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Evaluation of lattice distortion by Bi incorporation in CdTe

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1. Introduction

The introduction of Bi as dopant in CdTe crystals, has proven to be a very effective way to obtain high resistive material with high photo sensitivity, very important for their application in X and Gamma ray detection, and photo-refractive devices [1,2]. When the Bi concentration in the crystals is changed from $1x10^{17}$ at./cm^3 to $1x10^{19}$ at./cm^3, the resistivity change from $1x10^{10}$ Ω.cm to $1x10^5$ Ω.cm respectively. On the other hand, the conductivity type change from n-type for low dopant concentration, to p-type for high dopant concentration, suggesting a possible change in the Bi lattice position. Recently, lattice relaxation due dopant incorporation has been proposed as an explanation of low resistance p-type conductance and persistent photoconductivity in II-VI semiconductors [3]. Both effects have been observed in our crystals of CdTe doped with Bi [2].

Figure 1. shows the evolution of the lattice parameter with the temperature, for undoped p-type and n-type CdTe [4], measured by Neutron diffraction techniques. The lower lattice parameter for p-type crystals is explained by the presence of Cd vacancies, which forced to the contraction of the lattice.

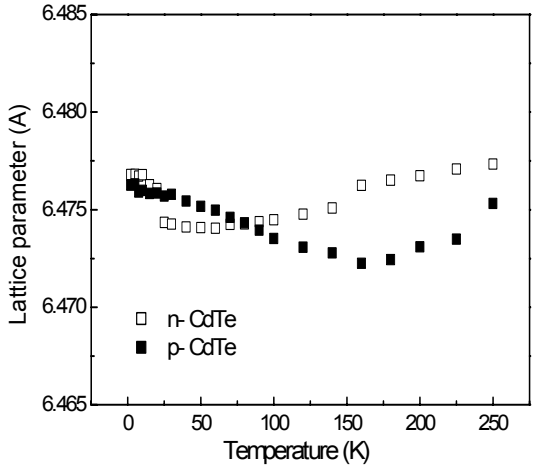

Figure 1. CdTe lattice parameter as a function of temperature for p-type and n-type material.

In consequence, the evolution of the lattice parameter with the temperature could be a very interesting way to demonstrate the Bi amphoter behaviour. For low dopant concentration, we think that Bi could occupy mostly Cd lattice positions, compensating Cd vacancies and leading to an increase in the lattice parameter impliying a lattice relaxation.

For high Bi concentration, Bi mostly occupy Te positions and no special changes in the lattice parameter are expected. Of course, the changes in the lattice parameter are less than 0.01 Å, and for this reason a very sensitive method of detection is needed. Therefore, the aim of the experiment is to support our hypothesis about the amphoter behaviour of Bi in CdTe, what it means the study of the lattice parameter as a function of the temperature. Also, an study of the Debye temperature with the Bi concentration is very interesting since provide the information about the mean displacement of the atoms, being useful for the evaluation of vacancies compensation [5,6]. Whit this experiment, we expected to evaluate the distortion level introduced by the Bi incorporation in the CdTe lattice, and to offer new evidences about their unusual behaviour, which will help to understand the very interesting electrical, photoelectrical and optical properties.

2. Experimental

The experimental set-up is coupled to the Beam Line SPline Nº25, consisting in a X-ray powder diffractometer, working in a temperature range between 80 K to 300 K. Glass capillaries 0.3 mm in diameter were filled with different CdTe powders (undoped and doped with different Bi concentrations), then mounted in the diffractometer. X-ray diffraction diagrams were obtained using the CdTe reflections: (111), (220), (311), (400), (331) and (442). Spectra analyses were performed using the standard program of the SPline, fitting the different peaks to a pseudo-Voigt function and extracting the inter-planar distance. Using the Bragg law we determine the lattice parameter, as a function of the Bi concentration and temperature.

3. Results

CdTe lattice parameter shows an increment with the Bi concentration from 6.4819 Å for the undoped sample up to 6.4828 Å for the sample doped with 2200 ppm of Bi. This is an expectable results because the bigger diameter of Bi in comparison with the Cd and Te atoms. The lattice expansion is proportional with Bi concentration confirming the effective incorporation of Bi in CdTe. Conversely, the expansion coefficient decreases with the Bi concentration, suggesting a lost of free movement of the atoms in the host lattice.

In order to understand the effect of the Bi incorporation on the different crystal orientations, the evolution of the inter-planar distance with the temperature was studied. Crystallographic orientations exhibit a non uniform behaviour for the different dopant concentrations. For the undoped and most doped samples, the expansion coefficients of the lattice parameter and the corresponding to the (111) direction are very similar implying uniform expansion over the three directions of the space.

For the sample with 2.5ppm of Bi, with unusual electrical and optical properties, the (111) direction presents an unexpected behaviour of the expansion coefficient, being almost two times lower than the predicted value. Furthermore, the value is lower than the one calculated for the total lattice expansion. On the other hand, the coefficient determined for the (220) direction, is unusually higher compared with the other concentrations.

The only one mechanism capable to explain this experimental observation is taking into account that for the sample doped with 2.5ppm of Bi the dopant occupies Cd lattice positions, forcing the Te first neighbours to approximate to each others, forming like Te dimmers. This is due to the lower ionic character of the Bi-Te bonds in comparison with the Cd-Te bonds, approaching pairs of Te atoms. The lattice instability formed by the Te dimmers could introduce a deep donor level in the middle of the band-gap, which is the responsible of the high electrical resistivity and photoconductivity states [3].

In the case of highly doped sample, Bi also occupied Te sites (we have evidences that mostly occupied Te sites) forming a deep acceptor level in the bandgap and explaining the low resistivity and photoconductivity of this material.

We are working in correlates the electrical and structural measurements in order to achieve a complete model for explaining Bi behaviour in CdTe.

4. Concluding remarks

The evolution of the lattice parameter with temperature was analysed in the temperature range between 90 K to 300 K. Evidences of the formation of Te dimmers were obtained, indicating that this kind of defect could be responsible of the deep energy level observed in the middle of the CdTe band gap, which explain their high resistivity.

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