Numerical simulations of the dislocation dynamics in the very high-cycle-fatigue regime

Margarita LONGSWORTH

Supervisors: Marc FIVEL et Nicolas RANC (PIMM, Arts et Métiers ParisTech)

Friday 29th of October at 2:00 pm

Amphithéâtre de la Maison Jean Kuntzmann

Jury :
Monsieur Ghiath MONNET - Chercheur-ingénieur HDR, EDF, Rapporteur
Monsieur Alexander HARTMAIER - Professeur, Rühr-Universität Bochum, ICAMS, Rapporteur
Monsieur Edgar RAUCH - Directeur de Recherche CNRS, SIMaP, Examinateur
Monsieur Dan MORDEHAI - Professeur, Technion University, Examinateur
Monsieur Laurent DUPUY - Chercheur-ingenieur, CEA Saclay, Examinateur

Abstract: In order to investigate the Very High Cycle fatigue behavior of FCC metals using Discrete Dislocation Dynamics simulations, the present thesis proposes an improved model of cross-slip mechanism which has been implemented in the nodal DDD code NuMoDis (Drouet et al., 2014). The first step was to obtain the effect of stress on the activation enthalpy of cross-slip using discrete dislocation dynamics. The obtained results were compared with two modern cross-slip models, namely the numerical model of Kang et al. (2014) and the analytical model of Malka-Markovitz and Mordehai (2019). It was shown that both cross-slip models were in quantitative agreement with the results obtained using discrete dislocation dynamics simulations. Due to its easy calibration based on the unstressed energy barrier of cross-slip, the analytical model of Malka-Markovitz and Mordehai (2019) was preferred to be employed in the discrete dislocation dynamics code to effectively calculate the activation enthalpy of screw segments. The second step was to implement the recent cross-slip rate model proposed by Esteban-Manzanares et al. (2020) into the discrete dislocation dynamics code NuMoDis (Drouet et al., 2014). The obtained results were compared with the numerical values of the cross-slip rate estimated by Vegge et al. (2000) and Oren et al. (2017) using atomistic simulations. It was demonstrated that the proposed cross-slip modelling was able to reproduce atomistic results using only one free parameter, namely the unstressed energy barrier of cross-slip required to fit the analytical model
developed by Malka-Markovitz and Mordehai (2019). As a first application of the benchmarked simulation methodology, the firsts cycles of the gigacycle fatigue regime were simulated two different configurations, namely one isolated screw dislocation and a network of twelve mixed dislocations. It was found that the effect of cross-slip on an isolated dislocation was negligible, whereas it produced irreversible changes in the case of a dislocation network. With the aim of simulating a much larger number of cycles, a jump-in-cycles method was finally proposed in the last chapter.