Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Optical Investigations on The Transition Metal Selenides $Nbse_3$ And $(Tase_4)_2I$

H. P. Geserich [a] , G. Scheiber [a] , F. Lévy [b] , P. Gressier [c] & P. Monceau [d]

[a] Institut für angewandte Physik, Universität, Karlsruhe, Fed.Rep.of Germany

[b] Institut de physique appliquée, EPF, Lausanne, Switzerland

[c] Laboratoire de Chemie de Solides L.A., 279, Nantes, France

[d] Centre de Recherches sur les Très Basses Temperatures, C.N.R.S., Grenoble, France

Version of record first published: 20 Apr 2011.

To cite this article: H. P. Geserich , G. Scheiber , F. Lévy , P. Gressier & P. Monceau (1985): Optical Investigations on The Transition Metal Selenides $Nbse_3$ And $(Tase_4)_2I$, Molecular Crystals and Liquid Crystals, 121:1-4, 19-22

To link to this article: http://dx.doi.org/10.1080/00268948508074825

Mol. Cryst. Liq. Cryst. 1985, Vol. 121, pp. 19-22
0026-8941/85/1214-0019/$10.00/0

Printed in the United States of America

OPTICAL INVESTIGATIONS ON THE TRANSITION METAL SELENIDES $NbSe_3$ AND $(TaSe_4)_2I$ *

H.P.GESERICH and G.SCHEIBER
Institut für angewandte Physik, Universität Karlsruhe, Fed.Rep.of Germany

F.LÉVY
Institut de physique appliquée, EPF Lausanne, Switzerland

P.GRESSIER
Laboratoire de Chemie de Solides L.A. 279, Nantes, France

P.MONCEAU
Centre de Recherches sur les Très Basses Temperatures, C.N.R.S. Grenoble, France

Abstract The polarized reflectance spectra of $NbSe_3$ and $(TaSe_4)_2I$ and 300 K are reported. The experimental data are analyzed in terms of a Lorentz-Drude and a tight binding model.

INTRODUCTION

The one-dimensional metallic character of the transition metal chain compounds $NbSe_3$ and $(TaSe_4)_2I$ manifests itself by the formation of charge density waves which are closely connected with phase transitions and non-linear transport phenomena[1,2]. However, in spite of this common feature the structural anisotropy of both chain compounds is quite different. Whereas $NbSe_3$ shows an intrachain

* This work was supported by the Stiftung Volkswagenwerk.

metal-metal distance of 3,48 Å and interchain metal-metal distances between 4.25 and 4.45 Å, the corresponding values in $(TaSe_4)_2I$ are 3.21 Å and 6.7 Å, revealing a clearly higher anisotropy[3,4]. In the present contribution the transport properties of both compounds along the metallic axis are compared by optical investigations.

EXPERIMENTAL RESULTS AND DISCUSSION

Fig.1 shows the polarized reflectance spectra with a metallic plasma edge for the polarization direction parallel to the metallic chains, and the nearly constant re-

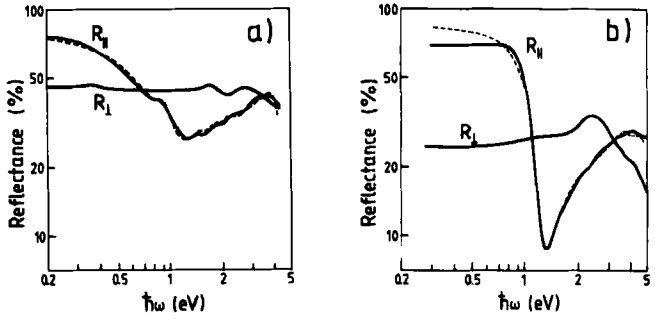

FIGURE 1 Polarized reflectance spectra of $NbSe_3$(a)[5] and $(TaSe_4)_2I$ (b). Dashed lines: Lorentz-Drude fit.

flectivity of a semiconductor for $R_\perp$. The smoother plasma edge of $NbSe_3$ indicates a shorter collision time of the free carriers in this material. Analyzing $R_\parallel$ by a Lorentz-Drude model, the spectral distribution of the real and the imaginary part of the dielectric function, $\varepsilon_1(\hbar\omega)$ and $\varepsilon_2(\hbar\omega)$, are obtained (Fig.2a,b). From the relation $\sigma(\hbar\omega) = \varepsilon_0\omega\,\varepsilon_2(\hbar\omega)$ one obtains the conductivity function, which can be extrapolated to zero energy, leading to an optical value for the dc-conductivity. As the free carrier concentration can be deduced from a discussion

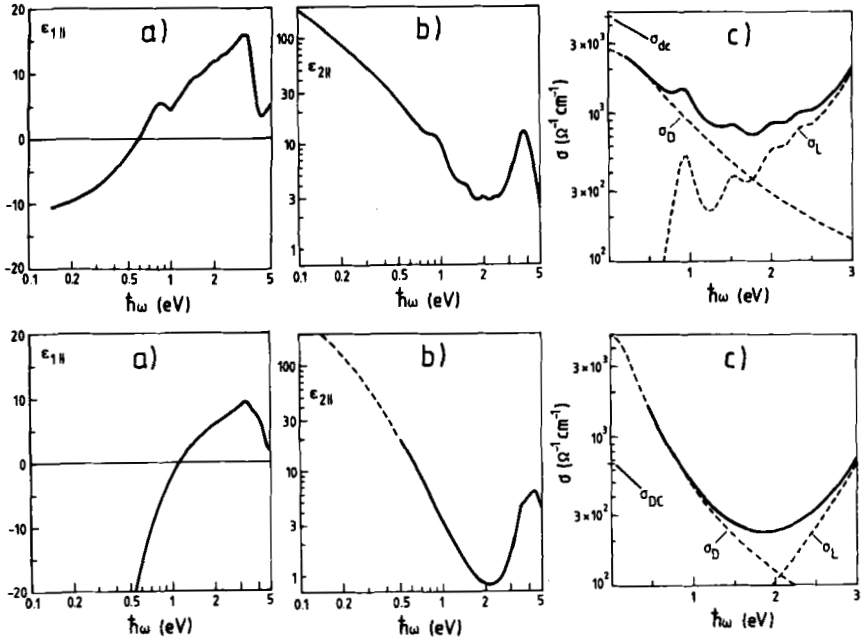

FIGURE 2 Dielectric function (a,b) and conductivity function (c) of $NbSe_3$ (upper part) and of $(TaSe_4)_2I$ (lower part). σ_D, σ_L and Lorentz contribution.

of the chemical bonds[1], also the effective mass can be calculated from the optical results. On the basis of a simple tight binding model follows further the band width 4t, the Fermi energy E_F, and the mean free path Λ.

TABLE I Transport properties of $NbSe_3$ and $(TaSe_4)_2I$

	N ($10^{21}/cm^3$)	$\frac{m^*}{m_o}$	τ (10^{-15}sec)	4t (eV)	E_F (eV)	Λ Å
$NbSe_3$	3.9	0.4	1	3.5	0.5	7
$(TaSe_4)_2I$	3.2	0.4	2	4.0	0.6	15

The most surprising results are the short mean free path of $NbSe_3$ and the high optical value of $4\times10^3(\Omega cm)^{-1}$ for the dc-conductivity of $(TaSe_4)_2I$, which is 6 times larger than the experimental dc-value.[2] The latter result, perhaps, indicates an influence of fluctuations, due to the phase transition at 263 K, onto the dc-conductivity at 300 K[6]. On the other hand, the value of the width of the conduction band of $(TaSe_4)_2I$ is in excellent agreement with band structure calculations if one takes into account that the tight-binding band must be folded back into a smaller Brillouin zone because the crystallographic unit cell contains four tantalum atoms along the chain axis[7]. On the contrary the width of the conduction band of $NbSe_3$ given her is considerably higher than the values of about 1.5 eV resulting from band-structure calculations[8-11]. This is presumbly due to the more complicated band structure of $NbSe_3$ with six nonequivalent metal chains.

REFERENCES

1. For a review: P.Monceau, J.Richard, M.Renard, Phys.Rev. B,25,931(1982) and J.Richard,P.Monceau, M.Renard, Phys.Rev.B,25,948 (1982).
2. Z.Z.Wang, M.C.Saint-Lager, P.Monceau, M.Renard,P.Gressier, A.Meerschaut,L.Guemas, and J.Rouxel,Solid State Comm., 46, 325 (1983).
3. P.Monceau, N.P.Ong, A.M.Portis, A.Meerschaut and J. Rouxel, Phys.Rev.Lett., 37, 602 (1976).
4. P.Gressier, L.Guemas, and A.Meerschaut, Acta Cryst.B, 38, 2877 (1982).
5. H.P.Geserich, G.Scheiber, F.Lévy, and P.Monceau,Solid State Comm., 49,335 (1984).
6. M.Maki, M.Kaiser, A.Zettl, and G.Grüner,Solid State Comm. 46, 497 (1983).
7. P.Gressier, M.H.Whangbo, A.Meerschaut, and J.Rouxel, to be published.
8. R.Hoffmann, S.Shaik, J.C.Scott,M.H.Whangbo, and M.J.Foshee, J.Solid State Chem., 34,263 (1980).
9. D.W.Bullet, J.Phys.C.,15,3069 (1982).
10. N.Shima,J.Phys.Soc.Jap., 52, 578 (1983).
11. M.H.Whangbo and P.Gressier, to be published.