Faceting and EDX chemical analysis in core-shell Ge-Si nanowires

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1. INTRODUCTION

Semiconductor nanowires attracted a great deal of attention during the last decades. Despite a large number of studies dedicated to their fabrication and physical characterization, the electronic properties have still not been up to expectations. At present, most of the studies switched to core-shell nanowires that are expected to have more revolutionary properties. Theoretical demonstration of a direct band gap metamaterial for specific core-shell Si-Ge NWs has boosted the number of studies. The composition profile, morphology and core-shell aspect ratio could fully modify the band structure of the NWs and should be determined accurately. The determination of all these parameters remains a major challenge using conventional nanocharacterization techniques. In this study we perform the growth of core-shell Ge-Si nanowires by CVD and we observe them by STEM. EDX analysis showed the core-shell Ge-Si structure is very well defined. The intensity profile of Ge and Si exhibit a slight dissymmetry which is stronger in the core. Two models of the section of the nanowires are proposed and compared to the experimental data and the presence of facets on the core is shown to be a possible cause for this dissymmetry.

2. RESULTS

2.1 Results

The NWs investigated here are fully relaxed and the shell exhibits a polycrystalline structure. Figure 1 shows a typical STEM dark field image of a nanowire and the corresponding EDX maps for silicon and germanium respectively. On these maps, we can immediately remark the total absence of Ge in the shell of the NW and the abruptness of the core-shell interface. An accurate determination of the core-shell configuration can be provided by nanoscale composition profiling by EDX.

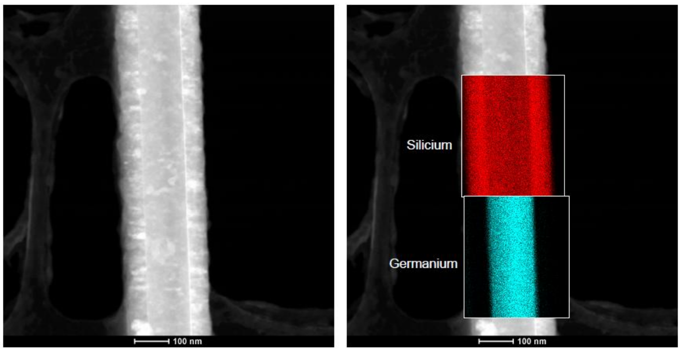

Figure 1. STEM dark field image of the core-shell Ge-Si nanowire and the corresponding EDX maps corresponding to Silicon and Germanium. The germanium forms the core and the silicon the shell.

Figure 2 shows such an EDX profile perpendicular to the axis of the nanowire. Both silicon and germanium relative compositions are represented on the graph. At first glance, they present the typical shapes expected for a core shell structure when the beam goes through the entire core-shell structure [1]. However, a slight dissymmetry is observed, especially in the core of the nanowire. The understanding of this dissymmetry is of crucial importance to determine the core-shell configuration. We then compare this experimental profile to the ones expected from two simple geometrical situations: a cylindrical shape and a faceted shape. In the latter we only consider the equilibrium facets that commonly form along the Si NWs, i.e. (111) and (100) facets.

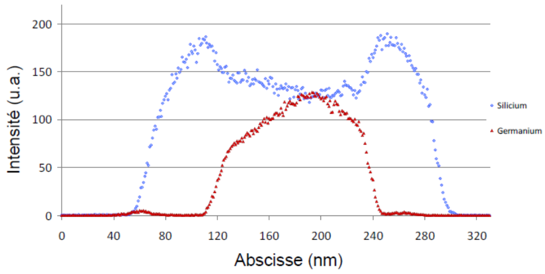

Figure 2. EDX profile for silicon and germanium perpendicular to the axis of the nanowire

2.2 Analysis

Figure 3 gives a schematic representation of two models for the section of the core-shell structure. The circular section explains qualitatively the general shape of the experimental profile but lacks of course the dissymmetry observed in the core. In the faceted case, a dissymmetry is observed on the profile, which fits well the experimental data on the core, but it gives a too large dissymmetry in the shell.

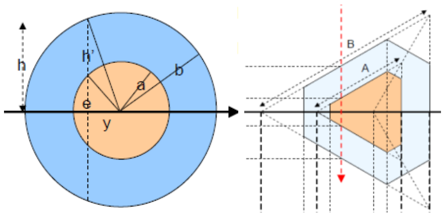

Figure 3. Schematic representation of the two simple configurations considered for the core-shell structure: cylindrical shape and faceted shape.

Figure 4 shows comparison of experimental profiles with two calculated ones resulting from a mixture between the two previously proposed models. The compositional profile fits a lot better the experimental results. This good agreement proves that the core-shell NW investigated here should have facets, but the shell is probably smoother.

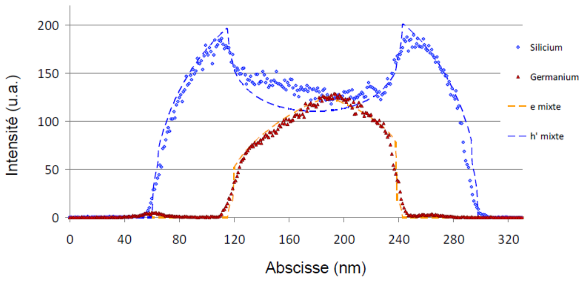

Figure 4. Experimental data superimposed on two profiles calculated from a mixture between both proposed models. The profile of the core has a mixing coefficient of 0.6 while the one of the shell is only 0.1, which means the core is probably more facetted than the shell.

3. CONCLUSION

Chemical analysis was performed by EDX on core-shell Ge-Si nanowires grown by CVD. The intensity profiles of Ge and Si present the overall expected shape for a core-shell structure but there is a slight dissymmetry in the core. These experimental data were compared to two profiles calculated from two simple configurations for the section of the core-shell structure: A cylindrical shape and a facetted one. The cylindrical model produces a shape profile very close to the experimental data of the shell but does not explain the dissymmetry observed in the core while the faceted configuration exhibits a strong dissymmetry. We show that the dissymmetry of the Ge profile could only be explained by a faceted Ge core, while the shell seems to maintain during growth a non equilibrium cylindrical shape probably due to the growth dynamics.

4. REFERENCES

[1] Varahramyan et al., *Applied Physics Letters*, 95, 033101 (2009) DOI:10.1063/1.3173811