The Warsaw Doctoral School in Natural and Biomedical Sciences and the Institute of Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Combining advanced ion beam and X-ray scattering theories to model ion implanted single to polycrystalline materials

given by

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on 25th June 2024, 10:30 at the IF PAN Auditorium

Duration: 45 min + question time

The event will be available on ZOOM also, at this link

All Warsaw-4-Phd students (and others) very welcome!

Abstract of the talk:

Recent progress in the growth techniques makes it possible to fabricate low-dimensional structures, e.g., thin films (planar multilayers), mesoscopic structures and nanostructures (lateral surface and multilayer gratings, quantum wires and dots). The opto- and micro-electronics are among the fields where the resulting novel properties of homo(hetero)-epitaxial growth of semiconductors are more significant. The optimization of the fabrication process and the physical understanding of the samples requires non-destructive structural studies of the materials. Improving the properties of the as-grown quantum materials is also fundamental from the point of view of the Nanotechnology. An example of controlled process to change the properties of materials is the ex-situ incorporation of ion species. The possibility to control dopant concentrations, depth profiling and the high purity through mass selection turn ion implantation into a silicon industry ready-to-use tool. However, the stochastic nature of the process in which energetic ions collide and penetrate the semiconductor, results in lattice damage. Although the crystal degradation is partially reversed after thermal or pressure annealing's, vacancies and point defects introduced and rearranged after annealing create a strain field which does not disappear completely. Complementary to the direct local probing methods (atomic force microscopy, transmission electron microscopy (TEM), high angle annular dark field (HAADF) or phase analysis to determine the strain in quantum materials), the X-ray elastic scattering methods probe locally the reciprocal space, thus providing relevant information about the statistical properties of the structural parameters averaged over a large volume of a sample. X-ray diffraction (XRD) and reflectivity (XRR) in the specular and non-specular geometries are relevant techniques for these structural studies of both crystalline and amorphous systems. They are highly sensitive to the distribution of the lattice parameters (diffraction) and refractive index (reflectivity). This presentation explores the synergy between ion beam implantation and X-ray scattering techniques to advance the understanding of implanted crystalline materials. Several examples of implanted single and polycrystalline crystals will be presented following by an overview of the required theoretical principles underlying both techniques. To predict the decrease of the crystalline induced by the ion implantation, a new approach to the interpretation of the diffraction data of implanted crystals will be presented. The novel methodology considers the effects of the variations of the atom's positions in the lattice instead of employing the static Debye-Waller, strictly related to thermal vibrations. The new method, supported by preliminary molecular dynamics simulations, is tentatively applied to chromium implanted Ga_2O_3 and carbon implanted 4H-SiC bulk-crystals and to argon implanted GaN thick layers grown by MOCVD on sapphire-c substrates. Finally, a brief description of the MROX software, acronym for Multiple Reflection Optimization package for X-ray scattering used to simulate the XRD data, is highlighted.

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Sérgio Nuno Canteiro de Magalhães *(ORCID number: 0000-0002-5858-549X; Web of Science ResearcherID: A-6709-2018) is a DL57 researcher under the 16/IPFN contract at Instituto Superior Técnico in Lisbon, Portugal. This contract was awarded for the development of models aimed at studying the effects of ion-implanted nano-materials using X-rays and ion beams.*

Sérgio Magalhães's journey into the realm of crystal growth began with the exploration of recent advancements in techniques, which have revolutionized the creation of low-dimensional structures. These structures, encompassing thin films, mesoscopic forms, and nanostructures, hold immense significance for Condensed Matter Physics, particularly in opto- and micro-electronics. Their uniqueness stems from the epitaxial growth of semiconductors, facilitated by cutting-edge crystal growth methods.

Sérgio Magalhães's fascination with enhancing the attributes of these materials led to delve into the realm of Nuclear Sciences. Here, Sérgio Magalhães discovered the pivotal role of controlled processes in modifying materials, particularly through ex-situ incorporation of ion species. This method allows for precise manipulation of dopant concentrations, depth-profiling, and ensuring high purity through mass selection, thereby positioning ion implantation as a key tool for integration into the silicon industry. However, the journey is not without its challenges. On the on hand, the stochastic nature of ion implantation brings forth lattice damage as energetic ions interact and penetrate the semiconductor lattice. While thermal or pressure annealing offers partial relief, the introduction of vacancies and point defects during this process leaves behind residual strain fields that persist beyond annealing. On the other hand, the advanced measurements acquired from X-ray scattering and ion beam techniques demand equally sophisticated computer software tools to simulate their data. In response to this need, the MROX (Multiple Reflection Optimization) package for X-ray diffraction/reflection software has been recently developed. It should be emphasized that program made by Sérgio Magalhães allows to simulate XRD data of advanced semiconductor structure systems (superlattices, nanowires, quantum-dots, thin layers, ion implanted structures) what is impossible in commercial available XRD software. Already, MROX program has been credited in 16 research manuscripts published in reputable international peer-reviewed journals.

Driven by the quest to unravel these complexities and enhance material properties, Sérgio Magalhães embarked on a mission to conduct non-destructive structural investigations. Leveraging X-ray and ion beam techniques, Sérgio Magalhães's goals are to gain deeper insights into the mechanisms of damage accumulation in crystals. The success has been bolstered by over 60 research publications, facilitated by numerous international collaborations, including partnerships with esteemed institutions such as the Institute of Physics at the Polish Academy of Sciences.