



Identification of the hydrogen diffusion parameters in bearing steel by Evolutionary Algorithm



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ABSTRACT

A novel mathematical method for the identification of hydrogen diffusion parameters in metals has been implemented. This method is based on a clustering-based Evolutionary Algorithm which provides robust and efficient optimization of the diffusion parameters. It is assumed that hydrogen diffusion obeys the McNabb–Foster equations, and by using the Evolutionary Algorithm the 1D time-dependent solution is calibrated to the experimental curve measured by the two cells permeation test. The original McNabb–Foster diffusion model, including reversible and irreversible traps, was simplified to the models with only reversible or irreversible traps and the calibration quality was tested. Due to the random nature of Evolutionary Algorithms, multiple calibration sets were identified, which corresponds to the non-uniqueness of calibration by the McNabb–Foster diffusion model. The definition of the invariant diffusion parameters describing uniquely the material and the test is the main novelty of the proposed study.

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1. Introduction

It is well known that hydrogen has a detrimental effect on steels and other metals. Even small amounts of hydrogen dissolved in metal can significantly change the material response in a plastic regime by reducing ductility [1]. The damaging effect of hydrogen on metals is typically associated with the loss of toughness – the phenomenon termed as “hydrogen embrittlement”.

Hydrogen atoms, being extremely small, can easily penetrate into the metal crystal, decreasing the surface energy [2] and degrading the metal's resistance to crack initiation and propagation. Other theories state that the embrittlement occurs due to the accumulation of gaseous hydrogen in micro-voids which raise the internal pressure in the material [3], or due to the formation of a brittle hydride phase [4]. Some experimental and theoretical works showed that hydrogen, by changing the dislocations mobility, can increase the yield strength [5] and hardness [6]. On the contrary, other studies claim that hydrogen causes softening and enhances localized plasticity (see e.g. Ref. [7]). Recently, based on molecular dynamics simulations, the detrimental role of hydrogen was explained in terms of the ductile-to-brittle transition caused by the

suppression of dislocation emission at the crack tip due to the aggregation of hydrogen [8].

Hydrogen has a detrimental effect on bearing steels, and the typical damage associated with hydrogen in rolling contact fatigue is the so-called “brittle flaking”, which is frequently accompanied by white etching areas [10]. A subsurface crack surrounded by a white etching area is shown in Fig. 1. The detrimental role of hydrogen has become evident from observations of flaking damage in bearing components where the measured amount of hydrogen was high [11], and from observation of the same type of failure in test rig specimens, which were pre-charged by hydrogen [12]. The tension–compression and fatigue properties of bearing steel were investigated in Ref. [13], demonstrating that the reduction of fatigue strength was in direct correlation with the diffusible hydrogen content.

To be able to predict the degradation of mechanical properties due to a growing amount of hydrogen, the process of its transport into the bearing components should be theoretically studied [14]. Hydrogen transport in metals is a complicated process of which the physical interpretation and mathematical description are rather complex. Generally speaking, hydrogen atoms are absorbed in metals in two ways [15]: in lattice interstitial sites and in so-called hydrogen traps, which are typically crystallographic defects like atomistic vacancies, dislocations and grain boundaries.

The mobility of the lattice and of trapped hydrogen is different. The hydrogen transport through the lattice can be considered as the

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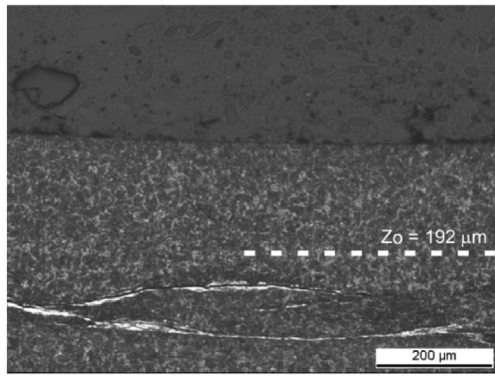


Fig. 1. Microstructure of the inner ring of bearing (cross-section), hydrogen charged, tested for 1.9×10^6 revolutions before failure [9].

mass diffusion process, which is mathematically described by the linear differential equation, obeying the classical Fick's law:

$$\frac{\partial C_L}{\partial t} = D_L \nabla^2 C_L \quad (1)$$

In Eq. (1) C_L is the lattice hydrogen concentration and D_L is the lattice diffusion constant. The trapped hydrogen has very limited mobility compared to the lattice, but exchange between the lattice sites and the traps can occur. If a hydrogen atom can move from the lattice to the trap and back, then the trap is called “reversible”, and if the atom cannot return to the lattice it is called an “irreversible” trap. This exchange can be described mathematically by the set of the so-called McNabb–Foster (MF) equations [16], which in addition to the diffusion process account for the hydrogen exchange between lattice and traps. The mathematical description of the lattice–traps exchange according to the MF equations requires additional material parameters.

The simplistic way to account for the trapping effect is to replace the lattice diffusion constant, D_L , and the lattice hydrogen concentration, C_L , in Eq. (1) by the equivalent diffusion constant, D , and the total (lattice and trapped) hydrogen concentration, C . The common experimental technique for measuring D is the two cells permeation test, which was established in 1962 by Devanathan and Stachurski [17]. This method is based on the electrochemical effect which allows recording of the hydrogen flux through the membrane in terms of electric current. The two cells permeation test has been used in myriads of works for the estimation of diffusion constants in different metals and for study of the temperature, stress [18] and strain [19] effects on the hydrogen transport. This test and thermal desorption spectroscopy (TDS) are the main experimental techniques (see e.g. Ref. [20]) used for study of the hydrogen diffusion and trapping in metals.

However, treating hydrogen transport by the linear model (governed by a single parameter D) can lead to oversimplification, especially when the traps density is high and their effect is not negligible. Typically, it occurs at the crack tip, where local high stresses cause plastic flow, which in turn is a source of new hydrogen traps [21]. The MF equations were used for the analysis of hydrogen diffusion at the crack tip in Refs. [22] and [23]. In the latter work it was theoretically found that the hydrogen distributions evaluated by the MF equations were drastically different from the distributions predicted by simpler formulations. Similar effects can relate to rolling contact fatigue, in which micro-plastic deformation and phase transformation appearing in bearing steels with the growing amount of loading cycles [24] can increase the density of hydrogen traps [25].

The two cells permeation test can be used for the identification of the MF parameters. For this, the diffusion parameters used in the MF equations have to be selected in such way that the experimentally measured and the theoretically predicted curves are as close as possible to each other. An attempt at such calibration was done in 1989 [26] for chromium martensitic stainless steel. In this work, it was done only for one material, so the authors of [26] did not focus on using any efficient calibration algorithm (probably, it was also irrelevant for the low performance computers of those days). The calibration of the diffusion parameters for the MF equations should be done by any optimization method that minimizes the difference between the theoretical and experimental results. In the current work, this is done by a clustering-based Evolutionary Algorithm (EA).

EAs are a family of tools used to solve high-complexity computational problems. They help in optimization, simulation, modelling, design, and prediction purposes in science, medicine and technology. The use of EAs in materials science and engineering has become increasingly popular in the last few years. In materials science and related fields of science and technology, the EAs open up possibilities for materials design, studies of their properties or production at industrial scale [27].

In the current work, the clustering-based EA was applied for bearing steels. However, it can be used for the study of hydrogen permeation in any metal. This study can be useful in such industries as hydrogen energy, storage and transportation or in other industries where hydrogen diffusion and embrittlement play a role.

2. Problem description

As mentioned in the introduction, hydrogen diffusion through an ideal metal lattice obeys Fick's law, which, generally speaking, is not valid in the case of a real metal structure containing crystallographic imperfections. The mathematical model taking into account the effect of these imperfections is given by the MF equations (see Refs. [16,22,26]). This set of equations accounts for the hydrogen exchange between lattice and traps in addition to the diffusion process:

$$\frac{\partial C_L}{\partial t} = D_L \nabla^2 C_L - \sum_{i=1}^n N_i \frac{\partial \theta_i}{\partial t} \quad (2a)$$

$$\frac{\partial \theta_i}{\partial t} = k_i C_L (1 - \theta_i) - p_i \theta_i \quad (2b)$$

The first two terms in Eq. (2a) correspond to the classical Fick's law (see again Eq. (1)), describing the hydrogen diffusion through the metal lattice. And Eq. (2b) describes the hydrogen exchange between lattice and traps of type i ; the number of exchange equations is equal to the number of trap types considered in the model. N_i is the volume density of trap i and θ_i is the fractional occupancy level of these traps. The parameter θ varies from 0 (all traps are empty) to 1 (the traps are full). The parameters k_i and p_i are the trap entry and exit rate constants, respectively. If a trap is irreversible then $p = 0$, meaning that the hydrogen atom, being trapped, cannot return to the lattice.

The permeation test setup is presented in Fig. 2. It consists of the charging and detection cells, divided by a membrane specimen made of the metal whose diffusion properties are being tested (see Fig. 2b). One side of the membrane acts as cathode and the other as anode. Hydrogen atoms are generated at the cathode side by reducing protons from an aqueous solution in the charging cell. Most of the hydrogen produced in this way combines to form hydrogen gas (H_2) bubbling away from the electrode, but a small

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