TEM characterization of axial CdTe/ZnTe nanowires and simulation of strain induced diffusion by finite element method

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Nanowires (NWRs) are one-dimensional objects of only some 10 nm in diameter and up to several micrometers in length. NWRs of semiconductor material exhibit unique physical properties opening new fields of applications. For applications in the infrared range of light a combination of CdTe/ZnTe is chosen. Such NWRs were fabricated via a vapor-liquid-solid (VLS) growth process generated in a molecular beam epitaxy system. Liquid droplets of a gold-based eutectic catalyst promoted the NWR growth. In a first step, ZnTe NWRs were grown. After a growth interruption Cd and Te were provided for the further growth process resulting in NWRs with a CdTe/ZnTe interface. For the TEM characterization the NWRs were harvested from the substrate and transferred to a holey carbon film. The TEM investigations were performed at a JEOL 2200FS operating at 200 kV.

The NWRs exhibit an unique shape showing a concentric buckling of the CdTe part close to the interface (see Figure 1). Three origins of the buckling can be considered. First, relaxation of lattice mismatch, second, lateral growth, and third, variation of the size/shape of the catalyst droplet. These aspects will be examined by means of quantitative high-resolution TEM (qHRTEM) and energy dispersive X-ray spectroscopy (EDXS).

The CdTe/ZnTe interface is free of misfit dislocations. Hence, the relaxation of the lattice mismatch has to be regarded as purely elastic. CdTe is compressed and relaxes within a certain distance from the interface (cf. Figure 2). Within the area analysed by qHRTEM the relaxation is still incomplete. The displacement of the 111 lattice planes corresponds to a Cd content of $x_{Cd} = 0.15$. Full relaxation of CdTe is achieved after a distance of more than 100 nm. At the same distance, the increase of the NWR diameter by far exceeds the maximum lattice mismatch of 6 %. This rules out relaxation as origin of the buckling effect.

EDXS line scans along the [111] growth direction reveal a strong smearing of the CdTe/ZnTe interface. Zn is detected about 100 nm away from the interface. The correlation of buckling and lateral growth was tested by EDXS line scans across the NWRs (cf. Figure 3). Lateral growth would result in a core-shell structure. The material grown in the last period of the growth process, viz. CdTe, should be enriched in the shell. The composition profiles in particular in the buckled region do not exhibit an enrichment of Cd at the lateral surface of the NWR. Hence, the buckling is not due to a lateral growth.

Finally, only a variation of either the size or shape of the catalyst droplet can cause the buckling. By altering the chemical composition of the droplet the properties of the liquid droplet are modified. This causes a different diameter of the circular contact area between liquid and solid phase. The NWRs grow in a buckled way until the lattice mismatch is

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relaxed, i.e., pure CdTe forms. Conclusively both, the buckling of the NWRs and the smearing of the interface have to be attributed to the container effect of the catalyst droplet.

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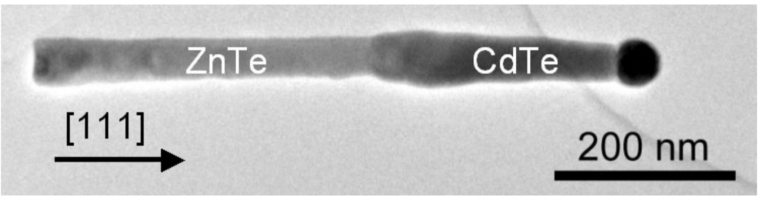

Figure 1. TEM bright-field image of a CdTe/ZnTe NWR.

a) b)

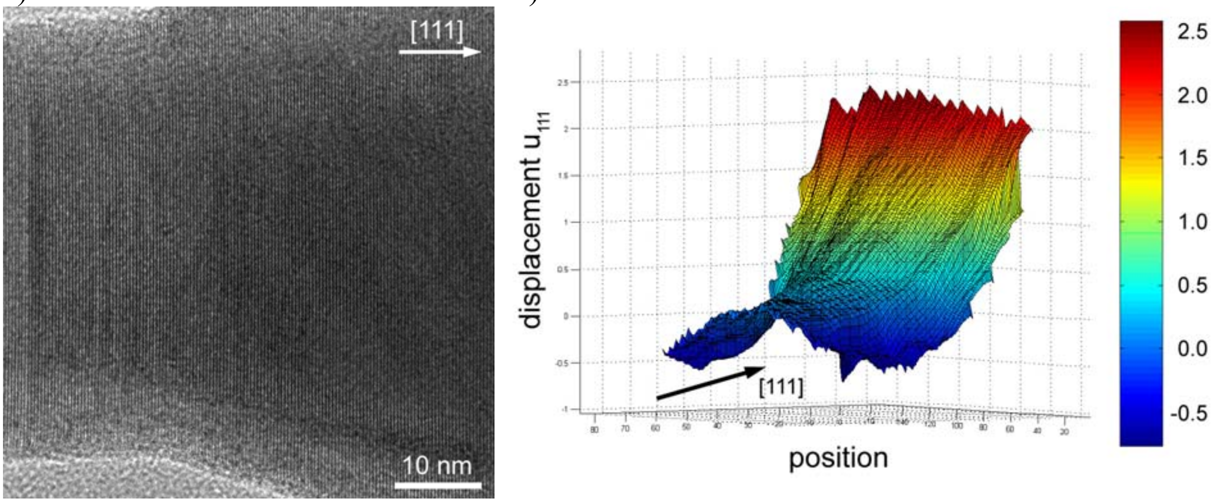

Figure 2. Strain analysis of the CdTe/ZnTe interface region of a CdTe/ZnTe NWR by qHRTEM: a) HRTEM image; b) relative displacement of the 111 lattice planes as revealed by peak finding method. For the analysis the area shown in Figure a) was selected.

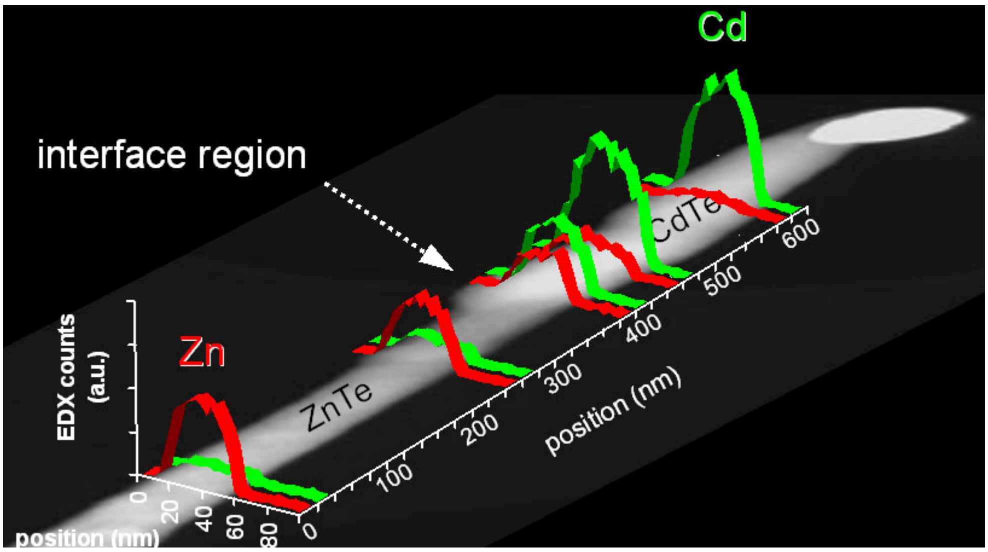

Figure 3. Composition profiling across a CdTe/ZnTe NWR acquired by EDXS.

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