AB INITIO CALCULATION OF LATTICE RELAXATION AROUND GA IN CDTE: EVIDENCE OF THE DX AND A CENTERS

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The lattice relaxation around Ga in CdTe is investigated by means of the density functional theory (DFT) calculations using augmented plane waves plus local orbitals (APW+lo) method. In addition, the calculations are done for DX and A centers in CdTe. The calculated results are in good agreement with the experimental data obtained from X-ray absorption spectroscopy and allow experimental identification of the DX and A center structures in CdTe.

1. Introduction

CdTe has been researched extensively in the past due to its interesting applications in optoelectronics. In order to improve the properties of CdTe dopants are often introduced, but this incorporation of impurity atoms is often followed by lattice distortions and formation of defect complexes, which can influence the electrical or optical properties of the system [1,2]. In highly doped crystals, apart from the substitutional position, Ga is expected to form an A-center (a complex with a nearby metal vacancy), but DX-centers [3] or anti-site defects [4] are equally possible. Such configurations differ considerably in their local distances. DX centers are an important type of defects that are considered responsible for limiting the doping efficiency in a broad range of semiconductors, but their experimental evidence is scarce. Apart from the x-ray absorption study where the photoinduced lattice relaxation around In in CdTe [5] was attributed to the presence of DX centers, the only direct evidence of the DX centers is given via the electric field gradient obtained in In doped CdTe [6], where the interpretation of the measurements had to be supported by DFT calculations. In this paper we report on direct measurements of the local structure relaxation around Ga in CdTe by EXAFS on samples doped with Ga under conditions that would make it feasible to achieve high concentrations of defect configurations, along with the normal substitutional one.

2.Experimental Procedure nad Results

We prepared two types of samples – one (S1) was prepared from the top of the CdTe<Ga> ingot with with galium concentration of ~ $9x10^{18}$ at/cm^3 in the melt and the other (S2) was made from CdTe<Ga> additionally saturated by Ga at 850 ^{0}C during 1.5 months. The estimated concentration of Ga in the latter case was 10^{20} at/cm^3. Thus, we expected increased concentration of Ga defect structures in the S2 sample. EXAFS experiments on the Ga doped CdTe samples were performed at the A1 beamline of HASYLAB with the absorption spectra collected at 20K. The absorption was measured at the Ga K-edge in fluorescence mode with a 7-segment Ge detector. The subsequent analysis was performed using the ATHENA/ARTEMIS software combination [7].

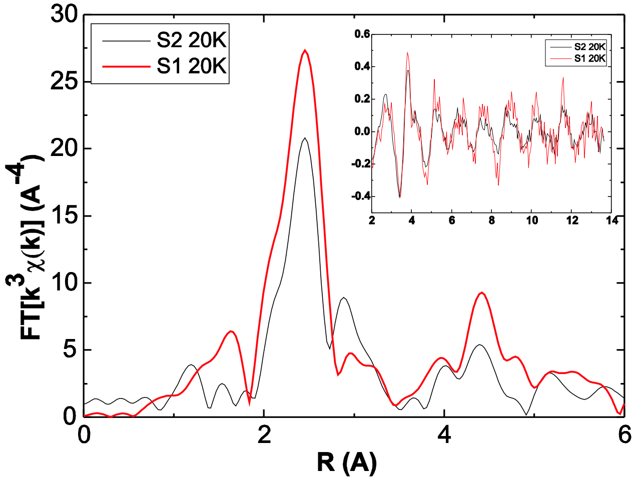

Figure depicts the Fourier transforms of the k^3 weighted experimental EXAFS spectra, $\chi(k)$, of the S1 and S2 samples. Qualitatively, the most important distinction between the two spectra is decrease in amplitude of the most dominant peak, and appearance of new peak around 3 Å in the heavily doped S2 sample. Given the theoretically predicted local configurations, the most likely reason for the decrease in amplitude can be the appearance of additional A-center and/or DX configurations, resulting in less sharply defined 4-fold neighborhood from a distorted NN shell. On the other hand, the shoulder around 3 Å can be traced down to contribution from local configurations which have undergone a deep relaxation, i.e., DX configurations. Fitting the data with only one substitutional fraction produces a satisfactory fit only for the S1 EXAFS data, while for the S2 we had to include contributions also from the other two assumed local geometries. The NN distances obtained from the fits compare relatively well with the calculated bond lengths.

3. Ab- initio Calculations

In order to complement our experimental work we performed DFT ab initio calculations with the WIEN code (LAPW method) [8]. Using the optimized lattice parameter of 6.33 A for CdTe, we constructed our 2x2x2 supercell in bcc symmetry. This procedure produced a supercell of 32 atoms used for calculation of the substitutional dopant position, where one of the Cd atoms was replaced with Ga. The same supercell was used also for the lattice calculation of the DX structures, after breaking the symmetry by moving the impurity in <-1,-1,-1> direction. For calculation of the structural relaxation of the A-center defect, in addition to substituting Cd with Ga, we removed one of the second nearest neighbor Cd atoms. We relaxed all the atoms in the supercell along the predefined symmetry directions with force criterion of 3mRy/a.u.. The results of our calculated distances, as well as distances obtained from the fit are presented in Table 1. The local structures obtained in this way were used as starting points for our ab-initio FEFF code [9], which produced the theoretical standards needed for the fitting procedure.

Table 1: Calculated and measured distances for the cases of Ga substitutional, DX and A centers

	distance (Å)	coordination number	distance obtained from EXAFS fit (Å)
Ga (Cd) neutral			
NN (Ga-Te)	2.83	4 (Te)	
NNN (Ga-Cd)	4.69	12 (Cd)	
Ga (Cd) 1+			
NN (Ga-Te)	2.72	4 (Te)	2.647 (1)
NNN (Ga-Cd)	4.69	12 (Cd)	
Ga (Cd) DX 1-			
NN (Ga-Te)	2.95	3 (Te)	3.1 (2)
NNN (Ga-Te)	3.61	1 (Te)	
NNNN (Ga-Cd)	3.95	3 (Cd)	
A-center 1-			
NN (Ga-Te)	2.66	1 (Te)	2.671 (9)
NNN (Ga-Te)	2.73	1 (Cd)	
NNNN (Ga-Te)	2.75	2 (Te)	

4. Conclusion

Our results indicate that the measured absorption spectra on the heavily doped CdTe:Ga sample cannot be explained using only one substitutional donor configuration only, whereas the inclusion of an additional DX and A-center local environments considerably improves the fits. The additional indication of the validity of this model is the good agreement between the fitted and calculated bond lengths.

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