The *Laboratoire d'Études des Microstructures et de Mécaniques des Matériaux* (LEM3) is a center for transdisciplinary experimental and theoretical research combining mechanics of solids and metallurgy, materials science, chemistry, and physics. The LEM3 opts since many years to contribute to materials research by developing new devices and new techniques for characterizing microstructures with electron microscopies.

The *Laboratoire lOrrain de Recherche en Informatique et ses Applications* (LORIA) is a CNRS/INRIA/Université de Lorraine/ CnetraleSupélec laboratory, which conducts research in computer science and information and communication technologies. The Orpailleur team is mainly interested in knowledge discovery in databases i.e. processing large volumes of data for discovering patterns that are significant and reusable.

To support our collaborative research, we are looking for a

Master Intern

Machine learning for coupling electron microscopy with polycrystal plasticity
(description next page)

Start date: **Mars 1st 2022**

Note that a security accreditation (minimal duration of the enquiry: 2 months) is mandatory before any access to LEM3. It may delay your starting date.

Your tasks

- You will perform cutting-edge techniques for characterizing microstructures, especially by electron microscopy.
- You will apply and test different machine learning methods on lab tests data.
- Your results will be discussed in the framework of materials physics.
- You will interact with researchers from several fields.
- You will share your time between LEM3 and LORIA, both located in Metz (France).

Your profile

- You must have a master's degree in materials physics, **passed with high honors**
- You must have good knowledge of materials physics, crystallography, metallurgy.
- You must have good knowledge in Machine learning.
- You have good written and verbal communication skills and enjoy working in a multi-thematic team.
- Good English language skills are required.

We offer:

- Dynamic international and multi-thematic environment
- Direct supervision by tenured senior academics (7 members)
- Cutting-edge experimental facilities
- The monthly gratuity will be paid by LEM3, according to the French law (https://www.service-public.fr/particuliers/vosdroits/F32131)
- This internship may lead to a doctoral researcher position (funding submitted).

Further information and application

For further information and application – **resume including addresses of referees and your exam scores (bachelor and master)** – please contact:

Dr. Antoine GUITTON, antoine.guitton@univ-lorraine.fr
Dr. Lydia BOUDJELOUD-ASSALA, lydia.boudjeloud@loria.fr

Application without enclosures mentioned will not be accepted.

Scope of the project:

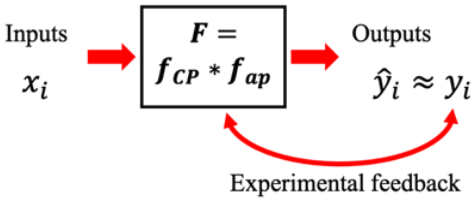
Developing new materials remains a main challenge to follow and predict the fast evolution of our society. Elaboration techniques must offer the possibility of developing such novel high-performance metals and alloys respecting environmental constraints. However, a mechanism-based tailoring of the performances requires constant improvements of experimental and theoretical techniques to unravel fundamental mechanisms controlling the macroscopic behavior. Plasticity is an important phenomenon which is considered here. It is closely related to the mechanical strength and formability and leads to progressive damage of components through non-reversible shape changes.

Most of used materials are generally polycrystalline, where grains are separated from their neighbors by Grain Boundaries (GBs). Grains cannot be deformed independently because the cohesion between them must be maintained. Dislocations glide through grains and interact with each other or with the GBs acting as sinks, traps, obstacles, and sources of dislocations. GBs are very important from the mechanical properties point of view.

Nowadays, we almost know how a dislocation interacts with a specific GB. But, understanding the collective response of several real GBs (contained in a real polycrystalline specimen) after receiving numerous dislocations is still a major scientific challenge. The difficulty becomes highly challenging when we consider the influence of the distribution of GBs, other types of interfaces, shape and orientation of grains, *i.e.* the microstructure.

In this context, our present objective is to explore a multi-level scale ranging from electron microscopy to micromechanics thank to machine learning methods. In this way, at the electron microscopy level we will develop new procedures for capturing statistically footprints of deformation mechanisms. At the micromechanics level, crystal plasticity models based on deep learning algorithms will be considered for suggesting specific microstructural parameters able to achieve targeted macroscopic mechanical properties. This project will have a major impact in current societal issues by enabling energy savings and limited costs associated with the tuning of microstructures targeting specific mechanical performances.

Supervised deep learning based on classification and/or regression is a machine learning approach known for being very efficient for treating numerical data. At first time, we will focus on the prediction of fundamental deformation mechanisms (slip, twinning, climbing, cross-slip) with respect to the specimen microstructure. In a mathematically simplistic way (see Figure), it requires, on one hand, to identify the relevant input (e.g. Euler angles…) and output (e.g. slip systems…) variables (let us call them $x_1, x_2, \dots, x_n, y_i$), and on the other hand the classifier F giving $\hat{y}_i = F(x_1, x_2, \dots, x_n)$, an "approximate" quantity tending towards the experimentally "true" measured value y_i. This classifier F must be based on a crystal plasticity law (f_{CP}), having a physical meaning, coupled ($*$) to a machine learning algorithm (f_{ap}) for its optimization. This aspect is the main originality of our strategy. During the learning phase, F will be trained to match at best the outputs y_i, experimentally measured, using the inputs x_i. Therefore, two work packages are necessary:



(i) feature engineering of the experimental datasets for feeding classifiers (F);
(ii) development of classifiers (F) adapted for polycristalline plasticity.