LMS Seminar

24 November 2022 at 2:00 pm - Room Jean Mandel

Hydrogen embrittlement of metallic alloys: atomistic simulations and microtensile experiments

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ABSTRACT

Recent small scale experiments will be briefly mentioned to give a sense of the advances made in the community towards "understanding Hydrogen embrittlement", namely : plasticity at crack tips [1], ductile to brittle (DTB) transition due to nano voids [2], the effect of co-segregation on fracture [3] and (almost) atom-scale resolution images of hydrogen trapped at precipitates by cryo-APT [4]. Then atomic scale simulations of the formation of voids, at a strained grain boundary, will be presented together with the effect that a fine distribution of such cavities has on fracture. A heterogeneous cohesive zone model was used to analyze the simulations and a criterion for DTB, based on the maximum curvature of the crack opening profile, will be given [5]. The time dependence of the opening of the nano fracture process zone will be discussed. In the last part of the seminar, an experimental study of crack propagation in AlZnMg alloy 7108 will be presented. Hydrogen is introduced in the material prior to straining the samples in air, under an optical microscope. DIC was used to measure local crack velocities at sub grain scale, crack opening angles and equivalent strain maps with a spatial resolution of 1 μm. Globally, the velocity decreases with the crack opening angle, as expected, but the measurements are largely scattered. In particular, sharp cracks can be slowed down which is interpreted as an effect of the many grains below the surface. The characteristics of the plastic zone ahead of the tip (the secondary plastic zone) were measured for different fracture mechanisms (transgranular, intergranular) and different degrees of embrittlement obtained by changing the conditions of hydrogen uptake. No clear correlations could be established, which might come from limitations of the DIC method used [6]. A way to overcome these limitations, by tracking gold nano droplets on the surface with SEM, will be discussed [7].

BIOGRAPHY

Döme Tanguy is Chargé de Recherche at CNRS, working at the iLM (Institut Lumière Matière), Université de Lyon. He did his PhD at the Ecole des Mines de Saint-Etienne with Thierry Magnin, on the stress corrosion of Al5%Mg (5XXX) alloys. Before his PhD, he worked at CEA Saclay in George Martin's lab where he simulated the segregation and precipitation of Mg on a simple grain boundary by a "Monte Carlo by Markov Chains" method (MCMC Monte Carlo Markov Chain). Afterward we worked as a postdoctoral fellow in the "Centre Européen de Calcul Atomique et Moléculaire", CECAM, on the plasticity induced by a shock wave by doing large scale Molecular Dynamics simulations with several stays at the Los Alamos National Laboratory. Döme then joined the CNRS at the Ecole des Mines de Saint-Etienne in 2001, with a hybrid simulation/experimental project. Over the years, he contributed to the quantification of the mechanisms proposed in the literature for the effect of hydrogen in metals: gap-hydrogen clustering, loss of cohesion, the effect of hydrogen on dislocation emission at crack tip. In 2010 he moved to the iLM (Institut Lumière Matière). Since 2017, He is developing an experimental activity in micro-mechanics, oriented to the study of fracture: small scale field measurements. The objective is to contribute to the modeling of embrittlement by bringing physics-simulations-experiments closer together.

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[3] Hydrogen-enhanced intergranular failure of sulfur-doped nickel grain boundary: In situ electrochemical micro-cantilever bending vs. DFT, T. Hajilou, F. Christien, A. Barnoush at al., Mat. Sci. Eng. A 794 (2020) 139967

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[7] Mesures de champs de déplacement par suivi individuel de nanoparticules d'or, Antoine Ollivier et al. cfm2022 hal-03738056