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Numerical simulation of hydrogen permeation in steels

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Abstract

The McNabb-Foster model was used to simulate the permeation curves, based on the proposed method and Oriani's equilibrium theory, by varying the characteristics of hydrogen trapping sites and the apparent hydrogen solubility. The simulated permeation curves were analyzed using lag time and breakthrough time methods to obtain effective diffusivities, which were finally utilized to reproduce the permeation curves according to Fick's diffusion laws. The discrepancies between the simulated and reproduced permeation curves were valued and analyzed. The influence of hydrogen apparent solubility and hydrogen trapping site characteristics, such as trapping sites density and hydrogen-trapping sites binding energy, on the permeation curves were studied and discussed.

Keywords: Modelling; Diffusivity; Hydrogen Trapping; Permeation Curve

1. Introduction

The hydrogen embrittlement susceptibility increases with the material's strength, in general. For example, it has recently been reported that for some steels, such as dual-phase (DP), quenching and partitioning (Q&P), and twinning-induced plasticity (TWIP), and advanced high-strength steels (AHSS), the negative influence of hydrogen on their mechanical properties increases with strength [1]. Hydrogen segregation, diffusion, and effusion processes have been widely investigated to clarify the underlying mechanisms of hydrogen embrittlement [2]. Reliable information