PhD offer at LMGP Lab.

Investigating the polarity related properties of well-ordered ZnO nanowires for piezoelectric devices: The issue of defects & hydrogen

Topic

The development of semiconductor nanowires (NWs) is of great basic and technological interests owing to their high aspect ratio at nanoscale dimensions, giving rise to novel, remarkable properties, as well as a broad range of potential applications. Among them, ZnO as an abundant and biocompatible compound semiconductor with attractive properties has been receiving increasing interest over the last decade. It crystallizes into the strongly anisotropic wurtzite structure, which is both polar and piezoelectric. Its ability to grow as NWs oriented along the polar and piezoelectric ±[0001] (*i.e.*, *c*) axis by a number of deposition techniques including the low-cost and low-temperature chemical bath deposition is of great importance for its use in nanoscale engineering devices. The efficient integration of ZnO NWs into the engineering piezoelectric devices to name a few requires the precise control of the uniformity of their structural morphology over large surface areas. This is typically achieved by selective area growth using pre-patterned nucleation surfaces by technological processes in a cleanroom environment (*i.e.* advanced lithography and etching).

Two correlated fundamental properties that have crucial effects on the piezoelectric device performances are the polarity and the nature and the defect density. We have shown, for the first time, in 2014 the formation of O- and Zn-polar ZnO NWs, opening the way for more deeply analyzing their effects, which are critical as reported in ZnO single crystals and films. Interestingly, the nature and the density of the defects are related to surface terminations at the NW top facet and thus to polarity. However, these characteristics are not known in ZnO NWs, although they drastically govern the performances of the engineering devices. In particular, hydrogen has recently emerged as a major source of defects in ZnO NWs, but very little is currently known about this subject.

The thesis project aims at elucidating the present polarity as well as the nature and density of defects (especially defects in connection with hydrogen) on well-ordered O- and Zn-polar ZnO NWs formed by combining selective area growth with chemical bath deposition in LMGP by correlating advanced characterization experiments as transmission electron microscopy, Raman spectroscopy, Fourier Transformed infrared spectroscopy, tunnel microscopy equipped with local probes, X-ray photoelectron spectroscopy with *ab initio* calculations to simulate the position of H inside the ZnO structure. Following this fundamental investigation, the fabrication of piezoelectric devices will be considered to directly show the beneficial effects on the device performances.

Scientific environment:

The applicant will work in the LMGP, Materials and Physical Engineering Laboratory inside the Nanomaterials and Advanced heterostructures team in close collaboration with the Aristotle university of Thessaloniki, Physics department in Greece for the *ab initio* calculations and neighbour laboratories in Grenoble (i.e. Institut Néel, …) for specific characterisation techniques.

Located in the heart of an exceptional scientific environment, the LMGP offers the applicant a rewarding place to work.

LMGP Web Site: http://www.lmgp.grenoble-inp.fr/
PhD thesis duration: 36 months from Fall 2019

Required background

The applicant should have an Engineering degree and/or a Master of Science in materials physics and chemistry, nanosciences, and/or semiconductor physics. Specific skills regarding team work and English abilities will be required for her/his integration into the team and for taking part in the ongoing international collaborations.

Fundings: IMEP-2 Doctoral School (priority PhD thesis topic)

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Closing date for applications: 27th of May 2019