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

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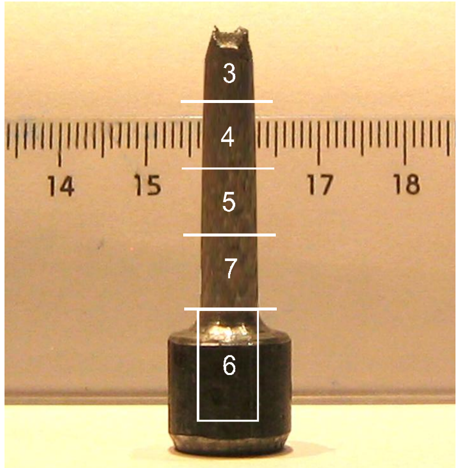
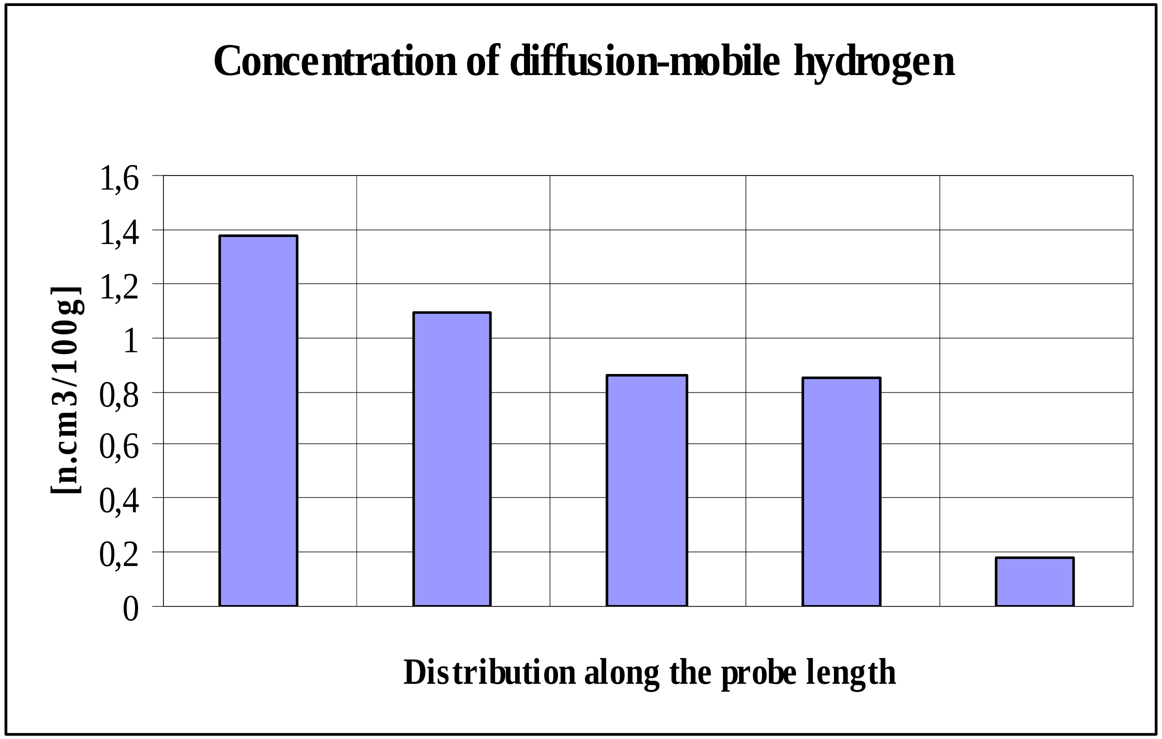
Content

Introduction

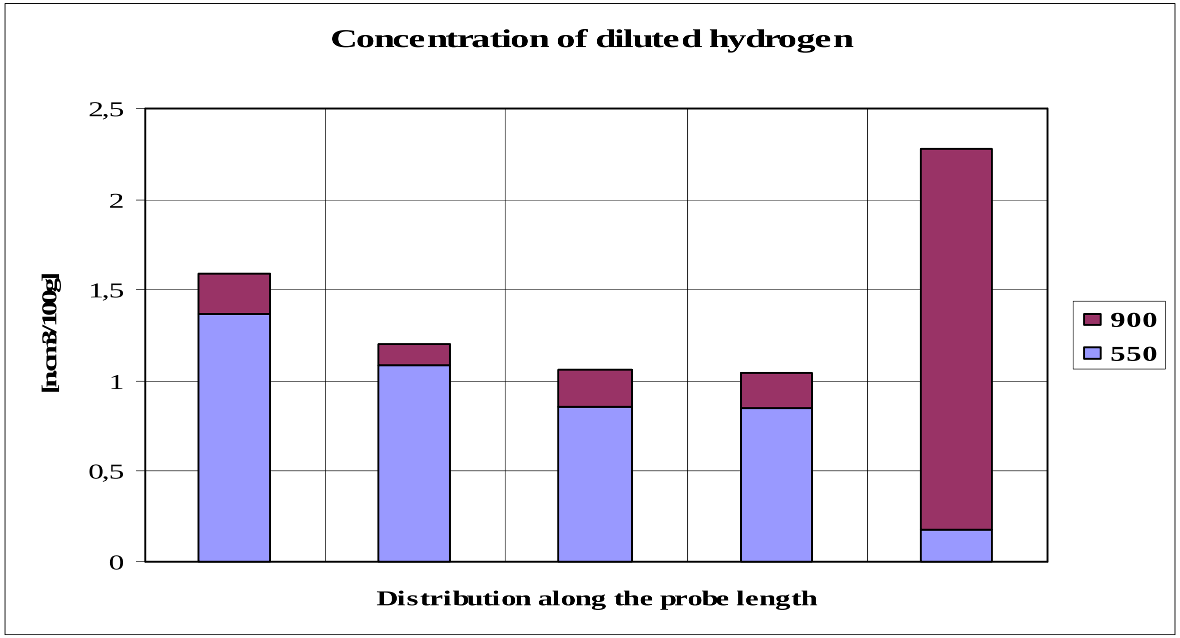
The experimental foundations of the theoretical models



Uniaxial tensions of the steels



The probe of St3 broken under longitudinal stretch and the scheme of cutting of the probes for testing. The upper part is the destruction zone, and the lover part is the zone of fixation of the probe in the breaking machine.



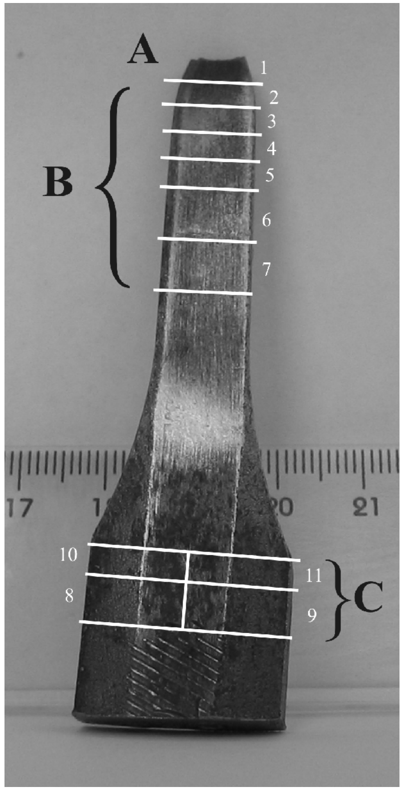
Distribution of concentration of diffusion-mobile (550) and tightly bound (900) hydrogen along the probe length. The upper level of columns shows the total concentration f hydrogen in the probe. Left, the breaking point; right, the part turned from not deformed probe.

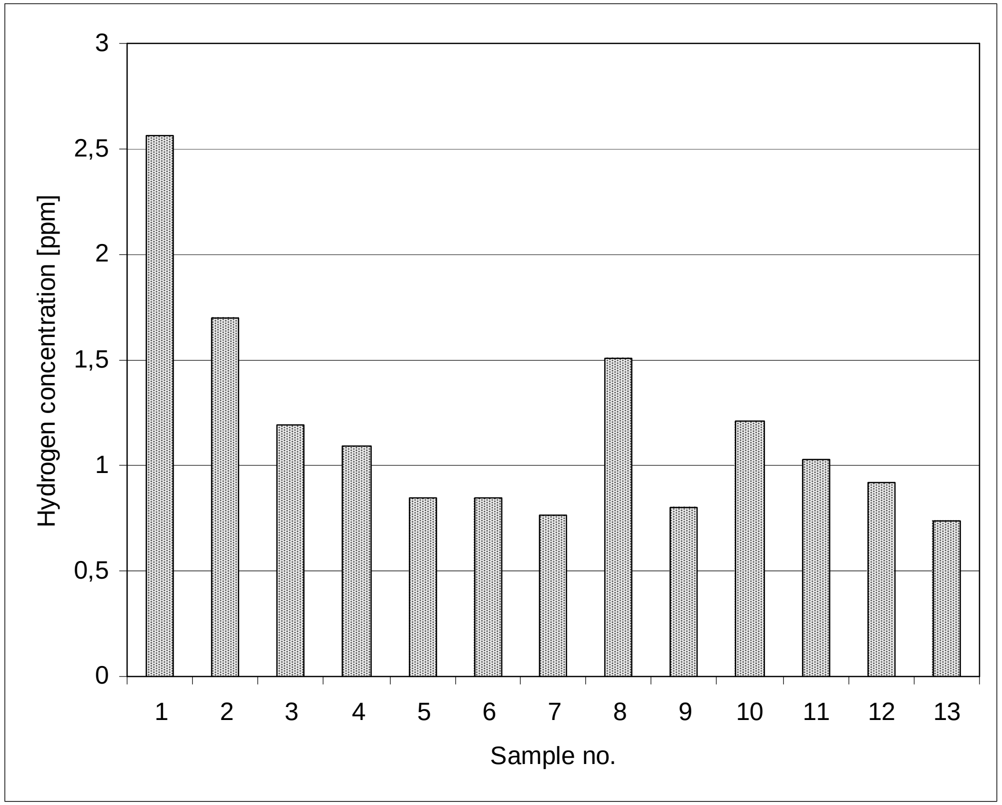
Relative values of maximum stretching tensions and concentrations of diffusion mobile hydrogen

Probe number	Ratio of maximum mechanical tensions to those in probe #6	Ratio of concentrations of diffusion-mobile hydrogen to those in probe #6	Relative spread of relative values for single probe (%)
3	8,6	7,8	10,0
4	5,6	6,2	10,0
5	4,9	4,9	0,0
7	4,7	4,8	1,7
6	1,0	1,0	0,0

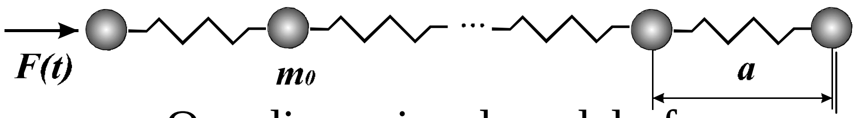
The sample of 35G2 steel fractured under axial tension showing the schematic of test sample cutting.

Upper part (zone A) - zone of fracture, lower part (zone C) - sample grip zone in the test bed

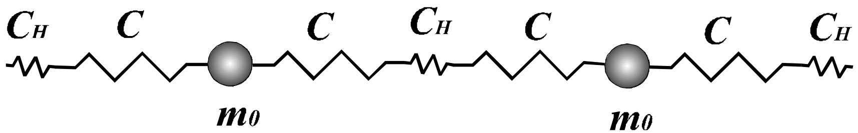




Model of the two component's continuum



One dimensional model of
homogeneous continuum



One dimensional model of the two
component's continuum with hydrogen

$$E_{\Xi} = \frac{E_o E_H}{n_0 E_H + n^+ E_0}$$

$$n_0 = \frac{N_0}{N_{\Xi}} \qquad n^+ = \frac{N_H^+}{N_{\Xi}} \qquad n_0 + n^+ = 1$$

N_{Ξ} -Total atoms number

N_0 -The number of atoms with non hydrogen links

N_H^+ - The number of bind hydrogen atoms

One-dimensional dynamic equation

$$\frac{\partial s^{(1)}}{\partial x} = r^{(1)} \frac{\partial v^{(1)}}{\partial t} + J_{12} v^{(1)} + R_{12}$$

$$r^{(1)} = r^{(0)} + r_H^{(+)}$$

$$r^{(0)} >> r_H^{(+)}$$

$J_{12} v^{(1)}$ - jet force

R_{12} - internal force determines reaction of interaction between the first and second components of the considered continuum

The equation determining dynamics of the mobile hydrogen particles

$$-\frac{\partial p}{\partial x} = r^{(2)} \frac{\partial v^{(2)}}{\partial t} + J_{12} v^{(2)} + R_{21}$$

$$r^{(2)} = r_H^{(-)} = m_H \cdot N^-$$

N^- -The number of the mobile hydrogen particles

The state equation determining the dependence between pressure and density

$$p - p_0 \cong r_H^{(-)} \cdot C_H^2 = m_H N^- \cdot C_H^2$$

The mass-balance equations

The mass-balance equations for bound hydrogen

$$\frac{\partial N_H^+}{\partial t} + \frac{\partial (N_H^+ v^{(1)})}{\partial x} = \frac{J_{12}}{m_H}$$

The mass-balance equations for diffusely hydrogen

$$\frac{\partial N^-}{\partial t} + \frac{\partial (N^- v^{(1)})}{\partial x} = \frac{J_{21}}{m_H}$$

The liner model of diffusely hydrogen flow

$$R_{12} = -R_{21} = k \frac{N^- m_H}{D(e)} \left(v^{(2)} - v^{(1)} \right)$$

$D(e)$ -diameter of the diffusion channel

k - linear coefficient

Let the source linear depend on concentration

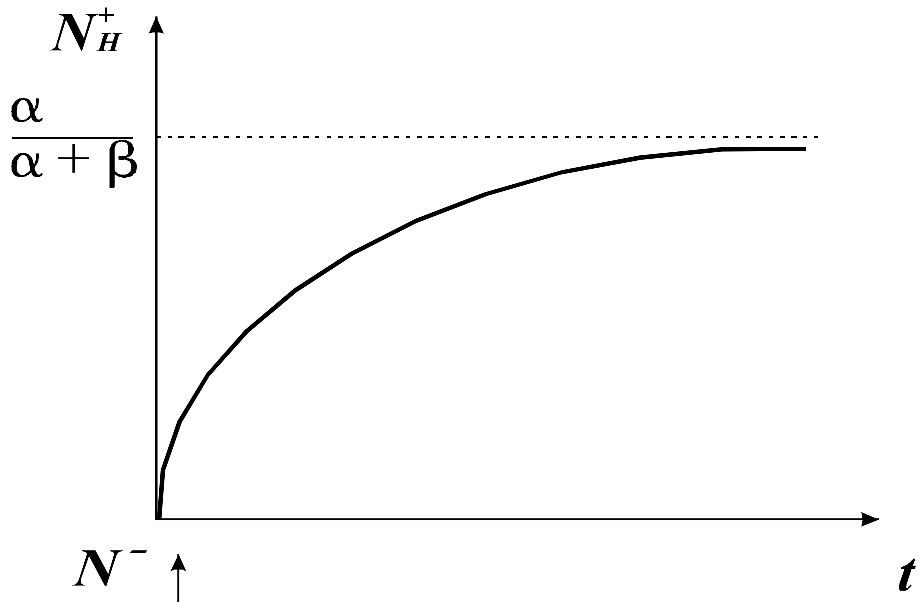
$$J_{12} = -J_{21} = aN^- - bN_H^+$$

The equation of the hydrogen concentration relaxation

$$\frac{dN_H^+}{dt} = a\,N^- - b\,N_H^+$$

$$\frac{dN^-}{dt} = -a\,N^- + b\,N_H^+$$

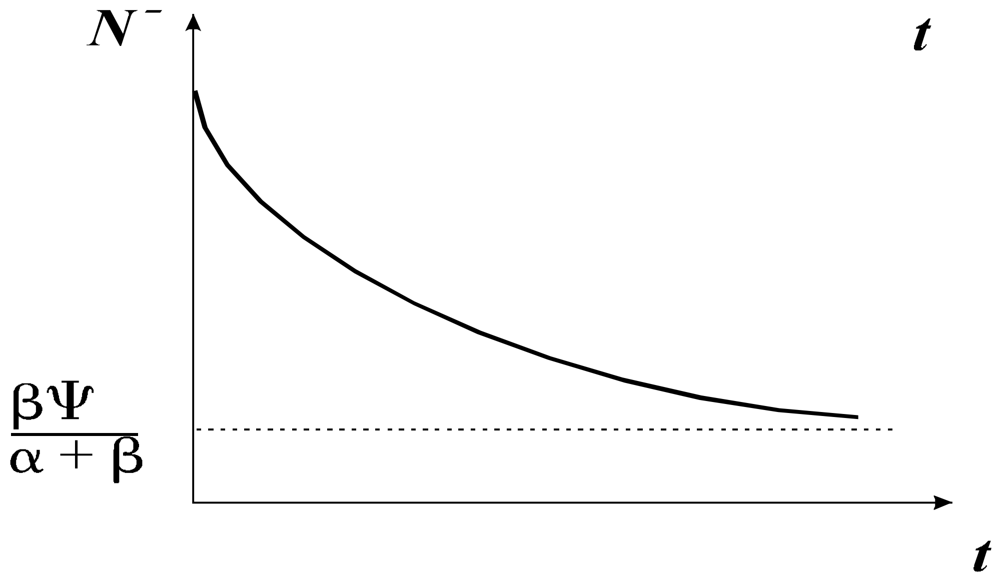
$$N^-(0) = \Psi\,; \qquad N_H^+(0) = 0$$



Solutions

$$N^- = \frac{1}{a+b}a\Psi(1-e^{-(a+b)t})$$

$$N_H^+ = \Psi\left[1-\frac{1}{a+b}a\,(1-e^{-(a+b)t})\right]$$



The total equation system for model of the two component's continuum

$$\frac{\partial s^{(1)}}{\partial x} = \rho^{(1)} \frac{\partial v^{(1)}}{\partial t} + J_{12} v^{(1)} + R_{12},$$

$$\rho^{(1)} = \rho^{(0)} + \rho_H^{(+)}, \qquad \rho_H^{(+)} = m_H N_H^{+}, \quad s^{(1)} = \frac{E_o E_H}{n_0 E_H + n^{+} E_0} e, \quad n_0 = \frac{N_0}{N_0 + N_H^{+}}, \quad n_0 = \frac{N_H^{+}}{N_0 + N_H^{+}},$$

$$-\frac{\partial p}{\partial x} = \rho^{(2)} \frac{\partial v^{(2)}}{\partial t} + J_{12} v^{(2)} + R_{21},$$

$$\rho^{(2)} = \rho_H^{(-)} = m_H \cdot N^{-}, \qquad p - p_0 \cong \rho_H^{(-)} \cdot C_H^2 = m_H N^{-} \cdot C_H^2,$$

$$\frac{\partial \rho^{(0)}}{\partial t} + \frac{\partial(\rho^{(0)} v^{(1)})}{\partial x} = 0,$$

$$\frac{\partial N_H^{+}}{\partial t} + \frac{\partial(N_H^{+} v^{(1)})}{\partial x} = \frac{J_{12}}{m_H},$$

$$\frac{\partial N^{-}}{\partial t} + \frac{\partial(N^{-} v^{(1)})}{\partial x} = \frac{J_{21}}{m_H},$$

$$R_{12} = -R_{21} = k \frac{N^{-} m_H}{D(e)} \left(v^{(2)} - v^{(1)}\right), \qquad J_{12} = -J_{21} = a N^{-} - b N_H^{+}.$$

Strain-stress equation $$s^{(1)} = E_0 \left[1 - \frac{n^{+}}{n_0 E_H / E_0 + n^{+}} \right] e$$

The dynamics of the diffusely mobile component

$$e = e_{st} + \tilde{e}(x,t), \quad v^{(1)} = 0 + \tilde{v}^{(1)}, \quad v^{(2)} = 0 + \tilde{v}^{(2)}$$

$$N_H^+(x, e_{st} + \tilde{e}, t) = N_H^+(x, e_{st}, t) + \left.\frac{\partial N_H^+}{\partial e}\right|_{e=e_{st}} \tilde{e}(x,t)$$

$$s = s_{st} + \tilde{s} = \left[1 - \frac{n^+}{n_0 E_H / E_0 + n^+}\right] e_{st} + E_0 \left[1 - \frac{n^+}{n_0 E_H / E_0 + n^+}\right] \tilde{e}$$

The equation of the stress dependence

$$\frac{\partial s^{(1)}}{\partial e}\frac{\partial e}{\partial x} + \frac{\partial s^{(1)}}{\partial n_H^+}\left[\frac{\partial n_H^+}{\partial e}\frac{\partial e}{\partial x} + \frac{\partial n_H^+}{\partial x}\right] = r^{(1)}\frac{\partial v^{(1)}}{\partial t} + J_{12} v^{(1)} + R_{12},$$

In the first approximation:

$$\frac{\partial s_0}{\partial e}\frac{\partial e_{st}}{\partial x} = 0 \qquad \frac{\partial \tilde{s}^{(1)}}{\partial x} = r^{(1)}\frac{\partial \tilde{v}^{(1)}}{\partial t} + J_{12}\Big|_{e=e_{st}} \tilde{v}^{(1)} + R_{12}\Big|_{e=e_{st}} - \left.\frac{\partial s^{(1)}}{\partial n_H^+}\right|_{e=e_{st}} \left.\frac{\partial n_H^+}{\partial x}\right|_{e=e_{st}}$$

$$R_{12}\Big|_{e=e_{st}} = k\frac{N^- m_H}{D(e)} v^{(2)}$$

The equation for the second component

$$-\frac{\partial p}{\partial x}=k\frac{N^{-}m_{H}}{D(e)}v^{(2)},\quad p-p_{0}=p=m_{H}N^{-}\cdot C_{H}^{2}$$

After changing of variables

$$n_{H}^{-}=\frac{N^{-}}{N^{-}+N_{H}^{+}},\; n_{H}^{+}=\frac{N_{H}^{+}}{N^{-}+N_{H}^{+}}$$

New form of the equation for the second component

$$v^{(2)}=\frac{\cdot C_{H}^{2}}{kn_{H}^{-}}D(e_{st})\frac{\partial n_{H}^{-}}{\partial x}$$

The particles balance equation

$$\frac{\partial^2 n_H^+}{\partial t^2} + (a + b)\frac{\partial n_H^+}{\partial t} - \frac{C_H^2}{k} D(e_{st})\left[b\frac{\partial^2 n_H^+}{\partial x^2} + \frac{\partial^3 n_H^+}{\partial t \partial x^2} \right] = 0$$

Initial conditions

$$n_H^+(0,x) = 0, \quad n_H^-(0,x) = \frac{\Psi^-}{2}\left(1 + \cos\frac{2px}{l}\right), \quad \dot{n}_H^+(0,x) = a\frac{\Psi^-}{2}\left(1 + \cos\frac{2px}{l}\right)$$

λ – parameter of the inside structure

Take the solution in the form

$$n_H^+(t,x) = q(t)\frac{\Psi^-}{2}\left(1 + \cos\frac{2px}{l}\right)$$

.

The equation for *q(t)*

$$\ddot{q} + \dot{q}(a + b + G(e_{st})) + qbG(e_{st}) = 0$$

The solution of the particles balance equation and the strain-concentration equation

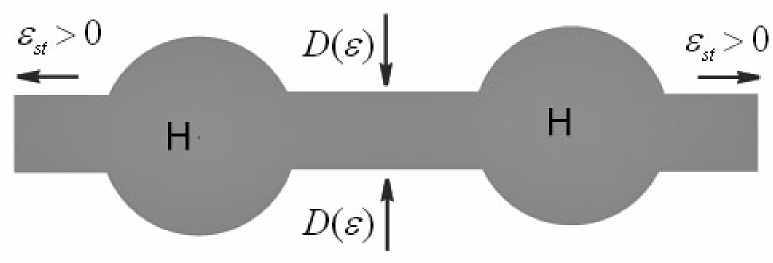
$$q(t) = \frac{a}{a + G(e_{st})} \Psi^{(-)} \left(e^{-\frac{fG(h_{st})}{a+G(e_{st})}t} - e^{-\frac{aG(h_{st})}{a+G(e_{st})}t}\right),$$

$$G(e_{st}) = \frac{C_H^2}{3k} D(e_{st}) \left(\frac{2p}{l}\right)^2$$

The strain-concentration equation

$$\frac{\partial n_H^+}{\partial e} = -\frac{C_H^2}{3k} \frac{\partial D(e_{st})}{\partial e_{st}} \left(\frac{2p}{l}\right)^2 \frac{a}{a + G(e_{st})} \Psi^{(-)}$$

The mechanical model of the hydrogen diffusion channel



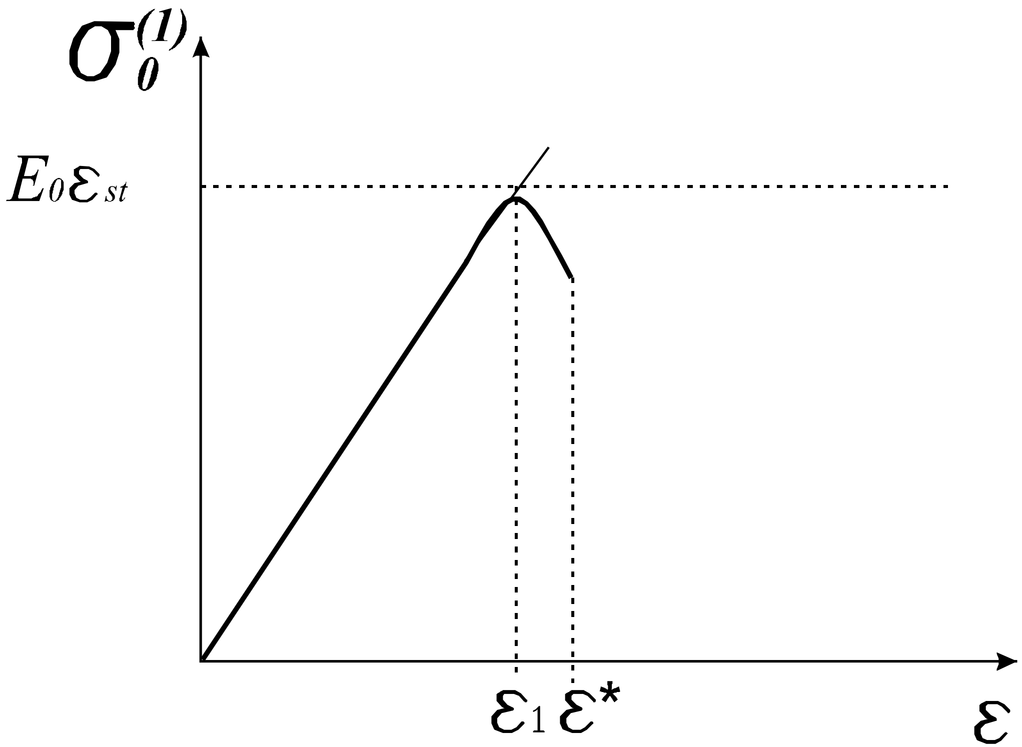
Model of the hydrogen embrittlement

$$s_0^{(1)} = E_0 e_{st} \cdot \frac{k}{\dfrac{a}{a + D(e_{st})}\Psi^{(-)} + k}$$

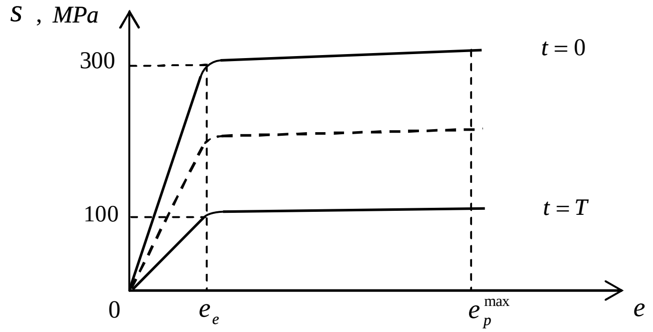
For steels

$$\left.\frac{\partial s_0^{(1)}}{\partial e}\right|_{e=e_1} = 0 \Rightarrow e_1 = e^* \left(1 - \sqrt{a\frac{\Psi^{(-)}}{k}\frac{kl^2}{c_h^2}D_0 l^2}\right)$$

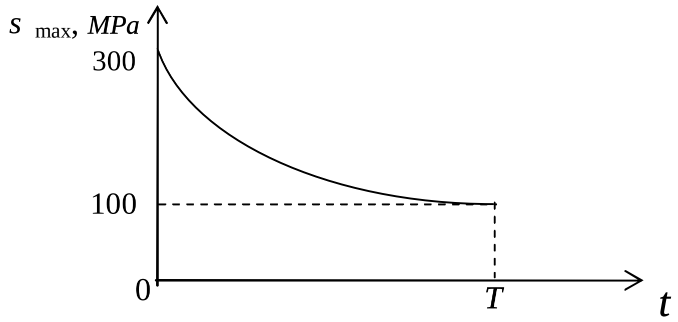
$$\Psi^{(-)} = 10^{-6}, \quad k = 10^{-7} \div 10^{-8}$$



Model of the stress-strain relaxation in finite elements calculations

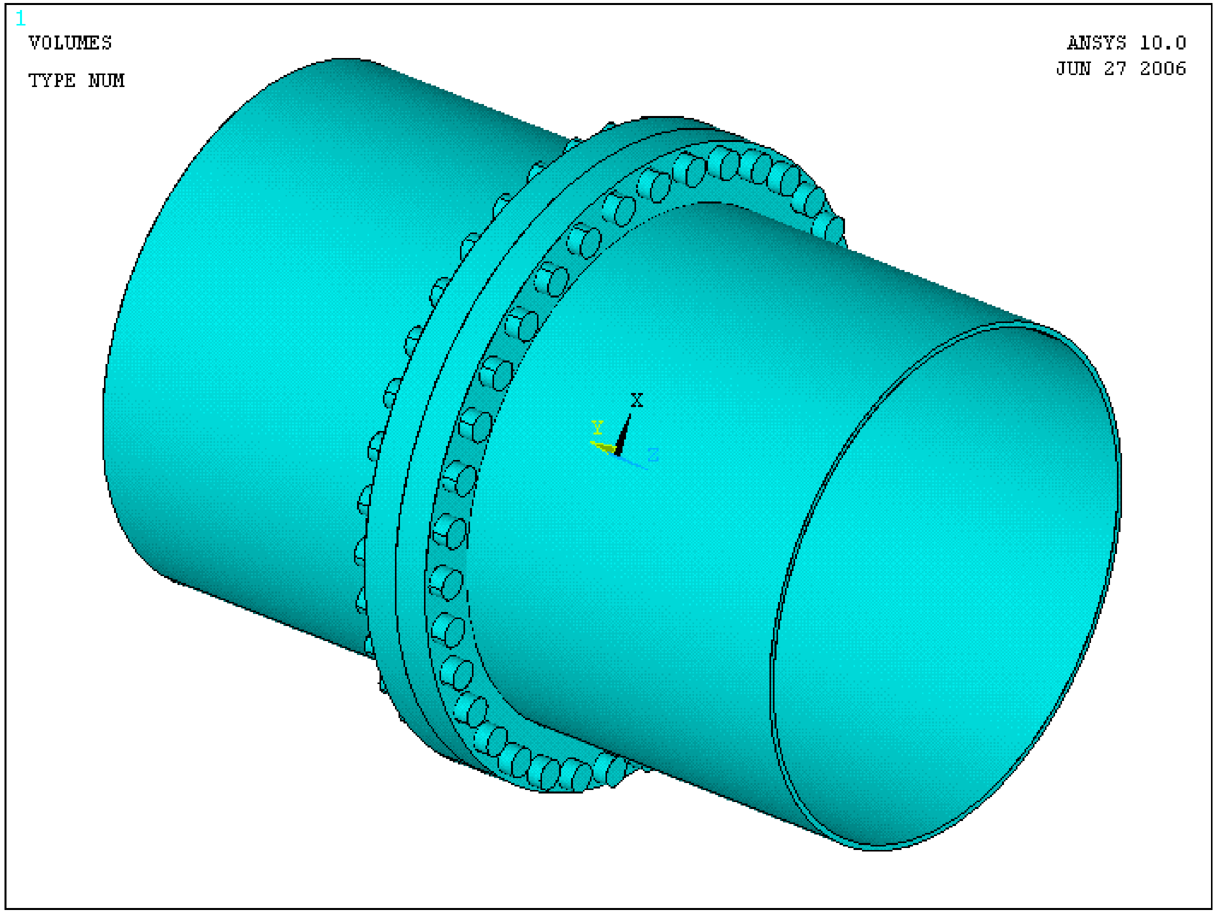


The stress-strain curve for steel



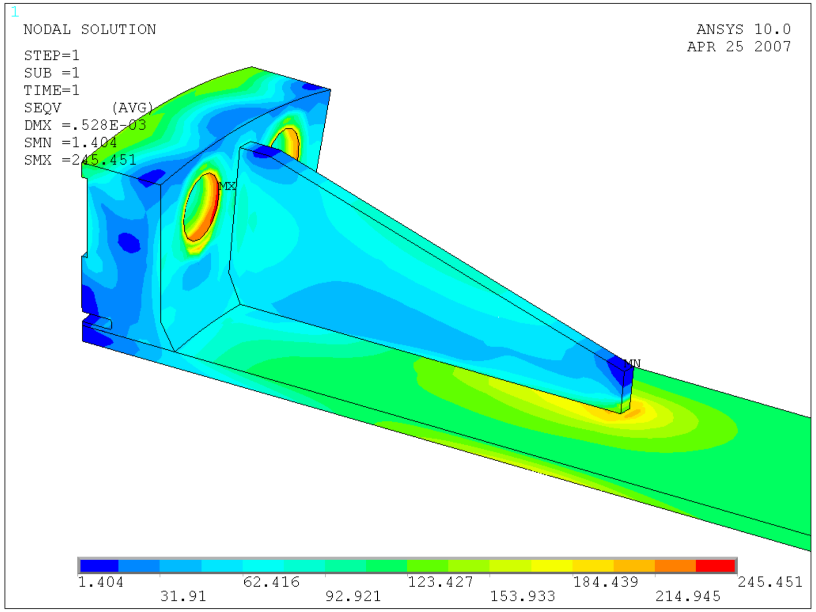
The relaxation of the yield stress in steel with time in the presence of hydrogen

Design the steel butt joint with hydrogen redistribution and accumulation inside the material

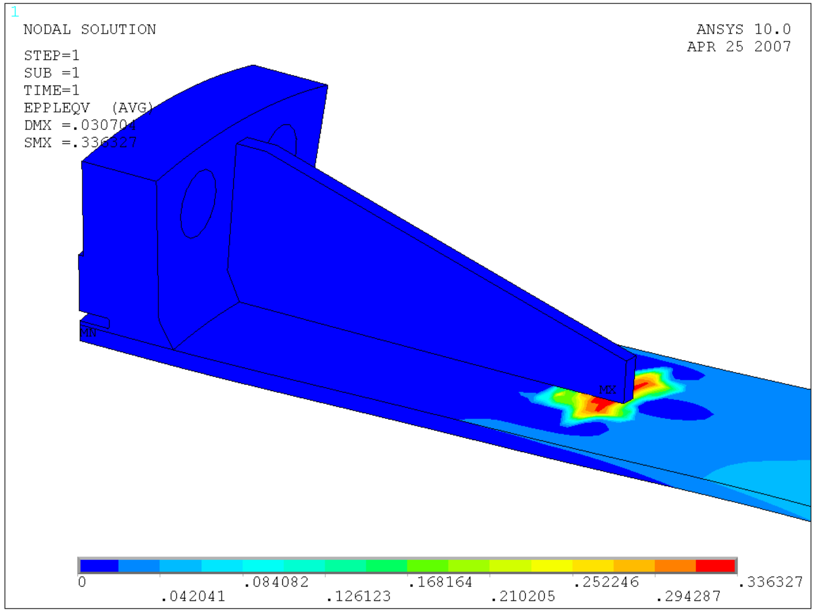


Relaxation of the stress with reinforcing plate

The distribution of the von Mises stress

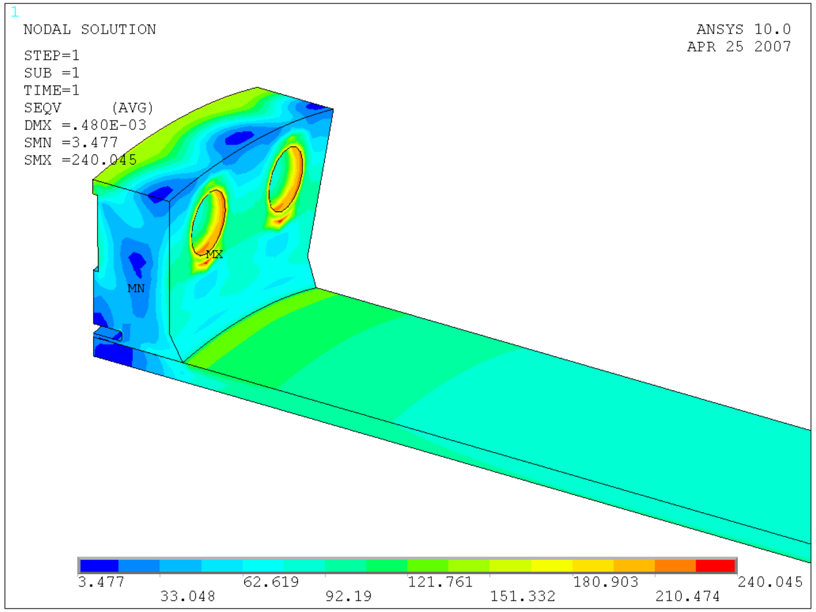


The distribution of the strain after hydrogen saturation

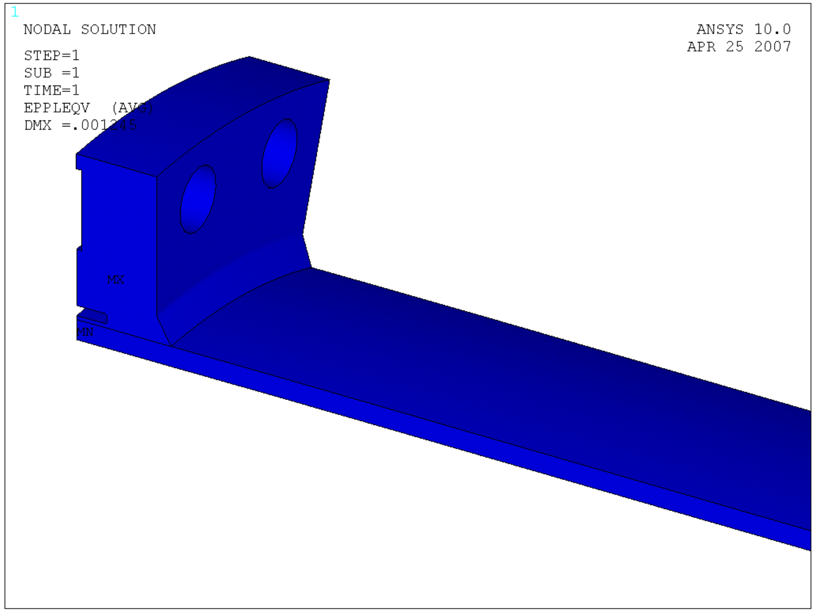


Relaxation of the stress without reinforcing plate

The distribution of the von Mises stress



The distribution of the strain after hydrogen saturation



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..