NanOX-ML project is a joint French-Austrian academic research project funded for 4 years by the ANR and FWF agencies. It brings together 6 academic labs. It focuses on the understanding of the coupling between phase transitions, local compositional fluctuations and strain distributions in dense nanostructured oxide polycrystals subjected to very high temperature thermal loading. Most of oxide based refractory materials are made of polycationic oxides in the form of solid solutions. Phase separation processes occur during thermal treatments, as a result of the coupling between local variations of composition at the nanometer scale and strain relaxation mechanisms. These transformations significantly affect the structural integrity (creeping, cracking, etc.) of the materials. The approach proposed in this project is based on x-ray diffraction (XRD) performed at synchrotron radiation facilities which allows analyzing quantitatively, in situ, at high temperature the evolutions at the nanometer scale of dense oxide polycrystals. The increasing efficiency of modern synchrotron radiation sources poses new challenges, not only in terms of the huge data throughput making human-based approaches unfeasible, but also regarding the development of smarter data collection schemes. At the core of the NanOX-ML are the development of machine learning (ML) codes able to solve this issue, via the development of new algorithms enabling, on the one hand, the development of agile and versatile data collection procedures and, on the other hand, the ability to analyze data in real time.

Recruitment of a Post Doc fellow (f/m)

"Computing X-ray diffraction data from polycrystalline materials for AI training"

1. Your responsibilities:

The project focuses on the analysis of the nanostructure of oxide polycrystalline materials, in particular using the upgraded Laue microdiffraction (µLaue) station of the European Synchrotron Radiation Facility (ESRF) IF beamline. µLaue is a powerful method to quantify strain at the local scale (~ 300 nm) and, with the recent development of deep learning-based indexing algorithms [1], it is able to operate in real time during *in situ* measurements even at high temperature [2]. One of the goal of this project is to push this technique further and analyze the intensity distribution in the vicinity of the x-ray diffraction (XRD) peaks so as to be able to quantify local strain, compositional gradients and defect densities. Computing XRD data is a two-step process. The first step involves the generation of realistic microstructures in the form of numerical cells. The second step is to compute the scattered intensity from the cells, considering the geometry of the experiment. Based on our previous work [3], this methodology will be applied to µLaue data, using numerical cells with simple model defect structures. Your work will therefore imply:

- ✓ generating numerical crystals with defects (point defects, dislocations, twin boundaries,...)
- ✓ computing the diffracted intensity in the µLaue geometry

Depending on the progress of the project, convolutional neural networks will be designed and trained with the data generated, and tested with real data recorded at ESRF.

[1] R. R. P. Purushottam Raj Purohit, S. Tardif, O. Castelnau, J. Eymery, R. Guinebretiere, O. Robach, T. Ors, J.S. Micha "LaueNN: Neural network based hkl recognition of Laue spots and its application to polycrystalline materials" J. Appl. Cryst. 55 (2022) 737-750.

[2] R.R.P. Purushottam Raj Purohit, D. Fowan, S. Arnaud, N. Blanc, J.S. Micha, R. Guinebretière, O. Castelnau, "Laue microdiffraction on polycrystalline samples above 1500 K thanks to the QMAX furnace" J. Appl. Cryst. 57 (2024) 470-480.

[3] A. Boulle, A. Chartier, A. Debelle, X. Jin, J. -P. Crocombette, "Computational diffraction reveals long-range strains, distortions and disorder in molecular dynamics simulations of irradiated single crystals", J. Appl. Cryst. 55 (2022) 296-309.

2. Your qualifications:

We are looking for a motivated applicant holding a PhD in condensed matter physics, material science, crystallography or other closely related fields. The successful candidate should be familiar with XRD and Python programming. She/he will have good communication skills and team spirit. The ability to work in a collaborative international environment is essential.

3. We offer:

The post doc fellow will be employed by the CNRS in Limoges (IRCER lab) and will work in close collaboration with the PIMM lab. in Paris and the scientific staff of the IF beamline in Grenoble where the experimental work will be done. This full-time position is aimed to start in spring 2025 and is offered on a fixed-term **18 months** contract.

4. Your application:

Applications, consisting of a detailed scientific CV and a letter of motivation, should be sent to the following addresses: rene.guinebretiere@unilim.fr, alexandre.boulle@cnrs.fr and damien.andre@unilim.fr before April 18, 2025. Contact information for 1 or 2 references are welcome.