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Cellular automata modeling of nitriding in nanocrystalline metals

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ABSTRACT

Severe plastic deformation has made it possible to alter the grain size of metal surface to nanoscale. With refined nanograins, the grain boundary effect on diffusion and phase transformation cannot be neglected. Consequently, the widely used conventional 1D nitriding model is not applicable. In this study, a 2D model considering grain boundary diffusion has been developed to investigate nanocrystalline nitriding. As a multi-physical process, both phase transition and diffusion are modeled. Cellular automata method was used to integrate the two models, and more importantly to deal with the moving 2D interface induced by grain boundaries. The phase transition model and diffusion model were validated with experimental data and the Maxwell–Garnett effective diffusion model, respectively. After validation, nitriding of nanocrystalline iron at low temperature (300 °C) was simulated and compared with nitriding of coarse-grained (μm level) iron. In addition, the growth kinetic, composition and spatial distribution of the nitride layer in nanocrystalline nitriding, with different temperatures, surface nitrogen concentrations and different grain sizes, were studied. It has been found that these parameters could significantly affect the growth rate as well as the composition of the nitrided layers. The results also demonstrated that the presence of nanoscale grain can not only decrease nitriding temperature and nitriding duration making low temperature nitriding possible, but also increase the volume fraction of ϵ and γ' phases in the nitride layer and therefore a better nitriding quality.

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1. Introduction

Nitriding, as an important surface engineering technology, has been widely used to process steels in order to improve the hardness, the fatigue performance and the corrosion resistance. After nitriding, a compound layer (white layer [1]), with the combination of ϵ-Fe phase (Fe_3N) and γ'-Fe phase (Fe_4N) can be formed on the steel surface. Beneath the white layer, there is a "diffusion zone", where nitrogen diffused into the matrix. Such surface structure gives rise to better wear resistance and longer fatigue life than the untreated. However, the nitrogen diffusivity is extremely low in coarse-grained material. For example, the nitrogen diffusivity in iron nitrides is at 10^{-12} m^2/s level at 570 °C [2]. As a result, long duration (7–10 h) and high temperature (around 600 °C) are needed in nitriding processing. Long duration processing at high temperature may cause unexpected consequences such as distortion and precipitation of alloying element. To improve nitrogen diffusivity and therefore reduce the processing duration and temperature, one potential method is to increase the fraction of grain boundaries because of the high diffusivity at grain boundaries.

To substantially improve the fraction of grain boundaries, one needs to refine the grain size of material to nanoscale. Conventional grain refinement, like forging, extrusion and heat treatment, can only decrease the grain size to micro-scale. Recently, severe plastic deformation (SPD) [3] and fast quenching [4] have been proposed to decrease the grain size below micro-scale. The idea of SPD is to generate nanocrystalline structure in bulk material by introducing massive plastic deformation. As one of the SPD technique, surface severe plastic deformation (SSPD) [5] only introduces deformation on the surface. One advantage of SSPD is that it only alters the surface of the material so that its bulk properties are preserved. Another advantage is that the material does not need to go through high temperature compared with fast quenching so that the bulk geometry can be maintained. Both advantages are aligned with nitriding because the nitriding efficiency is only affected by surface condition. Based on these facts, SSPD is a promising candidate to generate nanostructure for nitriding. Depending on the specific way to induce surface plastic deformation, a few techniques have been developed including Surface Mechanical Attrition Treatment (SMAT) [6] and Ultrasonic Nanocrystal Surface Modification (UNSM) [7]. It is worth mentioning that, Tong and his colleagues have successfully lowered the nitriding temperature by generating surface nanocrystalline structure through SMAT [6], and the follow-up research works [8–11]

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have proven the possibility of this duplex process combining SSPD with nitriding.

In spite of the experimental endeavor, the mechanism of nitriding efficiency improvement is still unclear [12,13]. In addition, the properties of the treated workpiece, like hardness, wear resistance and corrosion resistance largely depend on nitrogen concentration. There is an urgent need to develop a numerical model to quantitatively predict the nitrogen concentration and provide better understanding of SSPD assisted nitriding.

The modeling work of nitriding can be traced back to the analytical model in Roy's work [14], which was initially proposed for carburizing of metals. Roy indicated that for those processes with small atom diffusion in the interstitial space of metal matrix, like carburizing and nitriding, diffusion of metal atoms is negligible. Therefore, only the diffusion of interstitial atom was considered. In addition, local thermal equilibrium assumption, which determines the concentration at the interface directly from phase diagram, and 1D planner interface assumption were also used in Roy's model. Based on these assumptions, a 1D multilayer diffusion model was built. Somers and Mittemeijer [15] applied this model in nitriding of pure iron and quantified the nitrogen diffusivity with experiments. With a linear approximation for the composition in the nitride layer, their prediction result fits well with the experiment data. Soon after their works, Torchane et al. [2] have conducted a comprehensive study on gas nitriding of pure iron with constant surface nitrogen concentration, and deduced an analytical model to predict the layer depth which was validated by their experiments. The finite volume numerical method was also introduced to solve diffusion equation and the nitrogen diffusivity in alloy was calculated using thermodynamic calculation [16]. To make the model more commercially practical, the relation between the equilibrium nitrogen concentration and the nitriding potential on the surface of iron based alloy also introduced in the numerical calculation [1].

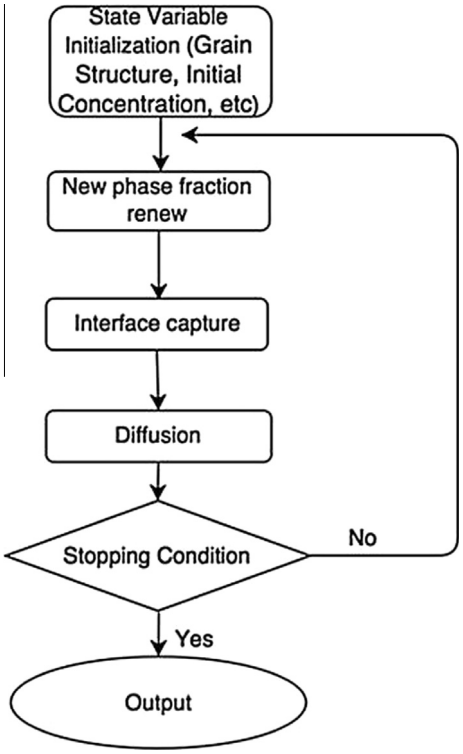

Fig. 1. Flow chart of the numerical model.

However, those models are 1D multilayer diffusion models and the grain boundary effects were ignored in their models. As a result, their models cannot be applied in nanocrystalline nitriding where the grain boundary plays an important role. Recently, some researchers have calculated the effective diffusivity of nanocrystalline materials [17,18] and used such effective diffutivity in 1D nitriding modeling. Therefore these works are still limited in 1D multilayer model, failing to capture heterogeneous phase growth and phase transformation due to the existence of the nanoscale grain boundaries. A 2D model is in lack to fully represent the crucial physical processes resulting from refined grain boundaries. When grain boundaries in presence, the moving phase interface becomes irregular in 2D or 3D configuration, which raises a tremendous challenge for modeling. To the knowledge of the authors, there is no work in literature towards solving the numerical challenge in the context of nitriding.

In this work, for the first time, a 2D nitriding model considering the grain boundary has been developed to study nitriding of nanocrystalline metals. In Section 2, we described the details of the numerical method. The nitrogen diffusion was calculated by the finite volume method, and the interface tracking was realized by the cellular automata (CA) algorithm. In Section 3, we first validated the numerical model by comparing the numerical results with experimental data available in the literature as well as theoretical prediction (the Maxwell–Garnet model); we then systematically studied of the effects of grain boundaries in nitriding process.

2. Numerical modeling

2.1. Overall description of the numerical model

There are two fundamental processes, nitrogen diffusion and phase transformation in the nitriding model. The physical processes occur through the network of grain boundaries, which increases the computational complexity significantly. Moreover, the phase transformation in a 2D domain requires capturing the phase nucleation and the growth interface. Because the phase transition tends to occur along the grain boundaries, the growth interface also evolves along the grain boundaries. The irregular interface gives rise to tremendous numerical difficulty. To solve the problem, we innovatively introduce the cellular automata (CA) algorithm to track phase growth interfaces and grain boundaries. With the application of the CA method, for the first time, the modeling of nitriding in 2D grained structure becomes possible. The nitrogen diffusion process is modeled by the finite volume method (FVM). A flow chart of the model is presented in Fig. 1, and the details of each step will be discussed in the following.

2.2. The phase transformation model

In order to study the Fe–N binary system, a Fe–N phase diagram [19], which is extended to 300 °C, is used in this study. According to the binary Fe–N phase diagram (Fig. 2), ϵ phase, γ' phase nitrides and α phase can form at corresponding temperature and nitrogen concentration. Between different phase regime, two kinds of phase interfaces, α/γ' and γ'/ϵ interfaces, need to be considered. A few key assumptions are made here. (1) At the growing interface with two phases, the assumption of local equilibrium is applied, i.e., the nitrogen concentration at the interface is directly determined by the phase diagram (Fig. 2). (2) The diffusion of iron atoms are ignored, therefore the phase transformation at both phase interface and matrix relies on nitrogen diffusion and concentration. There is no need for nucleation model based on the fact that nucleation occurs much faster than diffusion. This assumption is also widely used in 1D nitriding simulations [2,14,15]. (3) Nitride dissociation

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