Fracture Mechanics in the Context of Hydrogen Embrittlement

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INTRODUCTION

As a result of the ongoing transition from fossil fuels to renewable energy, hydrogen is believed to become a key player as an energy carrier in the near future. Ensuring safe and efficient infrastructure for transportation of hydrogen to the market is vital for this to be possible. As the presence of hydrogen in steels causes material degradation, the HyLine project at SINTEF Industry aims to understand and quantify these effects to address the material challenges related to transportation of hydrogen. In collaboration with the team at SINTEF Industry, this ongoing project specifically focuses on modelling fracture processes in steel in the presence of hydrogen.

HYDROGEN EMBRITTLEMENT (HE)

Hydrogen induced degradation of material properties is amongst the most common forms of metal and alloy embrittlement and occurs through multiple mechanisms such as *Hydrogen Enhanced Decohesion* (HEDE) and *Hydrogen Enhanced Localised Plasticity* (HELP).

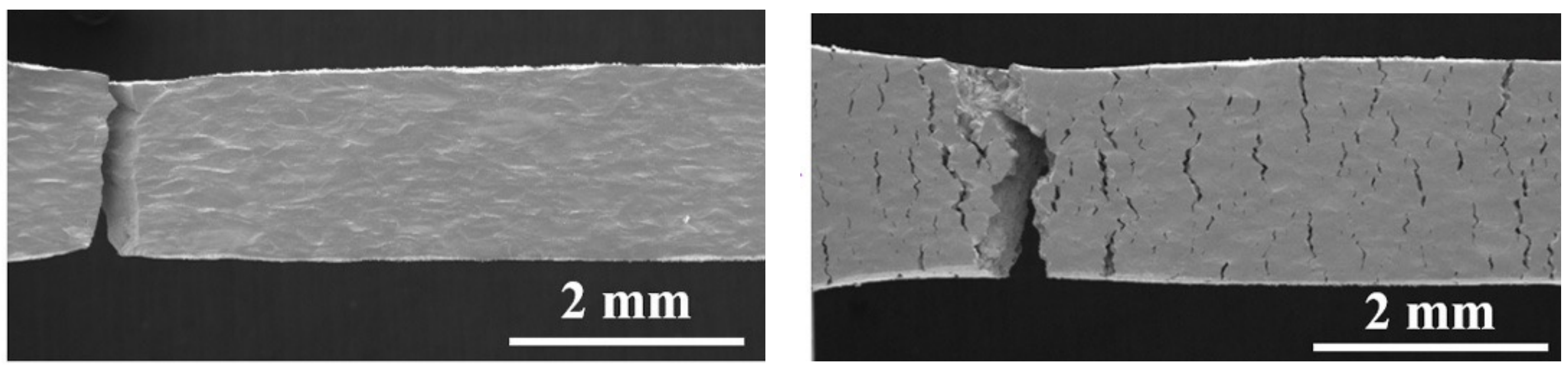


Figure 1: Fracture gauge surface of Fe–22Mn-0.6C (wt. %) TWIP steel samples with no hydrogen-charging (left) and 300 hours of hydrogen charging (right) [1].

The effect of a particular mechanism of embrittlement on the material degradation of a specimen depends on a range of factors such as i) material microstructure, ii) charging and trapping conditions of hydrogen, iii) global and local hydrogen concentration in the material sample and iv) mechanical stress applied to the sample locally and globally.

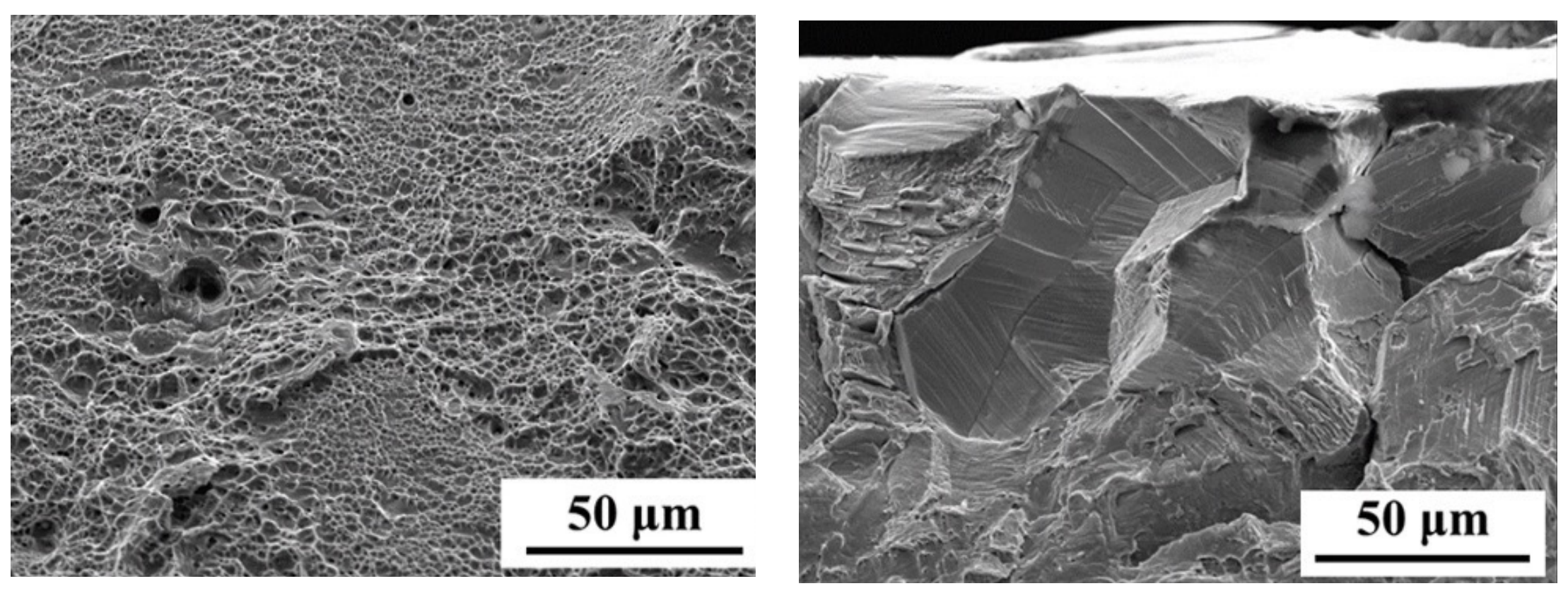


Figure 2: Fracture surfaces of tensile tested TWIP steel samples demonstrating the effect of embrittlement on the hydrogen charged sample (right) compared to the sample tested in vacuum [1].

EVOLUTION OF THEORETICAL COHESIVE STRENGTH

Inglis solutions to the stress concentrations at crack tip σ_C of an elliptical cavity with semiaxes *b* and c (with *b* << *c*) in a plate subjected to uniform stress σ_A.

$$\frac{\sigma_C}{\sigma_A} \simeq \frac{2c}{b}$$

Griffith criterion: *for a crack to propagate, the decrease in elastic strain energy must equal or exceed the energy required for creation of the new surface.*

Theoretical cohesive strength of perfectly brittle, ideal solids found from the Griffith criterion:

$$\sigma_{max} = \sqrt{\frac{E\gamma_s}{a_0}}$$

γ_s: surface energy
E: Young's modulus
a_0: atomic spacing

Cohesive strength when accounting for microscopic flaws (*Griffith flaws*) in materials:

$$\sigma = \sqrt{\frac{2E\gamma_s}{\pi c}} \approx \sqrt{\frac{E\gamma_s}{c}}$$

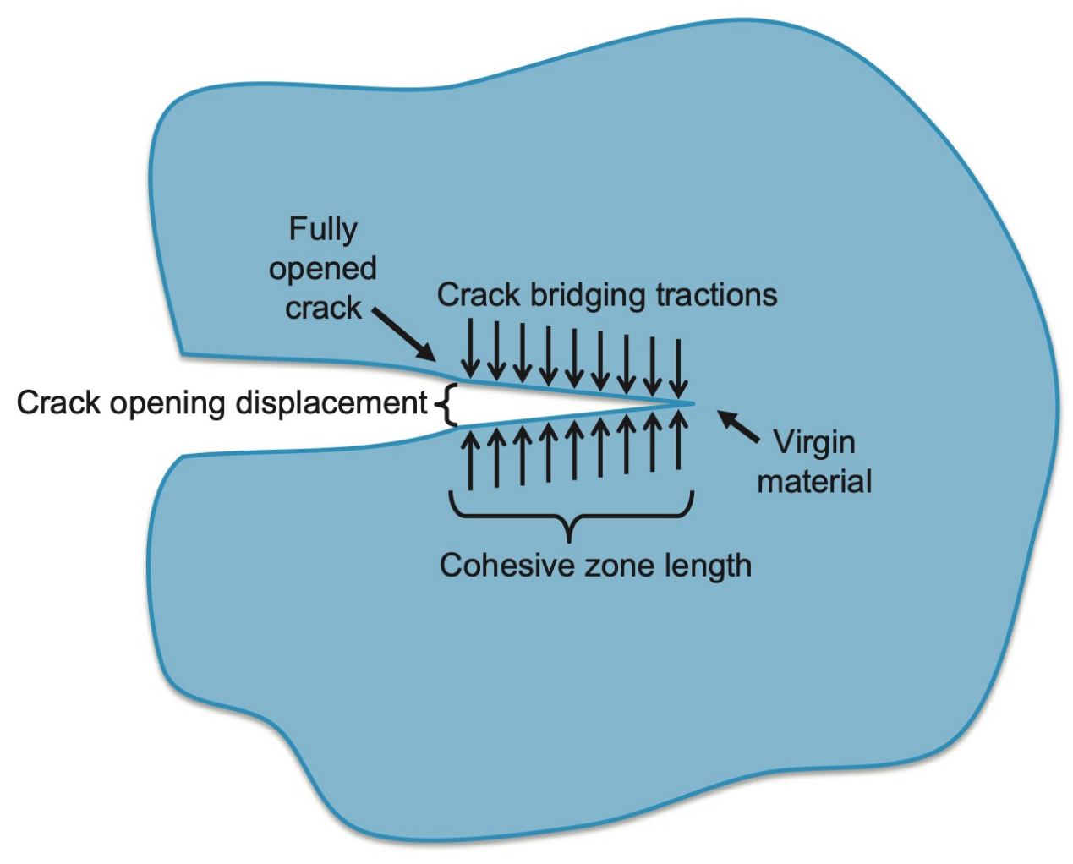
c: crack length of Griffith flaws

Irwin-Orowan extension for quasi-brittle fracture introducing the idea of plastic work:

$$\sigma = \sqrt{\frac{2E(\gamma_s + \gamma_p)}{\pi c}} \approx \sqrt{\frac{E\gamma_p}{c}}$$

γ_p: plastic energy term, $\gamma_p >> \gamma_s$

COHESIVE ZONE MODEL (CZM)



In the Griffith model, a stress singularity arises at the crack tip. Introducing finite nonlinear cohesive forces opposing crack formation solves this problem. These forces are described by a traction separation law (TSL). The work of separation per unit area is given by the area under this curve.

$$w = \int_{\delta_0}^{\infty} \sigma d\delta$$

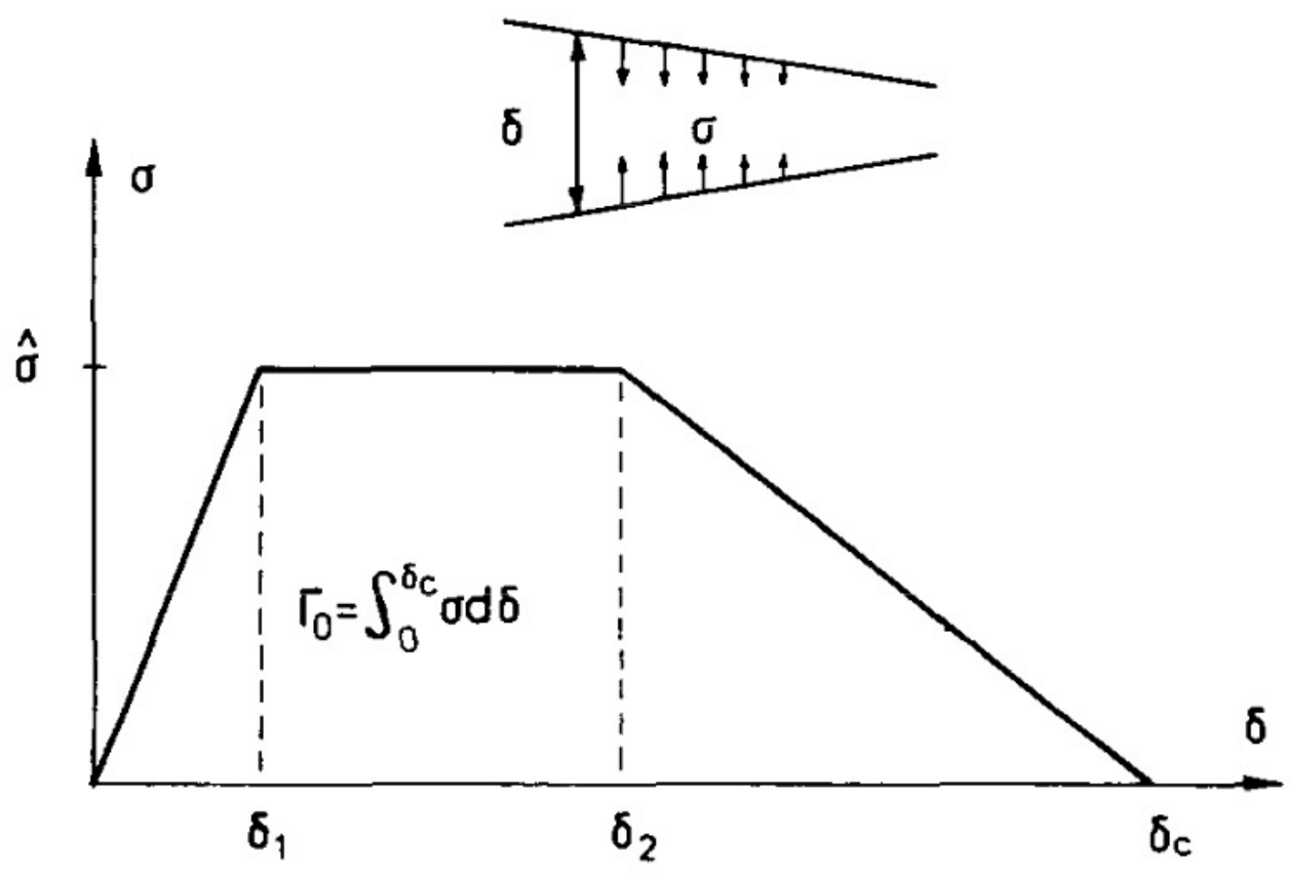


Figure 3: TSL for modelling a fracture process in an elastic-plastic solid with no adsorbed solute [2]. σ_{max}= [1,3]GPa

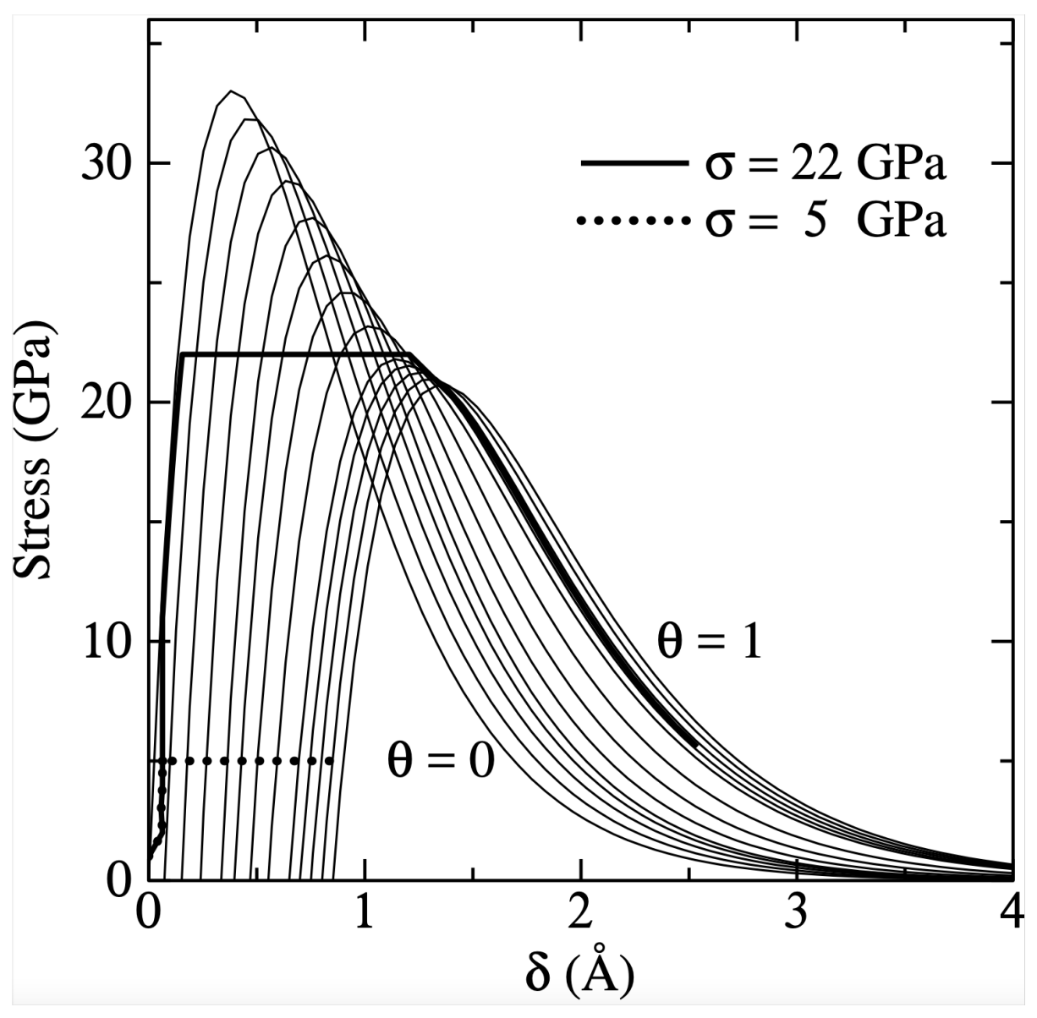


Figure 4: TSLs for a range of hydrogen occupancy values in the trap sites of the cohesive zone [3]. The thick solid line is the TSL at fixed hydrogen concentration of 1appm at fixed applied stress of 22GPa. σ_{max}= [20,30]GPa

The shape of the TSL in Tvergaard and Hutchinson's study (Figure 3) lends itself to the study of fracture in hydrogenated materials, however, the large gap in maximum stress between atomistic and engineering cohesive models remains an open issue.

FUTURE WORK

The focus of this project going forward is to examine how plasticity is implemented in Finite Element Models to study fracture. The aim is to investigate the disconnection between atomistic and engineering cohesive descriptions and suggest how a TSL can be implemented in a more transparent way such that it is clear how plastic work of fracture enters the model.

REFERENCES

[1] Wang, D., Lu, X., Wan, D., Guo, X. and Johnsen, R. (2021) *Effect of hydrogen on the embrittlement susceptibility of Fe-22Mn-0.6C TWIP steel revealed by in-situ tensile tests.* Materials Science and Engineering A. 802. 140638.

[2] Tvergaard, V. and Hutchinson, J.W. (1992) *The relation between crack growth resistance and fracture process parameters in elastic-plastic solids.* Journal of the Mechanics and Physics of Solids. 40(6) p. 1377 - 1397. DOI: 10.1016/0022-5096(92)90020-3

[3] Katzarov, I.H. and Paxton, A.T. (2017) *Hydrogen embrittlement II. Analysis of hydrogen-enhanced decohesion across (111) planes in α-Fe*. Physical Review Materials. 1. 033603. DOI: 10.1103/PhysRevMaterials.1.033603