# MM 33: Topical Session: Fundamentals of Fracture – Amorphous Metals

Time: Wednesday 15:45–18:00 Location: SCH A 215

MM 33.1 Wed 15:45 SCH A 215

**In situ measurement of plasticity accompanying Hydrogen induced cracking** — Leonel Stermann, Loïc Vanel, and •Döme Tanguy — Institut Lumière Matière, UMR5306 Université Lyon 1 - CNRS, Université de Lyon 69622 Villeurbanne cedex, France

Single crack propagation is studied in a Hydrogen embrittled aluminum alloy. Hydrogen is introduced in the system by electrochemical reactions in an acid aqueous medium. After Hydrogen charging, tensile tests are performed in air, on notched samples, with a micro-tensile machine. An optical microscope is used to follow single crack initiation and propagation at a high magnification. Digital Image Correlation gives the displacement field on the surface with a spatial resolution of about 1 micron. It enables the determination of the position of the crack tip and the local velocity at a sub-grain scale. The equivalent Von Mises strain is calculated and gives a precise measure of the local plastic field which accompanies crack propagation. In addition to the primary plasticity which is emitted from the crack tip or its immediate neighborhood in the form of two intense slip bands,It is systematically found a secondary plastic zone which spreads over several microns ahead of the tip. The characteristics of the plastic zone are measured, together with the velocity and the applied stress intensity factor. In addition, different fracture mechanisms are found on the fracture surface. In particular there are transitions in the fracture mode from intergranular smooth to transgranular parallel to the grain boundary plane. The local fracture mechanisms, in the vicinity of the surface, are linked to the local velocities and plastic deformations.

MM 33.2 Wed 16:00 SCH A 215

**Liquid metal induced fracture : modelling and supporting experiments** — Thierry Auger[1], Antoine Clement[1], Marco Ezequiel[2], •Eva Héripré[1], Ingrid Serre[2], Zehoua Hamouche[1], Julie Bourgon[3], Eric Leroy[3], and Maxime Vallet[4] — [1]PIMM/Arts et Métiers Technology Institute, CNRS, CNAM, 151 Bd de l'hôpital 75013 Paris, France — [2]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France — [3]ICMPE - UMR 7182 2/8, rue Henri Dunant 94320 Thiais, France — [4]MSSMAT, CentraleSupélec, University Paris-Saclay, France

Liquid metal embrittlement of an otherwise ductile material is an environmentally induced fracture phenomenon characterized by potentially high brittle crack propagation rate and deleterious effects on mechanical properties. Its phenomenology is still not well understood, in particular in terms of prediction of sensible couples and about the detailed intergranular fracture mechanisms. Here we will report on the study in the copper systems via both an energetic and QM/MM approaches at the atomic level to predict the sensitivity of model materials to liquid metal embrittlement. The main goal is to try to link micro-testing (flexion in FIB prepared samples or by in-situ TEM) to a sound modelling at the atomistic scale via fracture mechanics type sollicitations. The progress towards predictability of liquid metal embrittlement systems and understanding of fracture mechanisms will be presented along with a vision about their experimental validation.

MM 33.3 Wed 16:15 SCH A 215

**Microscale fracture behavior of Laves phases in the Mg-Ca-Al ternary alloy system** — •Anwesha Kanjilal, Uzair Rehman, James P. Best, and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Brittle intermetallic Laves phases often act as preferential sites for defects such as cracks in the Mg-Ca-Al alloys. This study investigates the nano- and microscale fracture behavior of C15 Al2Ca and C14 Mg2Ca Laves phases prepared as single-phase specimens. Spherical nanoindentation was performed at room temperature in grains of varying surface orientation to identify cleavage planes and orientation effects. Post mortem microscopic examination using electron channeling contrast imaging revealed cracks around indents in both Laves phases, and together with electron backscatter diffraction low index crack planes were identified using trace analyses. For C15 phase, further microcantilever bending and micropillar splitting geometries were fabricated using focused ion beam methodology, wherein fracture toughness Kc ~1-2 MPam^0.5 was obtained from in-situ testing. Fast screening methodology based on in-situ scratch and nanoindentation at temperatures from 25 to 500 °C was employed to determine brittle-to-ductile transitions in the Laves phases. The morphology of slip lines and cracks, and decrease in hardness during nanoindentation suggests probable transition ~0.5Tm for C15 phase, while studies on C14 are ongoing.

The authors gratefully acknowledge the financial support of Deutsche Forschungsgemeinschaft (DFG) within project B06 of Collaborative Research Center (SFB) 1394, project number 409476157.

MM 33.4 Wed 16:30 SCH A 215

**Fracture mechanics concepts in application to functionally graded coatings (FGCs) and FGC structures** — •Vera Petrova and Siegfried Schmauder — IMWF, University of Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany

The problem of thermal fracture of functionally graded thermal barrier coatings on a homogeneous substrate under the influence of thermomechanical loadings is analyzed. It is assumed that FGCs contain a pre-existing system of multiple cracks, edge and/or internal. The thermal and mechanical properties, as well as the fracture toughness of the FGC, are modeled by functions based on the rule of mixtures with a power-law coefficient as the gradation parameter. The problem is formulated using the method of singular integral equation, which are solved numerically. The following fracture characteristics are calculated: stress intensity factors, energy release rates, critical stresses and fracture angles. A series of computational experiments is carried out for FGC/homogeneous structures with typical systems of multiple cracks in the FGC at different gradation parameters and for different material combinations. It is known that the fracture resistance of a TBC can be increased by introducing dense vertical cracks in ceramic coatings; this mechanism is due to the shielding effect in these crack systems. These crack systems are studied and discussed. The goal of this study and the investigation based on the model is to find ways to improve the fracture resistance of FGC/homogeneous structures by avoiding certain critical crack systems.

MM 33.5 Wed 16:45 SCH A 215

**Nonlinear elastic effect on interacting crack paths in PDMS films** — •Loic Vanel[1], Osvanny Ramos[1], Thierry Biben[1], Stéphane Santucci[2], and Anthony Gravouil[3] — [1]ILM - UCBL, Villeurbanne, France — [2]LPENS - ENS Lyon, France — [3]LAMCOS, INSA Lyon, France

The observed repulsive behaviour of two initially collinear cracks growing towards each other and leading to a hook-shaped path questioned recently the validity of the Principle of Local Symmetry within Linear Elastic Fracture Mechanics theory [1]. Theoretical and numerical work has solved this dilemma, providing the precise geometric conditions for the existence of the repulsive phase and revealing a multi-scale behaviour of the repulsive/attractive transition [2].

Nonlinear elastic materials such as elastomers depart from the prediction of linear elasticity for interacting cracks. We performed experiments on PDMS film that indeed show a maximum angle of repulsion not only significantly smaller than the one of linear elasticity, but also smaller than the one observed in polymer films with a plastic process zone. Our FEM simulations on a Mooney-Rivlin material confirm that the nonlinear elastic response of PDMS modifies the crack path, reducing the repulsive strength between the two interacting cracks.

References [1] Dalbe, M.-J.; Koivisto, J.; Vanel, L.; Miksic, A.; Ramos, O.; Alava, M.; Santucci, S.; Phys. Rev. Lett. 2015 114, 205501 [2] Schwaab, M.-E.; Santucci, S.; Biben, T.; Gravouil, A.; Vanel, L. ; Phys. Rev. Lett. 2018 120, 255501.

**15 min. break**

MM 33.6 Wed 17:15 SCH A 215

**Modelling mechanochemical reactions in epoxy resins under tensile load using hybrid QM/MM/MD approaches** — •Christian R. Wick[1], Mattia Livraghi[1], Sampannah Pahi[1], Bariscan Arican[1], David M. Smith[2], and Ana-Sunčana Smith[1] — [1]FAU Erlangen-Nürnberg, PULS Group, Institute for theoretical physics, Erlangen, Germany — [2]Division of Physical Chemistry, IRB, Zagreb, Croatia

Epoxy resins are important thermosetting polymers in our everyday life with a large variety of applications, e.g. as structural materials in

airplanes, as coatings, flooring materials or adhesives. With the aim to understand these complex materials at the molecular scale, we investigate the formation and the mechanochemical response of epoxy resins, including the reactions taking place during curing and under tensile load, by means of quantum chemistry and hybrid Molecular Dynamics (MD) simulations. We present a block chemistry based AMBER force field,[1,2] which allows generation of fragment partial charges covering all states of curing and fracture, due to cleavage of molecular bonds. Further, we develop an on-the-fly hybrid QM/MM/MD Ansatz to identify bond rupture events in bulk epoxies to improve our understanding of the mechanochemical behavior of these materials.

[1] M. Livraghi, S. Pahi, P. Nowakowski, D.M. Smith, C.R. Wick, A.-S. Smith, Block Chemistry for Accurate Modeling of Epoxy Resins, chemrxiv, 2022 [2] M. Livraghi, K. Höllring, C.R. Wick, D.M. Smith, A.-S. Smith, J. Chem. Theory Comput. 17 (2021) 6449

MM 33.7 Wed 17:30 SCH A 215

**Machine Learning of fracture in glasses** — Francesc Font-Clos[1], Marco Zanchi[1], Stefan Hiemer[2], •Silvia Bonfanti[3], Roberto Guerra[1], Michael Zaiser[2], and Stefano Zapperi[1,4] — [1]Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy. — [2]Institute of Materials Simulation, Department of Materials Science Science and Engineering, Friedrich-Alexander-University Erlangen-Nuremberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [3]NOMATEN Centre of Excellence, National Center for Nuclear Research, ul. A. Sołtana 7, 05-400 Swierk/Otwock, Poland — [4]CNR Consiglio Nazionale delle Ricerche, Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia Via R. Cozzi 53, 20125 Milan, Italy.

Being able to predict the failure of materials based on structural information is a fundamental issue with enormous practical and industrial relevance for the monitoring of devices and components. Thanks to recent advances in deep learning, accurate fracture predictions are becoming possible even for strongly disordered solids, but the sheer number of parameters used in the process renders a physical interpretation of the results impossible. Here we address this issue and use machine learning methods to predict the failure of simulated two-dimensional silica glasses from their initial undeformed structure. We show that our predictions can be transferred to samples with different shapes or sizes than those used in training, as well as to experimental images.

MM 33.8 Wed 17:45 SCH A 215

**Using deep neural networks to bridge the gap between statistical fractographic analysis and fracture toughness prediction for polymers** — •Guillaume de Luca[1,2], Mohammed Idri[2], and Laurent Ponson[1,2] — [1]Institut Jean le Rond d'Alembert, Sorbonne Universite, CNRS, 4 place Jussieu 75006 Paris, France — [2]Tortoise, 231 rue Saint-Honoré, 75001 Paris, France

We propose to deploy DNNs to bridge the gap between statistical fractography and the toughness $K_{Ic}$ prediction for polymers as well as shed light on the role played by the different structures on their fracture surfaces. We generate the fracture surfaces in laboratory through tensile fracture tests while using DIC (Digital Image Correlation) to locally measure and compute the sought mechanical properties along the crack. An interferometric profilometer extracts the topography from the fracture surfaces, and the resulting height fields are post-treated with tools from statistical fractography to be used as input, while the experimental data are used as labels for the regression problem.

By doing so, we can estimate from a scanned fracture surface a material toughness value $K_{Ic}(x)$ along the crack propagation direction. Furthermore, the advancements in explainable neural networks allow us to go one step further by making assumptions about what roughness elements present on the fracture surface influence the most the results coming out of the pipeline.