K at zero pressure. However, near 4.5 kbar a local increase in T_t is observed. Above 5 kbar T_t again decreases with pressure and the magnitude of the pressure derivative appears to be somewhat greater than at low pressures. This result is consistent with the neutron diffraction work of Smith and Sparks[1] who found that the a- and c-axis parameters show an anomalous increase for a small pressure interval near 5 kbar.

[1]F. A. Smith and J. T. Sparks, J. Appl. Phys. 40, 1332 (1969).

*Supported by grants from the Defence Research Board and the National Research Council of Canada.

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OF THE AMERICAN PHYSICAL SOCIETY

MARCH 1975

INCLUDING THE PROGRAM OF THE
1975 MARCH MEETING IN DENVER, COLO.
31 MARCH–3 APRIL 1975

Series II, Vol. 20, No. 3 (1975)
pp. 273- 528

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