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Sobotta H., Neumann H., Dreiling R., Syrbu N. N.

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*Fachbereich Physik, Universität Leipzig<sup>1)</sup> (a) and  
Faculty of Radioengineering, S. Lazo Polytechnic Institute, Kishinev (b)*

## Infrared Lattice Vibrations of TlAsS<sub>2</sub>

By

H. SOBOTTA (a), H. NEUMANN (a), R. DREILING (a), and N. N. SYRBU (b)

The ternary compound TlAsS<sub>2</sub> belongs to the family of TI–V–VI<sub>2</sub> semiconductors with V = As, Sb, Bi and VI = S, Se, Te that have been investigated rather extensively with regard to their phase diagrams, electronic band structure, and transport properties [1]. However, the emphasis of previous studies was mainly on the small-gap selenides and tellurides [1], recently also on TlSbS<sub>2</sub> ([2] and references cited therein), while the other sulphides of this compound family are less investigated. In the case of TlAsS<sub>2</sub> the experimental knowledge of the fundamental physical properties is limited to the gap energy deduced from optical absorption spectra of thin films [3] and some first results regarding the lattice vibrational properties obtained from unpolarized Raman scattering spectra on small single crystals and infrared transmission measurements on powdered polycrystalline material embedded in polyethylene [4]. It was the aim of the present study to get some more insight into the lattice vibrational characteristics of TlAsS<sub>2</sub> and their correlation with specific structural features of the compound by measuring and analysing polarization-dependent infrared reflectivity spectra on single crystals.

From structure studies reported in the literature [5, 6] it follows that TlAsS<sub>2</sub> crystallizes in a monoclinic lattice with space group C<sub>2h</sub><sup>2</sup>, with 8 molecules per unit cell, and with all atoms in general positions. Since the primitive cell is identical with the unit cell the phonon spectrum of the compound consists of 96 branches. According to group theory the irreducible representation of the 93 optical phonon normal modes at the centre of the Brillouin zone is given by

$$\Gamma_{\text{opt}} = 24A_g + 24B_g + 23A_u + 22B_u,$$

while the acoustic modes comprise the representations  $1A_u + 2B_u$ . Of the optical modes the  $A_g$  and  $B_g$  modes are Raman active, the  $A_u$  modes are infrared active for the polarization  $E \parallel c$  of incident radiation, and the  $B_u$  modes are infrared active for any polarization  $E \perp c$ .

The samples used in the experiments were needle-like single crystals grown by chemical transport. They had typical diameters of 1 to 2 mm, lengths of 8 to 15 mm, and revealed a number of small faces with different orientation which were optically smooth and, thus, directly suited for optical measurements without further surface preparation. X-ray diffraction was used to confirm the structure of the compound and to determine the crystallographic orientation of the various faces on the crystals. As a result we were able to select faces which allowed us to measure infrared reflectivity spectra for the polarization direction  $E \parallel c$  and for two different polarizations with  $E \perp c$ , namely  $E \parallel b$  and  $E \perp b$ . The

<sup>1)</sup> Linnestr. 5, O-7010 Leipzig, FRG.