A Machine Learning Approach to Predict the Susceptibility of Materials to Hydrogen Embrittlement

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Hydrogen is widely considered a promising energy carrier capable of mitigating the human impact on the environment while making the countries energetically independent in the long term. Nevertheless, safety aspects represent the major bottleneck for the widespread utilization of hydrogen technologies. Industrial equipment operating in a pure hydrogen environment is prone to a variety of material degradations. Hydrogen embrittlement (HE) is the best-known hydrogen-induced damage and manifests itself as a reduction in tensile ductility, fracture toughness, and fatigue performance of the affected materials. It may cause component failures at stress levels significantly below the nominal tensile strength of the material, often resulting in undesired releases of hazardous substances in the environment. The occurrence of HE relies on the synergy of several factors, such as the hydrogen concentration, the operating conditions (i.e., temperature and pressure), the level of internal and applied stress, and the microstructure and chemical composition of the material. However, the mutual influence of these factors is still difficult to evaluate, and this results in serious difficulties in planning inspection and maintenance activities of hydrogen technologies. In this study, the experimental data of tensile ductility tests carried out on several materials exposed to hydrogen under different operating conditions were analyzed through an advanced machine learning approach. This study aims to provide critical insights into the susceptibility to hydrogen embrittlement for various materials at different operating conditions. In particular, the embrittlement index was estimated to predict the likelihood of component failures. The model demonstrated accurate and reliable predicting capabilities. The outcome of this study can increase the understanding of hydrogen-induced material damages and facilitate the decision-making process in planning inspection and maintenance of hydrogen technologies.

Norwegian University of Science and Technology

A Machine Learning Approach to Predict the Materials' Susceptibility to Hydrogen Embrittlement

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H2
Hydrogen
H2
zero emission

High Risk
Failure Rate
Low Risk
Consequence

Prevention of hydrogen-related accidents

Hydrogen has the potential to become the **energy carrier of the future.**

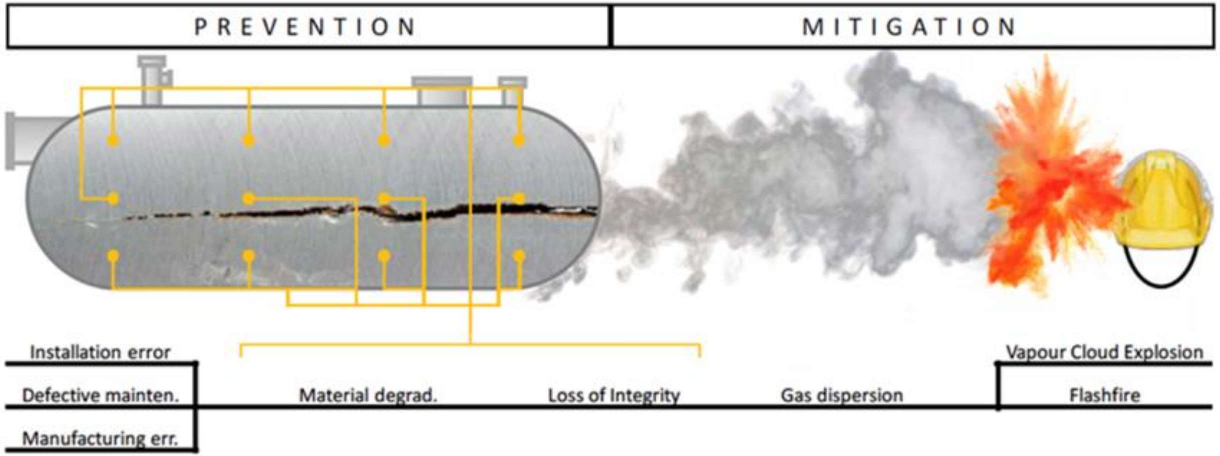
Safety is one of the **main bottlenecks** for a widespread rollout of hydrogen technologies.

Hydrogen is:

- Highly **flammable** and **explosible**
- Capable of **permeating** and **embrittling** metallic materials

Hydrogen-induced degradation of mechanical properties should be addressed with specific **preventive approaches**.

Careful material selection and **tailored inspection activities** are vital to ensure the physical integrity of equipment in a hydrogen environment.

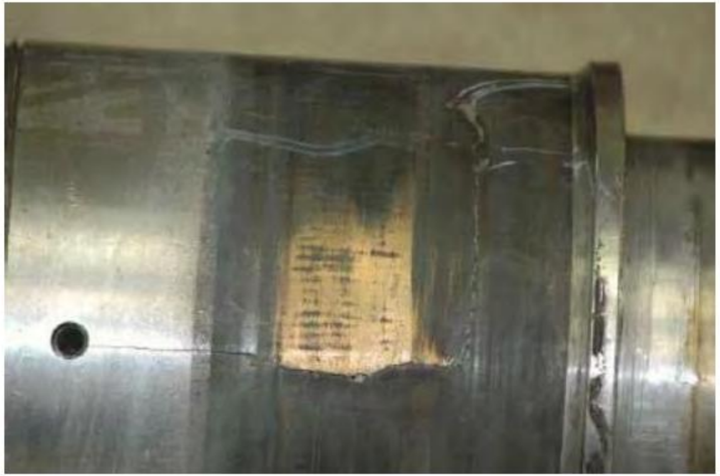


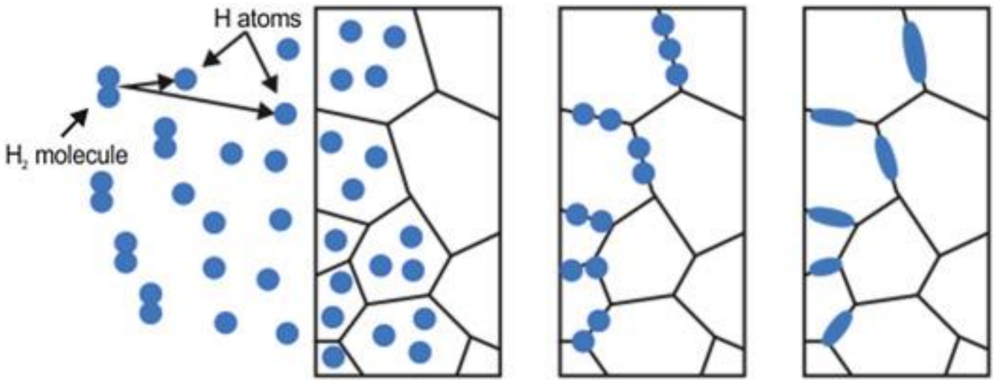
The issue of hydrogen embrittlement

Mechanical properties of metals are **degraded** by the interaction with hydrogen from the component’s working environment.

This phenomenon is known as **hydrogen embrittlement** (HE).

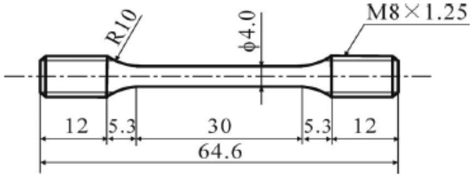
HE results from the combined action of **hydrogen** and residual or applied **stresses**.



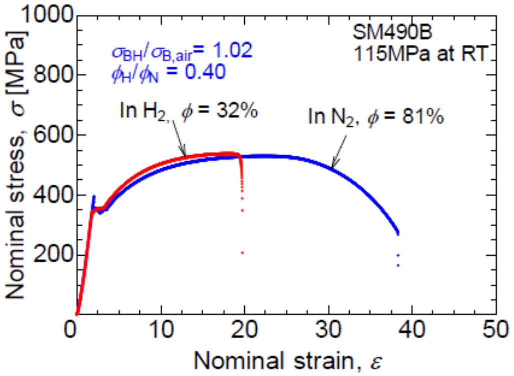


Effects of hydrogen embrittlement

Loss of ductility

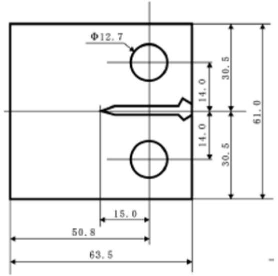


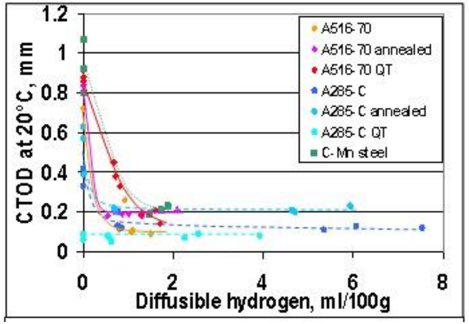
Tensile specimen



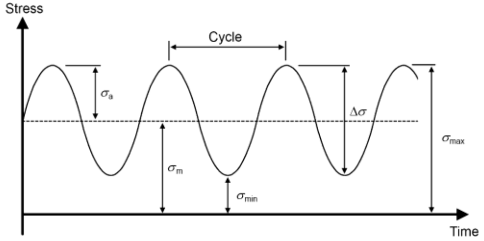
Stress-strain curve

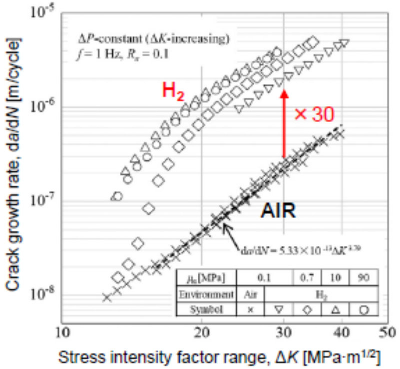
Reduction of toughness





Accelerated fatigue crack growth rate



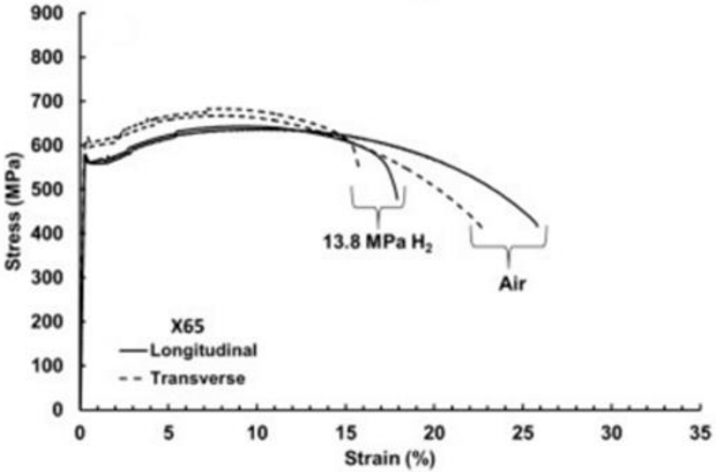


Ductility loss

Hydrogen-induced ductility loss is expressed as **reduced areas** after a tensile test obtained **with or without hydrogen charging**.

It is tested through **slow strain rate tests** (SSRT) or **linearly increasing stress tests** (LIST).

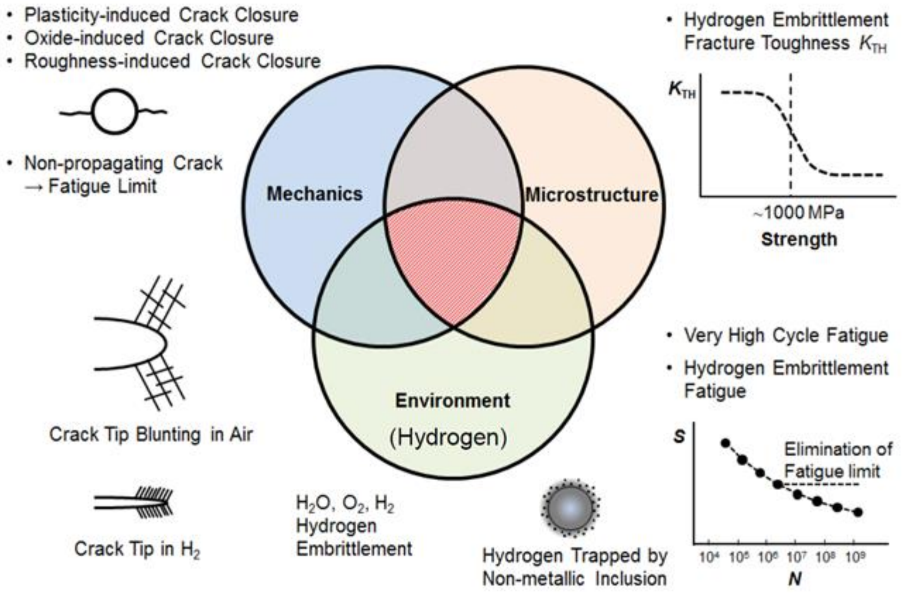
When the specimen undergoes tension, the stress concentration gradient causes the **migration of hydrogen**, possibly initiating a crack.



Susceptibility factors

HE relies on the **synergistic effect** of three factors:

- **Environment** → temperature, pressure, hydrogen purity
- **Material** → chemical composition, microstructure, strength, presence of weldments
- **Stress field** → stress concentrations, strain rate

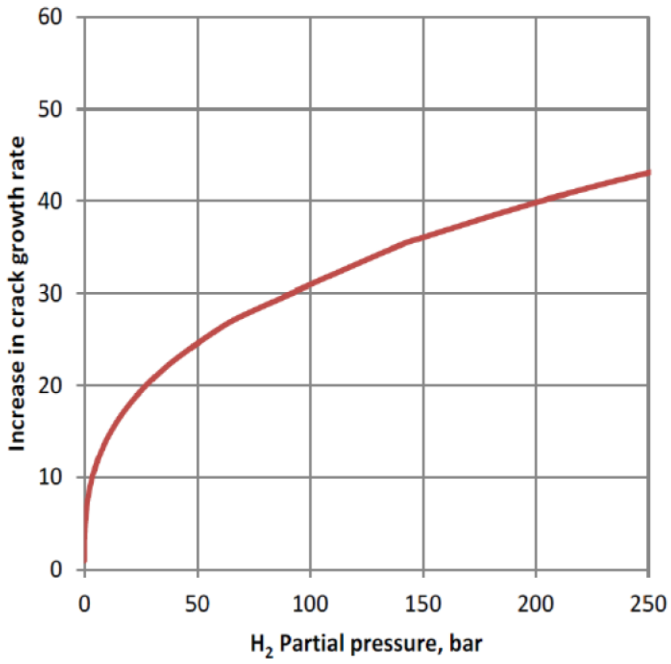


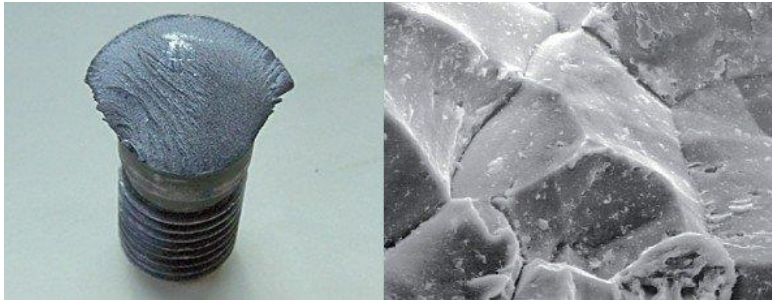
Environmental factors

Hydrogen concentration in the metal is **proportional to** hydrogen partial **pressure.**

Temperature affects the hydrogen **solubility, diffusivity, and trapping**.

The maximum HE is reached at **near-ambient temperature**.



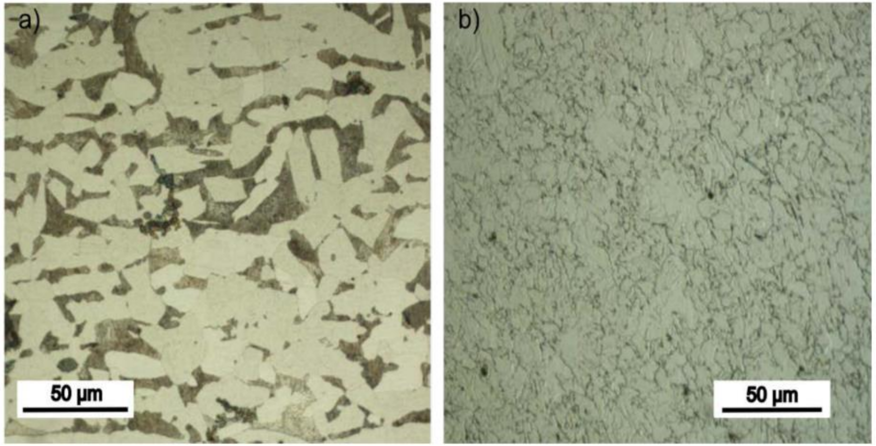


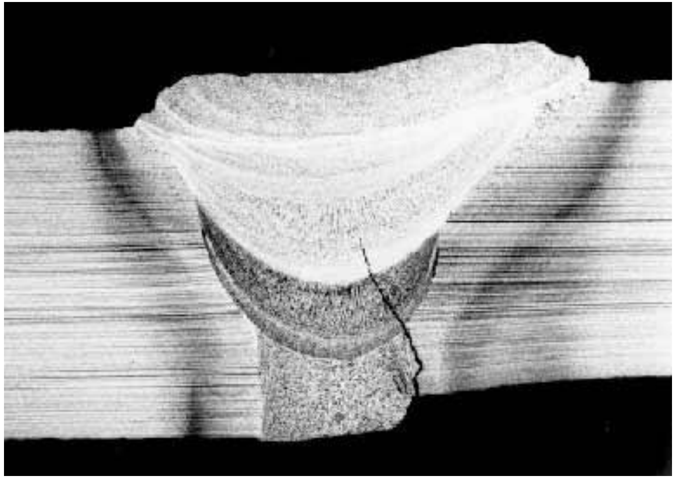
Material factors

Steels with **higher strength** tend to show a **more pronounced HE** degradation.

Martensite is the **most susceptible** microstructure.

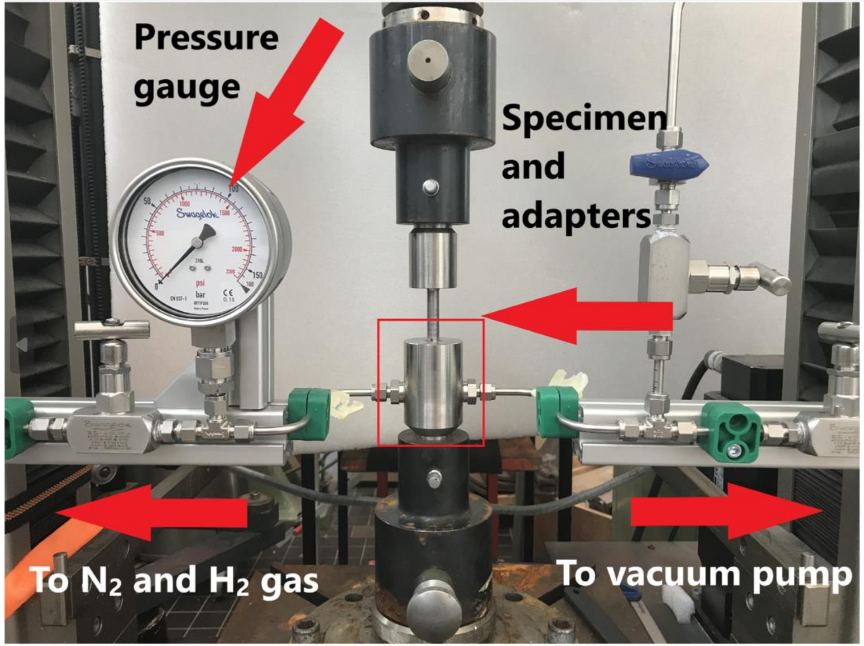
Welded areas and **heat-affected zones** (HAZs) are particularly prone to HE effects.

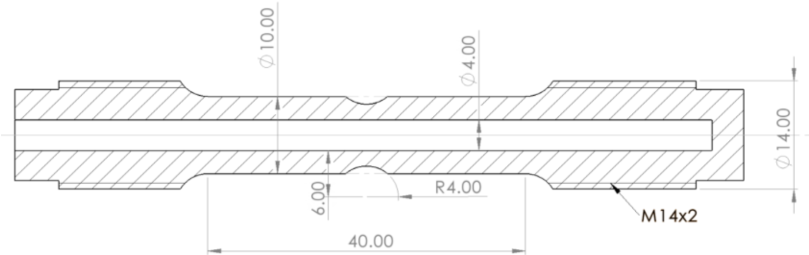




Stress factors

The **nominal strain rate** is the most important stress factor. It must be low enough to allow hydrogen to diffuse and accumulate in internal defects.



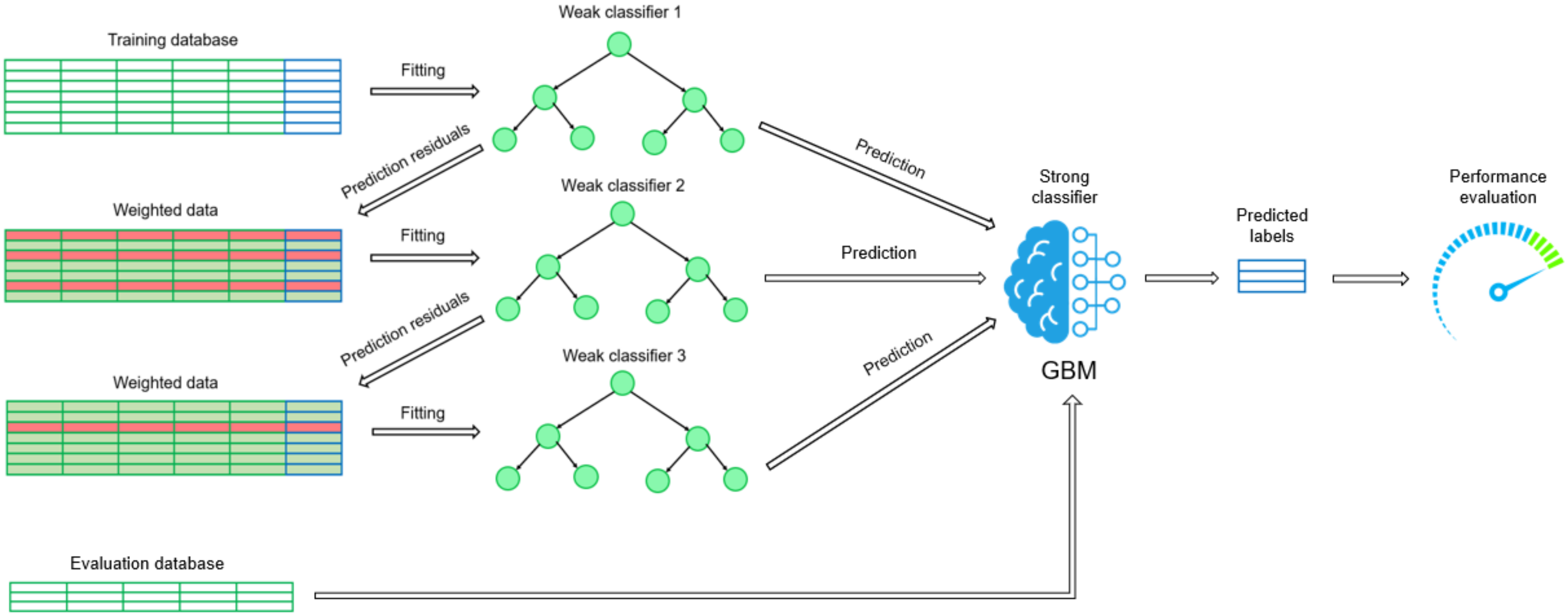


Machine learning approach

1. **Database creation and pre-processing**

2. **Target definition**

3. **Machine learning simulation**



Database creation and pre-processing

The database contains **tensile tests results**, conducted under **high-pressure hydrogen gas**.

The pre-processed database includes **200 tests** (i.e., rows) and **24 features** (i.e., columns).

Factor	Feature	Type
Environment	Pressure (MPa)	Numerical
	Temperature (°C)	Numerical
	Hydrogen purity (%)	Numerical
Material	Material: X80, X100, A515, A516, etc.	Categorical
	Composition: Fe, Cr, Ni, Mn, Mo, Nb, Ti, V, Al, Cu, Si, C, N, B, S, P, Co (%)	Numerical
	Microstructure: ferritic, pearlitic, bainitic, martensitic, austenitic	Categorical
	Type of weld or HAZ: EB, ERW, GMA, GTA, SA, SMA	Categorical
	Yield strength (MPa)	Numerical
	Ultimate tensile strength (MPa)	Numerical
Stress	Stress intensity factor	Numerical
	Nominal strain rate (s-1)	Numerical

Target identification

The **Embrittlement Index** is the target attribute to predict:

$$\mathrm{EI} = \frac{\mathrm{RA_{air}} - \mathrm{RA_{H_2}}}{\mathrm{RA_{air}}} \cdot 100$$

Two **susceptibility classes** are defined according to the classification provided in the technical report **NASA/TM-2016-218602**.

Susceptibility	Embrittlement Index	Material screening notes
Small / Medium / High (SMH)	$\mathrm{EI} < 50\%$	Recommended for hydrogen service at specific operating conditions and with tailored inspection and maintenance activities
Extreme (E)	$\mathrm{EI} \geq 50\%$	Not recommended for hydrogen applications in any temperature and pressure range

Results and metrics

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} = 0.886$$

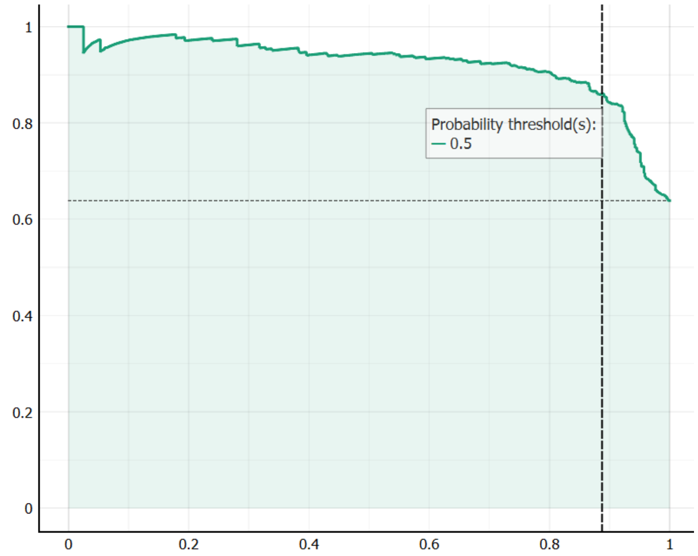
$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} = 0.860$$

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} = 0.889$$

Mislabeling an E susceptibility as a SMH is critical: it may cause an underestimation of the HE susceptibility, thus leading to **higher risk of component failure**.

Precision is the most meaningful metric for this task.

Actual \ Predicted	E	SMH
E	TN = 83.1%	FP = 11.1%
SMH	FN = 16.9%	TP = 88.9%



Implications

This study can aid to understand HE degradation in **equipment exposed to pure hydrogen**.

Inspection and maintenance of hydrogen technologies can be improved by risk-based approaches.

The collaboration between **material scientists** and **safety experts** must be strengthened to improve accident prevention.

Steam methane reformers

LH_2 cryogenic vessels

Electrolyzers

Hydrogen pipelines

GH_2 cylinders

Thank you for your attention

Contact

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