

Local structure around Te in heavily doped GaAs:Te using X-ray absorption fine structure

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The annealing of heavily doped GaAs:Te can significantly change the value of the free electron concentration in a reversible manner. These changes of electrical properties are accompanied by the structural changes of GaAs:Te solid solution [1]. In this contribution we present an attempt to determine local changes around Te atoms for different states of the GaAs:Te crystals caused by the annealing corresponding to different electron concentrations.

Extended X-ray Absorption Fine Structure (EXAFS) and X-ray Absorption Near Edge Structure (XANES) techniques have been employed to investigate the local structure around tellurium atom and its valence. Tellurium K-edge absorption has been measured in a fluorescence method at the X1 beamline in the HASYLAB. The samples were kept at the temperature of 80 K in order to minimize the thermal disorder.

Various models of Te defect complex have been used to fit the data for low concentration state: $V_{Ga} - Te_{As}$ complexes [2], $Te_{As} + Te_{As}$ pairs [1], as well as several DX-like configurations of tellurium. DX configurations have been calculated using density functional theory (DFT). The EXAFS and XANES spectra for different Te location have been simulated and compared with the experimental data. Multi-parameter fitting of the EXAFS data provided information on the local structure around Te (the bond lengths, the coordination numbers and Debye-Waller factor). The charge state of Te has been determined from the XANES data. The EXAFS and XANES were useful for ruling out the possibility of existence of GaTe and Ga_2Te_3 precipitations.

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References

- [1] T. Słupiński, E. Zielińska-Rohozińska, "Local order of Te impurity atoms and free electron concentration in heavily doped GaAs:Te," *Thin Solid Films* 367 (2000) 227-231.
- [2] D.T.J. Hurlle, "A comprehensive thermodynamic analysis of native point defect and dopant solubilities in gallium arsenide," *J. Appl. Phys.* 85 (1999)6957-7012.

