The Model of the Layer Boundary Diffusion in Multilayer Materials

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Abstract. The results of metallographic studies show the effect of the layers thickness of multilayer metal material on the diffusion depth after chemical heat treatment. The accelerate diffusion model of diffusible element along layers boundaries is proposed.

Introduction

A new class of structural metallic materials based on multilayer composite metal sheets may prove useful in engineering systems. Homogeneous materials consisting of hundreds or thousands of layers between large-angle boundaries are promising, as well as more traditional composites [1].

A method of producing multilayer samples (of sheet type) in which layers of two different grades of steel alternate has been developed on the basis of the research in [2]; the method employs hot rolling. This experimental technology permits the production of multilayer sheets with a laminar structure, characterized by the alternation of layers whose thickness is between 100 and 0.3 µm (according to calculations). The crystallographic disorientation of the layers is about 15°-20°; that corresponds to the large-angle grain boundaries in the initial steel [2]. In Fig. 1, we show the laminar structure of a 08X18H10+40X13 steel composite.

With appropriate choice of the initial composition that is, with the correct selection of the steel grades the laminar structure of the boundaries between the layers is retained up to the temperatures at which phase transitions begin in the initial steels.

Multilayer materials consisting of familiar steels are characterized by elevated mechanical properties along the layers in the structure [3]. They may be used as supporting elements in engineering devices. In that case, strengthening surface treatment, such as chemicothermal treatment, must be employed in the cross sectional planes of the samples that is, perpendicular to the direction of the layers.

The first experiments on chemicothermal nitriding in multilayer 08X18H10+08X18 steel composites showed that the depth of nitriding is greater in a multilayer material than in 08X18H10 steel [4]. It was found that the depth of nitriding increases with decrease in layer thickness in the samples of multilayer material treated in a single batch. In Fig. 2, we compare the depth of nitriding in the given multilayer composite with a layer thickness of 2 µm (Fig. 2a) and that of 08X18H10 steel in the same conditions (Fig. 2b).

The increase in thickness of the nitried layer in multilayer materials may be due to accelerated diffusion of nitrogen along the layer boundaries, with subsequent saturation of the layers from the boundaries. To confirm this hypothesis, in the present work, we propose a model of diffusion along the layer boundaries of a multilayer material, based on the Fisher model for grain boundary diffusion [5].
Fig. 1. Microstructure of the multilayer sheet sample of 08X18H10+40X13 steel composite after the first technological process: thickness of the sheet 2 mm; layer thickness ~20 µm; rolling perpendicular to the plane of the section [2].

Fig. 2. Nitrided layers: (a) in multilayer 08X18H10+08X18 steel composites (layer thickness 2 µm); (b) in 08X18H10 steel (control sample). Nitriding temperature $T = 540$ °C; time 45 h; $h$, depth of nitriding [4].

Model

Let us consider a system of parallel layers with thickness $l$ (Fig. 3). We assume that diffusion along the layer boundaries (LB) occurs in the same way as grain-boundary diffusion. In other words, at temperatures below 70% of the material's melting point, the diffusion coefficient $D_b$ along the layer boundaries is much greater than the diffusion coefficient $D$ within the volume of the layer. Note also that, as follows from microscopic research, the layer boundaries are continuous over their whole length and do not undergo any structural changes during the diffusion processes in the given conditions (chemicothermal treatment of the external surface, with the penetration of the hardening element, nitrogen, within the multilayer material).

In this work the diffusion model on LB of the multilayered material, based on Fisher's model for grain boundary diffusion [5] is considered.

Let some substance diffuses from an external surface of a multilayered sample on system of parallel LB, each of which have thickness $\delta$ (Fig. 3). Concentration of substance on an external surface is constant and equal to $c_0$. LB thickness also as thickness of the grain boundaries (GB) doesn't exceed 2-3 interatomic distances in crystal lattices of adjoining layers. Thickness of the layers divided by boundaries are identical and equal $l/\delta$. On Fig. 3 the direction of diffusive fluxes along LB and in the parties in adjoining layers is shown. We will designate diffusion coefficient on LB $D_b$, coefficients of volume diffusion in adjoining layers - $D_1$ and $D_2$. We consider
that diffusion on LB happens similar to diffusion on GB, and at temperatures values 0,7 are lower
temperatures of melting of a multilayered material diffusion coefficient on LB - \( D_b \gg D_1 \) and \( D_b \gg D_2 \). We consider that LB doesn’t undergo structural changes in the conditions corresponding
to considered diffusive processes.

![Diagram of diffusive fluxes](image)

Fig. 3. The directions of diffusive fluxes at diffusion along layer boundaries

We will consider two possible versions of model of diffusion on LB.

**Version 1.** Coefficients of volume diffusion in alternating layers are identical, \( D_1 = D_2 = D \). Thus
we will use all assumptions which are available in Fisher’s model. Then the diffusion model for
separately taken LB and for one layer will have an appearance

\[
\frac{\partial c_b}{\partial t} = D_b \frac{\partial^2 c_b}{\partial y^2} + \frac{2}{\delta} \frac{\partial D c_b}{\partial x} \bigg|_{x=\frac{\delta}{2}}
\]

(1)

\[
\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}
\]

(2)

c_b – concentration of diffuses element in LB, with – concentration in volume of a layer. Difference
of this option of model from Fischer's model [5] that diffusion in a layer is defined by two sources,
two layer boundaries, i.e. it will depend on layer thickness, \( l \).

Taking into account entry conditions - \( c (0, y, 0) = c (l, y, 0) = 0 \) and boundary conditions - \( c(x, 0, t) = c_0 ; c(0, y, t) = c_b \) solution of the
Eq. 2 at \( t > 0,05\delta^2/D \) (\( Dt/\delta^2 > 0,05 \)) with accuracy of 1 %
can be submitted in following form:

\[
\frac{c(x, y, t)}{c_b} = 1 - \frac{4}{\pi} \exp\left(-\frac{\pi^2 Dt}{\delta^2}\right) \sin\left(\frac{\pi x}{l}\right)
\]

(3)

Then we will find the solution of the Eq. 1 for a quasistationary case, we will receive:
\[ c_b = c_0 \exp \left[ \frac{8D}{D_b} \left( \frac{1}{8l} e^{-b} \right)^{0.5} y \right] \]  

(4)

where \( b = \frac{\pi^2 Dt}{l^2} \)

From the solution (4) it is possible to express the diffusive length of \( L_b \)

\[ L_b = \left( \frac{D_b \delta}{8D} e^{b} \right)^{0.5} \]  

(5)

For definition of position of the diffusive front in any point of a layer it is necessary to receive the common solution of the Eq. 1 and 2. It has the following appearance

\[ c(x, y, t) = c_0 \exp \left( -\frac{y}{L_b} \right) \left( 1 - \frac{4}{\pi} \exp(-b) \sin\frac{\pi x}{l} \right) \]  

(6)

At known values \( D, D_b \) and \( l \) the Eq. 6 allows to construct a profile of the diffusive front through all layer from \( x = 0 \) to \( x = 1 \).

With the help of the Eq. 6 we can estimate the nitriding depth of of composition 08X18H10+08X18 with layer thickness \( l = 5 \mu m \). Mode of nitriding we will choose the same that it was used in experiences for this composition in work [4] – \( T = 540 \) °C, exposure of 45 hours. For an assessment of the diffusion depth during the nitriding of process we will accept that the relation of diffusive length of volume diffusion to the average thickness of a layer value – \( (Dt)^{1/2}/l \) is only slightly greater than one, for example 1,1. On layers boundaries of \( D_b \) we will consider diffusion coefficient close to diffusion coefficients on grains boundaries that means that \( D_b/D \approx 10^3 \).

According to the Eq. 6 way of penetration on the middle of each layer \( L_V \) is determined by the expression

\[ L_V = L_b \left[ 1 + \ln \left( 1 - \frac{4}{\pi} e^{-b} \right) \right] \]  

(7)

Substitution of all provided data in expression (7) leads to estimated value of \( L_V \approx 320 \) microns. This value is close to the experimental data obtained for the layer nitrated depth of the composition 08X18H10+08X18 [4].

**Version 2.** Coefficients of volume diffusion in alternating layers are unequal, \( D_1 \neq D_2 \). The diffusion Eq. in LB will have thus an appearance

\[ \frac{\partial c_{b_1}}{\partial t} = D_b \frac{\partial^2 c_{b_1}}{\partial y^2} + D_1 \frac{\partial c_{b_1}}{\partial x} \bigg|_{y=-\delta/2} + D_2 \frac{\partial c_{b_1}}{\partial x} \bigg|_{y=+\delta/2} \]  

(8)

where with \( c_{x_1} \) and \( c_{x_2} \) – concentration in the layers located at the left and to the right of LB respectively (see Fig. 4). Two last expressions in the Eq. 8 show outflow of diffusing substance in the layers which are on the different parties from LB.
Distribution of diffusing substance from LB in adjoining layers can be described as follows:

\[
\frac{\partial c_x}{\partial t} = D_1 \frac{\partial^2 c_x}{\partial x^2}
\]  

(9)

\[
\frac{\partial c_x}{\partial t} = D_2 \frac{\partial^2 c_x}{\partial x^2}
\]  

(10)

The further solution of the Eq. 9,10 shows outflow of diffusing substance from LB in volumes of adjoining layers. The solution of a quasistationary problem in Eq. 8 was passed also as in version 1. As a result expression for concentration in LB was received

\[
c_x = c_0 \exp \left[ -\frac{4}{D_b} \frac{1}{\delta l} (D_1 e^{-b_1} + D_2 e^{-b_2}) \right]^{0.5} y
\]  

(11)

where \( b_1 = \frac{\pi^2 D_1 t}{l^2} \), \( b_2 = \frac{\pi^2 D_2 t}{l^2} \).

Diffusive length on LB - \( L_{b1,2} \), for this case is defined by expression

\[
L_{b1,2} = \left( \frac{D_b \delta l}{4(D_1 e^{-b_1} + D_2 e^{-b_2})} \right)^{0.5}
\]  

(12)

**Summary**

The depths penetration relation of diffusing substance along LB in versions 2 and 1 can be presented as follows

\[
\left( \frac{L_b}{L_{b1,2}} \right)^2 = \frac{D_1 e^{-b_1} + D_2 e^{-b_2}}{2D e^{-b}}
\]  

(13)
Estimates show that these depths can differ considerably (several times) if coefficients of diffusion differ in tens and hundreds times, and diffusive lengths of volume diffusion are small - $\sqrt{D_2t} \ll l$. That is at rather small times of process of diffusive penetration into a multilayered material diffusive zones of the next layers can differ considerably. At long exposures diffusive zones are leveled. It is in a qualitative consent with the experimental data obtained at nitriding of multilayered composition 08X18H10+08X18 [4], chemical heat treatment duration in these experiences made 45 hours.

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