Modeling hydrogen redistribution in steels containing retained austenite

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Hydrogen embrittlement remains a critical challenge limiting the reliability and durability of advanced high-strength and duplex steels with multiphase microstructures containing retained austenite. The susceptibility of such steels to hydrogen-assisted crack initiation and propagation is strongly governed by microstructural heterogeneities, phase interactions, and grain boundary characteristics evolving across multiple length and time scales. Because direct experimental observation of hydrogen at the microscale is difficult due to its small atomic size and high mobility, physics-based computational modeling provides an essential pathway for understanding and predicting the hydrogen redistribution processes.

In this work, a multiscale, multiphysics finite element framework is developed to systematically investigate hydrogen transport and accumulation in steels with complex austenite–martensite and ferrite–austenite microstructures, respectively. The modeling approach integrates stress-assisted hydrogen diffusion, reversible and irreversible trapping mechanisms [1], grain boundary diffusion, and orientation-dependent interface properties within a unified numerical formulation implemented in Abaqus. In addition, strain-induced martensitic phase transformation is incorporated to capture the strong coupling between evolving phase fractions and hydrogen redistribution. Particular emphasis is placed on hydrogen redistribution during transformation of metastable retained austenite to martensite, where differences in hydrogen solubility between phases promote local enrichment and increased embrittlement susceptibility. The framework is further extended to include three-dimensional grain boundary effects, enabling microstructure-resolved representation of transport pathways and interface-controlled accumulation processes. The latter are governed by the energy landscape across the interface, which is determined by means of ab initio calculations.

The modeling strategy is supported by in-situ hydrogen charging experiments performed at the synchrotron [2], where lattice expansion measurements provide indirect quantification of hydrogen uptake in austenite. These observations are reproduced using microstructure-resolved simulations that explicitly account for trapping and grain boundary transport, and are validated by X-ray diffraction measurements of hydrogen redistribution during charging.

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