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# Theoretical Model for the Hydrogen-Material Interaction as a Basis for Prediction of the Material Mechanical Properties

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*A two-continuum model of the hydrogen-solid body interaction is suggested. This model describes the relaxation of the stresses and degradation of the material properties under the mechanical loading in hydrogen-contained environment. The application of this model provides one with the instrument for prediction of the time resource and the mechanical properties of the aggregates of machines and mechanisms. The effect of the hydrogen-material interaction in the gas pipeline modeling is demonstrated.*

## Introduction

The hydrogen is contained in any metal. The hydrogen concentration is very low (about 1 atom of hydrogen in 100 000 atoms of the metal matrix), nevertheless its influence on the mechanical properties of the metals is of the crucial importance. As a rule, the hydrogen is accumulated in the metals during their exploitation. The main source for the hydrogen appearance in metals is water however the hydrogen diffusion for the gas and other hydrogen-containing substances is feasible.

In the metals, the hydrogen is contained in the traps with various bounding energies. It has been established, cf. [1], that thermo-mechanical loading results in the hydrogen redistribution over the traps. Diffuse hydrogen accumulates mostly in the aluminum alloys while strongly bounded hydrogen accumulates mostly in the titanium alloys.

A number of papers were concerned with the influence of hydrogen on the mechanical properties of metals, see e.g. [2]. Nearly all papers use phenomenological models and the redistribution of hydrogen over the traps is not described. The degradation of mechanical properties is carried out by means of empirical dependences

The two-continuum model of solid [3] allows one to describe the influence of small concentration of hydrogen on the mechanical properties of materials in terms of changing the bonding energy of the second continuum, the latter being responsible for the hydrogen concentration. The results obtained with the help of simple models should be generalized in order to make the account of small hydrogen concentration on the mechanical properties of materials available for the engineering practice.

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## Method of analysis

### A two continuum model

Basic principles of the above mentioned hypothesis can be illustrated on example of analysis of the one-dimensional chain consisting of identical particles which are the point mass $m_0$ (the atom mass in the crystal lattice of a material). They are connected to each other by the identical nonlinear springs of the length $a$, cf. Figure 1.

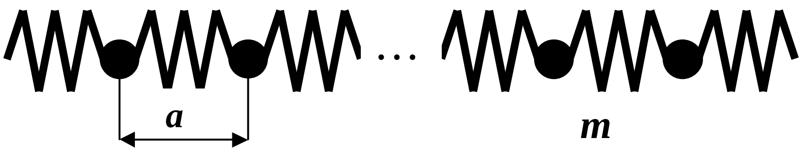


**Figure 1**: The schematics of the material model

The basic equation of the motion in the long-wave approximation is given by, cf. [2]

$$m_0 \ddot{u} = -a[f(a(1+u'))]' \qquad (1)$$

where a dot denotes the time derivative. As for small deformations $e = \partial u / \partial x$ we arrive at the following equation

$$\ddot{u} - J_0^2 u'' = 0, \qquad J_0 = a\sqrt{c/m} \qquad (2)$$

since $f[a(1+e)] \approx -Cae = -Ca\partial u / \partial x$.

The weakening of the internuclear bonds caused by “landing” of the hydrogen particles (or other mobile internal elements of structure) can produce the chain formations of new internuclear bonds, see Figure 2, as the consecutive connections of elastic bonds of the basic lattice and the introduced elastic bonds of new elements (e.g. hydrogen particles). Obviously, such chain is possible under the assumption that the mass of particles of a mobile structure is small, i.e. $m_0 >> m_H$ .

Equivalent rigidity of the new bond can be obtained from the equation

$$\frac{N_\Sigma}{C_\Xi} = \frac{N_0}{C_0} + \frac{N_H^+}{C_H} \qquad N_\Sigma = N_0 + N_H^+ \qquad (3)$$

The constitutive equation for this medium is as follows

$$s^{(1)} = E_\Xi e, \qquad E_\Xi = \frac{E_0 E_H}{n_0 E_H + n^+ E_0}, \qquad n_0 = \frac{N_0}{N_\Sigma}, \qquad n^+ = \frac{N_H^+}{N_\Sigma}, \qquad n_0 + n^+ = 1. \qquad (4)$$

Here $N_\Sigma$ denotes the total number of the particles in the elementary volume, is the number of the particles connected by the weaken bonds, $N_H^+$ is the number of hydrogen particles attached to the lattice with the bonds of rigidity $C_H$. Finally, $n_0$, $n^+$ are the concentrations of the corresponding particles.

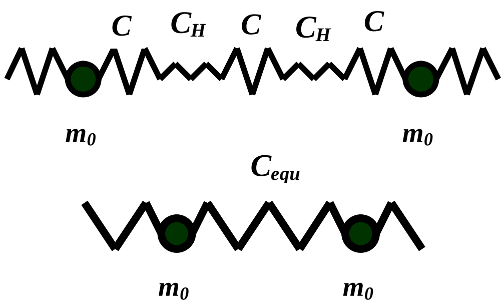


**Figure 2**: The model of the material with hydrogen particles

For small deformations the nonlinear force $f$ in Eq. (1) can be introduced as

$$f = -C_\Xi a e = -E_\Xi e \tag{5}$$

The equivalent modulus of the lattice $E_\Xi$, see Eq. (4), can be decreased essentially, since $E_H << E_0$ ($c_H << c_0$), and has a strong dependence on the concentration of the attached particles $n^+$.

The number of the lattice settled by the hydrogen particles depends on the stress state of the lattice at every point and, in general, on time. The unknown functional dependence of $E_\Xi$ on $n^+(e,x,t)$ should be determined with the help of the model of two-component continuum.

The details of the theory of two-component continuum can be found in [3]; therefore we are presenting here only the final results with some necessary explanation of the processes.

From the state equation we have $s = s(e, n^+(e,x,t))$, thus,

$$s = E_0 e \left[ 1 - \frac{n^+}{n^+ + n^{(0)} E_H / E_0} \right], \tag{6}$$

and the essential dependence of the stress state on concentration of the bonded hydrogen becomes evident.

The hydrogen concentration is described by the equation for $n^+$

$$\frac{\partial^2 n_H^+}{\partial t^2} + (a+b)\frac{\partial n_H^+}{\partial t} - A\cdot D(e_{st})\left[ b\,\frac{\partial^2 n_H^+}{\partial x^2} + \frac{\partial^3 n_H^+}{\partial t \partial^2 x}\right] = 0 \qquad (7)$$

Here $A = c_H^2 kj$, $a$ and $b$ are some constants, and $D(e_{st})$ denotes the hydrogen diffusion constant.

The equations (6) and (7) form a system for modeling the hydrogen influence on the dependence $s(e)$ for the material.

The stress-strain curve for steel is changing due to the hydrogen saturation which is displayed in Figure 3. Figure 4 demonstrates the relaxation of the yield stress in steel with time in the presence of hydrogen. It is easy to see that the yield stress decreases which leads to the exponential weakening of the material strength as time progresses, [3].

Hydrogen saturation time depends strongly on the temperature and varies in the range of tens minutes at the temperatures about 900°C up to several months at the temperature near 20°C.

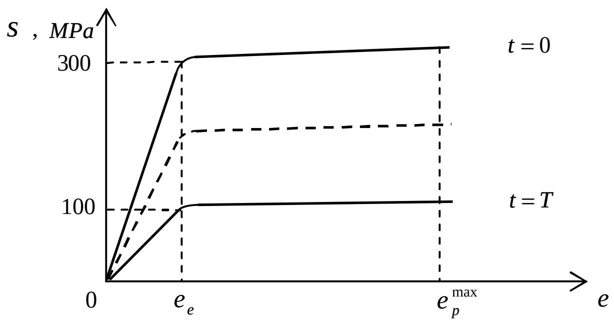


**Figure 3**: The stress-strain curve for steel

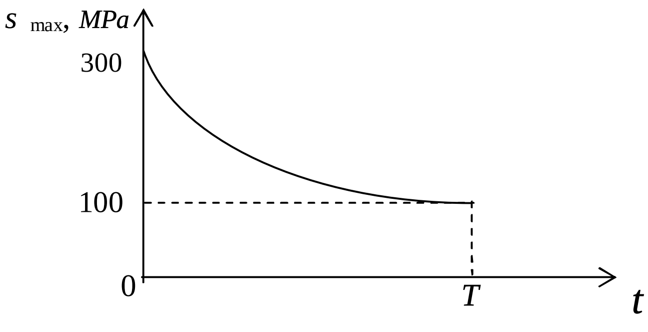


**Figure 4**: The relaxation of the yield stress in steel with time in the presence of hydrogen

## Results and Discussion

Mechanism of the gradual hydrogen embrittlement is demonstrated on the example of the flange connection of the pipeline part under high gas with hydrogen pressure. The analysis of pipeline hydrogen saturation is made by means of the three dimensional finite element code.

The flanges on the high diameter pipe (up to 2 meter) are very often supported with the stiffening ribs. The von Mises stress distribution in the fragment of the flange connection with the stiffening ribs after is shown on Figure 5.

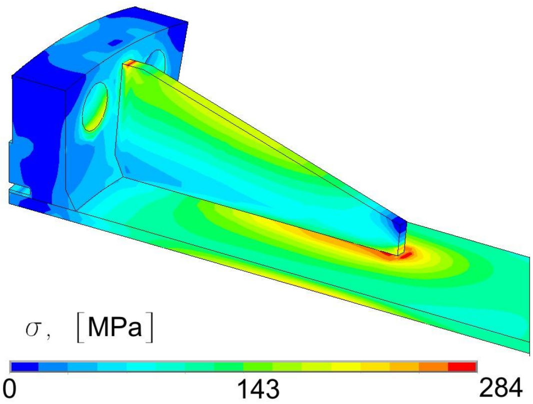


**Figure 5**: The distribution of the von Mises stress in the flange connection of the steel pipe line

The stress concentration is easily seen however the maximum stress 284 MPa is under the yield stress 300 MPa. The stress field is redistributed after the relaxation time ***T***. The hydrogen is accumulated in the zones of the tensile stress. After several successive calculations of the stress and hydrogen's accumulation we can calculate the final picture of the stress and the strain. The strain field is shown in the Figure 6. A very high strain level $\varepsilon$ = 33% is observed at the place of welding of the support to the pipe. This means that the welding will be totally destructed. So the hydrogen redistribution inside the steel leads to destruction of the flange connection.

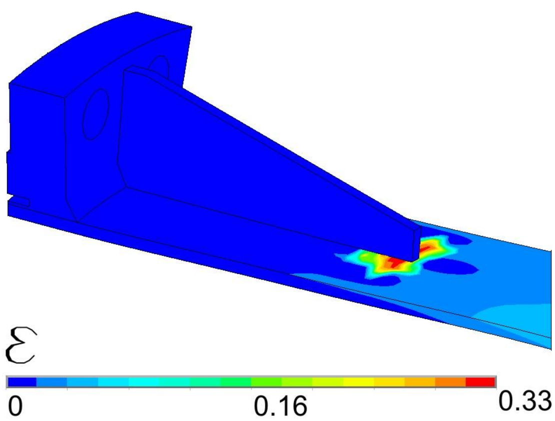


**Figure 6**: The strain distribution in the flange connection after the hydrogen saturation

The relaxation time constant T can be rather high, that is the saturation process is rather slow. The hydrogen saturation depends on the initial concentration of the hydrogen, diffusion constants temperatures, environment hydrogen concentration etc. In the present paper we made only a first calculation of the effects of hydrogen influence. Such calculation can be carried out by means of the empirical models of the material properties [2]. The present approach provides us with the possibility of developing an adequate multiple-factor model.

## Conclusions

A model is suggested which allows one to describe the kinetics of hydrogen in metals. The model is also appropriate for estimating the hydrogen transition from the mobile state to the bonded state depending upon the stresses and describing the localization of the bounded hydrogen. The result is destruction of the material at the localization places.

The constructed models enables describing very different effects of the hydrogen embrittlement such as the hydrogen concentration, diffusion rate, material temperature and the stress character in the framework of the same approach. This result allows one to predict the lifetime of the material in the hydrogen-containing environment.

The calculation of the stress field of the pipeline flange has clearly demonstrated that the two-component model can be successfully applied for engineering estimations of metal structures.

## Acknowledgements

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