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The Application of Phase Field Method in Microstructure Evolution Simulation

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Abstract. The physical properties and mechanical behaviour of metals are determined by their microstructure frequently. The microstructure is referred to the size, shape and spatial arrangement of phases, grains, etc. These microstructure features have the mesoscopic length scale. How to obtain the desired microstructure is one main task of metal alloy design. However, it is difficult because the microstructure evolution is influenced by the chemical driving force during phase transformation, the composition of the alloy, etc. With the development of computing power and computer modelling, the computational material science is playing an important role in the microstructure design. Especially the kinetic phase field method is a powerful tool which is fast developed and widely used in these years. The phase field method is a phenomenological approach based on classical thermodynamic and kinetic theories. It describes a microstructure by using field variables. In this paper, the basic principle and application of this method are presented.

1. Introduction

The metal alloy design has started from thousand years ago. However, the influence of microstructure on materials' properties is known until hundred years ago. Nowadays, the microstructure design of metal alloy is popular. Especially, the microstructure tailor through computational materials science is a vital method to obtain the required properties of materials.

The computational materials science is quickly developed in these years due to the fast improvement of the computing power. The phase field method which is one of the computational material sciences has shown strong power in the microstructure design from the beginning of its development.

The phase field method is a phenomenological approach based on classical thermodynamic and kinetic theories. It describes a complicated microstructure (chemical and structural non-uniformities) as a whole using a set of field variables that are spatially continuous and time dependent [1-5]. In the following sections, the basic principle and application of this method's will be presented.

2. Principle of the phase field method

The spatial distribution and time-evolution of the microstructure can be described by non-conserved structural order parameter fields, $\eta_p(r, t)$ as a function of position and time, where $p = 1 \sim n$. The number n is determined by the structural characters. For example, the system shown in figure 1, there are two phases, i.e., the red phase on the left and the blue phase on the right. Therefore, two variants are needed to describe the microstructure evolution, h1r and h2r. The profile of these two variants along the Z direction through the central axis is shown in figure 2(a). The concentration profile is shown in figure 2(b). The growth process of variant h1r is shown in figure 2(c). It indicates that the red phase grows by consuming the blue phase. In brief, the microstructural evolution of alloys can be

expressed by these two kinds of variants, i.e., the structural order parameter and concentration parameter. For example, the red phase indicates the water and the blue phase indicates the ice in Fig. 1,while the variants evolution shown in figure 2(c) means the melt of ice.

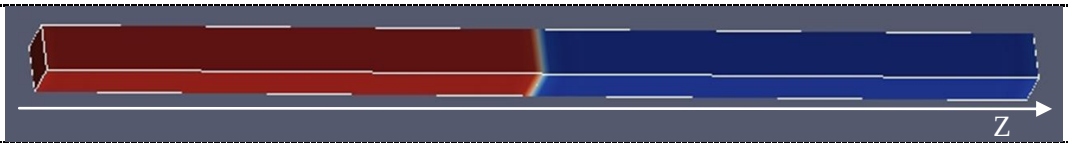

Figure 1. The red phase on the left and blue phase one the right in the system. The thin central layer is the interface of the two phases.

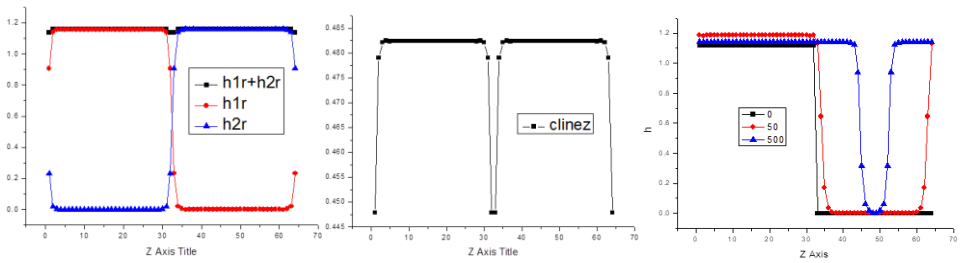

Figure 2. The structural order parameter profile (a) and concentration profile (b) of the two phases. The growth process of variant h1r (c).

The driving force of the microstructure evolution is the reduction of the total chemical free energy which consists of the local specific chemical free energy, the interfacial energy and the elastic strain energy. The local specific chemical free energy profile is shown in figure 3. It is a function of the structural order parameter and the concentration.

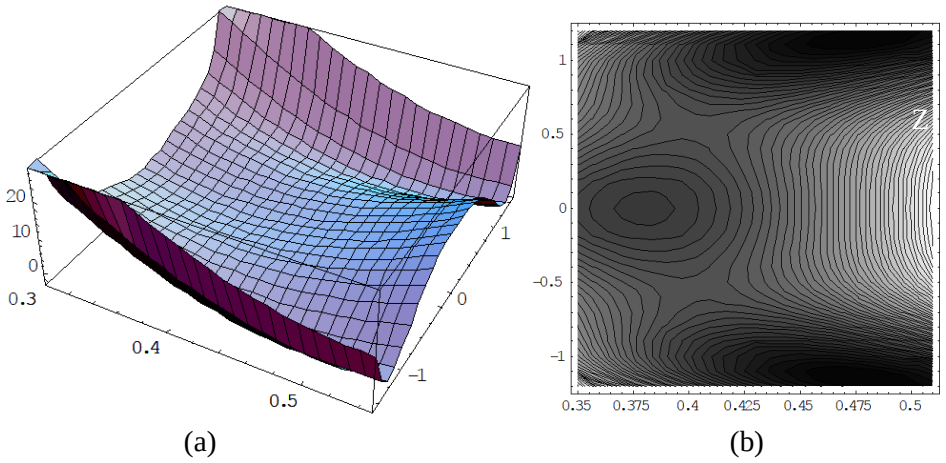

Figure 3. The local specific chemical free energy profile, (a) 3D view plot and (b) top view plot. This energy is a function of the structural order parameter and the concentration

The chemical driving force of the phase transformation is the energy difference between the phase alpha and phase beta shown in figure 4. The alpha phase is stable when the concentration is less than about 0.4, while the beta phase is stable on the other side.

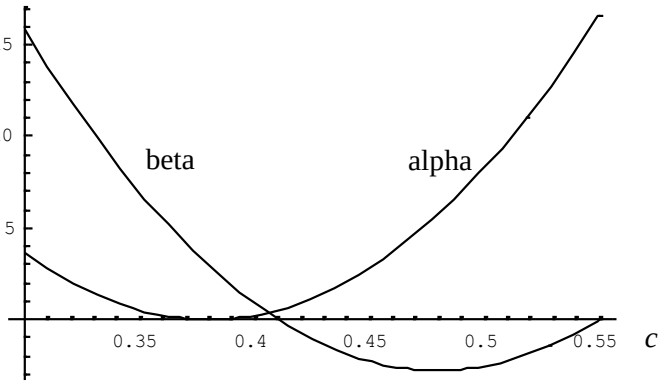

Figure 4. The chemical driving force for phase transformation.

The temporal evolution of the structural and the concentration fields are described by the time-dependent Ginzburg-Landau equation (1) and the non-linear Cahn-Hilliard diffusion equation (2) [1, 2], respectively,

$$\frac{\partial \eta_{\mathrm{p}}(\mathrm{r},t)}{\partial t} = -L\frac{\delta F}{\delta \eta_{\mathrm{p}}(\mathrm{r},t)} + \xi_p(\mathrm{r},t);\ \ p = 1,2,...,6 \tag{1}$$

$$\frac{\partial c(\mathrm{r},t)}{\partial t} = M\nabla^2\frac{\delta F}{\delta c(\mathrm{r},t)} + \zeta(\mathrm{r},t) \tag{2}$$

where L and M are kinetic coefficients characterizing structural relaxation and chemical mobility respectively (assuming that L and M are constants). F is the total free energy of the system, ξ_p(r, t) and ζ(r, t) are the random noise terms related to fluctuations in the structural order parameter and concentration, respectively.

The microstructure evolution process can be simulated with above variants selection, energy and governing equations formation. For example, the phase transformation of alpha to gamma has been investigated using the phase field method [6]. The detailed nucleation process is shown in figure 5. The nucleation and growth process is clearly seen from the simulation results. The twin nucleation is the main manner during alpha to gamma phase transformation. The twin frequency can be obtained with detailed statistical analysis, shown in figure 6. Furthermore, the influence of input parameters, such as the elastic energy coefficient, on the twin frequency can be obtained.

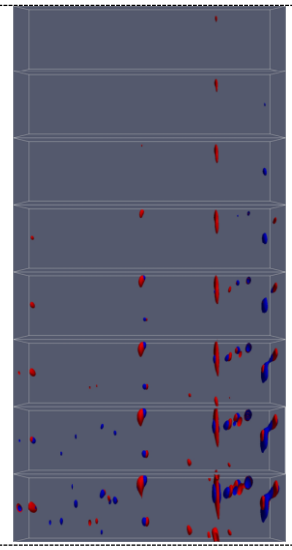

Figure 5. The nucleation process in the phase transformation of alpha to gamma.

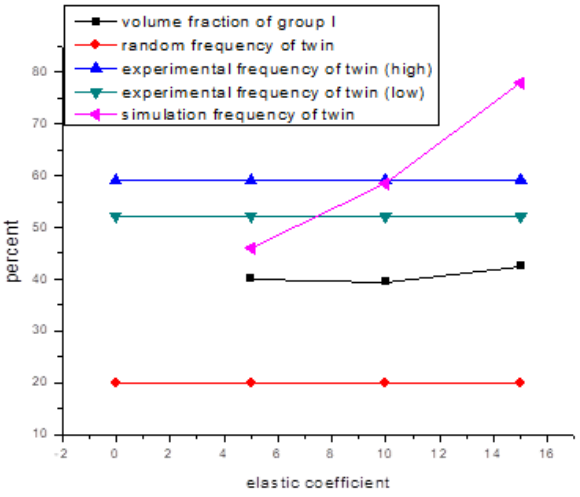

Figure 6. The statistical results of the nucleation process.

3. Discussions

The phase field simulation methods can be utilized in the research of solid phase transformation, liquid-solid phase transformation and the ferroelastic/ferroelectric/ferromagnetic phenomenon. Besides the phase transformation research in materials science and engineering, the application area of phase field simulation has been extended to biological research etc. in these years.

Though the phase field simulation method has success in the past years in the application of some research and industry sections. It is still in its very beginning stage. The existing phase field models can not satisfy the great demands of the materials design and other applications.

One problem is the lack of common and commercial phase field simulation software. The simulation program must be developed by the professional researchers. This difficulty in actual application restricts the wide and rapid spread of the phase field method.

Another problem is the difficulty in obtaining the input parameters of the phase field simulation. The accuracy of the phase field model depends on the accurate input parameters, such as the interfacial energy and elastic energy. Especially, the input parameters deviation with the change of temperature and composition, etc.

Therefore, more and more phase field models in different application aspects and more efficient algorithm should be developed in the upcoming period. Furthermore, the development trend of the computational materials science is integrating different simulation methods in different time scales and length scales.

It is a long way go and it is needed great effort on the development of the phase field simulation method before its easy and high efficient usage. Anyway, nothing can stand in the way of the phase field method becomes a powerful tool in microstructure evolution simulation.

4. Conclusions

The phase field method is a powerful tool in microstructure evolution simulation. The size, shape and spatial arrangement of phases, grains and so on can be obtained by this method. It will help the researchers tailor the microstructure of alloys. The relationship between the microstructure and the chemical driving force, the interfacial energy and the elastic strain energy can be explored in detail. With the development of computing power the phase field method will plays more and more important role in the microstructure design. Furthermore, the phase field method itself can be developed quickly.

5. References

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