Morphology dependent strain relaxation in horizontally grown semiconductor core-shell nanowires and its effect on electronic band alignment

Martí-Sánchez, S.[1], Oksenberg, E.[2], Koch, C.[1], Grau-Carbonell, A.[1], Joselevich, E.[2] and Arbiol, J.[1]

[1] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology (BIST), Spain, [2] Dept. of Materials and Interfaces and Chemical Res. Supp., Weizmann Institute of Science, Israel

Over the last years, bandgap engineering in semiconductors has played a key role in the development of new nanoscaled semiconductor materials thanks to their potential into new improved electronics. Among all the advantages that reducing the size of the employed materials present there is the ability of interfacing highly mismatched materials while keeping a high crystallinity, allowing the combination of the most suitable materials [1].

Horizontal guided growth was employed to obtain ZnSe@ZnTe planar nanowires [2], which present a 7.4 % mismatch between them. The materials form radial p-n heterojunctions that exhibit great optoelectronic properties, with dark currents below the detection limit and upon illumination a rectifying behavior with photovoltaic characteristics.

The growth of these materials has been done on sapphire substrates cut in different directions, and thereby having different mismatches with the materials grown on top. The formed structures present complex strain relaxation mechanisms in order to relax the high mismatched shell on top of the core of the nanowire that involve plastic and elastic deformations. An extended study involving Geometric Phase Analyses with modelling and HAADF-STEM image simulation has been employed to study these relaxation mechanisms. We have found how morphology of the core directly affects the strain distribution on the material, creating plane bending in the case of circular cores that form an angle between the dipoles in the structure that reach up to 4, and thereby, creating electrostatic potential barriers that affect the electronic band structure of the material. On the other hand, faceted-planar cores do not show any bending with respect to the core so there is no appearance of this potential barrier. Understanding and controlling the strain-induced band alignment modification has a key role in the understanding of the final properties of material and further operation of the corresponding devices.

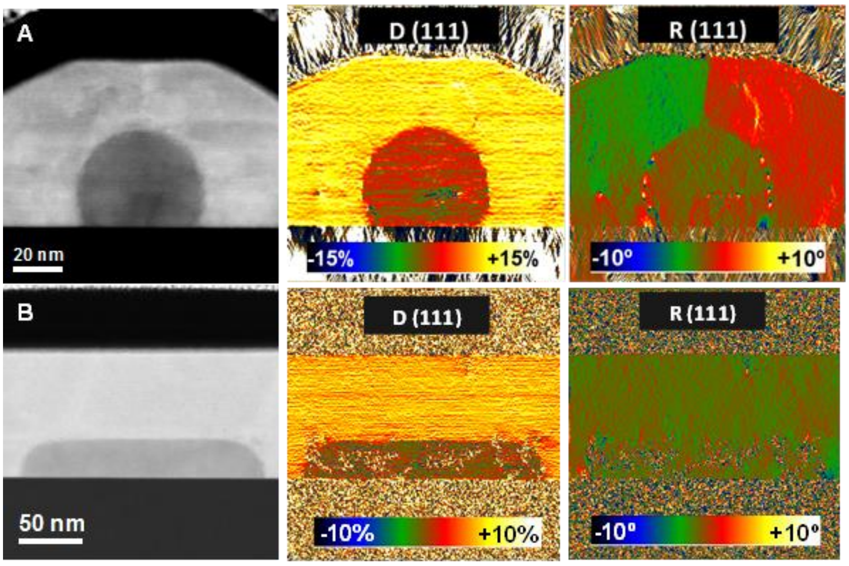

Figure. HAADF-STEM micrographs obtained on A) cylindrical core and B) flat core and dilatation and rotation of (111) planes obtained through GPA in both cases. A ±2 plane bending is found at both sides of the nanowire in the case of cylindrical core.

SMS acknowledges funding from "Programa Internacional de Becas "la Caixa"-Severo Ochoa", from Generalitat de Catalunya 2014 SGR 1638 and the Spanish MINECO e-TNT (MAT2014-59961-C2-2-R). ICN2 acknowledges support from the Severo Ochoa Program (MINECO, Grant SEV-2013-0295). Part of the present work has been performed in the framework of Universitat Autònoma de Barcelona Materials Science PhD program.

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[2] E. Oksenberg et al., ACS Nano, **11**, 6155-6166 (2017)