

PREPARATION AND SOME PHYSICAL PROPERTIES OF $Al_2In_{12}S_{21}$

B. ETLINGER

"Rudjer Bošković" Institute, Zagreb, Yugoslavia

PREPARATION: Crystals of $Al_2In_{12}S_{21}$ ($Al_2S_3 + 6In_2S_3$) are prepared by modified SSD (synthesis, solute, diffusion) technique¹. A schematic diagram of the apparatus and its temperature profile is shown in Fig. 1. Aluminum (6N) and indium (6N) are mixed together in 1 to 6 ratio. A crucible containing aluminum and indium is located at the upper portion of a reaction vessel at the temperature gradient ($50^\circ C/cm$). The upper surface of indium-aluminum melt is held at temperature, T_H , higher than the temperature at bottom part of the crucible. Temperatures at any part of the crucible are held below the melting point of $Al_2In_{12}S_{21}$. Sulfur is placed at the bottom part of the vessel at constant temperature, T_S . The temperature T_S is usually maintained at $500^\circ C$, so that the sulfur vapour pressure is 2 atmospheres, which is probably, higher than the dissociation pressure of $Al_2In_{12}S_{21}$ at T_H . While these temperatures are maintained in the vessel, sulfur vaporizes and reacts with aluminum and indium at the surface of the melt and $Al_2In_{12}S_{21}$ is formed as a film at the surface which dissolves and the solute, sulfur, diffuses into the indium-aluminum melt towards the lower temperature portion. The concentration of the solute increases to saturation at the bottom of the crucible, and then crystal starts growing there. The diffusion coefficient of sulfur was obtained from the growth rate and found to be $4.7 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ at $1060^\circ C$.

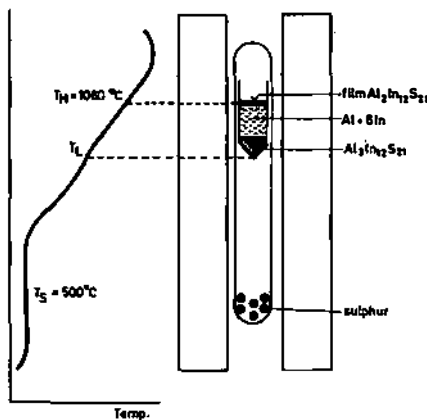


Fig. 1. Schematic diagram of the apparatus of $Al_2In_{12}S_{21}$ crystal growth by SSD method and its temperature profile.

PHYSICAL PROPERTIES: The polycrystals obtained were compact, with relatively large crystalline grains (1-2 mm), and reddish in appearance (transparent for wavelengths higher than 5800 \AA). Density was determined to be 4.32 g cm^{-3} . X-ray diffraction analysis has shown that

$\text{Al}_2\text{In}_{12}\text{S}_{21}$ belongs to the $I4_1/amd$ space group with unit cell $a=7.49 \text{ \AA}$

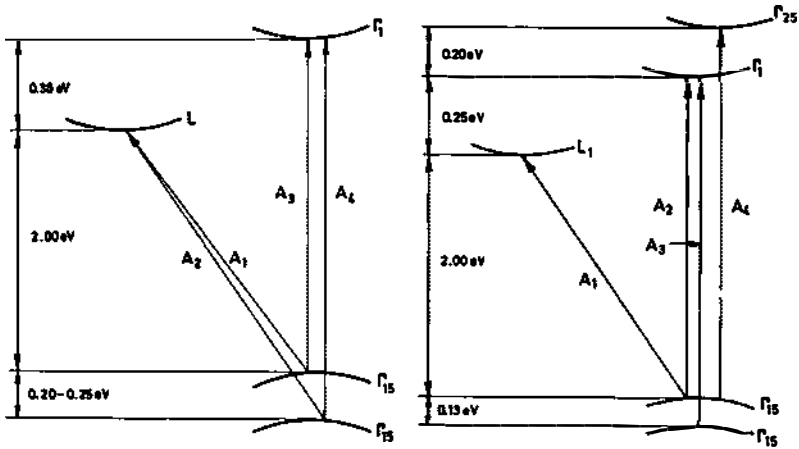


Fig.2. Models of the energy band structure of $\text{Al}_2\text{In}_{12}\text{S}_{21}$.

and $c=31.76 \text{ \AA}$. Conductivity of undoped $\text{Al}_2\text{In}_{12}\text{S}_{21}$ is very low at room temperature i.e. $9.0 \times 10^{-11} \Omega^{-1} \text{ cm}^{-1}$, somewhat higher for copper ($1.1 \times 10^{-10} \Omega^{-1} \text{ cm}^{-1}$) and bismuth ($6.5 \times 10^{-10} \Omega^{-1} \text{ cm}^{-1}$) dopands, and much larger ($4.8 \times 10^{-7} \Omega^{-1} \text{ cm}^{-1}$) in the case of cadmium-doped crystal (in all cases doped with 10^{17} atoms/cm³). The TEMF probe showed n-type conductivity in the case of cadmium-doped sample, and the energy level located at 0.50 eV below the conduction band. The spectral response of photoconductivity (taken from 4200 to 8000 Å) at room temperature shows four prominent peaks at 2.00, 2.25, 2.38 and 2.58 eV. Those results are in qualitative agreement with those obtained so far for In_2S_3 and CdIn_2S_4 , but the peaks are shifted to the wavelengths shorter than in the case of In_2S_3 . The peaks indicate the existence of the indirect transition in the energy gap and the appearance of the spin-orbit splitting in valence band. Fig.2. shows two possible models of the energy band structure of $\text{Al}_2\text{In}_{12}\text{S}_{21}$.

REFERENCES

1. K. KANEKO and all, J. Electrochem. 121, 557 (1974).
2. B. ETLINGER, Proc. of XIII Inter. Conf. of Physc. of Semiconductors, Roma, 30.8.-3.9.1976., Italy.
3. S. I. RADAUTSAN, Phys. Stat. Sol. (a) 15, 295 (1973).