

STUDY OF BONDING IN ZnSe AND CdTe BY COMPTON SCATTERING TECHNIQUE

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In this paper we report on the application of Compton scattering technique for the study of bonding in II-VI semiconductor compounds ZnSe, and CdTe. 59.54 keV gamma rays from a 5 Ci Am²⁴¹ source were scattered by the samples at about 170° and analysed by the high purity Ge detector. The overall momentum resolution of the spectrum was about 0.6 a.u. Since all abovementioned compounds have same number of valence electrons, so we have compared the ionicity factor in these compounds using equal-valence-electron-density (EVED) profiles. The EVED profiles were also compared with ZnTe. The analysis of EVED profiles of ZnSe and its isovalent compounds namely ZnTe and CdTe shows that the ionicity factor in CdTe is more than ZnSe and ZnTe, respectively.

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1. Introduction

Tetrahedrally bonded II-VI semiconductor compounds are technologically important materials. Their widespread applications in optoelectronic devices, detectors and photoelectrochemical reactions have stimulated strong interest in the properties of these materials. This interest has led to a number of optical measurements, thermoflectance, electroreflectance studies and band structure calculations. The II-VI semiconductor compounds are used as a detector material in X-ray and γ -ray spectroscopy and are also used in optoelectronic devices. Consequently, these compounds have been widely studied from both theoretical as well as experimental point of view.

In this paper, we are presenting the Compton scattering study of semiconductor compounds ZnSe and CdTe. We have compared the experimental data of ZnSe with another isovalent compound ZnTe [1] and CdTe with a view to compare the nature of bonding in the three compounds.

2. Experimental Procedure and data analysis

In this work, a 59.54 keV γ – ray spectrometer of 5Ci Am²⁴¹ source [2] is used for the measurement of a polycrystalline ZnSe and CdTe samples. The sample is held vertically by affixing it on the back of a brass slab covered by lead sheet in front. The sample was kept in an ampoule and mylar windows. The chamber is evacuated to vacuum of about 10⁻² mm pressure is obtained in the chamber with rotary oil pump to reduce the contribution of air scattering. The gamma rays of 59.54 keV were allowed to scatter from the powder sample, through a mean angle of 170°(±2°). The scattered radiation energy was analysed using HPGe detector with an overall momentum resolution of 0.6 a.u. The detector operates at –1000 volts. To reduce both the noise of preamplifier and the dark current of the crystal, this detector is operated at liquid nitrogen

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temperature (77^0 K). The spectrum was collected on a multi channel analyser (MCA) within 4096 channels giving a channel width of 20eV, which corresponds to about 0.03 a.u. of momentum. During the measuring time of 24 hours, about 26,500 counts were collected at the Compton peak for ZnSe and 30,000 counts were collected on Compton peak for CdTe in 53 hrs of measuring time. The background, from electronic noise, scattering from channels and stray cosmic background etc., was measured while placing the ampoule without powder, from about 17 hours. The stability of the system was checked atleast twice a day using a weak Am^{241} calibration source over the time of data acquisition, the drift in gain of the acquisition electronics was found to be negligible. To obtain the experimental Compton profile from the raw data, it was processed through several corrections. The measured background was subtracted from the raw data point by point scaling it to the actual counting time. Then the measured profile was corrected for the effects of detector response function, energy dependent absorption and scattering cross section, according to the scheme described by Williams [3] and other authors [4]. The data reduction for the detector response function was restricted to stripping the low energy tail of the resolution function and smoothing the data, leaving the theory to be convoluted with a Gaussian (0.6 a.u. FWHM). Then the absorption correction is applied from the sample. After converting the profile to the momentum scale, a Monte Carlo simulation of the multiple scattering was performed. The profiles were then normalised to free atom Compton profile [5] area of 27.133 electrons in case of ZnSe and 39.23 electrons in case of CdTe in the momentum range of 0 to +7a.u.

3. Results and discussion

Interestingly, Zinc Selenide, zinc telluride and cadmium telluride have equal number of valence electron. Therefore, a comparison of the behaviour of bonding electrons can be made, by studying their valence Compton profiles normalized to equal electron density, as suggested by Reed and Eisenberger [6]. To a first approximation, these profiles should be identical for compounds with ideal bonding. To compare the actual behaviour of valence electrons and the Compton profiles of these compounds, we have plotted the equal-valence-electron-density (EVED) [$J(p_z) \cdot p_F$] experimental profiles (in units of p_z/p_F , where p_F is the Fermi momentum) in Fig 1. In the case of ZnTe, we have considered the measurements of Sharma *et. al.* [1]. The figure shows that the profile of ZnTe is higher at $J(0)$ than that for ZnSe and CdTe. Further, there is a difference between these profiles on other points also. So, the bonding of ZnTe is different than the ZnTe and CdTe. After $p_z = 1.0$ a.u., the value of profile for ZnTe is rapidly decreasing compared to ZnSe and CdTe. Since sharing of electrons is responsible for covalent bonding, which increases localized charge in the direction of bonding which results in a sharper Compton line shape, therefore we can conclude that ZnTe is less ionic than ZnSe and CdTe.

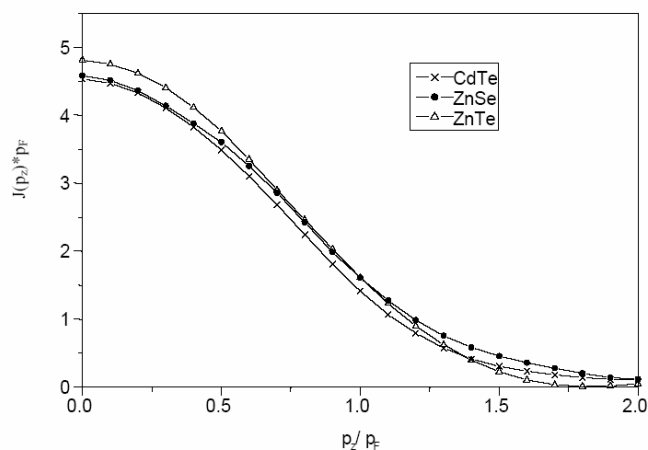


Fig. 1.

Phillips *et. al.* [7] and Walter *et. al.* [8] have also concluded that the ionicity of ZnSe is greater than ZnTe. According to Phillips and Van Vachten [7] ionicity factor can be written as,

$$f_i = \frac{C^2}{E_g^2}$$

The value of $f_i = 0$ denote completely covalent character of compound and $f_i = 1$ means completely ionic compound. E_g is average energy gap, given as $E_g^2 = E_h^2 + C^2$, where E_h and C are homopolar and heteropolar energy gaps, respectively. Phillips *et. al.* [7] has given values of E_h and C of some tetrahedrally bonded materials.

For CdTe, these values are: $E_h = 3.08$ eV and $C = 4.9$ eV. Thus, the ionicity factor comes out to be 0.71. For ZnSe, values of $E_h = 4.29$ eV and $C = 5.6$ eV. Thus the ionicity factor is 0.63. For ZnTe, $E_h = 3.59$ eV and $C = 4.48$, so the ionicity factor for ZnTe is 0.61. This calculation confirms that the ionic behaviour of CdTe is more comparative to ZnSe & ZnTe respectively.

4. Conclusions

In this paper we have presented the experimental Compton profiles of IIB-VIA compound semiconductor ZnSe and CdTe, using Am^{241} gamma ray source Compton spectrometer. To check the ionic character we have compared our data of ZnSe and CdTe with ZnTe experimental data by EVED method. By this comparison, we have observed that the ionic character of CdTe is little bit of large comparative to ZnSe and ZnTe.

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