PhD offer
"Micro-mechanics of fracture : how do voids nucleate in metals ?"

LABORATORY : iLM institut Lumière Matière

IN COOPERATION WITH : PIMM Arts et Métiers Paris Tech, CEA

TEAM : MMCI

WORK PLACE: Villeurbanne

CONTRACT TERM : 3 years

EXPECTED START DATE : september 1st 2026

WORK QUOTA : 100%

SALARY : 2 300€ gross per month

FUNDING : ANR DUTIFREE

LEVEL : Applicant skills : Strong background in condensed matter physics or materials science, some knowledge of C programming (or equivalent). The application should include a CV, a statement of interest and master's degree transcript (marks and ranking if available).

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KEYWORD(S) : physics of crystalline defects, atomistic simulations, small scale mechanics

SCIENTIFIC CONTEXT : Clarifying the process leading to void formation in metals will be useful for a number of applications such as ductile fracture, fatigue [3], damage related to hydrogen storage, dewetting of thin films, cavitation by electromigration in microelectronics… Fracture initiation is qualitatively well understood in metallic alloys which contain micron size inclusions. It occurs by decohesion of either the inclusion itself or its interface with the matrix. The voids grow by emitting dislocations and finally the ligaments between them break by plastic thinning. On the contrary, the mechanism is still controversial when the particles are in the nanometer range or when the alloy is pure [2]. Recent experiments (Fig. 1 a and b) have shown that voids appear preferentially at the dislocation

boundaries formed during straining. However they are detected only when they are already relatively large, 20 to 50 nm in diameter, and few information is known on the first stages of their formation within the dislocation boundaries.
The question is to determine if these voids can nucleate by vacancy condensation.

MISSIONS : In this research project, we propose to study void nucleation in various well chosen crystalline defects to unravel the mechanism of void formation. The methods used will be atomic scale simulations (Monte Carlo [5] and Machine Learning interatomic potentials). The work is part of an ANR project and therefore will benefit from interactions with partners having complementary competences. In particular, the atomistic simulations will have inputs from micro-mechanics simulations (stress levels from 3D discrete dislocation dynamics [6] performed at CEA) and from experiments (observations of microstructures produced by deformation, such as the one in Fig. 1a, and voids location) performed at PIMM Arts et Métiers Paris Tech, as well as at iLM (tensile tests within SEM, FIB slicing).

OUTLOOKS / PERSPECTIVES : /

BIBLIOGRAPHY :

[2] “Void nucleation during ductile rupture of metals: A review” P. J. Noell et al. Prog. Mat. Sci. **135** 101085 (2023) [3] “Fatigue damage of ultrafine-grain copper in very-high cycle fatigue region” P. Lukáš et al. Mat. Sci. Eng. A **528** (2011) pp. 7036-7040 [4] “Nanoscale conditions for ductile void nucleation in copper: Vacancy condensation and the growth-limited microstructural state” P. J. Noell et al. Acta mater **184** (2020) pp. 211-224 [5] “Sampling vacancy configurations with large relaxations using Smart Darting” **D. Tanguy** Phys. Rev. Mat. **8** 033604 (2024) [6] “On the role of cross-slip and collinear annihilation in dynamic recovery annihilation” **R. Madec**, B. Devincre and L. Kubin, Modelling Simul. Mater. Sci. Eng. **33** 015010 (2025)

IMAGE D’ILLUSTRATION :

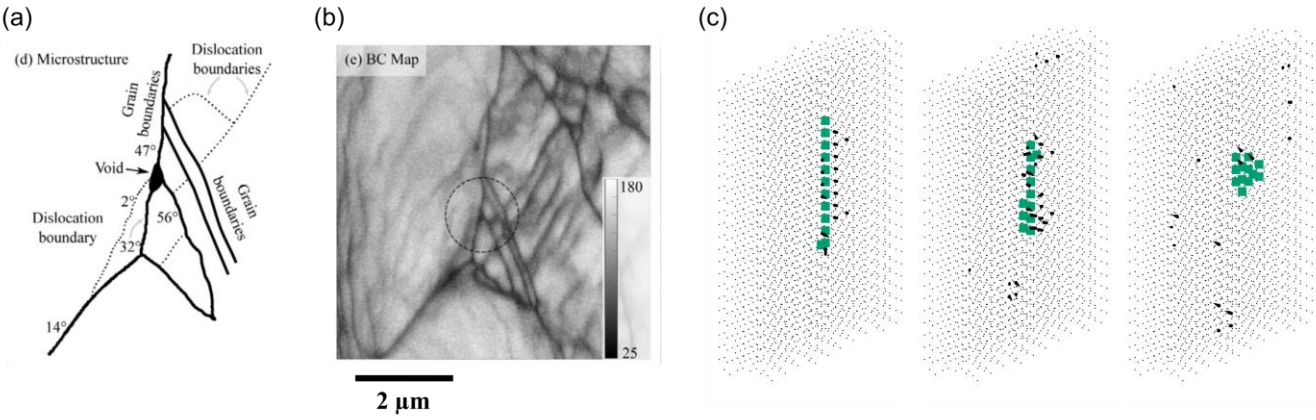

Fig. 1: (a) and (b) dislocation structure in pure Cu after about 50% strain [4]. A void is located on a triple grain boundary junction. (c) Initial (linear cluster), saddle and final configuration (void) for a cluster of 12 vacancies (green) in pure Al extracted from an atomic scale simulation of the nucleation process in a tilt grain boundary. Simulations done in our group.

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