## Simulation of Hydrogen Transport and Hydrogen-Induced Damage of High-Strength Steel Concepts

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## **Abstract**

The prediction of material damage induced by hydrogen transport mechanisms is a major challenge for the development of new steel concepts. Especially the ultra-high strength steel concepts (UHSS), like dual phase and martensitic steels, can exhibit a higher vulnerability to hydrogen induced damage. The main reason for this is the complex microstructure, including a large number of several features. To evaluate the security of possible material applications in respect to the hydrogen context, an innovative combination of physically motivated simulations and representative experiments has been realized.

Initially, experiments such as permeation measurements and slow strain rate tests (SSRT) have been performed for UHSS grades to generate fundamental material parameters. In particular the effective diffusion constants, the initial hydrogen contents and the material based flow properties were determined. Based on these parameters finite element (FE) simulations of 3D structural mechanic models by COMSOL Multiphysics® software were used to examine the hydrogen-repositioning induced by different global loads and hydrogen charging conditions. A physically motivated hydrogen transport model presented by Krom et al. [1] was implemented, which is based on the equilibrium theory of Oriani [2] and the transport model of Sofronis and McMeeking [3]. The added model considering effects of stress gradients, plastic strain and hydrogen trapping and allows evaluating influence factors for hydrogen induced fracture. Furthermore, by the option to connect several physical models with structural mechanic simulations critical component areas can be localized. The simulations are based on a simultaneous calculation of the time-dependent stress field and local hydrogen concentration.

The impacts of the hydrogen-repositioning process were examined by testing and simulating different tensile specimen geometries. Figure 1 presents the material behavior of UHSS shear load samples exposed with various initial hydrogen contents. The sample on the left side of the image illustrates comparatively low hydrogen exposures, while the sample on the right side contains high hydrogen concentrations. It becomes clear that the fracture behavior is strongly influenced by the local stress condition, strain state and hydrogen content. In addition, the change between ductile and brittle damage behavior can be visualized by the preferred direction of the crack. Ductile fracture takes place in the

area of maximum plastic strain, while brittle fracture initiates close to the shear slot and rises in direction of the highest hydrostatic stress. These results reflect the simulated maximum hydrogen concentrations areas.

In summary, the connection of a hydrogen transport model based on experimental investigations with structural mechanic simulations to characterize hydrogen-repositioning in UHSS materials is shown. Dynamic testing procedures can be analyzed by FE simulations with COMSOL Multiphysics to gain a better understanding of the hydrogen influence to fracture behavior. The prediction of material failure with respect to the hydrogen context will be realized by implementing damage models in further studies.

## Reference

[1] A. H. M. Krom et al., Hydrogen transport near a blunting crack tip, Journal of the Mechanics and Physics of Solids, Vol. 47, pp. 971-992 (1999)

[2] R.A. Oriani, The diffusion and trapping of hydrogen in steel, Acta Metall., Vol. 18, pp. 147-157 (1970)

[3] P. Sofronis and R. M. McMeeking, Numerical analysis of hydrogen transport near a blunting crack tip, J. Mech. Phys. Solids, Vol. 37, pp. 317–350 (1989)

## Figures used in the abstract

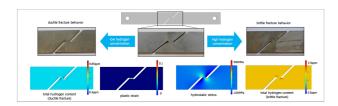


Figure 1