Interfacial phenomena in GaN core-AlN/GaN shell nanowires

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III-Nitrides core-shell nanowires (NWs) comprise non-polar $\{10\bar{1}0\}$ interfaces between the core and the shell, free from extended defects, allowing for a controlled band-gap and strain engineering in the development of novel optoelectronic devices. Transmission electron microscopy (TEM) methods were implemented to investigate the interfacial phenomena of GaN core- AlN/GaN shell NWs. The NWs were grown by plasma-assisted molecular beam epitaxy (PAMBE) on Si(111) with a thin AlN nucleation layer, consisting of a GaN base part, two intermediate, 10-15 nm thick, AlN spacers and a GaN cap layer. High-resolution TEM (HRTEM) observations revealed the core-shell structure with 2-3 monolayers (MLs) thick AlN shell around the GaN core and a second GaN shell overlaying the AlN one with a thickness of 7-10 MLs (Fig. 1). Quantitative measurements on the HRTEM images, along the growth axis, showed that this particular configuration imposes the *c*-lattice constant of the AlN shell to be adapted to the *c*-lattice constant of the GaN core. Therefore, a full elastic accommodation of the AlN on GaN is determined, considering the absence of misfit dislocations from the GaN/AlN interface. Regarding the AlN spacers, geometrical phase analysis (GPA) showed a gradual relaxation towards their central region, both along the axial and lateral directions, yet again without the presence of misfit dislocations. Finally, the core-shell NWs were investigated by Molecular Dynamics (MD) and Density Functional Theory (DFT) simulations of the experimental HRTEM images and the variation of the energy, stress tensors, strain components, displacement field and band-gap was calculated. The results shed light on the energetic, structural and electronic properties of the system.

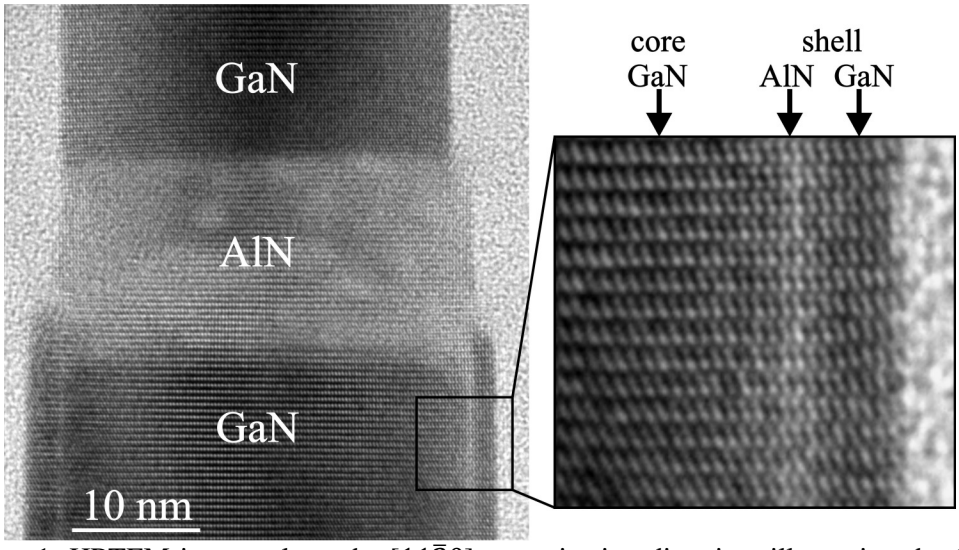

Figure 1: HRTEM image, along the $[11\bar{2}0]_{GaN}$ projection direction, illustrating the GaN core-AlN/GaN shell configuration.

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