

## Kinetic peculiarities of two-component diffusion saturation of titanium under rarefied nitrogen-oxygen-containing medium

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Previously, it was investigated the kinetics of single-component diffusion saturation of titanium by the interstitial elements (nitrogen or oxygen) [1]. It is clear that diffusion saturation of the materials by two and more components allows to change the properties of surface layers more considerably compared with single-component saturation. But it requires the theoretical knowledge about the kinetics of formation of diffusion zone, its composition and distribution of the elements. The aim of this work is to investigate analytically the peculiarities of simultaneous two-component (nitrogen and oxygen) diffusion saturation of titanium under rarefied controlled gaseous medium.

Kinetics of the compatible diffusion of nitrogen and oxygen in titanium is complicated and many-sided. The two-component (nitrogen and oxygen) diffusion saturation of titanium under rarefied controlled gaseous medium ( $P_N \gg P_{O_2}$ ) will be considered. Will be accepted that nitrogen  $\mu_1^G(P_N)$  and oxygen  $\mu_2^G(P_{O_2})$  potentials in gaseous medium (Fig. 1) such that concentrations of nitrogen  $C_1^S$  and oxygen  $C_2^S$  on the titanium surface equilibrium with the medium do not exceed their maximum solubilities, according to the phase diagrams. For  $T=800^\circ\text{C}$  they are 16 at.% and 33 at.%, respectively [2].

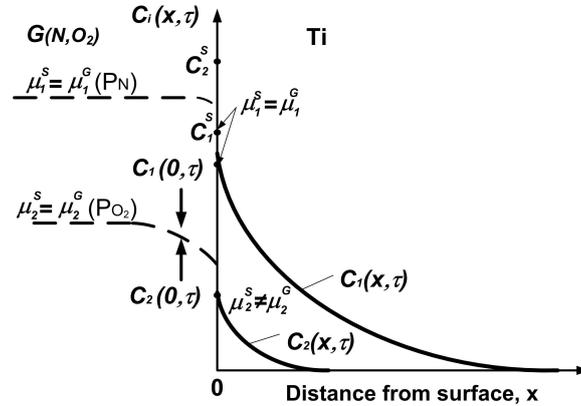


Figure 1: Scheme of mass transfer in system Ti-G(N, O<sub>2</sub>)

It should be noted that very often in the case of two-component diffusion the influence of one component is more significant than the other component. It will be accepted that oxygen (component 2) diffuses independently, while it affects the chemical potential ( $\mu_1(x, \tau) = d_{11}C_1(x, \tau) + d_{12}C_2(x, \tau)$ ,  $\mu_2(x, \tau) = d_{22}C_2(x, \tau)$ ) and diffusion ability ( $D_{12} = d_{12}L_{11}$ ,  $D_{21} = 0$ ,  $L_{11}$  – Onsager kinetic coefficient) of nitrogen (component 1). We have a system of the differential equations for description of the diffusion of these components:

$$D_{11} \frac{\partial^2 C_1(x, \tau)}{\partial x^2} + D_{12} \frac{\partial^2 C_2(x, \tau)}{\partial x^2} = \frac{\partial C_1(x, \tau)}{\partial \tau}, \quad D_{22} \frac{\partial^2 C_2(x, \tau)}{\partial x^2} = \frac{\partial C_2(x, \tau)}{\partial \tau}. \quad (3)$$

Since the aim of diffusion treatment of titanium is strengthening of its near-surface layers, then the half-space has been chosen as the object of investigation. The following boundary ( $x=0, x=\infty$ ) and initial ( $\tau=0$ ) conditions will be set for solution of a system of the differential equations:

$$C_1(0, \tau) + \lambda_{12}C_2(0, \tau) = C_1^S = \text{const}, \quad -D_{22} \frac{\partial C_2(x, \tau)}{\partial x} \Big|_{x=0} = H [C_2^S - C_2(0, \tau)], \quad (4)$$

$$C_1(x, 0) = C_2(x, 0) = 0; \quad C_1(\infty, \tau) = C_2(\infty, \tau) = 0, \quad \text{where } C_1^S = \mu_1^G/d_{11}, \quad C_2^S = \mu_2^G/d_{22}.$$

The condition of ideal contact ( $\mu_1^G = \mu_1^S$ ) on the surface was set in the boundary condition (2) for nitrogen. Surface concentration  $C_2(0, \tau)$  for oxygen was proposed to consider as a function of time. It is taken into account by mass transfer coefficient  $H$ . The solution of the system of equations (1) with the boundary conditions (2) is following:

$$C_1(x, \tau) = C_1^S - C_2^S[(\lambda_{12} + \alpha_{12})f_1(x, \tau) - \alpha_{12}f_2(x, \tau)], \quad C_2(x, \tau) = C_2^S f_2(x, \tau), \quad (5)$$

$$\text{here } f_1(x, \tau) = \operatorname{erfc}\left[\frac{x}{2\sqrt{D_{11}\tau}}\right] - \exp\left[\frac{H}{\sqrt{D_{11}D_{22}}}x + \frac{H^2\tau}{D_{22}}\right] \cdot \operatorname{erfc}\left[\frac{H\sqrt{\tau}}{\sqrt{D_{22}}} + \frac{x}{2\sqrt{D_{11}\tau}}\right],$$

$$f_2(x, \tau) = \operatorname{erfc}\left[\frac{x}{2\sqrt{D_{22}\tau}}\right] - \exp\left[\frac{Hx}{D_{22}} + \frac{H^2\tau}{D_{22}}\right] \cdot \operatorname{erfc}\left[\frac{H\sqrt{\tau}}{\sqrt{D_{22}}} + \frac{x}{2\sqrt{D_{22}\tau}}\right], \quad \alpha_{12} = \frac{D_{12}}{D_{22} - D_{11}}.$$

In particular, the time dependences of surface concentrations of components are following:

$$C_1(0, \tau) = C_1^S - C_2^S \lambda_{12} f(0, \tau), \quad C_2(0, \tau) = C_2^S f(0, \tau), \quad \text{where } f(0, \tau) = 1 - \exp\left[H^2\tau/D_{22}\right] \cdot \operatorname{erfc}\left[H\sqrt{\tau/D_{22}}\right]. \quad (6)$$

On the basis of obtained solutions (3), (4), the time dependences of surface concentrations of nitrogen and oxygen in titanium (Fig. 2a) and their spatial distributions in the diffusion zone (Fig. 2b) after saturation at  $T = 800^\circ\text{C}$  for 3h were calculated. The curves were plotted according to the following parameters:  $D_{11} = 1.2 \cdot 10^{-2} \cdot \exp(-45250/RT)$  cm<sup>2</sup>/s,  $D_{12} = \lambda_{12}D_{11}$ ,  $D_{22} = 0.8 \cdot \exp(-48000/RT)$  cm<sup>2</sup>/s,  $C_1^S = 16$  at. %,  $C_2^S = 33$  at. % [2],  $H = 5 \cdot 10^{-7}$  cm/s,  $\lambda_{12} = 0.5$ .

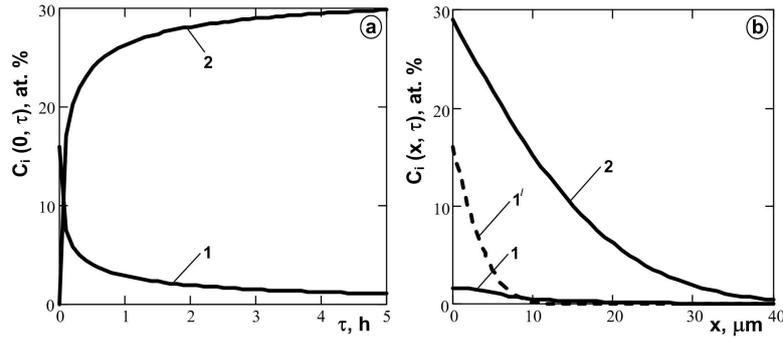


Figure 2: Time dependence of surface concentration of nitrogen and oxygen (a) and their spatial distributions in titanium after saturation at  $T = 800^\circ\text{C}$  for 3h. For nitrogen: curves 1 are for  $\lambda_{12} = 0.5$ , curve 1' is for  $\lambda_{12} = 0$ ; for oxygen: curves 2

Surface concentrations of oxygen and nitrogen depend on the saturation duration (Fig. 2a). The surface oxygen concentration (curve 2) increases gradually to equilibrium value with the medium because of slow oxygen delivery to titanium surface. The surface nitrogen concentration (curve 1), despite on the constant chemical potential on the surface, decreases with increase of exposure because of the increase of surface oxygen concentration. The diffusion zone with nonuniform distribution of oxygen and, especially nitrogen is formed in the near-surface layer of titanium as a result of gasing (Fig. 2b). The depth of the diffusion zone is determined by the distribution of oxygen concentration (curve 2), because the oxygen diffusion coefficient is two orders of magnitude larger than nitrogen diffusion coefficient. Distribution of nitrogen taking into account the influence of oxygen (curve 1) and without such consideration (curve 1') is different substantially. Nitrogen is pushed from titanium surface into the more distant zone because of the influence of diffusion dissolved oxygen. Under the certain time and temperature parameters the nitrogen distribution (curve 1) is nonmonotonic, its maximum concentration is not fixed on the titanium surface, but in the more distant zone from surface. Such character of nitrogen distribution is agreed with the experimental data [3].

## References

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