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Numerical modelling of free boundary dynamics in ‘metal-hydride’ phase transition

Yu V Zaika, N I Rodchenkova and K V Grudova
Institute of Applied Mathematical Research of the Karelian Research Centre of the Russian Academy of Sciences, Pushkinskaya St. 11, 185910 Petrozavodsk, Russia
E-mail: zaika@krc.karelia.ru, nirodchenkova@krc.karelia.ru, grudova@krc.karelia.ru

Abstract. One of the most important requirements for the reactor’s active zone materials (made of zirconium alloys) is low hydrogen absorptivity since hydrogen embrittlement may cause zirconium cladding damage. Depending on the hydrogen content and operation temperature, hydrogen may be present in zirconium alloys as a solid solution or as hydrides. Hydrides have the greatest embrittlement effect on alloys as they can form and enlarge cracks. The problem is to model the dynamics of the moving boundary of phase transition and to estimate the concentration distribution in hydride and in solution. This paper presents a mathematical model of zirconium alloy hydrogenation taking into account phase transition (hydride formation), and the iterative computational algorithm for solving the nonlinear boundary value problem with free phase boundary based on implicit difference schemes.

1. Introduction
The interest in the interaction of hydrogen with structural materials is multifarious [1–8]. It is sufficient to mention problems in power production, protection of metals from hydrogen corrosion, chemical reactor design, rocket making. Enthusiasts have been speaking about hydrogen economy along with hydrogen energy [4]. Some mathematical models of dehydrogenation and hydrogen permeability connected with this article are presented in [9–11]. One of the most important requirements for the reactor’s active zone materials (made of zirconium alloys) is low hydrogen absorptivity since hydrogen embrittlement may cause zirconium cladding damage. Depending on the hydrogen content and operation temperature, hydrogen may be present in zirconium alloys as a solid solution or as hydrides. Hydrides have the greatest embrittlement effect on alloys as they can form and enlarge cracks.

The mathematical research is based on the articles [12, 13]. The problem is to model the dynamics of the moving boundary of phase transition and to estimate the concentration distribution in hydride and in solution. This paper presents a mathematical model of a zirconium alloy plate hydrogenation taking into account phase transition (hydride formation), and the iterative computational algorithm for solving the nonlinear boundary value problem with free phase boundary based on implicit difference schemes.

2. Mathematical model of hydrogenation
We shall briefly describe the experiment (see details in [12]). A Zr–1Nb plate is polished on one side. The other side is nearly impermeable to hydrogen due to the presence of impurities, oxides.
and such. We disregard butt ends. Constant temperature of the sample $T$ and $H_2$ gas pressure $p$ are maintained during the experiment (sample cooling is carried out).

The alloy absorbs hydrogen quite well. A thin volume layer for which the hydrogen distribution can be considered uniform at a relatively high inflow pressure ($p \approx 2$ atm) is selected. Diffusion resistance starts to set only at a certain initial depth $\ell_0$. When the concentration of dissolved hydrogen reaches a certain value, nuclei of the hydride phase begin to appear, and this layer relatively quickly forms an initial hydride crust. This transient process ‘from nuclei to crust’ inside the near-to-surface layer is considered to be practically instantaneous on the time scale of the subsequent slow movement of the hydrogenation front to a considerable thickness. Further advance of hydrogen through the growing hydride layer proceeds at a much lower rate.

The notations are the following. $L$ is the plate thickness; $\ell_0$ is the thickness of the layer that absorbs hydrogen relatively easily and there is no diffusion resistance inside this layer yet (future initial hydride crust); $u(t)$ is the $H$ concentration in the $\ell_0$-layer ($1_H/\text{cm}^3$); $Q$ is the concentration at which the lattice is locally rearranged and nuclei of the hydride phase appear; $Q_h$ is the concentration of $H$ atoms in the hydride phase (chemically bonded hydrogen forming hydride as material); $c(t, x)$ is the concentration of dissolved $H$ in the $(L - \ell_0)$-layer; $\mu$ is the gas-kinetic constant. The plate temperature and inflow pressure are constant ($T = \text{const}$, $p = \text{const}$).

According to the gas kinetic theory, the particle flux density $J_p$ incoming to the surface (in this case the flux of $H_2$ molecules) is connected with the pressure $p$ by the Hertz–Knudsen formula: $J_p = p/\sqrt{2\pi mkT}$ ($k$ is the Boltzmann constant, $m$ is the mass of $H_2$ molecule). In the context of the experiment, it is convenient to select the following units $[x, t, L] = \text{cm}$, $[p] = \text{Torr}$. Then, we numerically obtain the dependence $J_p = \mu p$, $\mu(T) \approx 2.474 \cdot 10^{22}/\sqrt{T}$ ($[\mu] = 1_H/(\text{Torr}\cdot\text{cm}^2\cdot\text{s})$, $[T] = \text{K}$). Since the atomic hydrogen diffuses, for consistency we will calculate the flux in $H$ atoms: $J_p = 2\mu p$. Only a small part of $H$ will, however, be absorbed into the alloy: $J_{abs} = 2\mu sp$ ($s \ll 1$). Multiplier $s$ is the fraction of the incident $H$ that gets into the near-to-surface volume. We combine the elementary stages of physisorption, dissociation and dissolution itself into one stage: $s$ is the effective coefficient of absorption.

Stage I: hydrogen dissolution in Zr–1Nb

For the diffusion $(L - \ell_0)$-layer, we formulate the standard boundary value problem:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}, \quad x \in (\ell_0, L), \quad t > 0; \quad c(0, x) = 0, \quad x \in [\ell_0, L]; \quad c(t, \ell_0) = u(t), \quad \frac{\partial c}{\partial x} \bigg|_{L} = 0. \quad (1)$$

The boundary condition $c(t, \ell_0) = u(t)$ indicates that the $H$ distribution with respect to sample thickness is continuous, while $\partial_x c \big|_{L} = 0$ indicates that the plate side $x = L$ is impermeable. Hereinafter, we assume that coefficients depend on the temperature in an Arrhenius way, in particular $D = D_0 \exp\{-E_D/[RT]\}$. The temperature $T = \text{const}$ is maintained throughout any one experiment.

From the fluxes balance we derive the differential equation for the concentration $u(t)$:

$$u(t)\ell_0 = 2\mu sp - bu^2 + D \frac{\partial c}{\partial x} \bigg|_{\ell_0}, \quad u(0) = 0. \quad (2)$$

The meaning of this equation is the following. The amount of $H$ atoms that have been absorbed through 1 cm$^2$ during 1 s due to hydrogen pressure is $2\mu sp$, but there are the opposing desorption flux $bu^2$ ($b$ is the effective coefficient of recombination) and the diffusion outflow. The imbalance between these flux densities determines the accumulation of hydrogen atoms within the $\ell_0$-layer ($\dot{u}\ell_0$). This equation should be considered together with (1), since $u(t)$ determines the boundary concentration in (1). When $p$ is not too large (without hydride formation), in the equilibrium situation (when all derivatives are zero) we have $2\mu sp - bu^2 = 0 \Rightarrow \tilde{u} = \Gamma\sqrt{p}$, $\Gamma \equiv \sqrt{2\mu sb^{-1}}$. 
Therefore, under static conditions, the dynamics of (2) is consistent with the Sieverts law \( \bar{u} \propto \sqrt{\bar{p}} \), where \( \Gamma \) is the solubility coefficient. Let us emphasize that we speak about the dissolved diffusion-movable atomic hydrogen. In the ‘saturation–degassing’ experiment, the total absorption of hydrogen is taken into account, including reversible capture and hydride phases — the coefficient \( \Gamma \) may have another meaning and numerical value. Technically, it is easy to add the reversible capture of \( H \) atoms in the \((L - \ell_0)\)-layer by different types of ‘traps’ (defects of the material), but in this problem we consider reversible capture to be a minor factor.

**Stage II: hydride formation and phase boundary movement**

When the concentration \( u(t) \) becomes equal to the threshold concentration \( Q = Q(T) \), hydride nuclei appear (\( \delta \)-phase). Further influx of absorbed atomic hydrogen is utilized for the growth of nuclei until a solid hydride crust is formed (with the concentration \( Q_h > Q \) of chemically bonded hydrogen) and for maintaining the level \( c(t, \ell_0) = Q \) in the \( \alpha \)-phase of the solution. At the same time, nuclei grow and connect faster at the input side, the total hydrogen concentration begins to exceed the level \( Q_h \) due to additional dissolution in the hydride. When the inflow to the hydride microlayer boundary \( x = \ell_0 \) begins to exceed the outflow to the \( Zr-1Nb \) alloy, a ‘driving force’ appears and the phase transition boundary begins to move and the hydride layer grows. We believe that this transition process is relatively fast. It is convenient to set a new time zero \((t = 0)\) when \( u(t) = Q \) in the \( \ell_0 \)-layer. The hydride crust with the concentration \( Q_h \) is rapidly formed. By this time, we have \( c(0, x) = \varphi(x) \) (the distribution of dissolved hydrogen in the \( \alpha \)-phase is taken from the previous stage), \( \varphi(\ell_0) = Q \). Now the hydrogen begins to diffuse through the hydride \( \ell_0 \)-layer. Denote by \( v(t, x) \) the concentration of \( H \) atoms in the hydride. We emphasize that \( v(t, x) \) is the concentration of diffusing as opposed to chemically bound hydrogen (the hydride is a new ‘independent’ material), the total concentration is equal to \( Q_h + v(t, x) \). We put down the diffusion equations for the plate with growing hydride crust \((x = \ell(t)\) is the phase boundary, \( \ell(0) = \ell_0 \):

\[
\frac{\partial v}{\partial t} = D_* \frac{\partial^2 v}{\partial x^2}, \quad x \in (0, \ell(t)), \quad v(0, x) = 0, \quad x \in [0, \ell_0],
\]

\[
\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}, \quad x \in (\ell(t), L), \quad c(0, x) = \varphi(x), \quad x \in [\ell_0, L].
\]

Here, \( D_* \) is the \( H \) diffusion coefficient in the new material (hydride). We write the ‘input-output’ boundary conditions similarly to stage I:

\[
2\mu_* p - b_* v^2(t, 0) = -D_* \frac{\partial v}{\partial x} \bigg|_{x=0}, \quad \frac{\partial c}{\partial x} \bigg|_{L} = 0.
\]

In the hydride, the concentration gradient appears almost immediately, since it is much harder to diffuse through the \( \delta \)-phase. There is no ‘cumulative’ layer (the analogue of the \( \ell_0 \)-layer in Stage I). When the ‘inflow–outflow’ balance becomes positive, the phase boundary \( x = \ell(t) \) begins to move and additional conditions at the interface \( x = \ell(t) \) are needed to ‘sew together’ the diffusion equations.

We begin with the Stefan type equation describing the dynamics of the free phase boundary movement:

\[
\left[ v(t, \ell(t)) + Q_h - c(t, \ell(t)) \right] \dot{\ell}(t) = -D_* \frac{\partial v}{\partial x} \bigg|_{\ell(t)} + D \frac{\partial c}{\partial x} \bigg|_{\ell(t)},
\]

A jump of concentrations occurs: \( v(t, \ell) + Q_h > Q_h > c(t, \ell), \quad \ell = \ell(t) \). Still, the concentration \( v(t, \ell) \) is negligible (the \( Zr \)-alloy ‘does not resist’ the penetration of hydrogen). We assume
that $v(t, \ell(t)) = 0$. The incoming flux from the $\delta$-phase is almost completely spent on the formation of a new hydride layer (movement of the boundary $x = \ell(t)$) and goes to the solution. When $c(t, \ell) < Q$, a thin hydride layer at the phase boundary becomes unstable and partially decomposes, so we assume $c(t, \ell) = Q$.

Thus, we accept the following conditions on the moving free phase boundary:

$$v(t, \ell(t)) = 0, \quad c(t, \ell(t)) = Q, \quad t \geq 0, \quad [Q_h - Q]\dot{c}(t) = -D_s \frac{\partial c}{\partial x}\Big|_{t=\ell}, \quad t \geq t_s > 0. \quad (6)$$

We emphasize that the Stefan equation (6) ‘is connected’ to the model when the right-hand side (fluxes balance) becomes positive. This is how we choose $t = 0$. The front moves ($t \geq t_s$) with the total concentration $Q_h$ towards $x = L$. Passing to the limit ($t \to 1$), we have $\ell(t) \to L$. The concentration distribution $c(x, t)$ tends to uniformity and slowly increases up to the limit value $Q$, when one can neglect the thin ‘residual’ $Zr-1Nb$ layer in calculations.

3. Model transformation to dimensionless form

Stage I. We transform time $t = L^2 D^{-1} \ell'$, where $L^2 D^{-1}$ is the characteristic diffusion time, and transform the independent variable $x = \ell_0 + z[L - \ell_0]$, \(c(t', z) = c(t(t'), x(z))\). We introduce appropriate normalization of concentrations and leave the same notation for the function $\hat{c}$:

$\hat{c} := \frac{c}{\mu_{sp}/b}, \quad \hat{u} := u/\hat{u}, \quad \bar{u} = \sqrt{2\mu_{sp}/b}$.

The boundary value problem (1)–(2) after the change of variables is

$$\hat{c} = \left[\frac{L}{L - \ell_0}\right]^2 \frac{\partial^2 \hat{c}}{\partial z^2}, \quad \hat{c}(0, z) = 0, \quad z \in [0, 1], \quad \frac{\partial \hat{c}}{\partial z}\big|_{z=1} = 0, \quad \hat{c}(t', 0) = \hat{u}(t'), \quad (7)$$

$$\frac{d\hat{u}}{d\ell'} = d_1(1 - \hat{u}^2) + d_2 \frac{\partial \hat{c}}{\partial z}\big|_{z=0}, \quad \hat{u}(0) = 0, \quad d_1 \equiv bL^2\bar{u}[D\ell_0]^{-1}, \quad d_2 \equiv L^2[\ell_0(L - \ell_0)]^{-1}. \quad (8)$$

Stage II. We transform time $t = \frac{L^2}{\sqrt{D\ell_s}}\ell'$ and the spatial variable:

$\text{(3): } x = \ell(t')y, \quad v \rightarrow \hat{v}(t', y); \quad \text{(4): } x = \ell(t') + z[L - \ell(t')], \quad c \rightarrow \hat{c}(t', z).$

We introduce appropriate normalization of concentrations and leave the same notation for the functions $\hat{v} := \frac{v}{\bar{v}}, \quad \hat{c} := \frac{c}{\mu_{sp}/b}, \quad \bar{v} = \sqrt{2\mu_{sp}/b}$.

Additionally, we introduce the function

$$\lambda(t') \equiv \frac{\hat{v}(t')}{\bar{v}} = \frac{d}{d\ell'} \ln \ell(t'),$$

where the dot denotes the differentiation with respect to $t'$.

The boundary value problem (3)–(6) after the change of variables is

$$\hat{\partial} = \sqrt{\frac{D_s}{D}} \left(\frac{L}{\ell}\right)^2 \frac{\partial^2 \hat{v}}{\partial y^2} + \lambda(t')(1 - z) \frac{\partial \hat{v}}{\partial y}, \quad t > 0, \quad y \in (0, 1), \quad \hat{v}(0, y) = 0, \quad \lambda(t') \equiv \frac{\ell(t')\hat{v}}{\bar{v}}, \quad \hat{v}(t', 1) = 0, \quad (9)$$

$$d_s \left[1 - \hat{v}^2(t', 0)\right] = \frac{\partial \hat{v}}{\partial y}\big|_{y=0}, \quad d_s \equiv \frac{b\ell(t')\bar{v}}{D_s}, \quad \hat{v}(t', 0) = 0, \quad (10)$$

$$\frac{\partial \hat{c}}{\partial t} = \sqrt{\frac{D_s}{D}} \left[\frac{L}{L - \ell}\right]^2 \frac{\partial^2 \hat{c}}{\partial z^2} + \frac{\lambda(t')(1 - z)}{L\ell^{-1}(t') - 1} \frac{\partial \hat{c}}{\partial z}, \quad z \in (0, 1), \quad (11)$$

$$\hat{c}(0, z) = \psi(z) \left[0 \leq z \leq 1\right], \quad \hat{c}(t', 0) = \frac{Q}{\bar{v}}, \quad \frac{\partial \hat{c}}{\partial z}\big|_{z=1} = 0, \quad (12)$$

$$\left[\frac{Q_h - \hat{c}(t', 0)}{\bar{v}}\right] \cdot \lambda(t') = -\sqrt{\frac{D_s}{D}} \hat{v} \left(\frac{L}{\ell}\right)^2 \frac{\partial \hat{v}}{\partial y}\big|_1 + \sqrt{\frac{D_s}{D}} \left[\frac{L^2}{\ell(t')(L - \ell(t'))}\right] \frac{\partial \hat{c}}{\partial z}\big|_{z=0} (t' \geq t_s). \quad (13)$$
4. Computational algorithm

Stage I. The main computational challenge is to solve the nonlinear boundary value problem with moving phase boundary (Stage II). Therefore, we only briefly describe here the general scheme for Stage I. The authors approximate the diffusion equation (7) (using a four-point pattern) and ODE (8) by implicit difference schemes of second–order accuracy. The algorithm is of iterative nature due to the model nonlinearity. Moving on to the next time layer, we use explicit schemes for the diffusion equation to calculate the initial approximation for the first three grid nodes with respect to the spatial variable. Knowing the current approximations of the concentration in the boundary nodes \((z = 0, 1)\), we used the Thomas algorithm for solving the system of algebraic equations with a tridiagonal matrix. After correcting the concentration values in internal nodes, the concentration in the boundary node \(z = 0\) is recalculated as a positive root of the quadratic equation (from the difference approximation of the boundary condition (8)). The iterations proceed until the distribution \(\hat{c}(t', z), z \in [0, 1]\) becomes stable. Then, we move on to the next time layer.

Stage II. We fix the time step \(\Delta t\) and choose uniform grids for spatial variables. The initial distribution \(\psi(z) (\varphi(x))\) is taken from the previous stage. Formally, one can forget about the physical meaning of function \(\ell(t')\) as the phase boundary and consider it as a functional parameter. All model coefficients are unambiguously determined using the solution \(\ell(t')\) (knowing \(\lambda(t', z)\)). Therefore, the computational algorithm will be based on the implicit scheme and will have an iterative character. Iterations are meant to more precisely define \(\lambda(t')\) at every time layer. We use a standard four-point pattern to approximate the diffusion equations (9), (12) and then solve the resultant linear equation systems applying the Thomas algorithm. We now describe the way to more precisely define the value of \(\lambda(t')\) at every time layer.

We use the value from the previous layer \(\lambda(t_n') \approx \lambda(t_{n-1}')\) as the initial approximation. The parameter \(\lambda(t_n')\) is subject to iterative improvement, the value of \(\ell(t_n')\) is known.

Moving on to the \((n + 1)\)-time layer, we use explicit schemes for the diffusion equation (9) to calculate the initial approximation for the first two grid nodes with respect to the spatial variable \(y = y_{1.2}\). We have a quadratic equation in (10) for \(\hat{v}(t_{n+1}', 0)\) and choose the positive root. Find the distribution (approximation) \(\hat{v}(t_{n+1}', y), y \in [0, 1]\) using the Thomas algorithm. Go back to the improvement of \(\hat{v}(t_{n+1}', 0)\) in virtue of (10) (the values of \(\hat{v}\) at \(y = y_{1.2}\) used to calculate \(\partial_y \hat{v}|_{y=0}\) have already changed). Proceed with this process until the distribution \(\hat{v}(t_{n+1}', y)\) becomes stable. The time step is small enough, so a few iterations will suffice.

Move on to the Neumann boundary value problem (11)–(12) returning to the previous time layer \((t' = t_n')\) and find the distribution \(\hat{c}(t_{n+1}', z), z \in [0, 1]\) applying the Thomas algorithm.

After these calculations we approximate the derivatives on the \((n+1)\)-time layer and substitute them into the boundary conditions (13). We find a new approximation of \(\lambda(t_{n+1}') > 0\) and return to the beginning of the described subalgorithm (Stage II). After some iterations, we obtain a steady-state value of \(\lambda(t_n')\). Further, we calculate \(\ell(t_n') = \lambda(t_n')\ell(t_n')\) and by virtue of

\[
\lambda(t_n') = \frac{d}{dt} \ln \ell(t')|_{t_n'} = \ln(\ell(t_n' + \Delta t')) \approx \ln \ell(t_n') + \lambda(t_n') \cdot \Delta t'
\]

we determine \(\ell(t_{n+1}'), t_{n+1}' = t_n' + \Delta t'\). Using \(\ln \ell(t_n')\), we find \(\ell(t_{n+1}')\) and go on to the layer \(t_{n+2}'\), taking \(\lambda(t_{n+1}') \approx \lambda(t_n')\) as the initial approximation. Next, we specify the value of \(\lambda(t_{n+1}')\) and the distributions \(\hat{v}(t_{n+2}', y), \hat{c}(t_{n+2}', z)\) according to the above scheme.

Numerical algorithm testing. The iterative algorithm is developed on the basis of implicit difference schemes and the Thomas algorithm. Computational experiments confirming the algorithm efficiency have been conducted. The input data, for example, are \(L = 6 \times 10^{-2} \text{ cm}, \ell_0 = 1.3 \times 10^{-3} \text{ cm}, p = 1520 \text{ Torr}, T = 593 \text{ K}, Q = 6.14 \times 10^{20} \text{ cm}^{-3}, Q_h = 6.14 \times 10^{22} \text{ cm}^{-3} D_0 =\)
2.2 \times 10^{-3} \text{ cm}^2 \text{s}^{-1}, E_D = 35 \times 10^3 \text{ J mol}^{-1}, D_{40} = 1.5 \times 10^{-3} \text{ cm}^2 \text{s}^{-1}, E_D^* = 59 \times 10^3 \text{ J mol}^{-1}, b = 5.5 \times 10^{-24} \text{ cm}^4 \text{s}^{-1}, b_5 = 3 \times 10^{-27} \text{ cm}^4 \text{s}^{-1}, s = 7 \times 10^{-7}, s_* = 6 \cdot 10^{-8}.

The modelling results conform to experimental data.

Conclusions
Zirconium alloys are the construction materials for critical elements in active zones of nuclear power reactors. During the operation of reactors such materials are subject to hydrogenation. Hydrogenation results in a decrease of alloy plasticity and cracking resistance. The formation of brittle hydrides at crack tips can result in severe embrittlement. One of the most important requirements for the reactor’s active zone materials is low hydrogen absorptivity.

Since dissolved atomic hydrogen represents an extremely mobile interstitial phase, it is practically impossible in experimental studies to determine time-dependent hydrogen distribution in the material (even within the experiment time scale) based on the available external measurements.

The article presents a model of a Zr-alloy plate hydrogenation taking into account the nonlinear dynamics of adsorption-desorption processes and the movement of free phase boundary (hydride–metal). In the asymptotic (under chemical equilibrium) the model corresponds to the experimental Sieverts law of solubility. The algorithm that allows to numerically model the dynamics of the phase boundary and the distribution of dissolved hydrogen concentrations across the hydride and the alloy layers is briefly presented. Particularly important is the model-based forecast on the time horizon much exceeding experimental capabilities.

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