PREPARATION AND FAR INFRARED PROPERTIES OF $CdIn_2Te_4$ AND $ZnIn_2Te_4$

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ABSTRACT: Semiconducting polycrystals of the compound, $CdIn_2Te_4$ and $ZnIn_2Te_4$, were obtained using the Bridgeman procedure. Crystallographic properties were measured and also far infrared reflectivity was measured in the range betwen 40 and 400 cm^{-1}.The experimental data were numerically analysed and ionic bonds in both compounds discussed. The influence on the ionic bonds of the replacement of Cd atoms with Zn was also analysed.

1. INTRODUCTION

Many papers about $A^{II}B_2^{III}C_4^{VI}$ componds have recently been published. However, attention has mostly been paid to $HgIn_2Te_4$ /1/, then $ZnIn_2S_4$ /2,3,4/ and partly to cadmium gallium chalcogenides for instance $CdGa_2S_4$, $CdGa_2Se_4$ and $CdGa_2Te_4$ /5,6,7/. All of them have the S_4^2 structure. The properties of these compounds can be studied by observing the properties of the two component compounds. Thus,for $CdIn_2S_4$ they are CdS and In_2S_3 /6/.

As far as we know there are only two published papers concerning $CdIn_2Te_4$ one about its crystallographic characteristics /8/ and the otherrecording some optical properties in the visible range /9/.

The compound $ZnIn_2Te_4$ has not been studied yet. Except that its crystallographicproperties were observed by Hahn /8/ a long time ago.

Generally, $A^{II}B_2^{III}C_4^{VI}$ compounds are studied because of their well exposed photoconductive properties.

In this work the way of preparation, crystallographic and far infrared optical properties of $CdIn_2Te_4$ and $ZnIn_2Te_4$ were investigated.

2. Experimental

Polycrystallinesamples of $CdIn_2Te_4$ and $ZnIn_2Te_4$ were obtained using the Bridgeman procedure. The elements of at least 99.9990% purity and in stoichiometric proportion were placed in a quartz tube which was evacuated to about lo^{-5} mmHg and then seeled off. The ampoules were put in a vertical furnace which was heated to about lo50°C. After several hours the ampoule was lowered down into the cooler zone at a speed of about lmm/h. It was confirmed that the produced crystals were single faced polycrystals by x-ray powder photography. The calculated values of lattice parameters were a=6.11 Å and c = 12.22 Å for $ZnIn_2Te_4$ and a= 6.205 Å and c= 12.405 Å for $CdIn_2Te_4$.

The speciemns for optical measurements were cut from ingots. Slices were between 0.5 and lmm thick. The samples were then polished on one side using a conventional polishing technique.

The far infrared reflectivity measurements were performed using a Beckmann FS 720 Fourier spectrometer. The variatbn of near normal incident reflectivity for $CdIn_2Te_4$ and $ZnIn_2Te_4$ are given in figures 1 a and 1 b respectively, where the experimental dataare represented by squares. The solid lines were calculated using the oscilator parameters, which were obtained by numerical analysis carried out withthe aid of a fitting procedure,

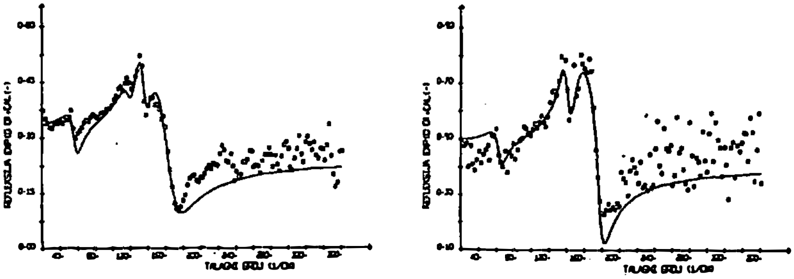

Fig. 1. Far infrared reflectivity of $CdIn_2Te_4$ (a) and $ZnIn_2Te_4$ (b). The solid line were calculated using the oscillator parameters given in Table 1 .

according to the Gervais four parameters model. /1o/. The values of transversal (ω_{TO}) and longitudinal (ω_{LO}) optical modes and their damping factors (γ_{TO} and γ_{LO}) for four oscillators of $CdIn_2Te_4$ and three oscillators of $ZnIn_2Te_4$ are given in Table 1. Table 1.

	$CdIn_2Te_4$				$ZnIn_2Te_4$		
	I	II	III	IV	I	II	III
$\omega_{TO}(cm^{-1})$	75.5	138	151	163.5	82	155	171
$\omega_{LO}(cm^{-1})$	78	140	156.5	189	85	163	200
$\gamma_{TO}(cm^{-1})$	13.5	13	12	22.5	14	8	11
$\gamma_{LO}(cm^{-1})$	9.5	1o	9.5	23.5	9.5	7	9
ε_∞	8.5				20		

The real /RE(EPS)(——--) / and imaginary /In(EPS)(-----)/ parts of the complex dielectric function for both compounds are given in figures 2a and 2b.

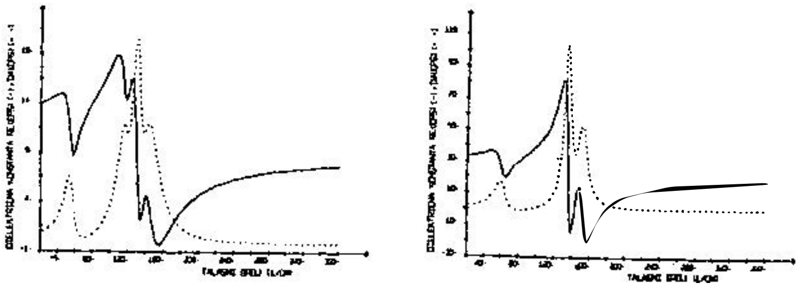

Fig. 2. Real and imaginary parts of the complex dielectric function of $CdIn_2Te_4$(a) and $ZnIn_2Te_4$(b)

3. DISCUSSION

The number of infrared and Raman active modes were calculated for $CdIn_2Te_4$ and $ZnIn_2Te_4$ using Adams-Newton Tables /11/. Since their tetragonal lattice structure, spaced group S_4^2 and Wyckof´s sites were known, the complete number of these modes was:

$$\Gamma = 3A+6B+6E .$$

The number of acoustical modes is $N_A=3$ and they have the symmetry (B+E). In that case there are three (3A) Raman active modes and 10 infrared active modes. (5B+5E), five for $E\perp c$ and five for E//c.

In this work we have observed only four and three infrared active modes for $CdIn_2Te_4$ and $ZnIn_2Te_4$, respectively. That means that the nonobserved oscillators should be much weaker compared with the observed ones. They probably were not observed for two reasons. First, the level of noisy was of a similar height to the signal and secondly the crystals were polycristalline so that oscillators for E//c and $E\perp c$ could overlap. It is very interesting to compare the oscillators with the highest wavenumber for both compounds. Judging by Fig. 1a and 1b it is about 163 cm^{-1} for $CdIn_2Te_4$ and about 170 cm^{-1} for $ZnIn_2Te_4$. This is as expected because Cd has a larger atomic weight than Zn. If we make a similar comparison between $CdIn_2Te_4$ and $CdGa_2Te_4$ we can see that the position of the observed oscillator is moved much further to about 21o cm^{-1} /12/. When the heavier atoms of In are replaced with the much lighter Ga.

From these data onecan conclude that the roles of the ionic bond between Cd and In atoms is relatively more important than that of the ionic bonds between these and the chalcogenide elements.

4. References

1. Miller A., er al., J.Phys. C:Solid State Phys. 9,2997-3011 (1976).
2. Gombia, E., et al., Phys. Stat.Soc. (a) 34, 651-5 (1976).
3. Radantsan S. I et al., Fiz.Teh. Poluprov. ., 9, 2278-83(1975).
4. Unger W.K., Solid St.Comm. 25, 913-15 (1978).
5. Randastan, S.I. et al., Soc. Phys. Semicond. 11, 38 (1977).
6. Radanstan S.I. et al., Fizika i tehn. Poluprov.,11, 69-74 (1977).
7. Nikolić, P., et al., Fizika 10,Suppl.2,362 (1978).
8. Hahn H., Frank G., Klinger W., Storger A.D. and Storger G., Zeit fur Anorg Chemie 279, Heft 5-6, 241-8(1955).
9. Radantsan, S.I., et al., Troinie poluprovodniki $A^{II}B^{IV}C_2^{V}$ and $A^{II}B_2^{III}C_4^{VI}$, "Štinca", Kišinev 230-33 (1972).
lo. Gervais, F. Pirov. B, Phys. Rev. BID, 1642,1974.
11. Adams D.M. and Newton D.C., "Tables for Factor Group and Point Group Analysis, Beckman, RIIC, 1970.
12. P.M.Nikolić, and S. Stoilkovic to be published.