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# Simulation of hydrogen diffusion affected by stress–strain heterogeneity in polycrystalline stainless steel

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## ABSTRACT

The effect of microstructure-induced strain–stress heterogeneity on the evolution of hydrogen distribution was studied on 316 L stainless steel. A crystal plasticity-transient hydrogen diffusion finite element analysis was developed. To reach the stress–strain heterogeneity, synthetic microstructures were computed under uniaxial loading. The results show that hydrostatic stress gradients is the main cause of the hydrogen redistribution and the strain rate has a crucial effect on the redistribution degree. Statistical analysis of H-segregation reveals clustering of H-enriched zones at the mesoscopic scale. Copyright © 2013, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.

## 1. Introduction

Among the problems related to the hydrogen used as a vector of energy, the particular one is the application of different materials in hydrogen production and storage systems [1].

The effect of hydrogen on material properties has been intensively studied since the 1950s. Hydrogen has a tendency to redistribute easily in the material microstructure during mechanical charging and to segregate at microstructural defects produced by plastic deformations such as dislocations,

micro-cracks, voids and others. This behaviour of hydrogen in a heterogeneous stress–strain field may result in an embrittlement of the material [2–4]. Therefore, hydrogen interaction with microstructure has to be studied properly, and theoretical basis for quantitative analysis of hydrogen evolution at the micro- and mesoscale is needed.

The numerical analyses in which stresses and trapping have been taken into account simultaneously were presented in [5,6]. The hydrogen transport problem was studied in conjunction with large elasto-plastic deformations in the vicinity of a blunting crack tip in bcc material (impure iron).

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Assuming that the strain field around H atoms in bcc metals has cubic symmetry [7], the effect of hydrostatic stress [5] and strain rate [6] on the H-diffusion were estimated. It was found that the total hydrogen concentration and plastic strain decreases with distance from the crack tip whereas the hydrostatic stress rises.

The model used in [5] and [6] is based on the approach proposed in [8] which assumes the local equilibrium of hydrogen in traps and in normal interstitial lattice sites. Another approach in which the kinetics of trapping is described in terms of probabilities to capture and to release a hydrogen atom by trap can be found in [9]. More general formulation derived from Boltzmann-type transport equations, including effects of trapping phenomena, diffusion obstacles, stresses, temperature and non-uniform solubility was presented in [10].

Since the local fracture event for the initiation of brittle fracture in the presence of hydrogen is stress-controlled [11], the stress field plays the crucial role in the hydrogen-assisted cracking. The resolution of an explicit microstructure of the material can precise the hydrostatic stress field and, hence, the hydrogen transport in the specimen during loading.

Due to elastic anisotropy, strong hydrostatic stress gradients at grain scale are expected to be encountered in polycrystalline materials under mechanical loading even without notch or crack. A hydrogen diffusion analysis was recently proposed in [12].

In the present work the influence of stress field on the evolution of hydrogen in the context of microstructural mechanics was investigated by a one-way coupled analysis. A new numerical scheme proposed in [13] for the resolution of hyperbolic and parabolic equations was used. The material microstructure was taken into account without considering specific mechanical or diffusion properties of grain boundaries (GBs). Hydrogen transport by dislocation was not considered [14–16]. The effect of microstructure-induced stress–strain heterogeneity on the hydrogen redistribution in artificial stainless steel 316 L polycrystals was estimated.

## 2. Methods and calculation

Synthetic 2D microstructures containing about 110 grains were obtained following a Voronoi tessellation based procedure described in [17,18]. In the present work we did not take into account specific properties of grain boundaries: GBs are simply geometrical lines separating neighbouring grains. Each aggregate contains about 20,000 linear triangular elements and 40,000 nodes. The structural analysis was performed using the code ZeBuLoN [19]. Random crystal orientation sets were used: distribution of disorientation angle for each aggregate is close to Mackenzie distribution. The kinematics used in the field of crystal plasticity conforms to the classical multiplicative decomposition of the deformation gradient into elastic and plastic parts. Cubic elasticity was considered for modelling the elastic response of the 316 L steel:  $E_{1111} = 206$  GPa,  $E_{1122} = 133$  GPa,  $E_{1212} = 119$  GPa. Plastic deformation is assumed to be solely related to the slip deformation occurring in discrete crystallographic slip systems [20]. The driving force for the plastic slip is based on the Schmid

law and the resolved shear stress,  $\tau^s$ , is computed for each slip system,  $s$ . The crystallographic slip rate,  $\dot{\gamma}^s$ , is expressed as a power law function of the slip system resolved shear stress,  $\tau^s$ , as follows:

$$\dot{\gamma}^s = \text{sign}(\tau^s - x^s) \left\langle \frac{|\tau^s - x^s| - r^s}{k} \right\rangle^n, \quad (1)$$

$$r^s = r_0 + q \sum_{r=1}^N h^{sr} (1 - e^{-br^r}), \quad \nu^r(t) = \int_0^t |\dot{\gamma}^r(u)| du, \quad (2)$$

where  $k$  (50 MPa s<sup>(1/n)</sup>) and  $n$  (25) are viscosity parameters,  $r_0$  (75 MPa) is the critical resolved shear stress,  $q$  (125 MPa) and  $b$  (2). These parameters were identified from the macroscopic uniaxial stress–strain curve.  $h^{sr}$  is a hardening matrix ( $h^{sr} = 1$ , Taylor hypothesis).

Kinematic boundary conditions consist of prescribed displacements on the top and bottom edges of the aggregate, simulating a tensile loading, up to 2.2% total strain. The strain rate effect on the H-diffusion was investigated by considering three strain rates:  $2.2 \times 10^{-5}$  s<sup>-1</sup>,  $2.2 \times 10^{-6}$  s<sup>-1</sup> and  $2.2 \times 10^{-7}$  s<sup>-1</sup>. After completion of the structural analysis, displacements, strains and stresses were transferred step by step to the in-house diffusion code. Hydrogen diffusion in the polycrystalline aggregates was modelled by the equation:

$$\frac{\partial(C_L + C_T)}{\partial t} - D_L \Delta C_L + \nabla \cdot \left( C_L \frac{D_L V_H}{kT} \nabla \sigma_h \right) = 0, \quad (3)$$

where  $C_L(x,y,t)$  is the H-concentration in normal interstitial lattice sites (NILS),  $C_T(x,y,t)$  is the H-concentration in traps,  $D_L$  ( $2.8 \times 10^{-16}$  m<sup>2</sup> s<sup>-1</sup>) is a diffusion coefficient independent of the concentration in this approach,  $\sigma_h(x,y,t)$  denotes the hydrostatic stress and  $V_H$  ( $1.65 \times 10^{-6}$  m<sup>3</sup> mol<sup>-1</sup>) is a partial molar volume of hydrogen,  $k$  ( $8.3144$  J mol<sup>-1</sup> K<sup>-1</sup>) denotes the gas constant and  $T$  (300 K) is the absolute temperature. Assuming that normal and trapped hydrogen populations are in local equilibrium [8] H-concentration in traps can be written as:

$$C_T = \frac{C_L N_T K_T}{C_L K_T + N_L}, \quad (4)$$

where  $N_L$  ( $1.69 \times 10^{29}$  m<sup>-3</sup>) denotes the number of NILS,  $K_T$  (224.146) is equilibrium constant. The parameter  $N_T$  (number of traps) is calculated from the dislocation density data at different amounts of equivalent plastic strains presented in [21]. The system of Equations (3) and (4) is discretized by the residual distribution scheme proposed in [13].

The polycrystalline aggregate is considered to be embedded in a hydrogen chamber [12] (see Fig. 1). It allows to avoid the effect of diffusion boundary conditions in the aggregate by imposing them on the edge of the H-chamber, away from the aggregate edges. The size of the aggregates is 0.1 by 0.1 mm (0.2 by 0.2 mm with H-chamber).

The initial trap density is assumed to be equal to zero. Uniform H-concentration in the chamber and in the aggregate as dictated by Sievert's law at the pressure of 20 MPa and temperature of 300 K was used as initial conditions:  $C_{L0} = 2.313 \times 10^{25}$  atom m<sup>-3</sup>,  $C_{T0} = 0$ . Boundary conditions on the edge of the hydrogen chamber:  $\vec{J} \cdot \vec{n} = 0$ , where  $\vec{J}$  - hydrogen flux and  $\vec{n}$  is the outward unit normal vector.

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