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Editorial

Hydrogen Embrittlement of Metals: Behaviors, Mechanisms, and Engineering Practice

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1. Introduction

Hydrogen is widely regarded as a clean and versatile energy carrier, and it has become a cornerstone of the energy-transition strategies of many countries around the world. However, the development and utilization of hydrogen energy involve a complex chain of dynamic processes—from production and storage to transportation and end-use application—and a large number of metallic materials are deployed at every link of this chain. When metals are exposed to hydrogen-containing environments, their mechanical behavior and failure resistance can be severely degraded [1]. Moreover, internal hydrogen introduced during casting, welding, and thermomechanical processing can persist in metallic components and exert a decisive influence on their long-term mechanical properties. These considerations make the study of hydrogen behavior and damage mechanisms in metallic materials a matter of both fundamental scientific interest and pressing engineering necessity.

Hydrogen embrittlement (HE) is one of the oldest and most conspicuous material challenges, and it remains one of the most complex [2]. Over more than a century of research, a number of mechanisms have been proposed to account for hydrogen-induced degradation, including hydrogen-enhanced localized plasticity (HELP), hydrogen-enhanced decohesion (HEDE), adsorption-induced dislocation emission (AIDE), and hydrogen-enhanced stress-induced vacancy (HESIV) formation [3–5]. A growing consensus holds that these mechanisms rarely operate in isolation; instead, they act synergistically and sequentially depending on the material, its microstructure, the local hydrogen concentration, and the mechanical loading conditions [6,7]. Despite substantial progress, the precise prediction of hydrogen-induced failure remains elusive, particularly for complex engineering alloys with heterogeneous microstructures, such as the ferrite–pearlite and martensitic steels used in energy infrastructure.

The purpose of this Special Issue "Hydrogen Embrittlement of Metals: Behaviors and Mechanisms" is to gather original research and critical reviews that advance our understanding of the behaviors and mechanisms of hydrogen embrittlement in metallic materials. The topics covered include hydrogen diffusion and permeation, hydrogen transport and storage, microstructure evolution in hydrogen-containing environments, the mechanisms behind hydrogen-induced material failure, and the development of hydrogen-embrittlement-resistant materials and technologies. The seven articles collected in this Special Issue address these themes through a combination of advanced experimental characterization, multiscale computational modeling, and data-driven approaches, with a strong

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emphasis on the engineering challenges posed by the transition toward hydrogen-blended natural gas infrastructure.

2. Results

The seven contributions published in this Special Issue can be broadly grouped into three interconnected themes: (i) experimental elucidation of hydrogen-induced microstructural and fracture-mechanism evolution in pipeline and structural steels; (ii) multiscale and data-driven modeling for the quantitative prediction of hydrogen embrittlement; and (iii) engineering-oriented assessments of the hydrogen embrittlement resistance of pipeline steels, welded joints, and protective coatings.

2.1. Mechanistic Insights into Hydrogen-Induced Damage

Two experimental studies provide detailed evidence of how hydrogen charging conditions alter the microstructure and fracture behavior of industrially relevant steels. Dyakova et al. (Contribution 1) investigated the effect of hydrogen charging time on a low-carbon ferrite–pearlite steel that had been in operation for over 30 years in natural gas transmission service. Despite negligible changes in the total hydrogen content, extended electrochemical charging produced a clear transition from ductile fracture to predominantly brittle fracture modes (quasi-cleavage, intergranular, and transgranular), accompanied by an increased dislocation density and the formation of prismatic dislocation-loop debris within the ferrite phase. Transmission electron microscopy analysis revealed a sequential activation of HE mechanisms: HELP initially dominates within ferrite grains, followed by HEDE, particularly at ferrite–cementite interfaces in pearlite colonies, with enhanced hydrogen trapping at ferrite–cementite boundaries, grain boundaries, and dislocation cores. This work underscores the importance of charging time—rather than total hydrogen content alone—in governing the degradation of legacy pipeline steels.

Complementing this study, Yanachkov et al. (Contribution 2) examined the effect of hydrogen content on the microstructure, mechanical properties, and fracture mechanisms of low-carbon lath martensite steel, combining experiments with atomistic modeling. A transition from transgranular to intergranular fracture was observed at a hydrogen content of approximately 0.44 wppm, with the most probable failure mechanism identified as HELP-mediated HEDE. As the hydrogen concentration increased, the dislocation density on specific crystallographic planes, such as (111) and (100), rose, and atomistic simulations indicated that quasi-cleavage cracks predominantly initiate at block boundaries with higher local hydrogen accumulation. Together, these two contributions illustrate how hydrogen re-routes fracture along microstructurally specific paths—from interfaces within pearlite colonies to block boundaries in martensite—and provide a mechanistic basis for interpreting hydrogen-induced failures in widely used structural steels.

2.2. Multiscale and Data-Driven Modeling

Quantitative prediction of hydrogen-induced failure has long been a bottleneck in engineering design. Two contributions in this Special Issue address this challenge from complementary perspectives. Katzarov (Contribution 3) developed a multiscale modeling framework that couples a continuum decohesion model with atomistic calculations to analyze hydrogen-enhanced decohesion across block boundaries in low-carbon lath martensite. By incorporating hydrogen mobility and segregation at low- and high-angle twist boundaries in body-centered cubic iron, the model quantifies hydrogen-induced reductions in cohesive strength under realistic hydrogen-flux boundary conditions. The simulations demonstrate that, in the presence of a hydrogen flux, separation across block boundaries occurs at tensile loads significantly lower than the critical stress required for

rupture in hydrogen-free martensite, providing a direct atomistic-to-continuum bridge for the prediction of HEDE.

In parallel, Gyaabeng et al. (Contribution 4) adopted a machine learning (ML) approach to model the impact of hydrogen embrittlement on the fracture toughness of low-carbon and low-alloy steels. Among the seven ML techniques initially considered, the k-nearest neighbors (KNN) model delivered the most reliable predictive performance. Parametric studies revealed that hydrogen pressure is the most influential variable, accounting for 32% of the variation in fracture toughness, with a pronounced decline at low pressures (0–6.9 MPa); beyond 6.9 MPa, the reduction in fracture toughness diminishes, reaching a plateau at approximately 8 MPa, which indicates a saturation point. Low concentrations of oxygen impurity in the hydrogen gas environment (<200 ppm) mitigate HE in X70 steel, likely by limiting hydrogen uptake. These findings demonstrate the considerable potential of data-driven approaches for the fast, physics-informed screening of material and environmental parameters.

2.3. Engineering Assessments for Hydrogen Infrastructure

The remaining three contributions focus on the practical assessment of materials and protection strategies for hydrogen-blended natural gas pipelines. Ghadiani et al. (Contribution 5) performed double cantilever beam (DCB) fracture tests on a vintage API X52 steel and a modern API X65 steel under simulated hydrogen exposure, with charging parameters derived from hydrogen permeation tests. The results reveal markedly different responses of vintage and modern pipeline steels to hydrogen in terms of fracture toughness and crack growth, providing essential quantitative data for the safe integrity assessment of pipelines intended to carry hydrogen–natural gas blends.

Tang et al. (Contribution 6) addressed the weakest link in welded pipelines by investigating the hydrogen embrittlement behavior of the heat-affected zone (HAZ) of X80 welded pipe. By dividing the HAZ into coarse-grained, fine-grained, and intercritical sub-regions, the authors showed that the degree of hydrogen damage varies significantly with strain rate: the coarse-grained HAZ exhibits the highest HE sensitivity at low strain rates, whereas the intercritical HAZ suffers the greatest hydrogen damage at high strain rates. These microstructurally resolved findings provide a scientific basis for assessing the feasibility of using X80 welded pipes in hydrogen-blended natural gas transportation.

Finally, Falat et al. (Contribution 7) evaluated the protective effects of electroless-plated copper and nickel–phosphorus coatings on the notch tensile properties of API 5L X42 pipeline steel under electrochemical hydrogen charging. Although the deposition process itself induced some degree of HE, the coated systems exhibited improved HE resistance—quantified by lower hydrogen embrittlement index (HEI) values—compared with the uncoated material after charging. However, hydrogen-induced deterioration of the coatings, including bubbling, flaking, and spallation, was observed, highlighting the need for improved surface quality and long-term durability, as well as validation under pressurized gaseous hydrogen conditions.

3. Conclusions and Outlook

Despite decades of research, several fundamental and practical gaps continue to limit the safe deployment of metals in hydrogen environments. First, the precise conditions under which different HE mechanisms—and their combinations—operate remain poorly quantified, particularly in complex, heterogeneous microstructures. Second, reliable quantitative relationships between hydrogen content, microstructure, and fracture properties such as fracture toughness are still lacking, hindering engineering integrity assessment. Third, the roles of time-dependent and rate-dependent effects, such as charging time, hydrogen

concentration, and strain rate, are frequently overlooked in laboratory testing. Fourth, welded joints, and especially their heat-affected zones, represent a persistent weak link that is not fully understood. Fifth, mitigation strategies, including protective coatings, have rarely been validated under realistic hydrogen-charging conditions.

This Special Issue makes tangible progress on each of these fronts. The contributions provide direct experimental evidence for the sequential HELP-HEDE activation in service-aged ferrite–pearlite steel (Contribution 1) and for hydrogen-induced fracture-mode transitions in lath martensite (Contribution 2); bridge the atomistic and continuum scales to quantify decohesion at block boundaries (Contribution 3); introduce a data-driven ML framework for fracture-toughness prediction (Contribution 4); supply engineering-level fracture-toughness data for vintage and modern pipeline steels (Contribution 5); resolve the strain-rate-dependent HE sensitivity of individual HAZ sub-regions (Contribution 6); and deliver a systematic assessment of electroless coatings as HE mitigation measures (Contribution 7). Collectively, these studies demonstrate that combining advanced characterization, multiscale modeling, and data-driven approaches is a powerful strategy for converting mechanistic understanding into engineering decision-making.

Several priority directions will shape the next generation of hydrogen embrittlement research. First, direct, quantitative observation of hydrogen at the microstructural scale remains a grand challenge; cryogenic atom probe tomography, combined with in situ TEM mechanical testing and advanced thermal desorption spectroscopy, can reveal where hydrogen resides and which trapping sites control failure, while standardized protocols are needed for transferable quantitative analysis. Second, physics-informed multiscale modeling integrating first-principles calculations, molecular dynamics, and crystal plasticity, and continuum damage mechanics offers a path toward predictive life assessment, though reliability depends on high-quality training data, physical grounding, and open benchmarked databases validated against component-scale experiments. Third, rather than merely mitigating embrittlement, future alloys should be designed with intrinsically hydrogen-tolerant microstructures, including engineered nanoprecipitates and carbides as stable trapping sites, grain-boundary engineering, retained austenite, and optimized dislocation substructures, while solute–hydrogen interactions deserve systematic investigation.

Finally, we are pleased to note the strong interest that this Special Issue has generated, having been viewed more than 20,000 times since its opening. The enthusiasm of the scientific community has prompted the launch of a second edition of this Special Issue, "Hydrogen Embrittlement of Metals: Behaviors and Mechanisms (2nd Edition)," and we cordially invite researchers to contribute their latest findings. We believe that continued collaboration between experimentalists, modelers, and engineers will be essential to transform hydrogen embrittlement from a longstanding challenge into a manageable engineering consideration, thereby accelerating the safe and sustainable deployment of hydrogen energy worldwide.

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