TEM investigations and MD/MS simulations of misfit dislocations in highly mismatched core/shell nanowires.

mgr inż. Dorota Janaszko

Abstract

The semiconductor nanowires (NWs) attracted much attention due to their high surface-to-volume ratio. Among II-IV semiconductors CdZnTe is an auspicious one, because of its great potential in many solid–state device applications. I would like to present the investigation results of the core/shell hetero-nanowires, where the lattice mismatch between the compounds exceeds 6,2%. The core was grown by Molecular Beam Epitaxy (MBE) using vapor-liquid-solid growth mechanism assisted with gold catalysts on GaAs or Silicon substrates. In the same MBE process, (Cd, Zn)Te shells were grown at low substrate temperatures, when the gold eutectic catalyst was solidified. The NWs were transferred onto holey carbon film and investigated using HRTEM and HRSTEM in planar view. Specimens were also fabricated by perpendicular cross-section with FIB and core/shell morphology was confirmed during EDS profiles and maps analysis. TEM and STEM images were analyzed using GPA (Geometric Phase Analysis) and DDT (Dislocation Density Tensor) to determine the lattice distortion state in projection. Among investigated nanowires two groups were distinguished. Strained NWs with ~40 nm CdTe core, and ~20 nm thick symmetric ZnTe shell, which were elastically strained , and the second group, the structures with ~80 nm core diameter and asymmetric ~10-40 nm thick shell, partially relaxed. In the second case, the misfit dislocation network on the core/shell interface becomes clearly visible in the GPA phase as well as in GPA amplitude images. When the thickness of the core and the shell is comparable the accommodation of the lattice mismatch occurs by elastic deformation. In the case of a more rigid (larger diameter) core, plastic relaxation occurs by the creation of misfit dislocation at the core /shell interface. It is found that the dislocation density on the CdTe/ZnTe interface in analyzed nanostructures depend on the shell thickness, symmetry, and core diameter. The Molecular Dynamics (MD) and Molecular Statistics (MS) simulations of investigated structures were performed with Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). Two different approaches were applied to find the best accuracy of misfit dislocation network simulation to the experimental observation: Bond Order Potential (BOP), and Stillinger-Webber Potential (SW). BOP is found to reproduce more accurately the dislocations' evolution, but requires more time and computational power, whereas SW potential, in literature used for the simulation of semiconductors, gives less precise results with less computational power and in shorter amount of time.