

NanOX-ML project constitutes a collaborative French-Austrian academic research project funded for 4 years by the ANR and FWF agencies. It brings together 6 academic labs and is centered on the understanding of the coupling between phase transitions, local compositional fluctuations and strain distributions in nanostructured oxide polycrystals subjected to thermal loading at very high temperatures. The majority of oxide-based refractory materials are constituted 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 (creep, nanocracks, etc.) of the materials. The overall 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 of the material at the nanometer scale. 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), 18 months

“Investigation of the stress field in nanostructured oxide materials during phase transformation by combining full-field modelling and X-ray diffraction”

1. Your responsibilities:

The objective of this postdoctoral position is to estimate the stress field that accumulates in an oxide material submitted to thermal loading. We will in particular study zirconium oxide (zirconia), which is extensively employed at an industrial scale as a refractory material in the glass industry, for dental implants, among other applications. Zirconia undergoes a **tetragonal → monoclinic phase transition** during cooling, starting around 1170°C. Modelling results will be compared with quantitative *in situ* high-temperature X-ray diffraction measurements performed at the **European Synchrotron Radiation Source (ESRF)**. **Stress levels in the GPa range** are expected at the grain (nanometric) scale [1] in this material. Such significant levels of stress lead to the formation of a nanocrack network. Moreover, the process of phase transition may be influenced by such stresses, for example by enabling the formation of a high-pressure orthorhombic phase. The relatively uncomplicated microstructure of the specimens (featuring 24 crystal orientations/variants) has been key to multi-year experiments at the ESRF from our group, enabling 3D scanning of the crystallographic reciprocal space [2] and surface imaging at 300 nm spatial resolution [3]. The responsibilities of the post-doctoral researcher will be twofold:

- The modelling of the stress field in monoclinic zirconia by employing a **spectral (FFT) full-field method** [4] during thermal loading is the subject of this study. In order to achieve this objective, random monoclinic **polycrystalline microstructures will be constructed** on the basis of established crystallographic rules for variant selection, in continuation of our previous work [5].
- The subsequent step will involve the extraction of **synthetic X-ray diffraction diagrams** from the model results, which will then be compared to the experimental ones. This comparison will be based on the experience of the team in this field [6]. Therefore, this position will also require **analysis of experimental datasets** to derive quantitative values suitable for comparison with the model results.

[1] R. Guinebretière, T. Ors, V. Michel, E. Thune, M. Huger, S. Arnaud, N. Blanc, N. Boudet, O. Castelnau, Coupling between elastic strains and phase transition in dense pure zirconia polycrystals, *Phys. Rev. Mater.* 6, 013602 (2022)

[2] R.R.P. Purushottam Raj Purohit, D. Pepin Fowan, E. Thune, S. Arnaud, G. Chahine, N. Blanc, O. Castelnau, R. Guinebretière, Phase transition and twinning in polycrystals probed by in situ high temperature 3D reciprocal space mapping, *Appl. Phys. Lett.*, 121, 181901 (2022).

[3] 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 achieved with the QMAX-microLaue furnace, *J. Appl. Cryst.*, 57 (2024), p. 470-480

[4] H. Moulinec, P. Suquet, A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Comput. Methods Appl. Mech. Eng.* 157, 69–94 (1998).

[5] L. Petrich, K. Derrien, V. Schmidt, R. Guinebretière, H. Moulinec, O. Castelnau, Thermo-elastic micromechanical modeling of tetragonal ZrO₂ with a herringbone microstructure inherited from the cubic phase, *Mater. & Design*, 257 (2025) 114425.

[6] 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 mechanics of materials, condensed matter physics, material science, or other closely related fields. The candidate should be familiar with numerical computation / Python programming, and possibly with crystallography and x-ray diffraction techniques. 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 Paris** (PIMM lab, France) and will work in close collaboration with the IRCER lab in Limoges (France) and the scientific staff of the D2AM and IF beamlines at ESRF (Grenoble, France) where the experimental work will be done. This full-time position is aimed to start ideally in January 2026 and is offered on a fixed-term **18 months** contract. The salary will follow CNRS standard and depends on your experience (~2535€/month for < PhD + 2years)

4. Your application:

Applications, consisting of a detailed scientific CV, a letter of motivation, and reports of the PhD defense, should be sent to olivier.castelnau@ensam.eu and katell.derrien@ensam.eu. The provision of contact information for 1 or 2 references is also welcome.

