



2-year postdoctoral position



## **Modeling of Ti-Zr-O thermodynamics from ab initio calculations**

A postdoctoral position is available in the laboratory of physical metallurgy in CEA Saclay (France) for two years starting this Fall 2020.

Among the various significant questions affecting titanium metallurgy, the effect of oxygen on the mechanical properties of titanium alloys remains one of the most critical issues. A small addition of oxygen is known to induce a strong hardening resulting in a large increase of strength but also a drastic drop of ductility leading to embrittlement. It has been shown recently that it is possible to add oxygen to a titanium alloy consisting of a binary Ti-Zr solid solution, to obtain the classical oxygen hardening contribution without any loss of ductility. The main objective of this postdoc is the accurate determination of the different phases existing in these new Ti-Zr-O alloys using thermodynamic modeling at the atomic scale and making use of ab initio calculations. We will in particular focus on the oxygen ordering tendency in titanium and on the impact of zirconium addition on this ordering, as the ductility loss induced by oxygen in titanium alloys is believed to be linked to the apparition of  $Ti_6O$  ordered compounds and/or to the development of short range order.

This postdoc is part of a project, ANR TiTol, involving four different French laboratories (IRCP Chimie ParisTech, ICMPE Univ. Paris Est, Diffabs Soleil and SRMP CEA Saclay). It will benefit from interactions with experimental work performed inside the project (alloy design, microstructural and mechanical characterization, synchrotron X-ray diffraction). In particular, predictions of the modeling approach will be directly compared to, but also guided by, X-ray diffraction experiments and resistivity recovery and calorimetry experiments

**Laboratory:** SRMP, laboratory of physical metallurgy, is part of CEA, the French atomic energy agency. The research center of Saclay is located 20 kilometers South of Paris to which it is connected by public transportation.

More information on CEA: <http://www.cea.fr/english>

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**Time frame:** The position is available immediately and the funding is for two years.

**Qualification:** The applicant should hold a Ph. D. Degree in solid state physics or materials science, with skills in one or more of the following simulation methods:

- Density functional theory
- Modeling of alloys thermodynamics

Experience in computer programming is also highly recommended.

**How to apply:** Candidates should send their application (statement of research interest, CV, names and contact information of two references) to [emmanuel.clouet@cea.fr](mailto:emmanuel.clouet@cea.fr)



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## Dislocation – precipitates interaction in Zr-Nb alloys

A postdoctoral position is available in the laboratory of physical metallurgy in CEA Saclay (France) for two years starting this Fall 2020.

Zirconium alloys, which are used for the cladding of the fuel rods in nuclear reactors, may contain niobium. Under irradiation, niobium enriched precipitates are formed. These precipitates, which are thermodynamically stable, improve the resistance to thermal creep after irradiation. This postdoc aims to understand how these Nb precipitates impact Zr plasticity, by studying their interaction with gliding dislocations in the zirconium matrix. In that purpose, we will perform molecular dynamics simulations using a newly developed Zr-Nb interatomic potential which is well suited to describe both dislocation properties in zirconium and properties of niobium precipitates. The elementary interaction mechanisms obtained at the atomic scale will be used then to develop dislocation dynamics simulations to describe the impact of a whole precipitate microstructure on dislocation glide.

This postdoc is part of a joined research project between CEA, EdF and Framatome. It will benefit from interactions with other parts of the project, including TEM characterization of plasticity in these Zr-Nb alloys and development of crystal plasticity models to describe post-irradiation creep behavior.

**Laboratory:** SRMP, laboratory of physical metallurgy, is part of CEA, the French atomic energy agency. The research center of Saclay is located 20 kilometers South of Paris to which it is connected by public transportation.

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<http://emmanuel.clouet.free.fr>

**Time frame:** The position is available immediately and the funding is for two years.

**Qualification:** The applicant should hold a Ph. D. Degree in solid state physics or materials science, with skills in one or more of the following simulation methods:

- Molecular dynamics simulation
- Crystal plasticity modeling at the dislocation scale

Experience in computer programming is also highly recommended.

**How to apply:** Candidates should send their application (statement of research interest, CV, names and contact information of two references) to [emmanuel.clouet@cea.fr](mailto:emmanuel.clouet@cea.fr)