



Review

A review on diffusion modelling in hydrogen related failures of metals



A. Díaz*, J.M. Alegre, I.I. Cuesta

Structural Integrity Group, Escuela Politécnica Superior, Avda. Cantabria s/n, 09006 Burgos, Spain

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ABSTRACT

Modelling of hydrogen embrittlement in order to prevent engineering failures requires a characterization of transport phenomena in the bulk metallic as a first step. Interstitial solid state diffusion can be described as a random phenomenon, however there will be also some drift forces biasing this behaviour so a modification in Fick's laws is needed. The potential energy landscape of the metal lattice characterizes the influence of imposed fields and microstructural defects in transport kinetics. Thus, considering the chemical potential as a driving force, the physical basis of diffusion will be translated into continuum equations. Finally the two-level models that take into account lattice and trapping sites for hydrogen will be reviewed.

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* Corresponding author.

E-mail address: adportugal@ubu.es (A. Díaz).

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1. Introduction

Hydrogen embrittlement is a common phenomenon which degrades metals [1–7]. A reduction in mechanical properties of metals and alloys occurs due to the inclusion of hydrogen as an impurity. The inserted atom is considerably smaller than the crystal atom so these phenomena fall under the category of interstitial solid solutions, in contrast to substitutional diffusion. This problem was documented over a century ago as a problem associated with the corrosion due to electrochemical reduction of hydrogen in aqueous media and also due to the gaseous hydrogen storage.

In literature there are plenty examples of hydrogen degradation associated with corrosion phenomena. For example, numerous failures attributed to hydrogen assisted cracking have been documented in pipelines transporting natural gas or oil [8]. Such petrochemical products typically contain H₂S which promote an aggressive environment in which hydrogen is produced and diffuses through the metal causing embrittlement. For this reason, API pipeline X grades steels has been thoroughly investigated and tested in hydrogen environments (e.g. X42 [9]; X60, X80 and X100 [10]).

Additionally, cathodic protection, sometimes used in order to avoid corrosion, for example in buried pipes or in marine environments, results in hydrogen production which can produce unexpected failures [11,12].

Similarly, hydrogen absorption might occur in parts that have been plated, e.g. Tanner documented failures of cadmium plated head cap screws during service and attributed them to hydrogen embrittlement [13].

Welding processes may also introduce significant amounts of hydrogen from materials in the electrode coating, in the flux or in the shielding gas, as well as from the moist environment [14]. This hydrogen insertion added to the usual presence of residual stresses in the weld frequently causes Hydrogen Assisted Cracking [15].

In recent decades, since hydrogen has been proposed as a promising energy carrier, the interest in the interaction between hydrogen and different types of materials for hydrogen storage has increased.

Several methods of storing hydrogen have been [16]: liquid hydrogen at cryogenic temperatures, by physisorption, as a metal hydride and in gaseous state at high pressures. The last is the least expensive and consist in storing H₂ in pressure vessels made of alloys or composite materials. However, although H₂ containers have been built for more than a century, embrittlement of the used alloys still is a problem. The explosion of some iron bottles storing gaseous hydrogen in an airship in 1894 [17] might be regarded as one of the first failure cases of hydrogen containers documented. Hydrogen assisted cracking produced the release of hydrogen, as a result supplying an explosive gas mixture.

Also in the space industry hydrogen embrittlement has been a concern since failures have been documented in high-pressure hydrogen storage vessels at NASA facilities from 70s [18].

Revisiting this and other failure cases shows the importance of integrity assessment and hydrogen embrittlement prognosis in storage systems.

Despite the efforts, a full understanding of the phenomenon has not yet been achieved and selection of suitable components for hydrogen service simply discriminates between especially susceptible alloys (high strength steels, and nickel alloys) and alloys hardly affected (austenitic stainless steels and aluminum alloys), as the Standard ANSI/CSA CHMC 1-2014 defines [19]. Such distinction has an empirical basis but lacks of a consistent microstructural and physical explanation. Therefore, assessment of hydrogen embrittlement must move towards a physical-based numerical modelling of the metal-hydrogen system.

Usually, the interaction of metal-hydrogen is divided into two parts: transport phenomena (absorption and diffusion) and damage mechanisms. Both phenomena are related, but in this paper only the mathematical models that try to establish constitutive equations of diffusion are reviewed. The ultimate aim of diffusion modelling is to obtain concentration profiles to predict where and how the fracture will begin or where the more severe damage will occur. In any case, a consistent theory of diffusion and the influence of the stress-strain fields on it will not only produce more accurate concentration profiles, but it will result in a better understanding of the damage micro-mechanisms.

The objective of this review is to develop a simplified continuum level model from the general physics fundamentals. Firstly, the multiscale and multidisciplinary character of materials science is underlined and in particular that of hydrogen embrittlement. Later, mass transport is physically explained and the interstitial diffusion mechanism is explained as a random motion at the atomic level.

Next, the importance of characterizing the energy landscape of the metal lattice is shown and what the factors are that influence the energy state of an inserted hydrogen atom. Spatial variations in such free potential energy are discussed as a driving force. This leads to defining and characterizing the chemical potential as a continuum function. In order to consider all the effects

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