

A simulation of Cr depletion in austenitic stainless steel with cellular automaton

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ABSTRACT

A cellular automaton modeling was developed to investigate the growth kinetics of Cr-rich carbides' precipitation and the three dimensional distribution of Cr concentration. The effects of solution treatment conditions and sensitization temperatures on Cr depletion were studied in detail. The results indicated that the amount of precipitate increased as sensitization temperature increased, decreasing along with the solution treatment temperature. Furthermore, the changing tendency of the precipitate's amount was in accordance with that of the degree of sensitization (DOS) obtained from the samples treated at the corresponding conditions.

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1. Introduction

The stainless steel has been widely used in various industries because of their excellent corrosion resistance. However, it is susceptible to corrosion and even leads to stress cracking corrosion when it is exposed in an environment with temperature between 450 and 900 °C. The main reason is that Cr-rich carbides and intermetallic phases precipitate along grain boundaries. Adjacent to the carbides, there is a chromium-depleted zone that can be preferentially attacked in corrosive environment [1–6]. In order to correlate intergranular corrosion (IGC) with the grain boundary characteristics, many studies have been devoted to evaluate the depleted zones quantitatively by empirical or analytical models [7–13].

Generally speaking, these models are successful to evaluate the stages of sensitization and desensitization to the IGC, but they can only produce the Cr concentration profiles rather than giving an overall view of the Cr distribution. So the intention of this work was to simulate the Cr distribution over a whole area.

As an important algorithm that describes the discrete spatial and temporal microstructure evolution on a mesoscale, cellular automaton (CA) has been applied to simulate recrystallization

[14–16], grain coarsening [17,18], phase transformation [19–21] and grain growth [22–25]. But there is so far no research about the precipitation evolution of Cr-rich carbides and the corresponding distribution of Cr concentration in austenitic stainless steel. Therefore, in this work, CA was used to simulate the precipitation process of Cr-rich carbides and the distribution of Cr concentration in a three dimensional way. The paper has also studied the effects of sensitization temperature and grain size on the precipitation.

2. Cellular automaton model

The solubility of carbon drops sharply when the temperature decreases, and it will precipitate in the form of Cr-rich carbides at grain boundaries. The nucleation will only occur at grain boundaries, considering that the diffusivity of C is several orders of magnitude higher than that of Cr. Based on the classical nucleation theory [19–21], the nucleation model can be described as follows:

$$I = K_1 D_\gamma k T \exp\left(-\frac{K_2}{kT(\Delta G)^2}\right) \quad (1)$$

where I is the nucleation density, K_1 is a constant related to the nucleation site density, K_2 is a constant related to all the interfaces involved in nucleation, D_γ is the Cr diffusion coefficient, k is the Boltzmann's constant, and ΔG is the driving force.

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Table 1

The key parameters used in the present model.

Parameters	M_0 ($\text{m}^4 \text{J}^{-1} \text{s}^{-1}$)	γ_m (J m^{-2})	θ_m	a (μm)	β	Q (kJ mol^{-1})	[12,17]
Values	1.56×10^{-11}	0.56	15°	1	0.137	245.7	

The growth of carbides is assumed to be controlled by both of the Cr diffusion and the interface mobility. As the interface moves during the precipitation, Cr atoms transfer from the matrix to the interface, and then they precipitate to the carbides. Consequently, the growth of carbides can be described as a free boundary problem for Cr diffusion in austenite and the dynamics of the interface. The Cr diffusion in austenite is described as follows:

$$\frac{\delta c}{\delta t} = \nabla \cdot (D \nabla c) \quad (2)$$

where c is the Cr concentration and D is the Cr diffusion coefficient. Usually, the interface velocity is determined by [17–25]:

$$v = MF \quad (3)$$

here M is the effective interface mobility, which includes the structural influence in interface mobility, such as pinning effects, setup of stresses or solute drags. F is the chemical driving force for interface migration. But allowing for the characteristics of precipitation of Cr-rich carbides, the mobility of interface is equal to the carbides' growth and the length of the interface covers can be expressed by [12,13]:

$$l = \beta \sqrt{Dt} \quad (4)$$

where t is the sensitization time and β is a constant. D is the Cr diffusion coefficient, which depends on the temperature as a thermally activated process [12,13]:

$$D = D_0 \exp\left(-\frac{Q}{RT}\right) \quad (5)$$

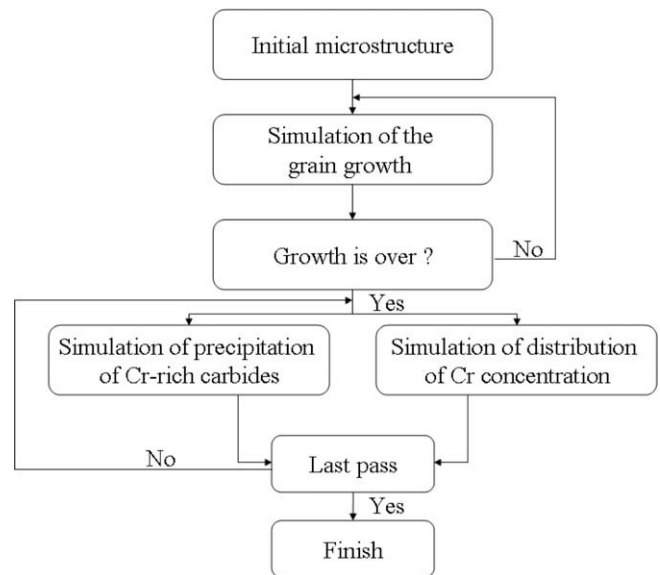
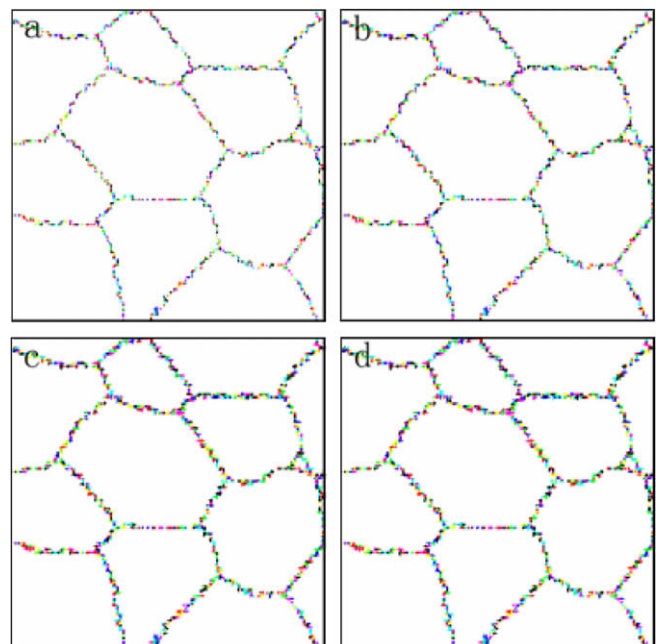
here D_0 is a pre-exponential factor, Q is the activation energy, R is the universal gas constant, and T is the absolute temperature. All the key parameters are listed in Table 1.

3. Results and discussions

Two kinds of different austenitic stainless steels were investigated in the present paper: AISI 304 and 316 austenitic stainless steels. Chemical compositions of these materials are given in Table 2. The heat treatment was carried out in a program control muffle (SXL-1208), and the changing range of temperature was $\pm 1^\circ\text{C}$. First, the muffle was heated to the required temperature, and then the samples were put into it after the temperature was stable and heated for a certain time. The samples (AISI 316) that were used to investigate the influence of sensitization temperature on Cr depletion were heated at 1100°C for 1 h, and then sensitized at 600, 650 and 700°C for 0–96 h. The 304 stainless steel was treated at 900, 1000 and 1100°C for 0–6 h and then sensitized at 650°C for 12 h in order to study the effect of grain size on Cr depletion.

After the heat treatment, the samples were tested by the electrochemical potentiodynamic reactivation (EPR) in a solution that

consisted of 0.5 M H_2SO_4 and 0.01 M KSCN [1,2,6]. A three-electrode set-up cell was used, with a saturated calomel electrode (SCE) as the reference electrode, two platinum plates as the counter electrode and the specimen as the working electrode. The electrode was stabilized in the cell for 10 min to determine the corrosion potential. Then it was polarized anodically to 0.3 V at 1.67 mV/s. As the maximum potential was reached, the scanning

**Fig. 1.** The flowchart of the CA simulation.**Fig. 2.** The microstructure of sensitization and desensitization obtained at different time: (a) 100 h, (b) 200 h, (c) 350 h and (d) 400 h.**Table 2**

Chemical composition of AISI 304 and 316 stainless steels.

	Elements (wt.%)							
	C	Mn	Ni	Si	P	S	Cr	Fe
304	0.055	1.00	8.48	0.60	0.029	0.005	18.28	Balance
316	0.043	1.68	12.13	0.56	0.024	0.024	17.60	Balance

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