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Structure defects in CdTe-based semiconductor heterojunctions

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The aim of this dissertation was the characterization of structure defects in CdTe-based heterojunctions grown for solar cells applications. The examined samples were obtained by the molecular-beam epitaxy (MBE) technique, under various conditions of stoichiometry, on two different substrates: (i) lattice mismatched by 14.6%, (001)-oriented GaAs and lattice matched, (001)-oriented CdTe. Two kinds of samples have been investigated: *p*- and *n*-type doped CdTe layers with metallic Schottky barriers and *p*-ZnTe/*n*-CdTe heterojunctions.

In order to determine the origin of the limited efficiency of solar-energy conversion in the CdTe-based heterojunctions the deep-level transient spectroscopy (DLTS) technique has been applied. The results of the DLTS studies revealed a presence of eight hole traps and three electron traps in the investigated samples. Considering the obtained emission activation energies, capture cross-sections and capture kinetics of charge carriers into the traps we have attributed the H2, H3, H6, E1 and E2 traps to the native point defects in CdTe: V_{Cd}, complex formed of V_{Cd} and Cd_{Te}, Te_I, Cd_I and Cd_{Te}, respectively. The logarithmic capture kinetics observed for the other traps strongly suggests their relation to electronic states of extended defects. The E3, H4 and H5 traps are worthy of special attention. The H5 trap was detected only in the close vicinity of the metal-semiconductors interface, indicating that the H5 trap is associated with acceptor states located at the CdTe surface. Both the H4 and E3 traps are associated with the *band-like* states of extended defects, most probably – the dislocation core states. The sum of their activation energies slightly exceeds the band-gap energy of CdTe suggesting that they are associated with electronic states of the same dislocation, which can act as effective recombination centers.

Transmission electron microscopy (TEM) was used to analyse the quality of GaAs/CdTe and CdTe/ZnTe interfaces, as well as to determine the type of dislocations and stacking faults observed in the measured heterojunctions. The structural quality, lattice parameters and misfit strain in the heterojunctions were evaluated from the high-resolution X-ray diffractometry (XRD) measurments.

Summarizing, the DLTS, TEM and XRD results, obtained for both the CdTe epitaxial layers with Schottky barriers and *p*-ZnTe/*n*-CdTe heterojunctions, point out that not the point defects but rather extended defects, in particular recombination centers associated with threading dislocations in CdTe layers, are responsible for the limited energy conversion efficiency in the CdTe-based solar cells.

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