High-Resolution X-Ray Diffraction Studies on MBE-Grown *p*-ZnTe/*n*-CdTe Hetrojunctions for Solar Cell Applications

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Heterojunctions based on cadmium telluride belong to the most promising devices for solar energy conversion into electricity. The investigated *p*-ZnTe/*n*-CdTe heterostructures were grown by the molecular-beam epitaxy (MBE) technique on two different substrates: (i) on highly lattice mismatched by 14.6%, (001)-oriented GaAs and (ii) on much more expensive, (001)-oriented CdTe. Initially, highly iodine doped *n*-type CdTe buffer layer was grown. Then it was covered by undoped CdTe absorber and afterwards, by nitrogen doped *p*-type ZnTe layer. Depositing *p*-type ZnTe layer with the free carrier concentration of above 10^{18} cm^{-3} facilitates for preparing low-resistivity contacts to the *p*-type side of the junction and increases the utilized spectral range of the solar spectrum.

The *p*-ZnTe/*n*-CdTe heterojunctions were investigated using high-resolution x-ray diffractometry (XRD). The structural quality, lattice parameters and misfit strain were evaluated from the measured reciprocal lattice maps and the rocking curves for the symmetrical (004) and asymmetrical $(\bar{3}\bar{3}5)$ reflections of Cu Kα_1 radiation.

The XRD results indicate that the CdTe layers, grown under compressive strain on GaAs substrate, are partially relaxed, by the formation of misfit dislocations at the interface, and display residual vertical strain of the order of 10^{-4}. Surprisingly, the relaxed lattice parameters of the CdTe layers are larger then those of bulk CdTe. The difference in thermal expansion coefficient between CdTe (4.8×10^{-6} K^{-1}) and GaAs (5.7×10^{-6} K^{-1}) would result in the opposite effect. Moreover, stoichiometric deviations or impurities should be also excluded as responsible for the increase in the relaxed lattice parameters because we observed the same effect for the layers grown under various conditions of stoichiometry, and both the iodine doped and undoped ones. In order to explain the observed results, we decided to examine heterostructures grown on CdTe substrate. Although the structural quality of CdTe layers grown on CdTe substrate is significantly better than that of the layers grown on GaAs substrate, our XRD investigations lead to the unexpected results of compressive strain existing also in homoepitaxial CdTe layers and the relaxed lattice parameters of the layers larger then those of the substrate. The mechanism responsible for those effects is not fully understood. However, the tendency for twinning during the homoepitaxial CdTe growth has been proposed as a favourite candidate for the explanation of the unusual strain [1]. In addition, our XRD measurements show that the ZnTe layers, grown under tensile misfit strain, display relatively good structural quality.

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[1] H. Heinke, A. Waag, M. O. Möller, M. M. Regnet, and G. Landwehr, *J. Crystal Growth* **135**, 53 (1994).