GaAs-based core/shell nanowires with extremely large lattice mismatch grown on Si substrates

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The geometry and high surface-to-volume ratio of nanowires offer unique possibilities for strain engineering in epitaxial semiconductor heterostructures with large lattice mismatch. In addition, the possibility to grow nanowires of high crystal quality epitaxially on Si substrates adds to their technological significance. In this work, we have investigated the growth of free-standing GaAs/$In_xGa_{1-x}As$ and GaAs/$In_xAl_{1-x}As$ core/shell nanowires on Si(111) substrates by molecular beam epitaxy, the accommodation of the lattice mismatch therein, and its effect on the nanowire properties.

Very thin GaAs core nanowires (20-25 nm in diameter) were grown in the self-catalyzed mode with a sufficiently low number density (to avoid beam shadowing effects) on SiO_x/Si(111) substrates, after an in situ treatment of the latter with Ga droplets. This resulted in zinc blende nanowires with their axis along the [111] crystallographic direction and six {1-10} sidewalls. Subsequently, conformal overgrowth of the $In_xGa_{1-x}As$ or $In_xAl_{1-x}As$ shell was obtained only under kinetically limited growth conditions that suppressed mismatch-induced bending phenomena.

The strain in the core and the shell was studied systematically as a function of the shell composition and thickness. To that end, we used Raman scattering spectroscopy, transmission electron microscopy and synchrotron X-ray diffraction, and compared the results with theoretical predictions based on continuum elasticity and density functional theories. Our results demonstrate that highly mismatched core/shell nanowires with defect-free interface can be obtained beyond what is possible in thin film heterostructures.

More interestingly, nanowires with strain-free shell and fully strained core can be grown under certain conditions. The large strain in the GaAs core is expected to have a strong effect on its fundamental properties. Here, we demonstrate a large shrinkage of the band gap, which can be as high as 35 % depending on the composition of the shell.

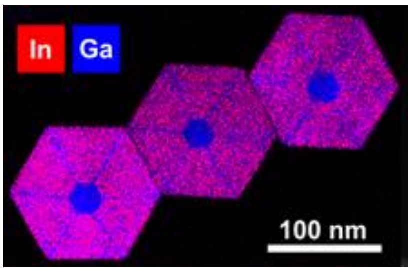

Fig. 1: Color coded elemental map showing the radial distribution of In and Ga in GaAs/$In_{0.20}Ga_{0.80}As$ core/shell nanowires as measured by energy-dispersive X-ray spectroscopy.

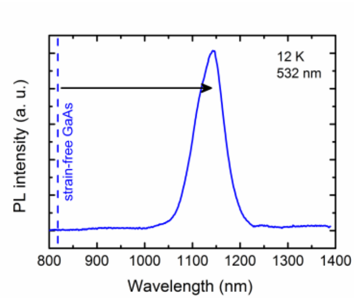

Fig. 2: Photoluminescence from GaAs/$In_{0.44}Al_{0.56}As$ core/shell nanowires showing the large band gap shrinkage of the tensely strained GaAs core.

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