Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration (HyWay)

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1. Introduction

Ensuring the safety of components used in the hydrogen infrastructure requires a comprehensive understanding of how hydrogen interacts with materials and how it alters or degrades mechanical properties. Once hydrogen atoms reach microstructure, interactions between hydrogen and advanced metallic materials start at the atomic level, affecting macroscopic mechanical properties. Hence, to acquire knowledge of these phenomena, academia and companies involved in constructing the hydrogen infrastructure need a multiscale methodology to assess hydrogen-material interactions. In this context, recent advancements in characterisation techniques can reveal hydrogen-material interactions from the atomic level up to the macroscopic scale. However, these characterisation tools still have limitations to be overcome by unifying multiple materials research disciplines:

1. The quality of characterisation results depends on the workforce's competence in tools operation. In this context, data-driven approaches and material modelling tools can support the multiscale characterisation campaigns, allowing a better interpretation of experimental data and providing more guidance on experiments.

2. Hydrogen-material interactions under actual service conditions are challenging to assess solely by experiments because of the time and cost required. To solve this research dilemma, we envision the multiscale and multiphysics material modelling platform as a solution to predict material behaviour under complex scenarios.

3. Typical problems when merging multiple materials research disciplines are data incompatibility and interoperability, demanding efficient Data and Knowledge Management Platform (DKMP) with ontology integration to establish relationships between domains, which follow Materials modelling - Terminology, classification, and metadata document.

The main objective of HyWay is to develop adaptive multiscale material modelling and characterisation suites for assessing interactions between hydrogen and advanced metallic materials and demonstrate their capabilities on hydrogen storage and

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transport components. Our ambition is to enable industries to be more efficient when developing and using new advanced materials, shorten the materials innovation cycle, seamlessly merge materials modelling and characterisation approaches along value chains, and create a robust material research ecosystem platform.

The realisation of multiscale materials modelling and characterisation suites for assessing interactions between hydrogen and advanced metallic materials for hydrogen storage and transport components relies on a seamless integrative approach involving immersive communication between physical and digitalised tools. To this end, the HyWay project consists of 3 key modules: Physical realm, Virtual world, and Data and knowledge management platform (DKMP).

2. HyWay Physical realm

Considering the complexities in the hydrogen-material interactions, it is imperative to use multiscale characterisation techniques and testing methods. We will materialise this using (a) multiple characterisation techniques, (b) mechanical testing at 3 different length scales, and (c) 3 different hydrogen charging methods. These experiments will be weaved together to understand the intricate structure-property correlations in advanced materials and to quantitatively evaluate the effect of hydrogen at the different length scales on the mechanical properties. These data will support development and validation of the multiscale and multiphysics materials modelling platform. To bridge the gap in the obtained experimental knowledge, we will incorporate the data-driven approaches to provide effective guidance on characterisation and improve the data interpretation.

3. HyWay Virtual world

Predicting the microstructure evolution and macroscopic properties changes of advanced materials under the complex boundary conditions along their entire life cycle requires a flexible and adaptive modelling scheme. We will develop a modularised multiscale and multiphysics material modelling platform for assessing hydrogen effects on advanced metallic materials' behaviour. Besides advancing in modelling, another emphasis will be on developing interchangeable modelling tools, allowing one to efficiently exchange data from each model depending on the end users' requirements. Once the platform is established, we will leave the modularised modelling platform open for further implementation by other researchers. The modularised multiscale and multiphysics materials modelling platform consists of 7 interdependent submodules: atomistic modelling toolset, hydrogen uptake models, hydrogen-induced phase transformation models, hydrogen transport models, continuum model of hydrogen effects on plasticity, hydrogen-aware fracture model, and macroscopic hydrogen-sensitive model. Besides an understanding of physical mechanisms obtained from the atomistic modelling, we will use it to derive material parameters for other simulation tools.

4. HyWay Data and knowledge management platform (DKMP)

Data generated from all materials characterisation techniques and multiscale and multiphysics material modelling tools to reveal hydrogen-material interactions under various conditions in HyWay will be massive and come from multiple sources, requiring a suitable materials ontology, which represents knowledge and information in a structured way using properties and relationships. We will advance the standardised data management platform by integrating a materials ontology to understand hydrogen-material interactions under actual conditions exposed to the hydrogen storage and transport components. Another benefit of having an ontology-based DKMP is its ability to facilitate data interoperability between different disciplines. DKMP will be compatible with further integration as well.