

Lattice relaxation in heavily In-doped CdTe films

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Heavily In-doped CdTe is a system that exhibits deep-level formation and persistent photoconductivity (PPC) [1]. The existence of PPC has been related to the appearance of lattice relaxations by some theoretical models [2–4]. In-doped CdTe is a good candidate for the observation of lattice relaxations created by the introduction of In. Another experimental observation that suggests the presence of lattice relaxation is the rapid decrease of the unit cell parameter as a function of dopant concentration [5]. Quite generally, the cell parameter of the host network varies systematically with the concentration of the foreign atoms. For isoelectronic substitutional atoms, the simplest geometrical model proposed initially by Vegard [6] explains these variations. However, for heterovalent substitutional atoms, the situation is not as clear, even when there is only a valence shift of one between the foreign and host atom. Often additional phenomena (e.g., deformation around defects) [3, 4, 7] are used to explain, but usually a satisfying model is still missing. In this letter, we report the results of these contributions to the variation of the lattice parameter relaxation to explain the very important effect of substitutional In incorporation in CdTe films.

The samples were prepared using close-spaced vapor transport combined with free evaporations [8] at a base pressure of 10^{-5} Torr. The raw materials were CdTe powder 99.99 at% and indium 99.999 at% purity from Balzers. Corning 7059 glass slides were used as substrates. The CdTe source was maintained at 600 °C during the growth procedure, while the In source temperature was varied between 550 and 725 °C to achieve different concentrations. The temperature of the substrate was fixed at 500 °C. The In concentration in the films was calculated from the measured energy dispersive X-ray analyzer (EDX, Jeol JSM-35C). X-ray diffraction (XRD) measurements were performed with a Siemens D5000 diffractometer fitted with a Cu anode. All the samples were found to be single phase with a cubic structure. These measurements show a linear decrease in the unit cell parameter with In con-

centration for the three crystallographic directions: [111], [220] and [311] (see Fig. 1). We note that the observed decrease is larger than the expected decrease obtained assuming a simple substitutional model, with a CdTe distance of 2.806 Å and an In–Te distance of 2.730 Å (the shortest reported In–Te distance for a compound containing both In and Te (see [9]; see Fig. 1). Such a rapid decrease in the cell parameter with dopant concentration has been reported in other II–VI doped semiconductors [5] and has been related to the presence of point defects [4, 5].

Following the Vegard's law, the evolution of the cell parameter is usually presented as

$$\Delta a/a_0 = \beta[c] \quad (1)$$

where $\Delta a = a - a_0$ and $[c]$ is the concentration per unit volume of the incorporated atom, In atom in our case. Fig. 2 shows the lattice strain versus the In

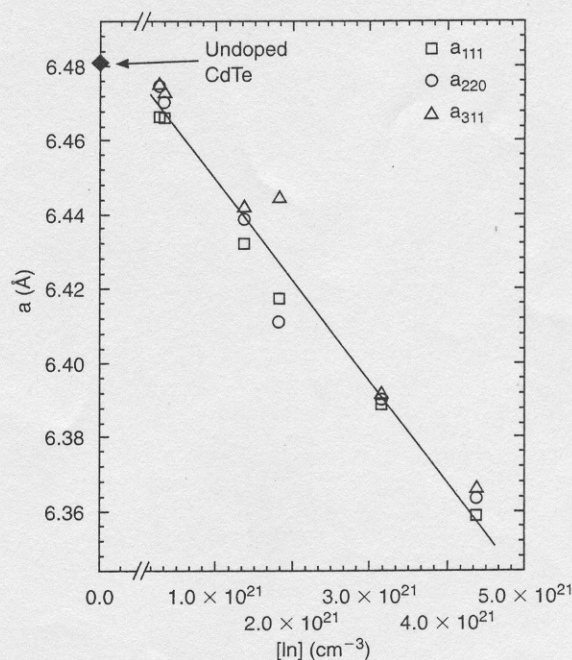


Figure 1 Lattice parameter as a function of In incorporation for the three crystallographic directions.

*Also with CICATA-IPN.

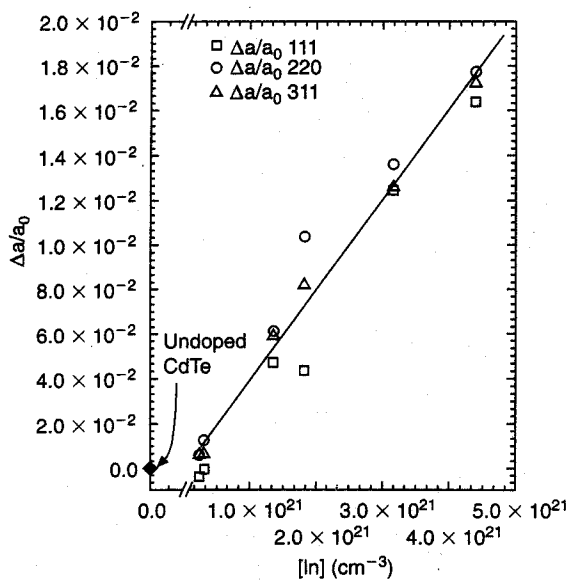


Figure 2 Cubic lattice parameter as a function of In incorporation, relative to the extrapolated value a_0 at $[In] = 0$ for the three crystallographic directions.

incorporated for the three crystallographic directions. To compare the different contributions with our results, an experimental mean value of β about $4.11 \times 10^{-24} \text{ cm}^3$ was chosen. According to these considerations, we get

$$\Delta a/a_0 = 4.11 \times 10^{-24} [In] \quad (2)$$

As we know, the substitution of atoms causes a lattice strain due to the different atomic size. By means of X-ray experimentation, the average strain resulting from the individual strain field around each In atom can be measured. In this consideration, the cumulative difference of covalent radii size of the doping (r_i) and host (r_{sc}) atoms is uniformly distributed among all sites, and therefore a linear variation of the lattice parameter with the doping atom concentration can be predicted and it can be expressed as

$$\Delta a/a_0 = \beta_{size} [N_i] \quad (3)$$

with

$$\beta_{size} = (r_i - r_{sc})/r_{sc} [N_{sc}] \quad (4)$$

where $[N_{sc}]$ is the concentration per unit volume of the semiconductor atom and $[N_i]$ is the doping concentration. In the case of substitutional incorporation of In in Cd vacancies into CdTe lattice predicts $\beta_{size} = -1.06 \times 10^{-23} \text{ cm}^3$, taking into account the covalent radii of the Cd atom ($r_{Cd} = 0.97 \text{ \AA}$) and the smaller one of the In atom ($r_{In} = 0.81 \text{ \AA}$). This negative value indicates a lattice contraction with In incorporation as we observe, but remains 2.5 times as large as the value obtained experimentally. If we assume an interstitial incorporation of In atom, β_{size} could be considered as:

$$\beta_{size} = (2r_i - r_{sc})/r_{sc} [N_{sc}] \quad (5)$$

in this case, $\beta_{size} = 4.32 \times 10^{-23} \text{ cm}^3$. The positive

value indicates a lattice expansion with In interstitial incorporation. This picture of incorporation in the interstitial site contradicts our experimental results, as is shown in Fig. 2.

Another contribution from a significant deformation around a defect has been introduced by Cargill *et al.* [10] to explain the effect of an electron empty of shallow donor levels (called DX centers) around Sn and Si in $\text{Al}_x\text{Ga}_{1-x}\text{As}$. Significant β values have been obtained, $\beta_{DX}(\text{Sn}) = (3.1 \pm 0.2) \times 10^{-24} \text{ cm}^3$ and $\beta_{DX}(\text{Si}) = (1.3 \pm 0.2) \times 10^{-24} \text{ cm}^3$. Supposing that the effect of the free carrier is negligible, a rough value of the $\beta_{DX}(\text{In})$ could be calculated in our case. The lattice deformation is therefore solely induced by the size effect, β_{size} , and the deformation around the In atoms, $\beta_{DX}(\text{In})$. We get:

$$\Delta a/a_0 = [\beta_{size} + \beta_{DX}(\text{In})][In] \quad (6)$$

From the experimental value of $\beta (4.11 \times 10^{-24} \text{ cm}^3)$ and the calculated one for $\beta_{size} (-1.06 \times 10^{-23} \text{ cm}^3)$, we obtain $\beta_{DX}(\text{In}) = 1.47 \times 10^{-23} \text{ cm}^3$. This value of $\beta_{DX}(\text{In})$ for In incorporation is about three times that for β and is similar to that for β_{size} . This is *a priori* unexpected, as the deformation around the In atom in CdTe is still expected to be large because In acts as a shallow donor in CdTe [1, 2].

In conclusion, the high-contraction $\Delta a/a_0 = 4.11 \times 10^{-24} [In]$ of the CdTe lattice from incorporation of In in the substitutional site is demonstrated. Vegard's law alone is not suitable, and additional contributions must be made to explain the decrease of the lattice parameter with In incorporation. A local deformation around the In atoms can be used to explain the decrease, even though a large deformation is unexpected because In is a shallow donor in CdTe. We also suggest a slight deformation of the lattice parameter (from residual defect or strain) to explain the different lattice parameter obtained according to the crystallographic direction. Therefore, the important effect of the deformation induced by the introduction of the In atom might be related only to the small length of the covalent bond in CdTe and the local deformation induced.

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