PhD thesis fall 2019

Laboratories : Institut Lumière Matière (iLM), Lyon (http://ilm.univ-lyon1.fr/) / CEA Saclay, Paris

Group : Modélisation de la Matière Condensée et Interfaces (MMCI)

Supervisors : Döme TANGUY (iLM), Maxime Sauzay (CEA)

Title : "Contribution of nanoscale cavities to the damage of metals: atomistic simulations and continuum mechanics calculations."

The formation of cavities is observed in numerous cases of damage in metals (intergranular creep, fatigue, enhanced ductile fracture triggered by irradiation, H embrittlement, see figure). Nevertheless, the microscopic mechanisms and the conditions leading to their production (local excess concentration of vacancies, stress, temperature, the nature of the sources, vacancy mobility) are poorly known. The classical models use a phenomenological theory of thermally activated nucleation and their predictions disagree with the experimental nucleation rates. Modern atomistic simulations can improve our understanding of the very first moments of the formation of cavities. The goal of the project is to use such techniques to study the absorption and aggregation of vacancies [1] in a broad choice of grain boundaries, under the influence of stresses. The stresses will be derived from continuum calculations of stress concentrators [2].

The project is part of the European project M4F ("Multiscale modeling for fusion and fission materials" http://www.h2020-m4f.eu/) which deals with the production of crystalline defects by irradiation, their effect on plastic slip and its consequences, in particular, the accelerated ductile failure where the formation of cavities is the initiation stage. The candidate will be recruited by CEA in Paris but will work in Lyon during the first half of the thesis.

The profile includes students holding a master 2-research in Materials Science or Solid State Physics (or graduated from an engineering school with an experience in academic research). The candidate will have the opportunity to learn atomistic simulation techniques: Density Functional Theory, Metropolis and kinetic Monte Carlo and Molecular Dynamics. Some experience in computer programming (Linux, C) will be appreciated. The position will remain open until the appropriate candidate is found.

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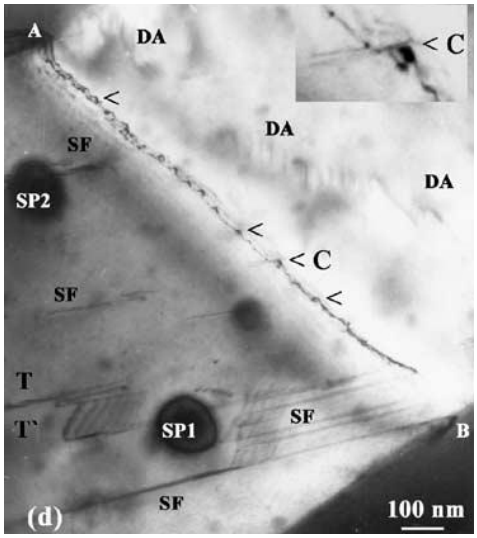
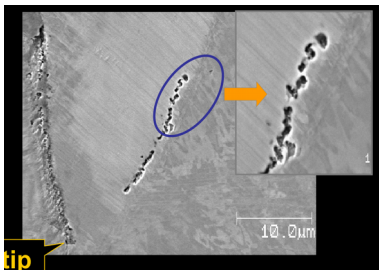
[1] D. Tanguy "Cohesive stress heterogeneities and the transition from intrinsic ductility to brittleness" **Phys. Rev. B 96** 174115 (2017)
[2] M. Sauzay, Ould Moussa M. "Prediction of grain boundary stress fields and microcrack initiation induced by slip band impingement" **Int. J. Fract., 184**, 215-240, (2013).



(a)



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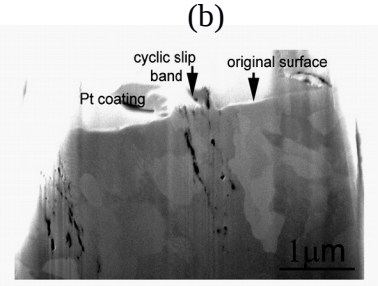

(c)

Figure: (a) nanoscale cavities at grain boundary ledges after severe plastic deformation in a superplastic Cu alloy (Gouthama Scripta Mater. **49** (2003) pp. 761-766), (b) intergranular creep cavity enhanced by the presence of hydrogen (Arioka Corrosion **71** (2014) p. 403), (c) copper submitted to cyclic deformation (Lukas Mat. Sci. Eng. A **528** (2011) pp. 7036-7040).