TOWARDS FULL MULTISCALE MODELLING OF FRACTURE: A NUMERICAL SIMULATION OF HYDROGEN EMBRITTLEMENT

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Environmental embrittlement is a long standing problem, and a particularly insidious form of it is hydrogen embrittlement (HE). In this work, we present results of numerical calculations of fracture properties for high strength steels embrittled by hydrogen.

We propose a method to coarse grain *ab initio* calculations of material properties that allows for the computation of fracture properties at the macroscopic level by means of cohesive surfaces, thrusting the application of multiscale calculations to fracture. The method involves several steps linked in succession, viz., a) calculation of atomic-level cohesive laws by first principles (e.g. density-functional theory), b) renormalization of the cohesive laws to account for many planes taking part in the fracture process, c) elastic correction to avoid double counting of elastic properties, d) embedding of the renormalized law into a finite element calculation with cohesive elements.

We discuss the application to the determination of the effect of several system parameters on hydrogen assisted cracking. In particular, we have analyzed the effect of varying yield strength, temperature, and hydrogen chemical potential in the environment, in terms of macroscopic -as crack propagation rate, stress intensity threshold, etc.- as well as microscopic -as hydrogen distribution- variables. The modification of atomic level cohesive properties induced by hydrogen leads to a very good agreement with experimental results at the macroscopic level.