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

In HEA, some specific features have been largely reported. Especially high solid solution and strain hardenings, unusual combinations of strength and ductility, slowed down phase transformation kinetics, as well as an improved irradiation resistance. Crystal defects such as dislocation's structure are obviously at the origin of many observed features. This present work 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. In this framework molecular dynamics (MD) will be the main simulation technique used. Static properties (dislocation core structure, stacking fault energy, dissociation of dislocations) will be studied, 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 (HERIA ANR PRCE).