$AddH_2$ – SP4: A Generalized FE-Framework for Hydrogen-Induced Ductility Loss in Porous Materials

Siddhi Avinash Patil, Stephan Roth, and Bjoern Kiefer
Professorship of Applied Mechanics – Solid Mechanics

Aims / Objectives

Exposing porous ceramic materials to a high-temperature hydrogen environment involves the synergistic action of several mechanisms, such as sintering, phase transformations, cracking, creep, grain boundary diffusion, and corrosion. To develop a material model that captures these complex effects, we have proposed a **modular framework** for the **ductile-to-brittle** transition in porous ductile materials (see Fig. 1), which can be easily extended to account for similar mechanisms in alumina. The underlying failure mechanism captured by the present framework is the nucleation, growth, and coalescence of microvoids. This fully-coupled mesh-independent framework combines **chemo-mechanics** with the **non-local** regularization of the well-known **Gurson-Tvergaard-Needleman** (GTN) damage model.

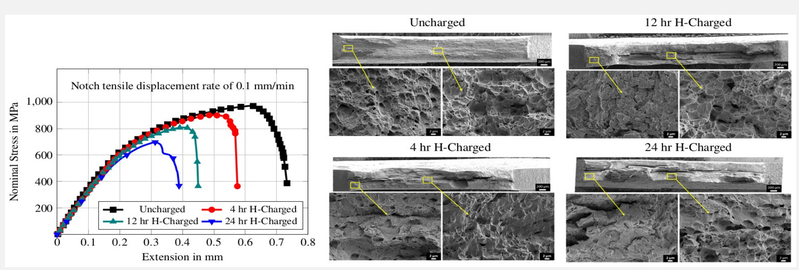

Fig. 1: Hydrogen-induced damage in a porous ductile material [1, 4].

Materials / Methods

- This multi-field model (see Fig. 2) is implemented as an **Abaqus user-defined element** in a small deformation setting to address the impact of hydrogen diffusion on the material's reduction in ductility, with the **finite element method** used for numerical analysis.
- The chemo-mechanical model is based on **Fick's law** for standard diffusion, adopting the **local condensation** approach from [5].
- The **linear scaling functions** $(1+\kappa_G \cdot c)$ and $(1+\kappa_N \cdot c)$ are introduced to account for the influence of hydrogen concentration c on the acceleration of **void growth and nucleation** in the original non-local GTN model [3]. Here, κ_G and κ_N are the hydrogen-enhanced void growth and nucleation acceleration parameters, respectively [2].

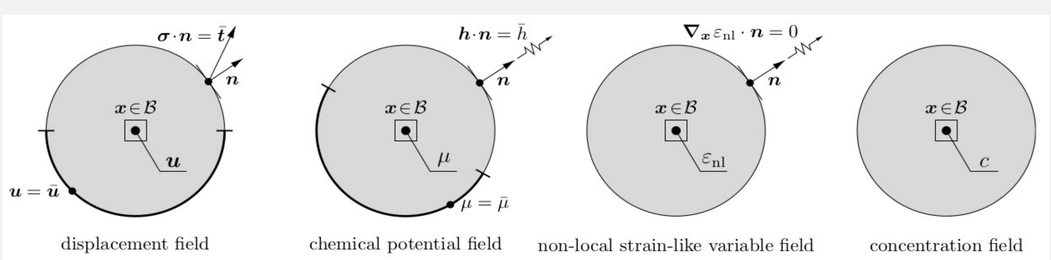

Fig. 2: Schematic of the multi-field formulation [1].

Results

- Investigation conducted using a 3D **notched tensile specimen** (see Fig. 3).
- **Mesh-independent** behavior is observed both with and without hydrogen (see Fig. 4).
- Enhanced **hydrogen-induced ductility loss** and **premature failure** are observed under slower loading rates (see Fig. 5) and higher pre-charging conditions (see Figs. 6 and 7).

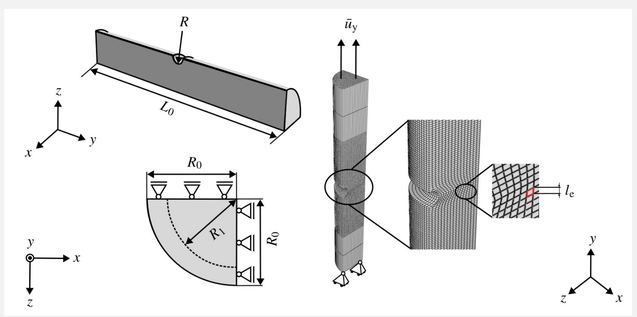

Fig. 3: Geometry and boundary conditions [1].

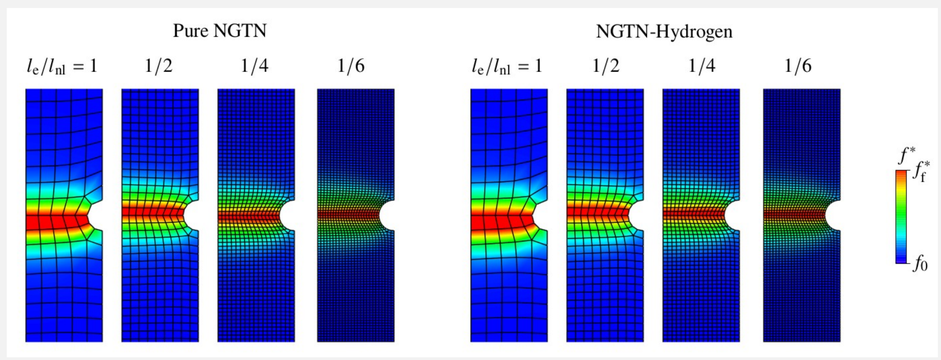

Fig. 4: Mesh convergence analysis [1].

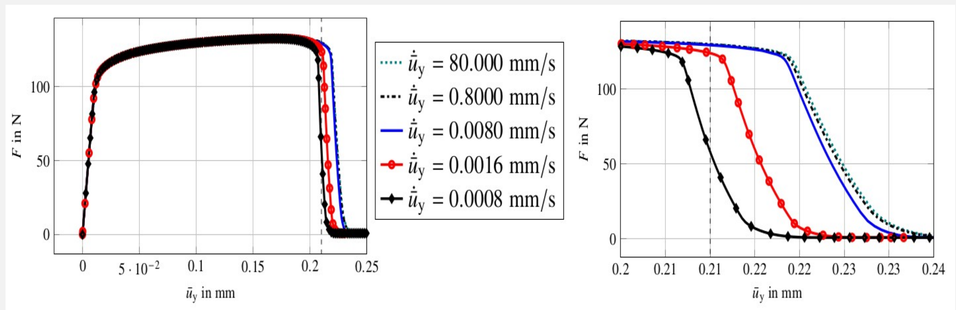

Fig. 5: Ductility loss at different displacement rates [1].

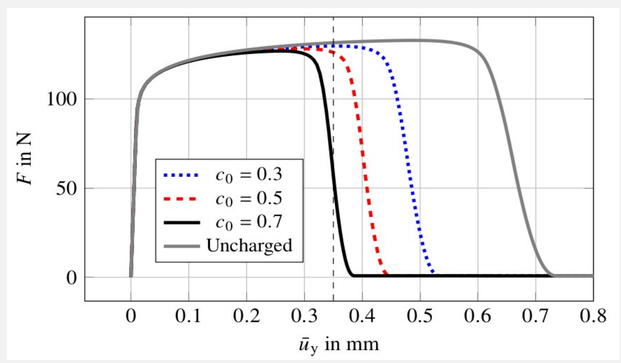

Fig. 6: Ductility loss under hydrogen pre-charging [1].

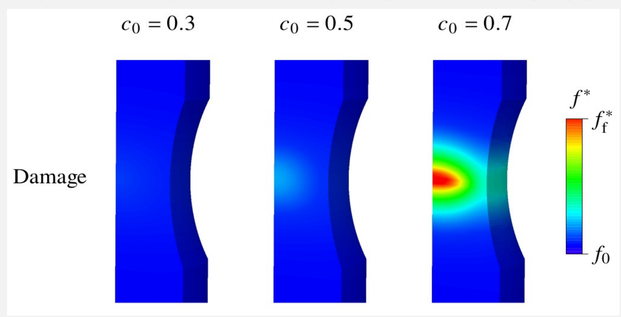

Fig. 7: Contour plots for hydrogen pre-charging [1].

Conclusions

- **A modular fully-coupled FE framework** for investigating **hydrogen-enhanced ductility loss** in porous ductile materials has been implemented.
- Hydrogen-promoted damage initiation and propagation, leading to **greater ductility loss** and **earlier component failure**, are predicted as a result of accelerated void growth and nucleation.
- The predicted response shows a **good qualitative agreement** with the literature.

References

[1] S. A. Patil, S. Prüger, S. Roth, and B. Kiefer. *A finite element framework coupling chemo-mechanics and the non-local Gurson-Tvergaard-Needleman model for hydrogen-induced ductility loss in steels.* In preparation.
[2] S. A. Patil, S. Prüger, S. Roth, A. Seupel, and B. Kiefer. *Implementation of a finite element framework coupling chemo-mechanics and the Gurson-Tvergaard-Needleman model.* Proceedings in Applied Mathematics and Mechanics, 2024, e202400168.
[3] O. El Khatib, G. Hütter, R. Pham, A. Seupel, M. Kuna, and B. Kiefer. *A non-iterative parameter identification procedure for the non-local Gurson-Tvergaard-Needleman model based on standardized experiments*. International Journal of Fracture, 241(1):73–94, 2023.
[4] A. Kumar, S. K. Paul, *Local strain evolution and microstructural characterisation of hydrogen-induced damage at different strain rates in dual phase (DP 780) steel*, Forces in Mechanics 13 (2023) 100237.
[5] C. Miehe, S. Mauthe, and H. Ulmer. *Formulation and numerical exploitation of mixed variational principles for coupled problems of Cahn-Hilliard type and standard diffusion in elastic solids*. International Journal for Numerical Methods in Engineering, 99(10):737–762, 2014.

Contact

M.Sc. Siddhi Avinash Patil
Dr.-Ing. Stephan Roth
Prof. Bjoern Kiefer, Ph.D.

Siddhi-Avinash.Patil@imfd.tu-freiberg.de
Stephan.Roth@imfd.tu-freiberg.de
Bjoern.Kiefer@imfd.tu-freiberg.de

ESF Plus
Project number:
100693906

Co-funded by the European Union

Freistaat SACHSEN

This project is co-financed from tax revenues on the basis of the budget adopted by the Saxon State Parliament