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A thermo-mechanically-coupled theory accounting for hydrogen diffusion and large elastic–viscoplastic deformations of metals

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ABSTRACT

In this paper we develop a thermodynamically-consistent coupled-theory which accounts for diffusion of hydrogen, diffusion of heat, and large elastic–viscoplastic deformations of metals. The theory should be of utility in the analysis of hydrogen diffusion in elastic–plastically-deforming solids, an analysis which is an essential prerequisite for theoretical and numerical efforts aimed at modeling the integrity of structural components used for hydrogen gas storage and distribution.

1. Introduction

Since the combustion of hydrogen produces only water as the combustion product, hydrogen is expected to play an increasingly important role as a "clean" fuel in the future.[1] However, hydrogen is a gas at ambient conditions, and the storage and distribution of hydrogen in its molecular or atomic form is a materials challenge (cf., e.g., Züttel et al., 2010). Atomic hydrogen, being the smallest of gaseous impurities, readily dissolves in and permeates through most materials. Hydrogen dissolution and permeation can be significant at high pressures which are expected to approach 100 MPa in some cases, and since hydrogen can embrittle materials it may affect the integrity of structural components used for hydrogen storage and distribution. Accordingly, it is important to understand and model the *coupled* diffusion-mechanics response of metallic components used to contain this gas, and this topic is receiving increasing attention because of its potential application to the development of the emerging technology of large-scale production, storage and distribution of hydrogen (cf., e.g., San Marchi et al., 2007; Dadfarnia et al., 2009, 2010).

The deleterious effects of hydrogen on the mechanical response of iron and steel are well-known (cf., e.g., Hirth, 1980). The precise microscopic mechanisms by which hydrogen embrittles steels are still not very well understood or modeled. This topic continues to be the focus of intensive theoretical and experimental research (cf., e.g., Serebrinsky et al., 2004; Ramasubramaniam et al., 2008; Novak et al., 2010; Dadfarnia et al., 2010),[2] and is *not the focus of this paper*. Instead, our focus here is on the development of a continuum-level theory for the diffusion of hydrogen, coupled with the thermo-elastic–plastic response of materials, which, as emphasized by Birnbaum and Sofronis (1994), is an essential prerequisite to any attempt to address the issue of hydrogen-embrittlement-related failures in structural components.

It has long been observed that there is an asymmetry between the kinetics of absorption and the kinetics of evolution of hydrogen in steels, in that absorption proceeds with a larger apparent diffusitivity than does evolution. This asymmetry in diffusivities is attributed to trapping of the hydrogen atoms at various microstructural "trapping sites," which include interfaces between the matrix and various second-phase particles, grain boundaries, and dislocation cores. A widely-used micro-mechanical model for describing this asymmetry in diffusivities, is that of Oriani (1970). His model is

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[1] Hydrogen is produced from water by electricity through an electrolyser, and the hydrogen so-produced is a "renewable" fuel only if it is produced directly from solar light, or indirectly from a renewable source, e.g., wind- or hydro-power (Züttel et al., 2010).

[2] As reviewed by Dadfarnia et al. (2010), research to date has identified the following two major mechanisms for hydrogen embrittlement: (i) hydrogen-enhanced decohesion—a mechanism induced by the segregation of hydrogen to microstructural interfaces such as grain-boundaries and particle/matrix interfaces, which leads to a reduction in the cohesive strength of the material; and (ii) hydrogen-enhanced localized plasticity—a mechanism induced by the segregation of hydrogen to dislocation cores, which leads to a reduction of the strength of barriers to dislocation motion, and thereby a reduction in the resistance to plastic flow.

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