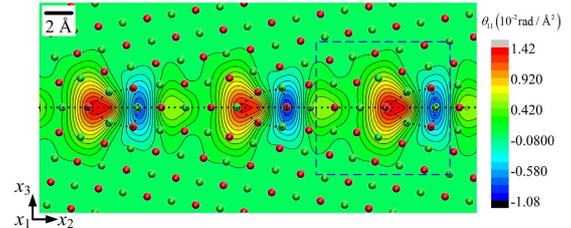


Master Internship

Discrete to continuous crossover characterization of interfaces in high-performance materials

Internship of 6 months for a Master student (under-graduate level), with gratuity around 570 €/month.

Interfaces like grain boundaries and phase boundaries play a major role in the deformation of crystalline materials such as rocks, metals or ceramics. Recently, a new framework has been developed to derive a continuous representation of the structure of grain boundaries from atomic-scale modelling [1,2]. This has opened new possibilities for the modeling of tailored materials microstructure with high-performance properties.



Disclination density field of a tilt grain boundary in Cu [1].

In this internship, we propose to use state of the art molecular static and molecular dynamic simulations based on semi-empirical potentials with the software LAMMPS, in order to obtain the atomistic structure of selected grain boundaries and interfaces in pure metals, lightweight Mg alloys and high-performance superalloys [3,4]. These interfacial configurations will be employed in a “bottom-up” approach to determine an accurate continuum field description based on dislocations, generalized-disclinations, etc. Within this internship, will aim at building the foundation of a generalized discrete-to-continuum crossover characterization for interfacial plasticity in high-performance materials.

References:

- [1] X.-Y. Sun, V. Taupin, C. Fressengeas, P. Cordier, *Int. J. Plast.* 77 (2016) 75–89.
- [2] X.-Y. Sun, V. Taupin, P. Cordier, C. Fressengeas, B.B. Karki, *J. Mater. Res.* 31 (2016) 3108–3114.
- [3] Y. Chang, W. Lu, J. Guénoles, L.T. Stephenson, A. Szczepaniak, P. Kontis, A.K. Ackerman, F.F. Dear, I. Mouton, X. Zhong, S. Zhang, D. Dye, C.H. Liebscher, D. Ponge, S. Korte-Kerzel, D. Raabe, B. Gault, *Nat. Commun.* 10 (2019) 942.
- [4] A. Prakash, J. Guénoles, J. Wang, J. Müller, E. Spiecker, M.J. Mills, I. Povstugar, P. Choi, D. Raabe, E. Bitzek, *Acta Mater.* 92 (2015) 33–45.

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The team

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Dr Vincent TAUPIN, CNRS research scientist HdR, expert in continuum modeling of material mechanics.

The laboratory

The Laboratory of study of microstructures, mechanics and material sciences (In French: *Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux*), also known as the LEM3, is a French laboratory of research located in Metz. As an interdisciplinary research center, the LEM3 combines solid mechanics, metallurgy, materials science, chemistry and physics. The scientific excellence of the laboratory is acknowledged by internationally recognized researchers and the combined authority of the CNRS, the University of Lorraine and the engineering school “Arts et Métiers ParisTech”. The LEM3 is part of the Carnot Institute ARTS and currently employs more than 150 persons.

Application

Please send a CV, an application letter and the grades of your last semester to both these emails:

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