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## Analysis and Containment of Defect Formation in Zn<sub>3</sub>P<sub>2</sub> Crystals: A Nanoscale Approach

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A study recently published in “Nanoscale” demonstrates that high-quality Zn<sub>3</sub>P<sub>2</sub> crystals, free of interface defects, can be fabricated with a nanoscale approach. It consists in using selective area epitaxy to grow nanowires of Zn<sub>3</sub>P<sub>2</sub>, a material of interest for application in solar and photovoltaic cells. This work, coordinated by ICN2 group leader ICREA Prof. Jordi Arbiol, also employs state-of-the-art microscopy techniques and 3D simulations to thoroughly investigate the formation of differently-oriented structures within the nanowires.

Zinc phosphide (Zn<sub>3</sub>P<sub>2</sub>) is a semiconductor whose properties, including the abundance on our planet of its components, a direct bandgap and a high capacity to absorb light in the visible range, make it an attractive candidate for use in solar cells as an absorber –i.e. the layer that produces free charge carriers as a result of light absorption. However, in-depth studies on it are limited because of the difficulties involved in fabricating high-quality material. In particular, crystals of Zn<sub>3</sub>P<sub>2</sub> are produced by epitaxial growth on a substrate, but the structural characteristics of this material make it hard to grow extended bulks of it without incurring in defects, which can hamper its performance.



A study published in [Nanoscale](#) uses a nanostructure fabrication strategy to produce nanowires of Zn<sub>3</sub>P<sub>2</sub> with reduced elastic strains, which results in much less defects at the interface with the substrate. Besides proving that this approach is favorable, the work also uses advanced microscopy, imaging and simulation techniques to analyse the growth process down to the atomic level and to investigate the characteristics and influence of other kind of irregularities appearing in the grown nanowires. This research was coordinated by ICREA Prof. Jordi Arbiol, leader of the [ICN2](#) Advanced Electron Nanoscopy Group, and Prof. Anna Fontcuberta i Morral, from the Ecole Polytechnique Fédérale of Lausanne (EPFL, [Switzerland](#)); first authors of the paper are Dr Maria Chiara Spadaro, postdoctoral researcher in Prof. Arbiol’s group, and Dr Simon Escobar Steinvall, previously at EPFL and currently postdoctoral

researcher at Lund University ([Sweden](#)).

The researchers grew Zn<sub>3</sub>P<sub>2</sub> nanowires on a substrate of indium phosphide (InP) by means of selective area epitaxy (SAE), a technique in which a mask is used to limit the growth to specifically designed openings and desired directions. The small contact surface between the two materials and the use of a mask allowed the fabrication of nanowires with no misfit dislocations at the interface, or in other words, no interface-related defects. In particular, two crystalline orientations were chosen to grow the nanowires, at 45° with respect to each other, and both exhibited the same high quality.

There are other defects, though, that can show up during the fabrication process –even using this nanoscale approach— and are actually more difficult to monitor and control. In fact, the authors of this study observed the formation of rotated domains in the grown material, which means that there are parts within the whole structure that present a different crystal orientation with respect to the rest. In order to analyse in detail this phenomenon and how it affects the quality of the Zn<sub>3</sub>P<sub>2</sub> nanowires, the authors of this study used state-of the art techniques (atomic resolution aberration corrected high-angle annular dark-field scanning transmission electron microscopy imaging, or AC-HAADF STEM) to collect structural information about the material down to the atomic level. They also used the data collected to create reliable 3D atomic models performing HAADF-STEM image simulation, to get deeper insight into the growth process.

They observed domains rotated 120° in both kinds of nanowires (of 0° and 45° crystalline orientation), whose interfaces though are very sharp. No dangling bonds or mid-gap electronic states formed at the rotated interface. They explained this phenomenon as a result of the simultaneous and independent growth of crystals with different orientations in separated parts of the mask openings. As growth continues, all parts merge in a unique structure and the dominant one completely integrate the others. Two animations were realized to illustrate this process in the two kinds of nanowires; they are available here (0° orientation) and here (45° orientation).

This study demonstrates that the nanoscale approach based on selective area epitaxy guarantees the fabrication of higher-quality Zn<sub>3</sub>P<sub>2</sub> crystals, i.e. its growth with no defects at the interface. It also proves the capabilities of advanced microscopy and imaging techniques (specifically, the abovementioned AC HAADF-STEM) and 3D atomic modelling and image

simulations to fully understand the defect formation and their impact on novel materials.

Read the [original article](#) on ICN2.