

## MS23-O2 Structure to property relations of single MBE grown GaAs and InAs nanowires onto silicon (111) studied by X-ray nanodiffraction

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Axial stacking faults separating zinc-blende and wurtzite entities are the major structural defects of MBE grown semiconductor nanowires (NWS). Structural composition, phase arrangement and residual strain of individual GaAs NWs grown on Si(111) can be investigated X-ray nano-diffraction employing a focused synchrotron. It is found that even neighbouring NWs grown on the same sample under the same growth conditions differ significantly in their phase structure. Moreover, the misfit strain at the substrate to NW interface releases within few monolayers due to relaxation towards the NW side planes [1]. The evolution of stacking faults is no constant but depends on growth time and the growth mode. In case of InAs NWs grown catalyst-free along the [111] we explored the dynamic relation between the growth conditions and the structural composition of the NWs using time-resolved X-ray scattering and diffraction measurements during the MBE growth. The spontaneous buildup of liquid indium droplet in the beginning of the growth process is accompanied by the simultaneous nucleation of InAs NWs predominantly grown in the wurtzite phase with low number of stacking faults. After nucleation the In droplets become consumed resulting in structural degradation of NWs due to the formation of densely spaced stacking faults [2]. For the first time the particular phase structure of single GaAs NWs could be correlated with their electrical properties. Here the V-I characteristics was measured in a dual Focused Ion Beam chamber the resistance and their effective charge carrier mobility was modeled in terms of thermo-ionic emission theory and space charge limited current model, respectively. Both resistance and inverse mobility show a qualitatively similar electric behavior comparing the inspected NWs. The same single NWs electrically measured have been inspected by X-ray nano-diffraction. The NWs were found to be composed by zinc-blende and twinned zinc-blende units separated by axial interfaces and a small plastic displacement. It turns out that the measured value of the extracted resistance and the inverse of effective mobility increases with the number of intrinsic axial interfaces, whereas the small plastic displacement has less influence on electrical properties [3]. We acknowledge support by BMBF and DFG.

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[2] Biermanns et al *Nano Lett.* 2014, 14, 6878–6883

[3] Bussone et al. *Nano Lett.* 2015, 15, 981–989

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## MS23-O3 Exploring crystal structure, size and stoichiometry of lead chalcogenide QDs by x-ray total scattering and the Debye scattering equation

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Colloidal lead chalcogenides Quantum Dots (QDs) are an increasingly important class of nanocrystalline materials. Due to strong quantum-size effects, they are very promising in fields of application as important as solar cells,[1] photodetectors[2] and thermoelectric devices.[3] Size-tunable QDs are typically synthesized using long organic ligands (controlling their growth and preventing from aggregation) providing metal-rich nanocrystals (NCs). Their complex functionality strongly depends on the structure and on the stoichiometry of the NCs. Many studies have concluded that they have a stoichiometric core and a Pb-terminated surface layer[4]. Using unconventional Wide-Angle X-ray Total Scattering techniques and a core-shell model relying on the Debye Scattering Equation, we characterized highly monodisperse PbS and PbSe – Oleate capped QDs (nominal sizes in the 3-8 nm range) in colloidal suspensions in terms of crystal structure, size and stoichiometry. Data were collected at the MS-XSA04 beamline of Swiss Light Source. Sample modeling was performed using the Debussy Suite[5]. The innovative approach enabled us to disclose novel and unexpected structural and compositional features, which will be presented in this communication.

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