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Modelling of Diffusion Saturation of (α+β) Titanium Alloy by Oxygen in Rarefied Gaseous Medium

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Titanium (α+β) alloys are considered as promising structural materials for modern air-craft and space industries. Thermodiffusion saturation by oxygen under low partial pressure is one of the effective methods of surface strengthening of titanium alloys [1]. The problems of optimization of phase-chemical composition of alloys, gaseous medium pressure as well as scientific-founded choice of the temperature - time parameters for the process are not completely solved.

The aim of the present research is to create a model for diffusion saturation of (α+β) titanium alloy by oxygen under rarefied atmosphere with taking into consideration singularities of interaction on the interface and to estimate the effect of temperature and time of process.

The interaction between (α+β) titanium alloy and rarefied oxygen is schematically shown by the following processes with corresponding parameters (Figure 1): A (left): supply of molecules to titanium surface with, further, their adsorption, dissociation and chemisorptions (h is the coefficient of mass transfer, [cm/s]); B (centre): oxygen segregation on defects in contact layer (with mass capacity ω, [cm]) due to the chemical interaction with metal (reaction rate – k, [cm/s]; C (right): diffusion dissolution of interstitial elements in metal (D is the diffusion coefficient, [cm^2/s]) [2].

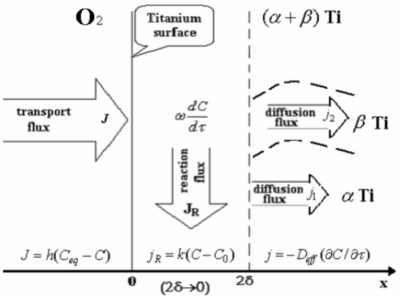

Figure 1: Scheme of mass fluxes in the vicinity of an interface (α+β)Ti / O_2.

It should be noted, that the processes mentioned in item A can be presented as two-stage reaction which includes diffusion stage described by rate constant h_D and stage of irreversible reaction (chemisorption) with rate constant h_R. Then, corresponding to summation of kinetic resistors $h^{-1} = h_D^{-1} + h_R^{-1}$, non-equilibrium processes mentioned above in points A and B should be described by an equation of the mass balance on the interface using adequate definition of boundary condition [2].

Phase-structural aspect mostly determines the diffusion dissolution of oxygen in metal core (point C). The two-phase structure is a feature of (α+β) alloy. That means that there are the regions with the different oxygen dissolution potential ability as well as with the different diffusivity of impurity. For instance, oxygen solubility in α-phase (area 1) is higher than in β-phase (area 2). However, oxygen diffusion coefficient in *β*-phase is one order higher than in *α*-phase [1]. Therefore, even in the case of small volumetric quantity of *β*-phase, these areas could be considered as, in a sense, the paths for enhanced diffusion which correct the kinetics of strengthened diffusion zone formation.

For the formulation of the corresponding diffusion problem a phenomenological approach was applied. This approach is based on a model of continuous spectrum in a medium consisting of two diffusion paths. The quasi-chemical reaction of transfer by oxygen $[O]_\beta \Leftrightarrow [O]_\alpha$ with corresponding coefficients (k_1 and k_2), which characterize the rate of such transfer, takes place between these channels [3]:

$$D_1 \Delta C_1 = \partial C_1 / \partial \tau + k_1 C_1 - k_2 C_2 \,, \; D_2 \Delta C_2 = \partial C_2 / \partial \tau - k_1 C_1 + k_2 C_2, \qquad (1)$$

Here, C_i and D_i (i =1, 2) are the concentration and the oxygen diffusion coefficient in the corresponding α and β areas. When we introduce the concentration $C=C_1+C_2$, the system of equations (1) can be reduced to a "non Fickian" differential equation of high order (fourth order following a spatial value) [3]. Assuming local dynamic equilibrium, such an equation attains a Fickian form, in which the effective diffusion coefficient of oxygen (D_{eff}) is presented by the relation:

$$D_{eff} \Delta C = \partial C / \partial \tau \;, \quad \text{where} \quad D_{eff} = (D_1 k_2 + D_2 k_1)/(k_1 + k_2) \qquad (2)$$

As the object of investigation the half-space ($0 \le x < \infty$), with the initial ($\tau=0$) oxygen concentration $C=C_0$ and the following boundary conditions, was chosen [2]:

$$\omega (dC/d\tau) = J - J_R - J_{dif} \quad \text{for} \quad x = +0, \quad C = C_0 \quad \text{for} \quad x = +\infty . \qquad (3)$$

It should be noticed, that the non-stationary boundary condition, Eq. 3, reflects the mass balance on interface (Fig.1). The difference between transport flux of oxygen $J(x=-0)$ and diffusion flux j_{diff} into the metal determines the kinetics of oxygen segregation on the interface caused by chemical reaction. The segregations take place in the contact layer on defects prototyped as "traps" for the diffusant [2]. The solution of diffusion problem Eq. 2, Eq. 3 was obtained in an analytic form.

Based on the obtained solution, the regularities and peculiarities of kinetics of diffusion saturation of (α+β) titanium alloys by oxygen have been illustrated. They correlate well with experimental results. It was shown that the depth of strengthened diffusion zone increases with increment of volumetric quantity of β-phase. The effect of temperature and time on the kinetics of the process is estimated. The peculiarities of oxygen redistribution on the interface in dependence on temperature of isothermal exposure are explored. It is established that, for the same duration of the process, an increase of temperature does not always tend to increase the impurity concentration on the interface.

References

[1]. Fedirko V. M. et al., Materials Science, 41, 2 (2005) 208-216.

[2] Prytula A., Pohreljuk I., Vedirko V., Matychak Ya., Defects and diffusion forum, 237-340 (2005) 1312-1318.

[3] Aifantis E.C. Acta Met., 27 (1979) 683-691.