Liquid metal embrittlement: from application of global energetical criterium to crack initiation stress intensity factors

Thierry Auger*[1], Antoine Clément[2,3], and Marco Ezequiel[4,5]

[1]Laboratoire Procédés et Ingénierie en Mécanique et Matériaux – Centre National de la Recherche Scientifique - CNRS – France

[2]Aalto – Finland

[3]Laboratoire Procédés et Ingénierie en Mécanique et Matériaux – École Nationale Supérieure d'Arts et Métiers (ENSAM) – France

[4]Unité Matériaux et Transformations - UMR 8207 – CNRS – France

[5]Laboratoire des Sciences des Procédés et des Matériaux – CNRS – France

Abstract

Liquid metal embrittlement (LME) 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. LME also encompasses fracture induced by the grain boundary wetting (GBW) phenomenon. The phenomenology of these phenomenons is still not well understood, in particular neither for the prediction of sensible solid/liquid couples, nor to decipher a priori potential fracture modes or fracture toughness.

We will illustrate what energetical criterium based on AbInitio modelling of solid-liquid interfaces can bring to the phenomenology of LME in terms of the prediction for systems classification (GBW versus standard LME with a ductile to brittle transition induced by environmental adsorption). Via a sound calculation of the wettability parameter S representing the driving force for GBW, the predicted trend for several systems from pure elements to high entropy alloy will be presented and we show a good match with experiments. The fracture toughness in Fe based systems showing LME will be also shown to compare favorably with the predicted trends by an energetical Griffith approach based on the modelling of solid-liquid interfaces. Taking all these results together, this brings confidence that energetical criterium based on AbInitio modelling can be used in LME for predicting at least the LME sensitivity of various systems.

At last, we will report on the study at the atomic level by QM/MM approach to go one step beyond and predict crack initiation stress intensity factors in a copper LME system. A methodology for comparison with experiment will be presented that show how mechanical quantities of interest in fracture could be infered from AbInitio modelling.

*Speaker