MODELING CAVITIES IN CRYSTALS AT THE NANOSCALE : ATOMIC AND MESO SCALE SIMULATIONS

LABORATORY : Institut Lumière Matière
IN COOPERATION WITH : CEA

LEVEL : M2
TEAM(S) : MMCI

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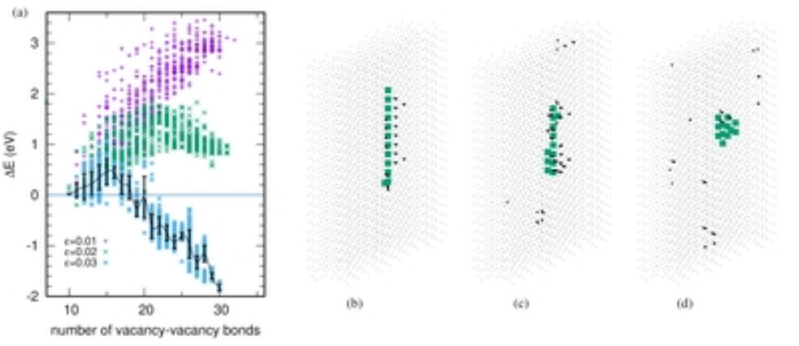
KEYWORD(S) : crystalline defects / atomic scale simulations / meso-scale dislocation dynamics

SCIENTIFIC CONTEXT :

Cavities are often at the origin of the damage of materials. Examples include : ductile fracture initiation in metals [1, 2], damage related to hydrogen storage, dewetting of thin films, cavitation by electromigration in microelectronics... Modeling the first stages of cavity formation is key to the development of more resistant materials.



Energy barrier for cavity nucleation and representative configurations (inital, saddle and final).

MISSIONS :

We have recently developed an atomic scale Monte Carlo (MC) method [5] capable of sampling the vacancy clusters configurations, within the framework of classical statistical mechanics, in complex crystalline structures, such as grain boundaries and including the effect of mechanical stresses. Preliminary results (Fig.) reveal that the interaction of the vacancy with the other defects, prior to the application of stress is of primary importance. Therefore, the code needs to be extended to more realistic defect configurations, for example, a dislocation impinged on a grain boundary. The second aspect of the problem will be explored by producing and analyzing three dimensional dislocation arrangements by a meso scale discrete dislocation dynamics code [6]. The idea will be to transfer the local stress levels from the dislocation scale to the atomic scale within the MC code.

OUTLOOKS :

Possibility of a PhD (funding already obtained).

BIBLIOGRAPHY :

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

[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)

published on 08/10/2025