Postdoctoral position

Lattice dynamics of point and extended defects in III-V semiconductor nanostructures from *ab initio* calculations

A 2 year post-doctoral position is available in the framework of an international French-German ANR-DFG project at the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), CNRS & Sorbonne Université, Paris.

Job description

Job title : Post-doctoral researcher on lattice dynamics of point and extended defects in III-V semiconductor nanostructures from ab initio calculations
Location : Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, 4 place Jussieu 75005 Paris, France
Required degree : PhD degree
Planned starting date : November 1st, 2024
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Scientific context

Electron Energy Loss Spectroscopy (EELS), as implemented in the Scanning Transmission Electron Microscope (STEM), is a widely-used technique based on the inelastic scattering of fast electrons (30-300keV) as they travel through a thin specimen. The spectrum, obtained by analyzing the energy lost by the transmitted electrons, reveals many excitations characteristic of the solid, ranging from phonons, excitons or plasmons to inner-shell ionizations. During the last 15 years, EELS has witnessed a revolution triggered by the availability of aberration correctors and monochromators which offered, for the first time, the possibility to carry out atomically resolved spectroscopic mapping with, now, a sub-10meV energy resolution [1-4].

The newly accessible energy loss range located between 15 and 500meV is of utmost importance in materials and nanosciences as it essentially matches the energy scale characteristic of atomic vibrations. Therefore, atomic scale measurements of these vibrations are now accessible and open tantalizing opportunities in research areas such as optoelectronics, where nanoscale thermal management of high-speed or high-power devices is becoming a central issue. For instance, atomic vibrations in nanowires (NW) with dimensions comparable to the phonon wavelength can be coherently scattered by surfaces, interfaces or structural defects, creating quite literally hot spots and eventually degrading the device efficiency.

Systems containing a very large number of atoms, such as those necessary to describe the structure of point or extended defects, often display complex behaviors, hindering a straightforward interpretation of their vibrational spectra based on a simple comparison with known references or empirical models. A proper assessment of the origin of the different structures observed experimentally and of the underlying physics therefore heavily relies on first-principles calculations [5,6]. Systems of a few thousand or even tens of thousands of atoms remain, however, impossible to handle with a standard use of the current available computational tools. The theory group of IMPMC recently developed a strategy based on the so-called *force constant matching* approach in which the

interatomic force constants calculated *ab initio* on smaller subsystems, are latter assembled to build the dynamical matrix of the entire system [2]. These developments have set the state-of-the-art in the field and are still unmatched in terms of accuracy and predictive power.

The goal of this postdoctoral project is thus to investigate computationally, using first-principles methods (DFT), the atomic scale vibrational properties of relevant point or extended defects (dopants, cluster of impurities, stacking faults, inversion domains, interfaces) in III-V semiconductors (mostly GaN and AlN) NWs used for optoelectronics applications. Part of this work will be devoted to the interpretation of high-resolution EELS experimental data acquired by the German partner of the project (Arbeitsgruppe Strukturforschung und Elektronenmikroskopie - Humboldt-Universität, Berlin) on a state-of-the-art NION HERMES microscope.

Project description

The candidate will investigate theoretically the vibrational properties of a series of well identified atomic scale defects occurring in III-V semiconductor nanowires (GaN/AlN), ranging from isolated and clustered dopant atoms (Si, Mg, Eu) to stacking faults and inversion domains. The strategy developed to tackle this challenging problem on the ground of *ab initio* methods will rely on the force-constant matching approach [2,7]. This strategy therefore implies the extensive use of codes based on Density Functional Theory, such as the suite of codes Quantum ESPRESSO [8], involving structural relaxation, in-depth electronic structure analysis and vibrational properties investigation of systems of small size, using finite-displacement or linear response techniques [8,9]. The candidate will then extend/adapt the codes already developed in the lab for constructing the dynamical matrix of larger systems containing up to a few tens of thousands of atoms providing a well converged, realistic model of the systems investigated experimentally. The analysis of the results will typically involve the calculation of quantities such EELS spectra, dynamic structure factors, phonon dispersions or projected phonon densities of states.

Surface phonon-polaritons, resulting from the coupling between light and phonons in polar materials such as GaN or AlN, are also measured in EELS when investigating nanostructures. The theoretical study of these localized excitations in III-V nanowires can be addressed in a second part of the project, depending of the candidate's skills and interest. These excitations can be very accurately described using the local continuum dielectric model, which consists in solving Maxwell's equations in a region of space containing the nanostructure and accounting for the inelastic scattering of the swift electrons within the framework of classical electrodynamics. Several aspects will be considered, such as the influence of the nanowire aspect ratio on the polariton energies or the existence of coupled phonon-plasmon polaritons in heavily *n*-doped nanowires.

The candidate will also strongly interact with our collaborators in France (IRIG, CEA Grenoble), responsible for the growth and characterization of the nanowires and in Germany (AG SEM Humboldt Universität, Berlin), responsible for the EELS measurements.

Working environment

The Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (*IMPMC*), located in the center of Paris (place Jussieu), is a world leading laboratory for the development and the modeling of light, X-ray and electron-based spectroscopies. Its worldwide recognized expertise ranges from core-level spectroscopies such as X-ray absorption spectroscopy, X-ray circular magnetic dichroism, X-ray Raman Scattering, to vibrational spectroscopies such as IR absorption, non-resonant inelastic X-ray scattering, Raman and vibrational EELS. The candidate will also benefit from the strong interaction with our collaborators in France (IRIG, CEA Grenoble, responsible the growth of the

samples) and in Germany (AGSEM, Humboldt-Universität zu Berlin, responsible for the high-resolution EELS experiments).

Required skills

- PhD degree in condensed matter physics or materials science;
- Prior experience in *ab initio* calculations (Density Functional Theory);
- Good programming language skills (Fortran, Python, etc.), Linux environment;
- Fluent English;
- Strong taste for solid-state and numerical physics.

How to apply

Qualified candidates should submit their application through the dedicated CNRS website (https://emploi.cnrs.fr/Offres/CDD/UMR7590-GUIRAD-003/Default.aspx). Additional information can be obtained directly from Guillaume RADTKE (guillaume.radtke@sorbonne-universite.fr) or Michele LAZZERI (michele.lazzeri@sorbonne-universite.fr).

References

[1] O.L. Krivanek *et al., Nature* **514** (2014) 209.
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