

High-throughput X-ray diffraction data analysis with deep-learning algorithms

This PhD position is offered within the framework of the SYNEART project, a multi-partner initiative funded under the France 2030 investment plan and the PEPR DIADEM exploratory program. The position is opened at IRCER (Institut de Recherche sur les Céramiques – Limoges, France) in close collaboration with GREMAN (Materiaux, Microélectronique, Acoustique et Nanotechnologies – Tours, France).

Context

Current Artificial Intelligence (AI) is constrained by the Von Neumann bottleneck, where the separation of processing and memory units leads to massive energy inefficiency. The SYNEART project aims to address this issue by leveraging the physics of relaxor ferroelectric thin films to produce neuromorphic devices. As compared to conventional ferroelectrics, relaxor ferroelectrics are characterized by polar nanoregions and a "flat" energy landscape, which allows them to experience multiple stable states, making them ideal candidates for building artificial synapses and neurons with much lower power consumption than traditional CMOS technology. To accelerate the discovery of optimal "composition/thickness/electrode" combinations, the project utilizes high-throughput synthesis (Combinatorial Pulsed Laser Deposition - CPLD) and AI-assisted characterization.

Objectives

The PhD student will specifically contribute to AI-accelerated high-throughput characterization and analysis. The primary objectives are:

- high-throughput XRD analysis: microbeam X-ray diffraction (XRD) will be performed on compositional libraries synthesized by CPLD, with a special interest for 2D and 3D reciprocal space maps (RSMs), recorded in several geometries. Efficient data handling workflows will be developed.
- deep learning implementation: a central challenge is the massive volume of data generated that poses a challenge to conventional analysis methods. The objective is to develop and implement deep neural networks to automate data analysis, enabling fast recognition of phases, symmetry (polar/non-polar, cubic, etc.), and lattice parameters.

The recruited student will be able to draw on the expertise of IRCER and GREMAN in the field of thin film growth and characterization [1, 2] and advanced XRD data analysis, including the development of deep learning algorithms [3, 4].

Profile of the applicant

Education: a Master's degree (or equivalent) in Materials Science, Solid State Physics, Crystallography, or Applied Mathematics/Data Science with a strong interest in physical applications.

Technical expertise: proficiency in programming for data handling and scientific computing.

Soft skills: ability to work in a highly interdisciplinary environment. Good communication skills for collaborating across the project's various research units (SPMS, IRCER, GREMAN, LPMC). A good command of the English language is required, both written and oral.

Salary, dates

The starting date of the 3-years PhD position is 1st October 2026. It is a fixed term contract (36 months) with a gross monthly salary of ~2300 €.

Contact

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References

- [1] C. Daumont, Q. Simon, S. Payan, P. Gardes, P. Poveda, M. Maglione, B. Negulescu, N. Jaber, J. Wolfman, "Tunability Investigation in the $BaTiO_3$ - $CaTiO_3$ - $BaZrO_3$ Phase Diagram Using a Refined Combinatorial Thin Film Approach", *Coatings* 11, 1082 (2021).
- [2] Nadaud, G. F. Nataf, N. Jaber, B. Negulescu, F. Giovannelli, P. Andreazza, P. Birmal, J. Wolfman "Enhancement of piezoelectric properties in a narrow cerium doping range of $Ba_{(1-x)}Ca_xTi_{(1-y)}Zr_yO_3$ evidenced by high throughput experiment", *ACS Applied Electronic Materials* 6, 7392 (2024).
- [3] A. Boulle, A. Debelle, "Convolutional neural network analysis of x-ray diffraction data: strain profile retrieval in ion beam modified materials", *Machine Learning: Science and Technology* 4, 015002 (2023).
- [4] A. Souesme, R. Guinebretière, O. Castelnau, A. Boulle, "High-throughput determination of crystallite size and microstrain from X-ray diffraction data with deep neural networks", to appear in *Machine Learning: Science and Technology* (2026).