HEXAGONAL AND TWINNED-CUBIC PHASE DOMAINS IN SILICON NANOWIRES

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Formation of hexagonal domains in group IV and III-V nanowires has been a point of intensive study in the last few years due to the dramatic influence of these domains on the electronic and optoelectronic properties of these nanostructures [1,2]. Wurtzite/Zinc-blende heterostructures have been found to influence the optical properties in III-V nanowires [3]. It is also expected that the presence of these heterostructures will change the transport properties [2].

The nanowires were grown by the Vapor-Liquid-Solid method, in which a metallic nanoparticle is used to catalyze the the nucleation and growth of the nanowires. Gold is the most widely used metal, because of its ease of implementation for the growth. Gold is an undesired metal for Si-based technology. As a consequence, the use of other catalysts such as Cu, In, Al or even catalyst-free nanowires growth have been studied [4]. Recently, after successful use of Ga as catalyst for III-V NWs [5], the use of Ga as an alternative catalyst for Si NWs growth has been also implemented [6]. The main benefit of using Ga is to avoid harmful contamination of the nanowires. Interestingly, in this case the Si nanowire morphology, growth direction and crystallization are affected. In particular, the appearance of rotationally twins and stacking-faults in the NW structure is a problem that must be studied in detail, as this phenomenon can have dramatic consequences for the physical properties of the grown nanowires.

Twin planes and, more generally, planar stacking faults are commonly found in group IV and III-V nanowires grown in the [111] direction. The formation and resulting morphology of randomly distributed stacking faults and twins in nanowires has been investigated by several authors. A rotationally twin plane in a zinc-blende (ZB) nanowire changes the atomic stacking locally and can be considered as a monolayer of the Wurtzite (WZ) phase. Formation of hexagonal domains in group IV and III-V nanowires has been the subject of intensive study in the last few years due to the dramatic influence of these domains on the electronic, optoelectronic and thermal conductivity properties of these nanostructures as elements for electronic device.

In the present work, we will present a detailed study of the formation of hexagonal domains in Si NWs when using different catalytic seeds (such as Ga, In, Cu and Au). Growth conditions (temperatures, pressures, etc.), as well as the material used as a catalyst and its deposited amount induce important changes in the NW crystallization, sometimes leading to the formation of twins and stacking-fault defects on the cubic structure. Periodicity of these faults, mainly twin defects, will be shown to create local areas of hexagonal structure. A detailed high-resolution transmission electron microscopy study of the different defect arrangements found in our nanowires will be shown. Several 3D atomic models and corresponding electron microscopy simulations will be also used for the understanding of the different structural configurations.

References:

[1] A. Fontcuberta i Morral, et al. Adv. Mat. **19** (2007) 1347.
[2] J. Arbiol, et al. J. Appl. Phys. **104** (2008) 064312.
[3] J. Arbiol, et al. Nanotechnology **20** (2009) 145704.
[4] J. Arbiol, et al. Nanotechnology **18** (2007) 305606.
[5] (a) A. Fontcuberta i Morral, et al. Appl. Phys. Lett. **92** (2008) 063112. (b) A. Fontcuberta i Morral, et al. Small **4** (2008) 899. (c) M. Heigoldt, et al. J. Mat. Chem. **19** (2009) 840.
[6] I. Zardo, et al. Nanotechnology **20** (2009) 155602.

Figures :

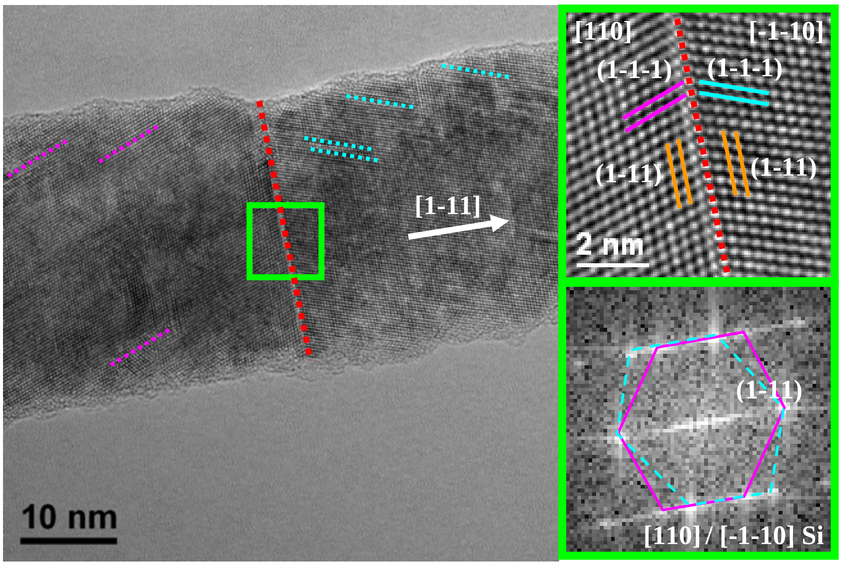

Figure 1 : (a) HRTEM micrograph of a Ga-seeded Si NW with presence of several twinned-cubic domains. (b) Magnified detail of the squared region in (a) showing the structure at both sides of the twin. (c) Power spectrum obtained in (b).