GaAs/AlGaAs core-shell nanowires for energy applications: A structural study

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III-V compound semiconductors based solar cells present much higher efficiencies, due to their increased light absorption and charge mobility. Incorporating the photovoltaic properties of III-V semiconductors into nanowire (NW) structures, efficiencies similar to today's best solar cells are expected, with much less material. Furthermore, by decoupling light absorption from carrier collection pathways in core-shell NWs, excellent optical quality and long carrier lifetimes can be achieved.
GaAs/AlGaAs core-shell NWs were grown on Si(111) by plasma assisted molecular beam epitaxy (PAMBE) via the vapor-liquid-solid mechanism. Their nanostructure was explored by high-resolution and scanning transmission electron microscopy (HRTEM-STEM). NWs are zinc-blende (ZB) single crystals that emerge directly from the Si surface despite the presence of the thin amorphous native oxide. Then, growth proceeds by a continuous succession of (111) mirror twins. The core-shell structure was revealed by both diffraction contrast TEM and annular dark-field (ADF) STEM imaging, showing that the AlGaAs shell occupies at least one half of the projected diameter of the NWs, ranging from 80 nm to 200 nm. The Al content of the shell was estimated at ~35-38% by energy dispersive X-ray (EDX) analysis (Figure 1). Moreover, molecular dynamics (MD) simulations of plan-view NW slices were applied to calculate the variation of the energy, the stress tensors, the displacement field and the strain components of the core-shell configuration.

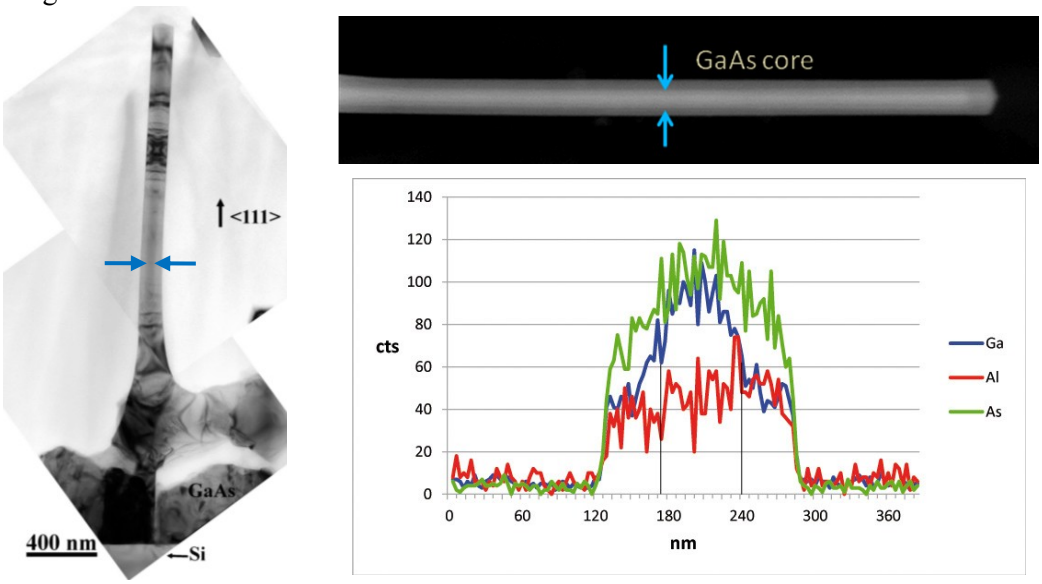

Figure 1. TEM image (left) of a GaAs/AlGaAs NW and the corresponding ADF image (top right). Arrows indicate the GaAs core. The EDX scan of the NW reveals the boundary between the core and the AlGaAs shell.

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