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OPTICAL PROPERTIES OF TIN DISULPHIDE IN THE FAR-INFRARED SPECTRAL RANGE

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Abstract. The far-infrared reflectivity of single-crystal SnS_2 has been measured with polarized light $\vec{E} \perp \vec{c}$ and $\vec{E} \parallel \vec{c}$, at a room temperature. By using the Kramers-Krönig analysis and four-parameter fitting procedure, the spectra obtained are numerically analyzed and infra-active TO and LO modes and damping factor determined. The Reststrahlen peaks were observed for the case $\vec{E} \perp \vec{c}$ and $\vec{E} \parallel \vec{c}$.

Introduction

Tin disulphide is a layered semiconductors from the group $A^{IV}B^{VI}_2$. It crystallizes in a hexagonal sistem with lattice parameters: a = 0,3639 nm and c = 0,5884 nm.[1,2,3]

The optical energy gap for polarization $\vec{E} \perp \vec{c}$ amounts to E_g^{opt} = 2,20 eV[4,5,6] and the change factor of the energy gap with the temperature for the same light polarization is $\partial E_g/\partial T = -9 \cdot 10^{-4}$ eV/K.[7,8] The refractive index SnS_2 has been experimentally determined within the spectral range 0,5 μm - 40 μm for both polarizations of light. The existence of Reststrahlen phenomena has been established and the optical modes determined.[9]

In this paper are given the results of measuring of reflectivity SnS_2 at a room temperature and within the spectral range 25-250 μm, for light polarization $\vec{E} \perp \vec{c}$ and $\vec{E} \parallel \vec{c}$.

The experimental date are numerically analized by using the Kramers-Krönig analysis and the fitting procedure.

Experimental

The reflection spectra SnS_2 were determined on monocrystal samples obtained by Bridgman method [8]. Room-temperature spectra were obtained using a BECKMANN FS 720 Fourier spectrometer.

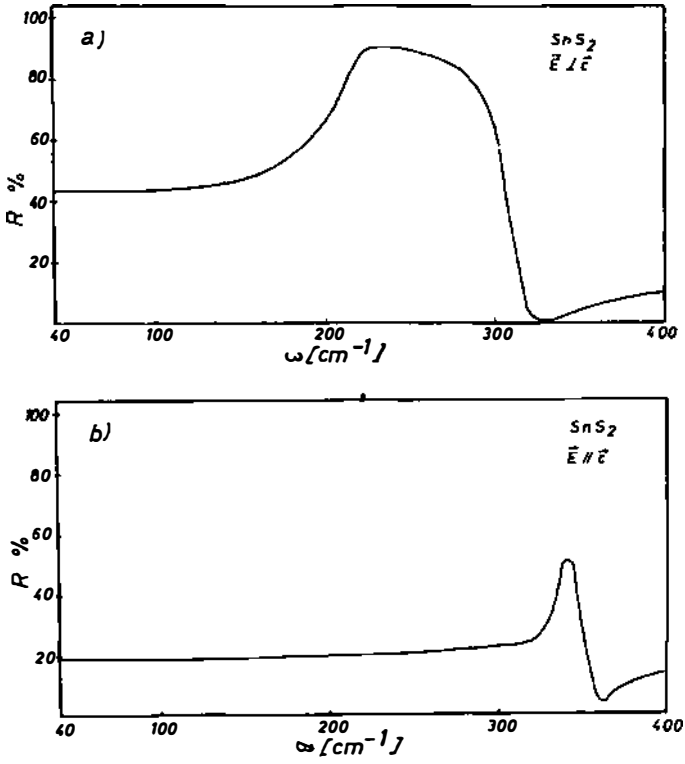

Fig.1. Room-temperature IR - reflectance spectra of SnS_2

The appearance of reflection spectra is given on Figs.1.a) and 1.b). Two Reststrahlen peaks are visible on reflection spectra one at each light polarization.

Using the dependence $R(\omega)$ as initial datum, the Kramers-Krönig integration gave the following values for optical parameters: wave numbers of ω_{LO} -longitudinal and ω_{TO} -transversal optical mode; γ_{LO} and γ_{TO} -damping factor of optical modes; dielectric permeability ε_o at low and ε_∞ at high frequencies. (Table 1.)

Further analysis of the reflection spectrum has been car-

ried out by the method of numerical fitting, by comparing the results obtained experimentally with the results obtained by applying the selected theoretical model, describing the phenomenon studied.

	ω_{TO} /cm^{-1}/	ω_{LO}/cm^{-1}/	γ /cm^{-1}/	ε_∞	ε_o	$\Delta\varepsilon$
$\vec{E}\perp\vec{c}$	204	318	11	5,8	16,5	10,7
$\vec{E}\parallel\vec{c}$	330	360	10	6,7	7,1	0,3

Table 1. The values of optical parameters SnS_2 obtained on the basis of Kramers-Krönig integration.

In this case the harmonic oscillator with damping is used as a model describing the lattice vibrations under the effect of infrared radiation.

On the basis of algorithm of Gervais and Piriou[10], where the starting parametar ω_{LO}, ω_{TO}, γ_{LO}, γ_{TO}, ε_∞, and the dielectric permeability defined by the expression

$$\varepsilon = \varepsilon_\infty \prod_j \frac{\omega_{jLO}^2 - \omega^2 + i\gamma_{jLO}\omega}{\omega_{jTO}^2 - \omega^2 + i\gamma_{jTO}\omega}$$

the following values are obtained for the stated optical parameters.(Table 2.)

	ω_{TO}/cm^{-1}/	ω_{LO}/cm^{-1}/	γ_{TO}/cm^{-1}/	γ_{LO}/cm^{-1}/	ε_∞	ε_o
$\vec{E}\perp\vec{c}$	206,5	313,5	12,5	10	7,6	17,4
$\vec{E}\parallel\vec{c}$	339	354,5	11,5	5	6,45	6,8

Table 2. The values of optical parameters SnS_2 obtained on the basis of four-parameters fitting procedure.

The experimental reflection spectra and the spectra obtained numerically are given on Figs. 2.a), and 3.a) for both light polarizations. Excellent matching of experimental results and those obtained numerically is noticeable. Figures 2.b), 2.c) and 3.b), 3.c) show the dispersion spectra the real and imaginary part of refractive index and the real and imaginary part of dielectric permeability for the stated polarization.

Discussion

The results of Kramers-Krönig analysis and the fitting proce-

dure have been compared through LST relation and the fitting procedure has given much better maching so we shall deal only with these results.

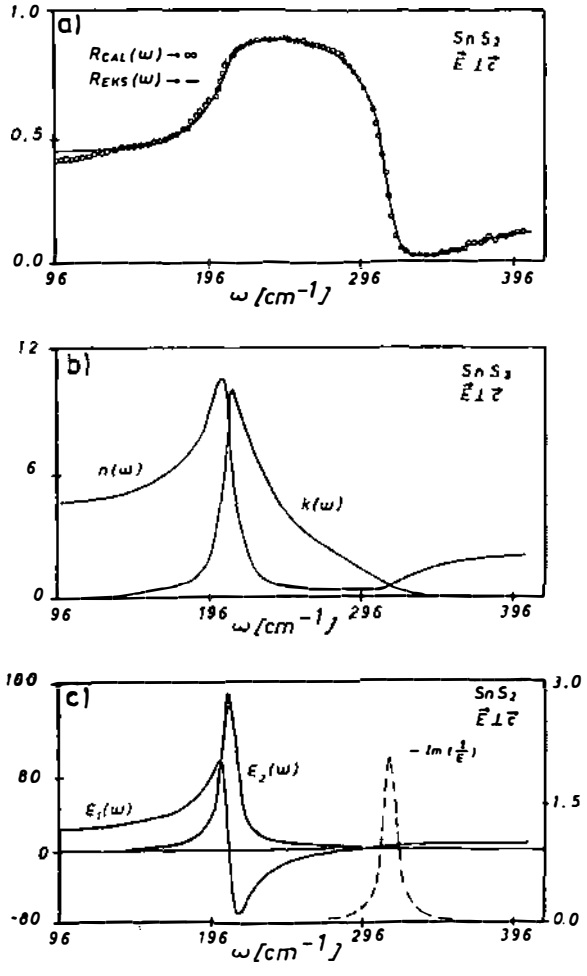

Fig.2. Frequency dependence of reflection coefficient R, optical constants n,k and dielectric permeability for SnS_2.

Considerable anisotropy of optical properties of SnS_2 subject to the observed direction in crystal has been noticed. By comparing of dielectric permeability at low and high frequencies is noticed in ionic contribution to dielectric permeability for the direction normal to $\vec{c}$-crystal axis and the direction parallel to $\vec{c}$-crystal axis. This shows that the chemical bonds in the direction normal to $\vec{c}$-axis are more of a ionic

character than the bonds to its $\vec{c}$-axis. This is also indicated by the calculated energy of the oscillator the values of which are given in Table 3.

	$\Delta\varepsilon = \varepsilon_0 - \varepsilon_\infty$	E_{0s} /cm^{-2}/
$\vec{E} \perp \vec{c}$	9,8	426 000
$\vec{E} \parallel \vec{c}$	0,4	48 000

Table 3. Ionic contribution to dielectric permeabilitu and energy oscillator of SnS_2.

The results were expected since the general characteristic of the layer material is that

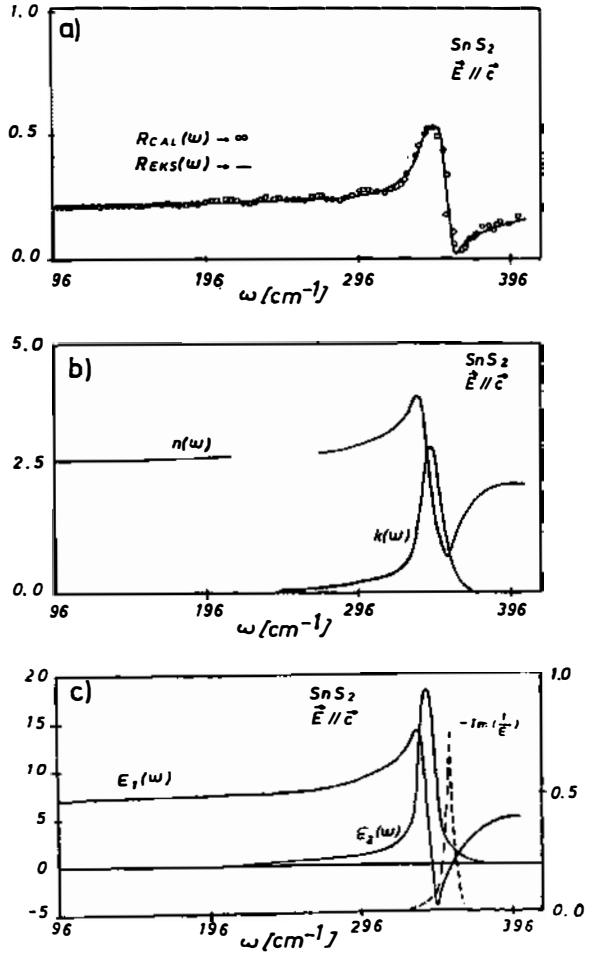

Fig.3. Frequency dependence of reflection coefficient R, optical constants n,k and dielektric permeability for SnS_2.

atoms within one layer are connected by strong bonds (ionic, covalent) and that the bonds between the layers are of Van der Valse type.

Acknowledgments

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References

1. Oftedal,I., Z.Physik.Chem.,(Leipzig),134,301, 1928.
2. Grenaway,D.L., R.Nitsche, J.Phys.Chem.Solids, vol 26,pp. 1445-1448, 1965.
3. Greenwood,N.N., Jonic crystals, lattice defects and non-stoichiometry, Butterworths, London 1968.
4. Domingo,G., R.S.Itoga, C.R.Kannewurf, Phys.Review, vol. 143, No.2, pp.536-541, 1966.
5. Lee,P.A., G.Said, R.Davis, T.H.Lim, J.Phys.Chem.Solids, vol.30, pp.2719-2729, 1969.
6. Murray,R.B., R.H.Williams, J.Phys. C, Solid state Phys. vol.6, pp.3643-3651, 1973.
7. Donetskikh,V.I., E.A.Kulyakhina, V.V.Solobev, V.I.Shatanov, S.G.Kroitoru, E.F.Zagainov, V.P.Zlomanov, Fiz.Tekh. Poluprovodnikov, 2. pp.250-255, 1976.
8. Mitrinović,M.D., P.M.Nikolić, Z.V.Popović, S.S.Vujatović, Fizika, vol.8, supplement, pp.82-85, 1976
9. Lucovsky,G.,J.C.Mikkelsen, W.Y.Jung, R.M.White, R.M.Martin, Physical Review B, vol.14, No.4, pp.1663-1669, 1976.
10. Gervais,F., B.Piriou, Phys. C, Solid state Phys., vol.7, pp.2374-2386, 1974.