MICRO-MECHANICS OF FRACTURE : HOW DO VOIDS NUCLEATE IN METALS ?

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : PIMM (arts et métiers Paris Tech), CEA

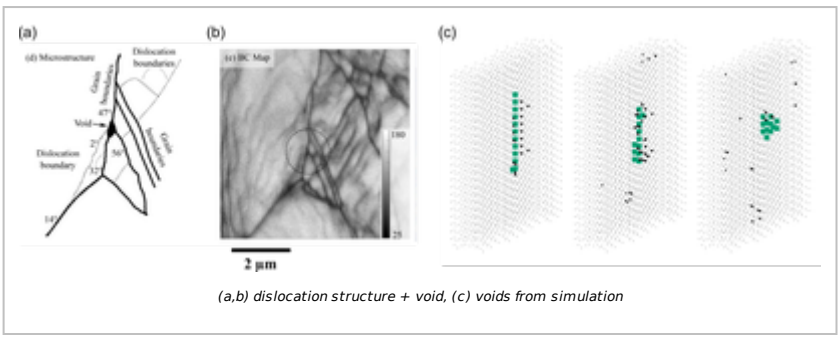
TEAM(S) : MMCI

CONTACT(S) : TANGUY Döme

CONTACT(S) DETAILS: dome.tanguy[at]univ-lyon1.fr / Tel. 0472431996

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

SCIENTIFIC CONTEXT :



(a,b) dislocation structure + void, (c) voids from simulation

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).

Applicant skills :

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

OUTLOOKS :

Salary : ~2300 euros gross, funding from ANR DUTIFREE

Work quota : 100%

BIBLIOGRAPHY :

[2] “Void nucleation during ductile rupture of metals” P. J. Noell et al. Prog. Mat. Sci. 135 101085 (2023)

[3] “Fatigue damage” P. Lukáš et al. Mat. Sci. Eng. A 528 (2011) pp. 7036-7040

[4] “Nanoscale conditions for ductile void nucleation in copper:” 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] Madec, Modelling Simul. Mater. Sci. Eng. 33 015010 (2025)

published on 23/02/2026