Grain-boundary nitrogen diffusion model in multilayer materials

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Abstract. The paper presents the dependencies for the formation of diffusion layers in materials having a laminar structure, when they are saturated with nitrogen. The influence of chemical composition on the thickness of the nitrided layer has been determined. Models for formation of diffusion layers depending on permeability of interlayer boundaries and chemical formula of the composition are proposed.

1. Introduction

It is known that various reactions in solids associated with the change in microstructure and the progress of phase transformations are due to diffusion processes. The diffusion rate is largely determined by the structure of the material and imperfections of the crystal lattice, especially by the grain boundaries, which are the main elements providing accelerated diffusion. Therefore, boundary diffusion plays an important role not only in recrystallization processes, but also in reinforcing processes of the surface saturation with interstitial elements, such as nitrogen.

Most mathematical models describing grain-boundary diffusion processes are based on the model first proposed by Fisher [1]. In this case, the grain boundary is a semi-infinite isotropic layer of equal thickness. According to the model, during diffusion annealing, the diffusant actively penetrates along the boundaries with subsequent outflow into the grain body. Since the diffusion coefficient along the grain boundary is significantly higher than in the grain itself, it is along the boundary that the diffusant penetrates deeper, and that is why the boundary becomes a kind of diffusion source, from where the diffusant penetrates into the surrounding grains.

In the development of Fisher's ideas, grain-boundary diffusion models were proposed, according to which three types of diffusant penetration into adjacent grains can be observed, depending on the volume diffusion coefficient [2, 3]. In the first case, there is a strong outflow of the diffusant into the layer due to a significant volume diffusion coefficient (type A). The case of an impermeable boundary can be considered as diametrically opposite, when the volume diffusion coefficient is zero, and the diffusant outflow into the volume can be neglected (type C). The case when the boundaries are taken for semi-permeable can be considered as intermediate. In this case, the substance diffuses into the layer from the boundary, the flows from the neighboring boundaries do not interact with each other and do not overlap (type B) (Fig. 1).
2. Materials and research methods

The purpose of the study is to analyze and update grain-boundary diffusion models using the example of multilayer steel materials obtained by hot pack rolling according to the previously developed process flow [4-5]. The study used samples of multilayer materials consisting of alternating layers of 08kp and 08Ch18N10, 08Ch18N10 and 08Ch18, 08kp and U8 steels with a layer number of 100 and a layer thickness of 100 μm nitrated at a temperature of 650 °C for 45 hours.

![Diagram](image)

Figure 1. Effect of volume diffusion coefficients on diffusion layer concentration profiles

3. Results and discussion

The analysis of the microstructure showed that the models described above are explicitly implemented in the studied objects, however, the formation of diffusion layers is observed in only one of the layers, in this case in the layer of 08Ch18N10 steel (Fig. 2).

At diffusion saturation, nitrogen, first of all, begins to penetrate along the interlayer boundary, after which the outflow into the layer begins when a certain concentration is reached. However, the solubility of nitrogen in pure iron (08kp steel) at a temperature of 590 °C is 0.1%, so the diffusant does not penetrate into the layers of 08kp steel from the boundary. In these layers, only volume diffusion is observed, resulting in the formation of a thin crust consisting of ε-nitrides (Fe₂N) [6-9]. Conversely, chromium increases the solubility of nitrogen in iron, so the main outflow from the boundaries occurs into the layers of austenitic 08Ch18N10 steel [10-12], the diffusion proceeds according to the type B
mode. The layers of this steel also show volume diffusion with the formation of a nitride crust and a clearly detectable concentration profile.

![Figure 2](image2.png)

**Figure 2.** Microstructure of multilayer material of the 08kp+08Ch18N10 composition after nitrogen saturation

If the multilayer material is obtained on the basis of 08Ch18N10 and 08Ch18 steels, the microstructure shown in Fig. 3 is observed. Analysis of the microstructure shows that during diffusion annealing, the diffusant also first of all actively penetrates along the interlayer boundary with subsequent outflow into the layer. Since the steel layers are alloyed with chromium, the outflow occurs both into 08Ch18N10 steel and into 08Ch18 steel, the diffusion proceeds according to the kinetic type A mode. Nickel reduces the solubility of nitrogen, as a result, a convex meniscus is observed in the layers of 08Ch18N10 steel, which indicates a lower rate of volume diffusion [13].

![Figure 3](image3.png)

**Figure 3.** Microstructure of multilayer material of the 08Ch18+08Ch18N10 composition after nitrogen saturation
With diffusion saturation of the multilayer material obtained on the basis of U8 and 08kp steels, the microstructure (Fig. 4) is of the type that is observed in the 08Ch18N10+08Ch18 composition, but in this case the diffusion layers are much smaller. This is due to the fact that 08kp and U8 steels have low nitrogen solubility. As a result, a crust consisting of iron nitrides is formed on the surface, which makes further penetration of the diffusant into the material impossible.

![Microstructure of multilayer material of the 08kp+U8 composition after nitrogen saturation](image)

**Figure 4.** Microstructure of multilayer material of the 08kp+U8 composition after nitrogen saturation

As a result of consideration of the proposed compositions, a refined model for formation of diffusion layers in multilayer steel materials can be formed depending on the chemical composition of the layers and the permeability of the boundary (Fig. 5).

![Model for formation of diffusion layers in multilayer materials](image)

**Figure 5.** Model for formation of diffusion layers in multilayer materials

(a) one boundary is permeable; (b) two boundaries are permeable; (c) both boundaries are impermeable
4. Conclusion
Thus, a grain-boundary diffusion model in multilayer materials has been obtained. The concentration profile and contribution from the grain boundary is only observed if there is at least one layer capable of dissolving the diffusing element.

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