LOCAL STRUCTURE IN Te DOPED GaAs

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Keywords: EXAFS, gallium arsenide, tellurium, dopant

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Tellurium doping of GaAs is used to provide n-type conductivity. Tetrahedrally coordinated Te substituting As is a shallow donor, and the electron concentration is usually close to the concentration of Te atoms. However, in heavily doped GaAs:Te reversible changes of the free electron concentration with the high temperature annealings were observed since early sixties of 20th century [1]. Various hypotheses were proposed to explain a deactivation mechanism in GaAs:Te. Fuller and Wolfstirn [1] suggested creation of "impurity molecules" which trap electrons. Gebauer *et al.* [2] identified V_{Ga}–Te_{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 the results of XAFS measurements in an attempt to determine local changes around Te atoms for different states of GaAs:Te crystals corresponding to different electron concentrations.

GaAs:Te crystal has been grown by Czochralski method with the tellurium concentration $(1.7\text{-}1.8)\times10^{19}$ 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 Te atoms concentration. For the samples BA and J3 free carrier concentration is 1.5×10^{19} cm^{-3} and 3.5×10^{18} cm^{-3} respectively. EXAFS measurements at the Te K edge have been carried out at the X1 beamline in the HASYLAB at room temperature and at 80 K. Due to the dilution of Te in our crystals ([Te] < 0.1%) multiple-scans were recorded in the fluorescence mode with a Si:Li detector. Fig. 1 shows the Fourier transforms of the EXAFS oscillations for three samples.

For the J1 and BA samples the substitutional Te_{As} model fits perfectly the EXAFS data with dilatation of the nearest-neighbour distance due to the difference in atomic radii of Te and As (from 2.43 Å for the As–Ga distance to 2.65 Å for the Te–Ga bond length). 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 (J1). 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.

Following the authors of the paper [3] we assumed that in the low concentration state (J3 sample) electrons are trapped by clusters of the Te pairs. We allowed a relaxation of two Te atoms towards each other in the <110> direction. We found that a model combining the substitutional Te_{As} with the Te pairs model in a proportion resulting from the electron concentration ratio provides a good fit to the EXAFS data with a Te relaxation of 0.8 Å. However, it has to be noted that the EXAFS itself is not able to provide a univocal evidence for the Te pairs model. We await a theoretical justification to support such a hypothesis.

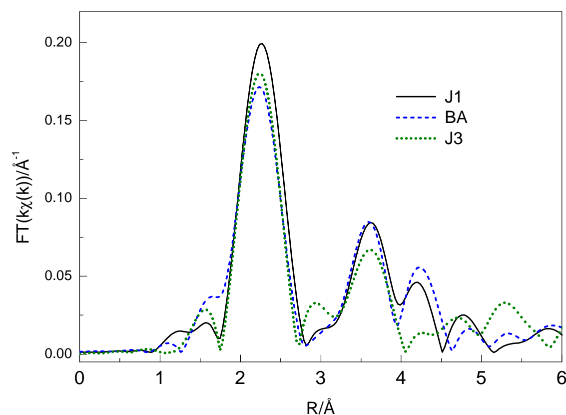

Figure 1. Fourier transforms of the EXAFS oscillations for 3 samples of GaAs:Te with [Te] = 1.7×10^{19} cm^{-3} subject to different thermal treatments.

References

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