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NUMERICAL SIMULATION OF NITROGEN DIFFUSION IN A SOLID CHROMIUM PARTICLE

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1. Introduction

A technological process for diffusive nitrogen saturation of pure metals and alloys has been developed in the Institute for Metal Science, Sofia [1]. The diffusion of nitrogen during this process takes place within a temperature range from $T = 1000^0$C to $T = 1300^0$C and for a pressure value equal to 1.5 MPa. In one of the variants of the above mentioned process metal spherical particles with radii 0.5 mm are saturated with nitrogen. Kinetics of diffusivity layers forming, the layers width and the time for which the particle becoms fully saturated with nitrogen, are subjects of interest for scientists and engineers during the above described technological process.

The surface nitrogen saturation of different metals and alloys is mainly discussed in the literature (see, for example [2,3], and references therein). Diffusivity coefficients for different pure metals and phase diagrams for metal-nitrogen systems are available in the above mentioned papers. The data, presented there, are obtained mainly within experimental works. The nitrogen concentration and graphics of different phase layers width versus time, are also subject of measurment in above mentioned papers.

A mathematical model, describing surface nitrogen concentration in a half-space, is described in [2]. It is welknown, that mathematical modeling allows the process to be investigated with less expences than in the physical experiments. Developing the

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mathematical model from [2], the process of nitrogen diffusion in a solid spherical chromium particle is numerically investigated in the present paper.

2. Mathematical Model

Let us consider the diffusivity process in a solid spherical particle from pure chromium (Cr), which is situated in a nitrogen gas medium with a given temperature. The nitrogen atoms penetrate deep into the crystal mesh of the chromium particle during the time. As a result, the so called "L-solid solution" is formed there. After the concentration of nitrogen atoms in the L-solid solution became greater than a given value, the forming of Cr_2N starts. The concentration discontinuity takes place at the interface between the two phases. The boundary values of the nitrogen concentration at the interface can be determined from the cromium-nitrogen phase diagram.

The above described process is governed by the following equation:

$$\frac{\partial C_i}{\partial t} = \frac{D_i}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) \tag{1}$$

Here $C = C(r,t)$ is the concentration, t – the time, D – the diffusivity coefficient, r – the radii. The index $i = 1$ denotes the nitrid phase, and $i = 2$ denotes the L-solid solution phase. As it was mentioned above, the boundary values for the nitrogen concentration at the interface are taken from the phase diagram.

$$C_1(\xi(t)+0,t) = C_{1\xi}, \tag{2}$$

$$C_2(\xi(t)-0,t) = C_{2\xi}, \tag{3}$$

where $\xi(t)$ denotes the boundary between phases. The nitrogen concentration at the chromium particle surface is supposed to be known:

$$C_1(R_p,t) = C_{1p} \tag{4}$$

The standard boundary condition is considered at $r = 0$:

$$r^2\frac{\partial C_2}{\partial r} = 0 \tag{5}$$

The interface front movement is governed by the welknown Stefan equation:

$$D_1\frac{\partial C_1(\xi(t)+0,t)}{\partial r} = D_2\frac{\partial C_2(\xi(t)-0,t)}{\partial r} + \Delta_c\frac{d\xi}{dt}, \tag{6}$$

where Δ_c stands for the discontinuity jump at the interface. It is supposed, that for $t = 0$ the nitrogen concentration in the particle is equal to zero:

$$C(r,0) = 0, \qquad 0 \le r \le R_p. \tag{7}$$

Here R_p stands for the particle radii.

3. Numerical Algorithm

Generally, two different approaches are used for solving moving boundary problems like (1)–(7). The first is the so called fixed grids approach, when all computations take place on a fixed grid, without explicit matching of the moving interface boundary. The second approach is based on the explicit matching of the interface boundary. A variant of the second approach, based on changing of variables, is used in this paper for solving the above system of partial differential equations.

Let us introduce a new variable in the region of nitrid phase with the equality:

$$R_2 = \frac{r}{\xi(t)}, \quad r = \xi(t) R_2.$$

Omitting some details, we will rewrite the diffusivity equation in the nitride phase as follows:

$$\frac{\partial C_2}{\partial t} - \dot{\xi}(t) \frac{R_2}{\xi(t)} \frac{\partial C_2}{\partial R_2} = \frac{1}{\xi^2(t)} \frac{D_2}{R_2{}^2} \frac{\partial}{\partial R_2} \left(R^2{}_2 \frac{\partial C}{\partial R_2} \right) \quad 0 \le R_2 \le 1, \ t \ge 0. \tag{8}$$

$$R_2{}^2 \frac{\partial C_2(0,t)}{\partial R_2} = 0, \tag{9}$$

$$C_2(1,t) = C_{2\xi}. \tag{10}$$

In the L-solid phase a new variable can be introduced by the equality:

$$R_1 = \frac{r - \xi(t)}{R_p - \xi(t)}, \quad r = \xi(t) + R_1 (R_p - \xi(t)).$$

In this case the diffusivity equation and boundary conditions can be rewritten as follows:

$$\frac{\partial C_1}{\partial t} - \dot{\xi}(t) \frac{R_1 - 1}{R_p - \xi(t)} \frac{\partial C_1}{\partial R_1} =$$

$$\frac{1}{(R_p - \xi)^2} \frac{D_1}{[\xi + R_1 (R_p - \xi)]^2} \frac{\partial}{\partial R_1} \left((\xi + R_1 (R_p - \xi))^2 \frac{\partial C_1}{\partial R_1} \right) \tag{11}$$

$$0 \le R_1 \le 1, \quad t \ge 0.$$

$$C_1(0,t) = C_{1\xi}, \tag{12}$$

$$C_1(1,t) = C_{1p}. \tag{13}$$

In the new variables Stefan condition has to be written as:

$$\Delta_c\dot{\xi}(t) = -D_2\frac{1}{\xi(t)}\frac{\partial C_2(1-0,t)}{\partial R_2} + D_1\frac{1}{R_p - \xi(t)}\frac{\partial C_1(1-0,t)}{\partial R_1}. \tag{14}$$

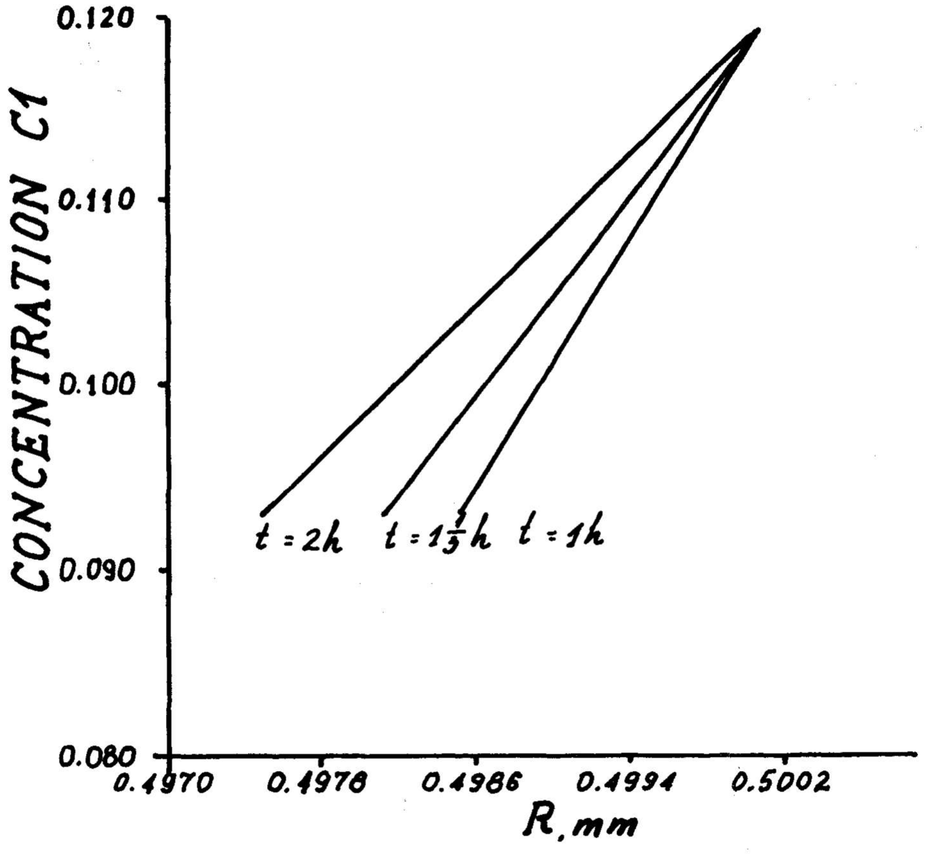

Fig. 1

Finite differences method [4] is used for solving the system of partial differential equations (8)–(14). Uniform grids are introduced on intervals $0 \le R_1 \le 1$ and $0 \le R_2 \le 1$. Partial differential equations for C_1 and C_2 are approximated, assuming that $\xi(t)$

and $\dot{\xi}(t)$ are known from the previous time step. TDMA is used at each time step for solving the obtained three-diagonal sets of linear algebraic equations in any of the two regions. After C_1 and C_2 have been computed at the new time step, the new position of the interface boundary $\xi(t)$ is computed, using explicit Euler method.

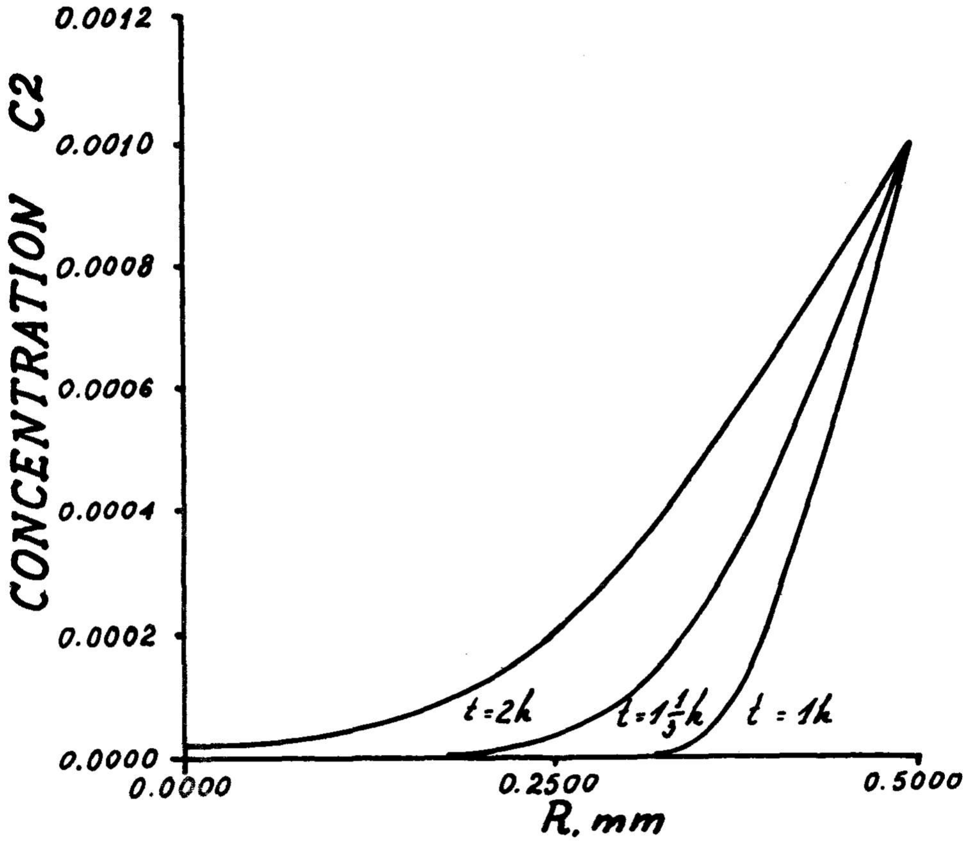

Fig. 2

4. Results from the Numerical Experiments

To verify the above algorithm, the vanadium nitride saturation in a half-space was computed and compared with the results from [2]. The phase transition position at $t = 90$ min, obtained in [2] is $\xi(90) = 5.2\mu$ and the one computed by us is $\xi(90) = 5.225\mu$. This result shows good compatibility with the mathematical model. It is necessary more extensive experimental tests to be carried out for this model in the future.

The distribution of the nitrogen concentration in the nitride layer is shown in Fig. 1. It is seen in the diagram that with increase of time the concentration profile spreads in depth from surface towards the centre. Fig. 2 presents the nitrogen concentration in the solid solution at different times from the begining of the process. With the increase of time the nitrogen penetrates to the centre of the particle. The motion of the chromium nitride – solid solution front $\xi(t)$ is shown in Fig. 3. At time 3 hours $\xi(3) = 0.4957mm$, or the tickness of the nitride layer is equal to 4.3μ.

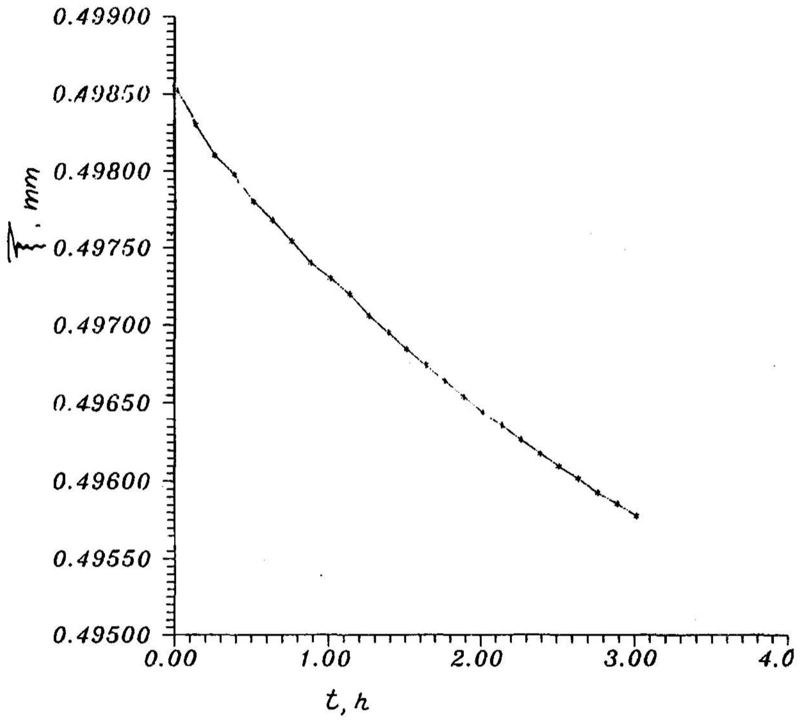

Fig. 3

Fig. 4 and Fig. 5 show the fields of nitrogen concentration at holding times 2 hours and 4 hours respectively. It can be pointed out that at time $t = 6$ hours the tickness of the nitride layer is 21μ, and the nitrogen concentration in the solid solution is constant which is equal to the value $C_2 = 0.001$ along all the radius of the particle.

As a conclusion it can be said that a mathematical model and a numerical method which enable the computation of nitrogen diffusion in solid metals accounting for phase formation, are developed. By means of this model concentration fields in spherical particles at various temperatures can be obtained.

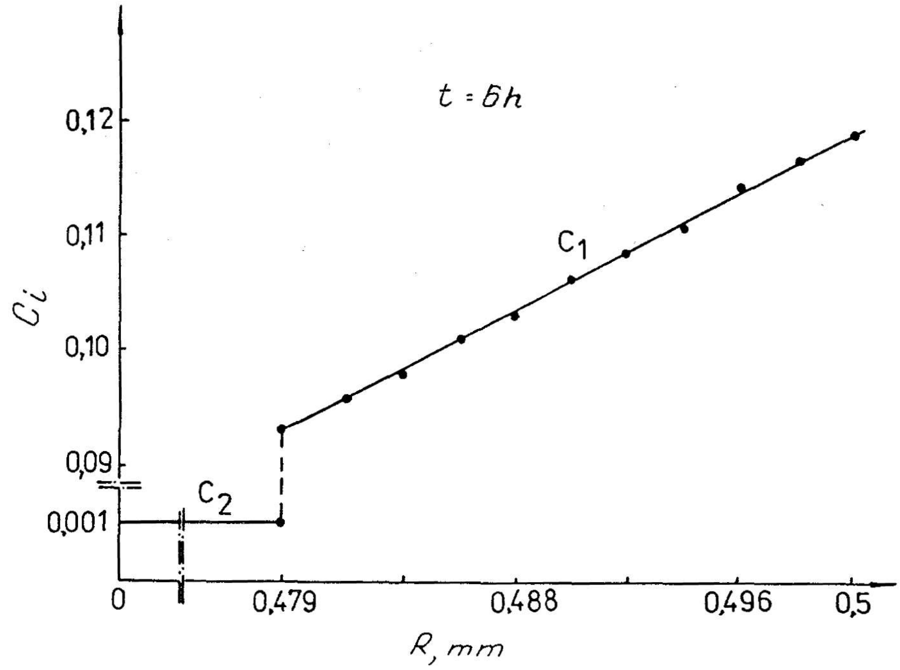
t = 6h
0,12
0,11
0,10
0,09
0,001
0
C_i
C_1
C_2
0,479
0,488
0,496
0,5
R, mm

Fig. 4

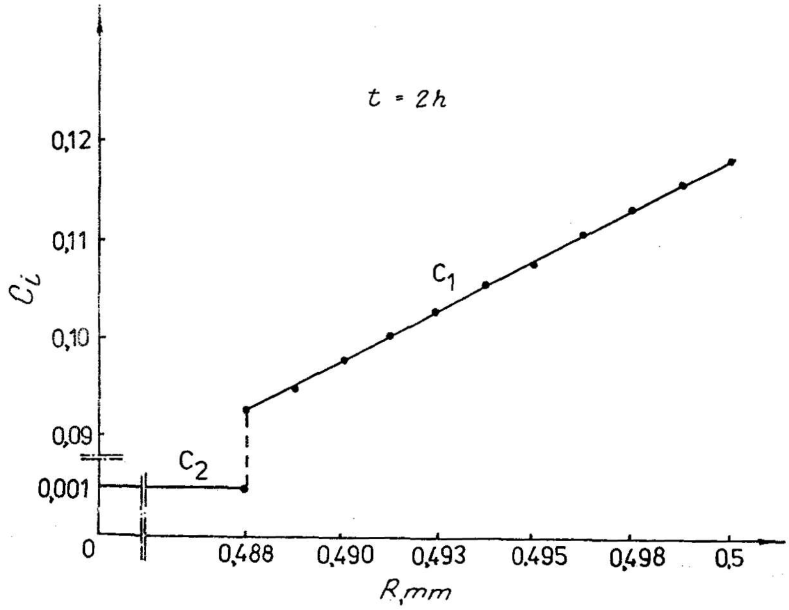
t = 2h
0,12
0,11
0,10
0,09
0,001
0
C_i
C_1
C_2
0,488
0,490
0,493
0,495
0,498
0,5
R,mm

Fig. 5

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