



Cellular automaton-based study of factors that affect dynamic solid phase transformation kinetics



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ABSTRACT

In this study, we simulated the β to α solid phase transformation in the preferred crystallographic orientation of TA15 alloy using a virtual front tracking modified cellular automaton model. The transformation kinetics were resolved by coupling the interface moving velocity and solute diffusion equations. The simulated phase transformation kinetics and microstructure agreed well with the results predicted by the Zener–Hillert equation and experimental data. We quantified the effects of temperature, interface curvature, preferred growth angle, and kinetic parameters, including solute diffusion and the interface mobility coefficient, on new phase morphologies and micro-segregation. Furthermore, diffusion/mixed/interface controlled transformations were distinguished by differences in the interfacial solute concentration from the initial solute concentration and the equilibrium solubility of the parent phase. Three transformation modes were simulated by varying the diffusion coefficient, interface mobility coefficient, and transformation driving force factor.

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1. Introduction

During hotworking or heat treatment processes with titanium, β to α or α' transformations lead directly to the arrangements and morphology of the constituent phases, which ultimately determine the mechanical properties of titanium products in engineering [1]. During solid phase transformation, the evolution of the microstructure is complex because it is affected by the heterogeneous grain size of the parent phase, asynchronous transformation in different zones at different times, crystallographic anisotropy, thermodynamics, kinetics, and other factors. This complexity makes numerical simulation increasingly attractive in this field. Previously, most microstructural simulations have focused on the transformation of austenite to ferrite in Fe–C and Fe–C–Mn steels [2,3], as well as other diffusion-controlled transformations [4–6]. It is still unclear whether there is a general solution for all types of phase transformations because many confusing problems still exist, i.e., para-equilibrium, solute drag, nonsteady state of interface frontier, sharp/continuous interface, and the corresponding transformation mode.

Scientists are always striving to obtain a better understanding of solid phase transformation models. The advanced models of solid phase transformation are divided mainly into the classic analytic solutions, finite element method, phase field,

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and cellular automata (CA). In the early stages, analytic solutions and their combination with the finite element method were applied widely [7,8]. Most of these models considered the complete diffusion-controlled transformation of interstitial solutions. The model outputs comprise the transformation fraction and interface moving velocity, but also the transient interface characteristics or phase morphology. The phase field does not have to track the moving phase boundary explicitly, but instead it uses a uniform continuous function as the governing equation for the phase state transition. Meozzi performed a phase field simulation of the transformation of austenite to ferrite in steels [9], where the chemical driving force of the transformation was linearly proportional to the difference in the carbon concentration of austenite at the interface compared with the equilibrium carbon concentration. Many studies have also used the conventional Gibbs energy formula, which is a function of the phase variable that implicitly represents the Gibbs energy change according to the phase state, i.e., by taking the Gibbs energy change as the driving force [10,11]. Loginova et al. [12] simulated the morphology of Widmanstätten ferrite with predefined anisotropy in the interface properties, where a transition was predicted from diffusion-controlled to massive transformation when the solute supersaturation (initial solute concentration) was very large. Huang et al. [13] simulated ferrite precipitation in a smooth globular shape. Nakajima et al. [14] simulated the formation of flake pearlite using multi-phase field model, which demonstrated carbon diffusion in ferrite, and the growth of cementite from ferrite increased the kinetics of the pearlitic transformation by a factor of four compared with growth from austenite only. Yamanaka et al. [15] calculated the interface energy and interface mobility determined by the phase state and grain angles to reproduce the austenite to ferrite transformation. However, the computational domain of the phase field was limited due to the extremely thin interfacial thickness.

CA is a popular method due to its computation efficiency, flexibility in multi-scale bridging, and physical consistency. There are many examples of its application but they mainly deal with the transformation of austenite to ferrite in multi-grains [16,17]. Quantifying the inherent transformation kinetics of solute diffusion and the interface mobility characteristics is of great importance for the practical applications of CA models. However, to the best of our knowledge, previous phase transformation CA models have not included sufficient information about the factors that control the transformation kinetics, especially the transformation mode. It is widely accepted that massive transformation is much faster than diffusion-controlled transformation, but solute partition is swallowed up by the fast moving interface in the former case. It is also known that as the interface mobility coefficient increases, the interface mode transformation shifts toward diffusion mode transformation, where both the transformation rate and solute partition are large. Obviously, the interface concentration is similar in massive transformation and interface mode transformation, whereas the transformation rate is completely different. Thus, we clarified this mechanism in the present simulation study.

In our previous study [18], we presented the virtual front tracking CA approach and verified that it was very successful when studying the crystallographic characteristics of transformation. In the present study, we focus on the numerical solutions of the CA model and its quantitative capabilities. The simulation was performed using a common transformation driving force model and a fixed transformation condition (constant temperature, diffusion, and interface mobility coefficient). To further extend this new model, we performed a quantitative analysis of the β to α transformation kinetics in terms of the factors that affect the transformation. We considered numerical and physical parameters such as the calculation grid size, time step, temperature, curvature effect, solute diffusion, interface mobility, and transformation driving force. We evaluated the transformation driving force models to obtain a more precise simulation. Three types of transformation are distinguished by a quantitative formula, i.e., diffusion, interface, and mixed transformation modes. We clarified the features of different transformation modes, including the interface moving velocity, solute flux around the interface, transformation driving force, and solute concentration gradient.

2. Models and simulation

2.1. Thermodynamics

In this study, we investigated TA15 alloy, which has a chemical composition of: Ti–11.26Al–0.644Mo–1.384V–1.105Zr–0.035Fe–0.132Si–0.138C–0.221H–0.176O–0.049 N (mole pct). Allotropic transformation is dominant during isothermal treatment or cooling from a high temperature [19], when the parent phase with a body centered cubic (bcc) crystal lattice transforms into a new phase with a hexagonal close packed (hcp) crystal lattice. The growth habit relations are $\{110\}_{\beta} // \{0001\}_{\alpha}$ and $\{1\bar{1}1\}_{\beta} // \{1120\}_{\alpha}$. The growth parallel to a certain crystallographic orientation is characterized by strong anisotropy in the interfacial properties, which results in the typical Widmanstätten structure found in metallurgy. Thermodynamics calculation of the multi-component TA15 alloy were performed using the Ti-Data database TT-Ti with Thermo-Calc software to consider the effects of the chemical elements listed in Fig. 1(a). The thermodynamic calculations indicated that β to α and reverse phase transformations in the TA15 alloy occur approximately between 980 and 776 °C. The equilibrium solubilities (molar fractions) of the α phase-stabilized element Al and the β phase-stabilized element Mo in two phases are shown in Fig. 1(b). The temperature-dependent solubility was fitted based on the corresponding values at different temperatures and the following formulae were obtained:

$$\begin{aligned} X_{Al}^{\beta} &= 1.26138 \times 10^{-4}T - 0.04547, \\ X_{Al}^{\alpha} &= 1.3X_{Al}^{\beta}, \end{aligned} \quad (1-1)$$

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