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A simple diffusion model for the growth kinetics of γ' iron nitride on the pure iron substrate

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Abstract

A simplified diffusion model designed to predict the thickness, microstructure of nitrided layer on the pure iron, and the nitrogen profile is reported. The error function model based on Fick's laws was used to study the growth kinetics of γ' phase during the gas nitriding process. The validity of the generated computer program was checked by comparing our simulation results with the experimental data taken from the literature and a fairly good agreement is achieved between calculated and experimentally measured values.
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1. Introduction

Gas nitriding is a technologically important surface treatment process which is well known to improve the tribological properties, the fatigue endurance and the corrosion resistance [1].

Depending on the composition of the nitriding atmosphere and the temperature, a compound layer that consists mainly of ε-$Fe_{2-3}N$ and/or γ'-Fe_4N is produced on the surface of the pure iron, and beneath the layer, a diffusion zone where nitrogen is dissolved interstitially in the iron matrix. Understanding of the gas nitriding of pure iron provides an essential, general basis for the subsequent modeling of gas nitriding of Fe–C alloys and alloyed steels. Hence, in order to optimize process control, it is necessary to have a clear understanding of the basic phenomenon which is the nitrogen diffusion.

In case of iron gas nitriding, several papers have been published [2–10] on the modeling of the

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monolayer growth kinetics of γ' phase. The comparison between the simulated results is rather difficult since they depend on the thermodynamic data used (i.e., the phase boundaries in the Fe–N phase diagram) as well as on kinetic data regarding the diffusion coefficients of nitrogen in α-Fe [11,12] and γ' [5–8] phases.

In the current work, a diffusion model based on Fick's laws, coupled with a thermodynamic description of the Fe–N binary system, was used for the study of the growth kinetics of γ' phase onto pure iron surface. Recently, the same model was successfully applied to the paste-boriding process [13]. Comparison of the simulation results obtained by this model with the experimental data from the literature was performed in order to validate the generated computer program used for simulation calculations. Particularly, this model was capable of predicting the nitrogen depth-concentration profiles for γ' phase as well as the locations of (γ'/α) interface.

2. Formation of γ' phase on the iron substrate

The growth of the nitrided case during the gas nitriding is assumed to be controlled by the diffusion of nitrogen atoms over the sites of their own sublattice (Fe–N phases [14] can be conceived as constituted of an Fe sublattice and an N sublattice: the latter is formed by the octahedral interstices of the Fe sublattice). Depending on the N activity imposed at the iron surface, the compound layer formed during the gas nitriding process, contains either γ' monolayer or (ε/γ') bilayer. When exceeding the maximum lattice solubility of N in the α-Fe phase, the formation of γ' phase becomes possible with an appropriate nitriding potential. The nitriding potential which is a fundamental parameter of the nitriding process, can be calculated from Eq. (1):

$$K_{\mathrm{N}}\,(\mathrm{atm}^{-1/2}) = \frac{p_{\mathrm{NH_3}}}{p_{\mathrm{H_2}}^{1.5}} = \frac{(1-y)}{(0.75y)^{1.5}} \tag{1}$$

where $p_{\mathrm{NH_3}}$ and $p_{\mathrm{H_2}}$ are partial pressure of NH_3 and H_2 respectively, and y is the fraction of dissociated ammonia which can be determined by the exit gas composition.

The so-called Lehrer diagram updated by Maldzinski [9], provides the composition range of iron nitrides as function of a reciprocal temperature and nitriding potential. A schematic illustration of the nitrogen-concentration profile is presented in Fig. 1 at a given temperature and under a nitrogen potential which allows the formation of γ' phase.

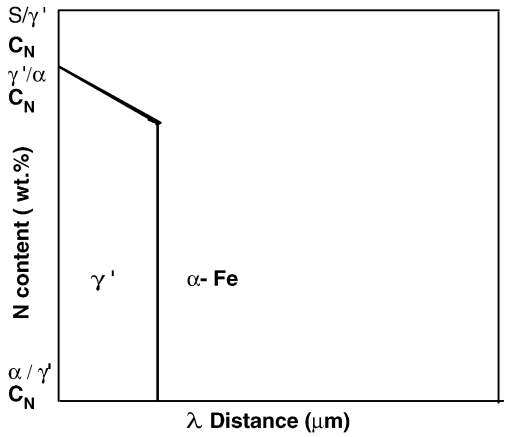

Fig. 1. Schematic illustration of concentration-depth profile for nitrogen diffusion controlled growth of γ' monolayer into α-Fe substrate.

3. Formulation model

As a result of nitrogen mass transfer from the ammonia gas to the iron surface, a nitrogen depth-concentration gradient is established. The evolution of atomic nitrogen in α-Fe phase obeys the Fick's second law which is the governing equation in modeling the gas nitriding process, i.e.,

$$\frac{\partial C_{\mathrm{i}}}{\partial t} = D_{\mathrm{i}}\frac{\partial^2 C_{\mathrm{i}}(x,t)}{\partial x^2} \tag{2}$$

where D_{i} is the effective diffusion coefficient for i phase, with i = (α or γ'), and $C_{\mathrm{i}}(x, t)$ is the concentration of nitrogen at a depth x after diffusion time t.

The following assumptions have been made in the formulation of the growth model:

- the model concerns nitrogen diffusion in the solid state, semi-infinite medium;
- the iron nitride γ' nucleates instantly on the iron substrate at $t = 0$;
- planar morphology is assumed for the (γ'/α) interface;

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