

Local structure in Te doped GaAs

R. Bacewicz, A. Pietnoczka, W. Zalewski, A. Antonowicz and ¹T. Stupiński

Faculty of Physics, Warsaw University of Technology, ul. Koszykowa 75, 00-662 Warsaw, Poland

¹Institute of Experimental Physics, Warsaw University of Technology, ul. Hoża 69, 00-681 Warsaw, Poland

Tellurium doped GaAs is an important material used in optoelectronics. In heavily doped GaAs:Te reversible changes of the free electron concentration with the high temperatures annealing were observed since early sixties [1]. Tetrahedrally coordinated Te substituting As is a shallow donor, and electron concentration usually equals to the concentration of Te atoms. However, for some thermal treatments the electron concentration drops significantly. Various hypotheses were proposed to explain this deactivation mechanism in GaAs:Te. Fuller and Wolfstirn [1] suggest creation of “impurity molecules” which trap electrons. Gebauer et al. [2] identified $V_{\text{Ga}}\text{-Te}_{\text{As}}$ complexes as responsible for the compensation effect. However, the latter hypothesis does not explain recovery of the electron concentration by the high temperature annealing. Using the X-ray diffuse scattering technique, the reversible changes of the concentration were attributed in [3] to the creation of the impurity pairs. In this contribution we report an attempt to determine local changes around Te atoms for different states of the GaAs:Te crystals corresponding to different electron concentrations.

GaAs:Te crystal has been grown by Czochralski method. Tellurium concentration was $(1.7\text{-}1.8)\times 10^{19}\text{ cm}^{-3}$. Three samples were cut from that crystal and annealed at 1185°C for 4 h (sample J1), at 1050°C for 39 h (sample BA), and at 800°C for 288 h (sample J3). For the J1 sample free electron concentration is approximately equal to the tellurium atoms concentration. (we call it a high electron concentration state). For the samples BA and J3 free carrier concentration is $1.5\times 10^{19}\text{ cm}^{-3}$ and $3.5\times 10^{18}\text{ cm}^{-3}$ respectively. We refer to the J3 sample as the low electron concentration state.

EXAFS measurements at the Te K edge have been carried out at the X1 beamline of the DORIS3 ring in the HASYLAB at room temperature and at 80 K. Due to the high dilution of Te in our crystals ($[\text{Te}] < 0.1\%$) multiple-scans were recorded in the fluorescence method and Si:Li detector was employed. Ifeffit package was used for the data analysis. Fig.1. shows the Fourier transforms of the EXAFS oscillations for 3 samples.

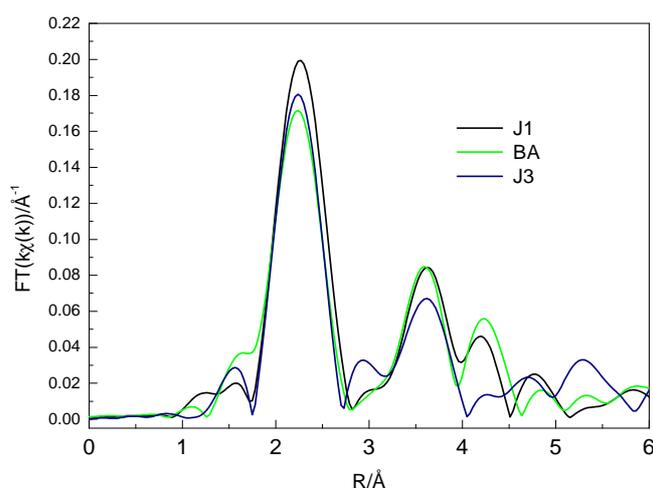


Figure 1: Fourier transforms of the EXAFS oscillations for 3 samples of GaAs:Te. Samples description see text.

For the J1 and BA samples the substitutional Te_{As} model fits perfectly the EXAFS data (Fig.2a), with dilatation of the nearest-neighbour distance due to the difference in atomic radii of Te and As (from 2.43 \AA for the As–Ga distance to 2.65 \AA (on average) for the Te–Ga bond length). Surprisingly, no significant increase in the interatomic distances is noted for the second- and third-neighbour shells. For the J3 sample the EXAFS from the first coordination shell is very similar to that of other two samples. Thus in a low electron concentration state, the close environment of Te atoms remains unchanged as compared to the high concentration state. We cannot see differences in the first-neighbour-shell ordering: the FWHM value of

the first peak is 0.58 Å for J1 and 0.57 Å for J3 sample. So, we have to reject those of DX models of Te impurity in GaAs which assume large lattice relaxation in the first-neighbour shell of Te impurity (e.g. [4]).

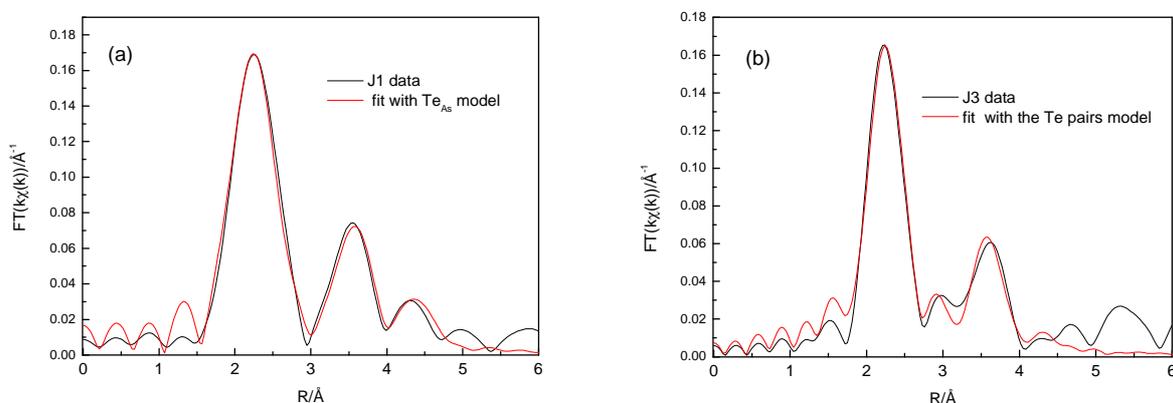


Fig.2. Comparison of the EXAFS data for the J1 sample with the Te_{As} substitutional model (a), and for the J3 sample with the combined model – isolated Te_{As} + Te_{As} pairs (b).

Some differences between the J3 sample and other two are visible in the second and third shell peaks. Especially the third shell peak (around 4.2 Å) is much lower for the J3 sample. We tried to find a model explaining these subtle differences. Following findings of authors of paper [3] we fitted the model representing pairs of Te atoms on neighbouring As sites including an arbitrarily chosen (0.9 Å) relaxation of Te atoms towards each other. This relaxation represents a sort of an attractive interaction between them leading to quasi-bonding of two Te atoms. We conserved a close environment of Te atoms shifting rigidly Ga tetrahedra together with these atoms. Since electron concentration for the J3 sample is approximately $\frac{1}{4}$ of the Te concentration we assumed that $\frac{1}{4}$ of Te atoms reside in isolated substitutional sites and $\frac{3}{4}$ are paired. The best fit for such a “combined” model is shown in Fig.2b. The peak at about 3 Å in the Fourier transformed EXAFS is due to the presence of Te atoms in the second-neighbour shell and the third shell amplitude is cancelled out. It is, of course, not unique choice of the Te atoms configuration leading to such effects. It solely demonstrates that it is possible to find a model based on Te pairing which explains qualitatively the EXAFS data. We realize that a proposed Te atoms displacement has to produce a lot of strain in the lattice. This is consistent with the observation of a huge number of dislocations in the crystals in the low electron concentration state.

We conclude that annealing induced deactivation of the electron concentration in GaAs:Te is not related to the changes in the first-neighbour shell of tellurium. As a hypothesis a Te pairing with a relaxation of Te atoms toward each other is proposed.

Acknowledgments

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