LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX

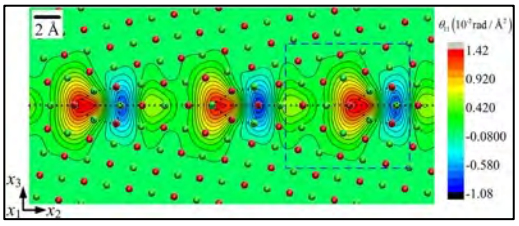
Contact emails:
julien.guenole@univ-lorraine.fr
vincent.taupin@univ-lorraine.fr

Master Internship
in numerical materials science and mechanics
2021

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

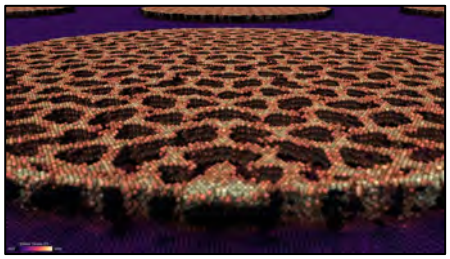
Internship of 6 months for a Master student (under-graduate level), with gratuity around 570 €/month.

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 microstructures 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 intermetallics [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, we aim at building the foundation of a generalized discrete-to-continuum crossover characterization for interfacial plasticity in high-performance materials.



Atomistic stress field of a high angle nano-twist defect by molecular dynamic simulation in a nanolayered intermetallic alloy.

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] A. Prakash, **J. Guénolé**, J. Wang, J. Müller, E. Spiecker, M.J. Mills, I. Povstugar, P. Choi, D. Raabe, E. Bitzek, Acta Mater. 92 (2015) 33–45.
[4] W. Yu, **J. Guénolé**, J. Ghanbaja, M. Vallet, A. Guitton, Scr. Mater. 191 (2021) 34–39.

Your skills

Required: Excellent knowledge in materials science and continuum mechanics of materials. Comfortable working with computers, including command lines.

Beneficial: Experience with scripting languages (python, bash…). Knowledge in data science and materials plasticity.

We offer

Dynamic international environment. Close supervision by CNRS scientist experts. Opportunity to develop cutting-edge numerical skills (high-performance computing, data management and processing…).

Possible continuation in a PhD program.

The team

Dr. Julien GUÉNOLÉ, CNRS research scientist, expert in atomistic modeling of material mechanics.

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: ***L**aboratoire d'**É**tude des **M**icrostructures et de **M**écanique des **M**atériaux*), 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, the DAMAS laboratory of excellence (*labex*) and currently employs more than 150 persons.

Application

Please send a **CV**, an **application letter** and the **grades** of your last semester to the **two emails** indicated in the header.

LABORATOIRE D'ETUDE DES MICROSTRUCTURES ET DE MÉCANIQUE DES MATÉRIAUX
LEM3 - UMR CNRS 7239
UNIVERSITÉ DE LORRAINE – SITE TECHNOPOLE
7 RUE FÉLIX SAVART – 57070 METZ - FRANCE
TÉLÉPHONE +33(0)3 72 74 78 00
LEM3-SAF-CONTACT@UNIV-LORRAINE.FR - WWW.LEM3.UNIV-LORRAINE.FR