Offre de thèse / PhD Project proposal

Elementary dislocation properties influencing mechanical behaviour of austenitic High Entropy Alloys (HEA)

HEA (***high entropy alloys***) are a new class of materials containing at least five elements in similar and significant fractions (5 to 35 at. %). In some of them specific features, like high solid solution and strain hardenings, as well as unusual combinations of strength and ductility have been found. Also, phase transformation kinetics is generally slowed down, whereas stable nanostructures are easily obtained. Besides, an improved irradiation resistance of some HEAs starts to be shown. Crystal defects (and especially : dislocations) structure seem to be at the origin of many observed features .
The proposed PhD project will search for better understanding of the **impact of dislocations elementary properties on the plastic behaviour of single phased HEAs** thanks to atomistic simulation techniques. Especially, a model of dislocation behaviour predicting specific properties of HEA as compared to classical austenitic steels, will be sought.
Molecular dynamics (MD) will be the main simulation technique used in this work. Static properties (dislocation core structure, stacking fault energy, dissociation of dislocations) will first be calculated, as a function of local chemical environment and temperature. Then, using a specific MD protocol and dislocation dynamics formalism, dislocation behaviour under stress will be evaluated, with focus on effects of temperature and local chemical composition on lattice stress and dislocation mobility, related to the defect's character (edge or screw segment). The so-obtained characteristics of dislocations will be used to describe the collective behaviour of defects which can be analysed on macroscopic scale (interaction coefficients and hardening), and compared with mechanical characterisation of the existing HEA, tested in the frame of the same research project*.

Candidates looked for:
Education: master in materials science, mechanics of materials or condensed matter physics;
Requested skills: good bases in computer programming, good knowledge of crystal structures and defects; basic notions of physical metallurgy; scientific English fluency.
Experience of dislocation dynamics would be an additional asset.

General information:
Work language : French or English are possible, non-French speaking candidates are welcome
Work place : MINES de St-Etienne, 42023 St-Etienne. Missions (a few weeks par year) in EDF Lab, Les Renardières, Paris region.

Work contrat type: 3-years PhD contract at MINES

Net salary: about 1700 € par month

Application: before the end of mai 2020

Expected starting date: 1st October 2020
Supervisors: Pr. Anna Fraczkiewicz (Laboratoire Georges Friedel, MINES St-Etienne), PhD supervisor. G. Monnet, C. Domain and G. Adjanor,EDF R&D :*co-supervisors*

Contact and application: Curriculum (1 page), cover letter (1 page) and recommendation letter. To be sent to anna.fraczkiewicz@emse.fr

This PhD project is part of wider experimental project involving the R&D divisions of three companies (EDF, Framatome, APERAM) and 4 research institutions (CNRS, ARMINES, CEA, IMN) funded by the ANR. It aims at further developing of original Co-free HEAs composition that have been designed in this consortium and their evaluation for application in nuclear applications.