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St. Petersburg Polytechnical University Journal: Physics and Mathematics 1 (2015) 305–314

www.elsevier.com/locate/spjpm

The description of deformation and destruction of materials containing hydrogen by means of rheological model

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Available online 7 December 2015

Abstract

The two-continuum rheological model taking account of a change in the hydrogen-binding energy has been proposed in this paper. As in the case of conventional approach our model makes it possible to describe the hydrogen transfer and its accumulation in the metals and to explain changes in the mechanical properties of metals that are caused by that accumulation. The proposed rheological model describes the hydrogen transition from a mobile state to the bound one, depending on the stress–strain state. Concurrent with this achievement our model describes the changes in the material matrix taking place as a result of the hydrogen addition to the matrix atoms. These processes lead to weakening and destruction of the material.

Keywords: Rheological model; Hydrogen embrittlement; Hydrogen concentration; Two-continuum model; Deformation; Destruction.

1. Introduction

Taking into account the effect of hydrogen on the mechanical properties of materials is an extremely crucial problem for science and modern practice. The interaction between hydrogen and solid materials is a good mechanical example of the effect of a small parameter. For instance, aluminum alloys with mean hydrogen mass concentrations of 0.4–0.8 ppm (part per million) display hydrogen-induced embrittlement.

Hydrogen embrittlement is the reason for numerous catastrophes, so its mechanisms are thoroughly studied [1–6].

It is impossible to design modern constructions without precise calculations carried out in advance. Since hydrogen strongly affects material strength, there are many studies concentrated on simulating this effect. Several basic approaches have been developed taking into account the effect of hydrogen on dislocation emergence and movement, and on crack formation. Approaches taking into account internal hydrogen pressure in metals and physical approaches have also appeared.

The emergence and movement of dislocations and their effect on localized plasticity (Hydrogen-Enhanced Localized Plasticity (HELP)) near crack tips leads to

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http://dx.doi.org/10.1016/j.spjpm.2015.12.002

(Peer review under responsibility of St. Petersburg Polytechnic University).

local plasticity occurring in the materials due to very high dislocation concentrations. The HELP mechanism was first described in Ref. [7]. Later, based on the physical considerations of the interaction potentials between hydrogen and dislocations, Refs. [8–10] formulated the constitutive equations modeling the local changes in material properties at the mouth of a microcrack.

At the same time, the calculations carried out in Ref. [8] indicate that substantial changes in the mechanical properties of a material occur for local hydrogen concentrations of about 9000 ppm, which is a very high value for most metals.

The constitutive equations assume an implicit power-law dependence on local hydrogen concentration that cannot be measured directly, i.e. the parameters of the equations (including the exponent) can be assessed only indirectly. Due to this circumstance, these parameters for specific materials cannot be found experimentally, which may result in significant errors in strength calculations.

To verify the model in Ref. [11], we calculated local plasticity for a crack with a spherical tip. We were able to demonstrate that even model local hydrogen concentrations are only 100 higher than the mean baseline data. Considering these means are commonly values of about 1 ppm, local concentrations do not exceed 100 ppm. Therefore, the test calculation does not confirm that local hydrogen accumulation in metals under external mechanical loads is possible for concentrations up to about 9000 ppm (i.e. steels).

Using modified Fick's law for the HELP model is another source for its possible errors [12]. This law explicitly includes the temperature dependence of the stress pattern coefficients but does not include the exponential dependence of the diffusion coefficient on temperature, which means there is no balance in taking into account the thermal velocities of hydrogen particles and the main matrix of a material. In other words, the effect of the temperature on the matrix is taken into account while its effect on hydrogen particles is not.

There are quite a number of uncertainties described by the authors of the model; in particular, there is a non-linear dependence of the inner potential on the stress intensity and on hydrogen concentration. Since this model implies dealing with large local concentrations many times higher than those observed in practice, all non-linearities must play a major role.

There is also the decohesion model (Hydrogen-Enhanced Decohesion (HEDE)) [13] that is similar to HELP. Their difference is that the HEDE model takes into account the decrease in the formation energy of free fracture surfaces that occurs with an increase in local hydrogen concentration.

Ref. [14] notes that the HELP model requires huge computational resources to solve any applied problem, so the only solution is using a continuum model of dislocation evolution. However, this substitute often proves inadequate, which is why the authors recommend using the submicrocrack growth criterion, by which they basically reduce all problems with hydrogen to modeling crack formation and decreasing crack resistance.

The evolution of hydrogen-induced cracks is modeled in Ref. [15]. Initially, it is assumed that the crack has already generated along a pipe's wall, while hydrogen is transformed into a molecular gaseous state and creates excessive pressure contributing to crack growth. The chemical potential gradient depending on stresses is considered to be the main cause of hydrogen diffusion. Additionally, a decrease in crack resistance due to parameter changes of the fracture criterion is taken into account when establishing the conditions for crack growth. Consequently, it is possible to calculate only the crack growth rate that is compared with the experimental results [16].

We should point out that there is no connection between the model and the real physical mechanism of hydrogen effect. Ref. [17] discusses two- and three-dimensional settings of the hydrogen-induced crack growth problem. Significant differences have been found in the values of maximum decohesion stress and threshold stress intensity used for describing metal properties when approximating the same experimental results. As it turns out, these must be set differently. For greater certainty, Ref. [18] recommends selecting these parameters based on only the 3D model.

Ref. [19] presents a theoretical calculation of the changes in the shear modulus and the crystalline lattice parameters of a platinum-zirconium alloy. This calculation was done using wave pseudopotential. The ratio where for each hydrogen atoms there are 3 or 4 matrix atoms (4000 ppm) was used as the calculation basis, which is absolutely improbable for ordinary construction materials. At these hydrogen concentrations hydrides form even in zirconium alloys, i.e., from a mechanical standpoint, the metal turns into a composite.

Ref. [20] takes into account the variation in the stress tensor due to internal pressure that hydrogen creates by penetrating the metal matrix. Tensile tests in samples were simulated by the finite element method (FEM), with the results compared to the experimental data [21]. In contrast with the previous studies, only the effect of hydrogen on the spherical part of the stress tensor was examined. With this approach, the effect of hydrogen is detected only for concentrations above 17 ppm, which, for steels, is a high value (according to the