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Multi-scale modeling in microstructure evolution of materials*

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Abstract: Intelligent design and control of the microstructure to tailor properties of materials is the dream that materials scientists have been worked hard for many years. Formation of research area of computational materials science paves the way to realize the dream. Simulation of microstructure evolution is a chief branch of the computational materials science and has caused great attention from materials researchers. Multi-scale modeling gets popular just within 5－6 years recently due to huge research works to try to shorten the distance between simulation and application. People have to command one or more classical simulation methods in order to do the multi-scale modeling so chief simulation methods will be discussed first and then more reviews in detail are given to the phase field simulation. The main part of the paper is carried out to introduce two key approaches to do the multi-scale modeling job. It is suggested that extension of the multiscale modeling is necessary to study the technologies to link microstructure simulation, processing simulation and property simulation each other as well as to build bridges between different simulation methods and between analytical models and numerical models.

Key words: materials computerization; multi-scale modeling; microstructure; materials simulation; phase field

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1 Introduction

Development of new materials depends on the try and error process for human beings in past long history. It is dreamed to design and control materials intellectually. Computational materials science can be believed beginning at 1964 if alloy design is assumed to be the first successful attempt to tailor properties of materials quantitatively[1]. However, computational materials science has become a popular research branch just within past ten years thanks to the intensive research activities and many achievements in the subjects in recent 20 years[2,3]. This is especially due to the great progress in computer industry and technology during the time as well as modern industries and technology require accurate control properties of materials and the highest quality of existing materials possible. Computational materials science is the symbol of a new materials science era that the properties of materials can be tailored quantitatively rather than

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qualitatively in the past. Many universities in the west have established their modeling laboratories to emphasize the subject as the strategy for a competitive materials discipline. Computational materials science may be classified into three main categories: microstructure simulation, properties calculation and processing modeling. All modeling work can be divided into two types: analytical and numerical. The concept of multi-scale modeling has been used only in microstructure simulation so far.

2 Main approaches to simulate evolution of microstructure in materials

There are several chief methods used to simulate the microstructure in literature: first principle, molecular dynamics, micro phase field, atomic Monte Carlo, front tracking, Monte Carlo, cellular automata and phase field[2-4]. The first two methods are typical analysis model to simulate materials behavior from each atoms and molecules. The phase field is also an analytical simulation based on thermodynamics of statistic rules of atom system rather than each atom behavior individually. However, the phase field simulation in real size requires free energy density data and mobility values of a system. The first two approaches are ideal if computers can deal with an atom configuration large enough to a size of real component, which is impossible at moment and also in a predictable future. Some numerical and phenomenological treatments have to be introduced into models in order to simulate real size microstructure of materials but in turn the methods are blamed not concrete. Most researchers use only one of above simulation methods, and the methods have competed each other in practice for many years but no one loses out so far. The hot word of multi-scale modeling is agreed in recent 5 years by majority of modeling workers to emphasize compromise and bridge between the methods to solve problems in applications. An illustrative summary is given in Fig. 1 to show the idea of multi-scale modeling.

3 The phase field modeling

The phase field method can be considered long distance diffusion and the elastic strain energy happened during phase transformation so that the simulated microstructure can be best closed to microscope observation. The early example of such simulation in solid phase transformation may be found in 1977[5] and the research group of Prof. Khachaturyan has shown leading authority in the technique[2]. There are a number of phase field simulations in publication such as on grain growth of two phase system[6], Martensite transformation[7] and precipitates in Ti-Al-Nb alloy[5].

Different phases are distinguished by non-conservative structural field variables $\eta_1(\boldsymbol{r}, t)$, $\eta_2(\boldsymbol{r}, t)$ and $\eta_3(\boldsymbol{r}, t)$ etc, which are called long-range structural order parameter (lro), whereas the concentration of an element in the phases can be described by a conserved field variable, $c(\boldsymbol{r}, t)$. The simulation is carried out by solving the time-dependent Ginzburg-Landau equations and the Cahn-Hilliard diffusion equation:

$$\frac{\partial \eta_p(\boldsymbol{u},\tau)}{\partial \tau} = -\left\{-\beta\nabla^2(\eta_p(\boldsymbol{u},\tau)) + \frac{\partial f_a}{\partial \eta_p(\boldsymbol{u},\tau)} + \varphi\frac{\delta E'_{el}}{\partial \eta_p(\boldsymbol{u},\tau)}\right\} + \xi'_p(\mathbf{u},\tau), \tag{1}$$

and

$$\frac{\partial c(\boldsymbol{u},\tau)}{\partial \tau} = \upsilon\nabla^2\left\{-\alpha\nabla^2 c(\boldsymbol{u},\tau) + \frac{\partial f_a}{\partial c(\boldsymbol{u},\tau)}\right\} + \zeta'(\boldsymbol{u},\tau), \tag{2}$$

where $\tau = L|\Delta f|t$ and $u_i = x_i/l$; Δf is the chemical driving force for the phase transformation under consideration and l is the length scale assigned to the computational grid size; $f_a(c, \eta_1, \eta_2, \eta_3)$ is the local specific chemical free energy of the system; E'_{el} is the elastic strain energy; $\xi'_p(\boldsymbol{u},\tau)$ and $\zeta'(\boldsymbol{u},\tau)$ are the Langivin random noise terms which are employed to simulate the stage of nucleation.

The free energy F consists of the chemical free energy (F_{ch}) and elastic strain energy (E'_{el}), i. e. $F=$

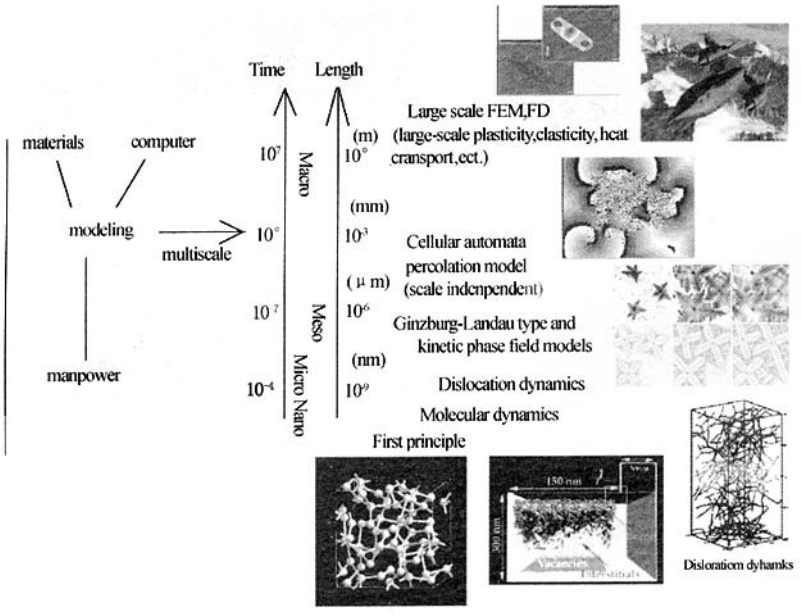

Fig. 1 Typical space and time scales and simulation methods in computational materials science

$F_{ch}+E_{el}$. The F_{ch} is mainly dependant on the f_a. A Landau type expansion polynomial is commonly used to approximate f_a:

$$f_a=\frac{a_1}{2}(c-c_1)+\frac{a_2}{2}\sum_{p=1}^{3}\eta_p^2-\frac{a_3}{4}\sum_{p=1}^{3}\eta_p^4+\frac{a_4}{6}\left(\sum_{p=1}^{3}\eta_p^2\right)^3, \tag{3}$$

where c_1 and c_2 are equilibrium concentrations for the phases respectively; a_1-a_4 are phenomenological constants which are chosen to fit the local specific free energy as a function of composition for the phases.

Two simulation examples are shown in Fig. 2 and Fig. 3 respectively.

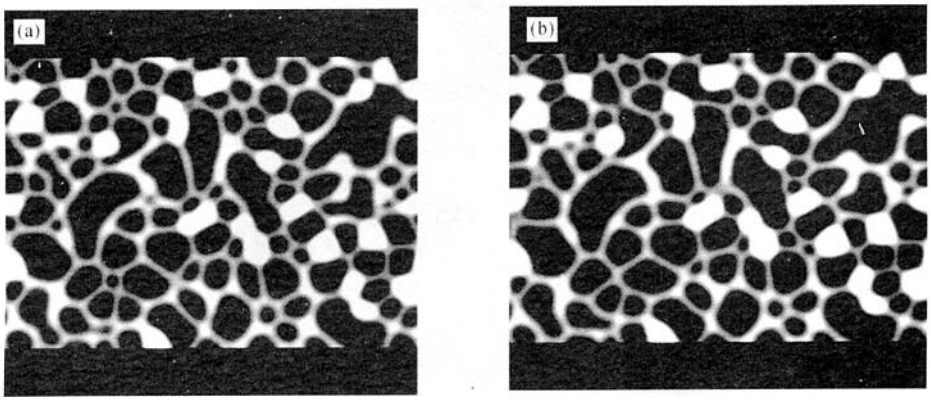

Fig. 2 Grain growth in Al_2O_3-ZrO_2 system simulated by phase field method and the ZrO_2 is 10% in volume fraction (a)t=800; (b)t=1000

4 Multi-scale modeling techniques

The idea of multi-scale modeling gets more and more popular in computational materials science and

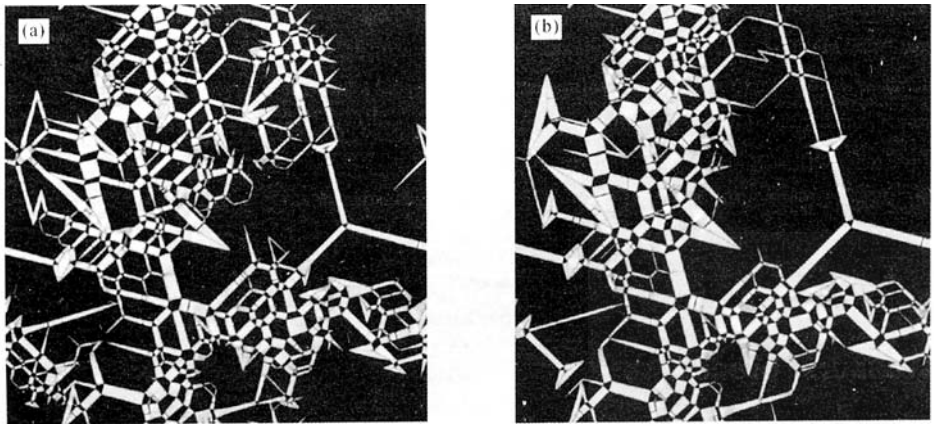

Fig. 3 Microstructure evolution in Ti-25Al-10Nb (at. %) alloy during $\alpha_2 \rightarrow O$ phase transformation simulated by phase field modeling

(a)t=3600; (b)t=10000

conventional modeling works are still very active as sprockets in the multi-scale modeling chain. There are only a limited number of research works reported to realize multi-scale modeling. The multi-scale modeling techniques may be divided into two types.

The first type is one step multi-scale modeling simultaneously developed by Shenoya *et al* in 1999[9]. The method is based on a semi-continuous mechanics and imbeds a first principle model into a finite element discretization. The local simulation results of a real atom congregation by the first principle model are interpreted into inner boundary conditions to the finite element model that can be in very large scale. Therefore, the simulation can be carried out in atom scale and macro scale simultaneously meanwhile the computational task is not heavy because only local atom structure is considered. The principle sketch of the method is given in Fig. 4.

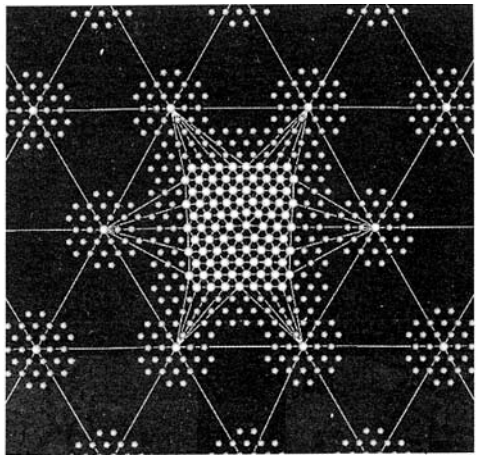

Fig. 4 Discretization used in the one step multi-scale modeling

The other method relies on several separate steps of modeling to realize the multi-scale simulation using several modeling techniques to a same material system. A good example was shown in reference[10]. The author calculated the free energy data of Al-Cu system by first principle method. The grain boundary energy was obtained by molecu-

lar dynamics simulation. Finally, phase field method was used to simulate the microstructure of the alloy. It is a very nice work with several modeling techniques to get the microstructure whereas conventional phase field simulation requires experimental data of free energy and other dynamic parameters such as grain boundary energy and mobility. The simulation results are shown in Fig. 5, Fig. 6 and Fig. 7[10]. The experimental micrograph in Fig. 7 is an Al-Si-Cu cast alloy aged at 230℃ for 3 h.

5 Discussion on extension of multi-scale modeling

The first principle simulation is based on electron theory to solve the Schrödinger equations with a solid physical background so that the results are ideal[11]. However, huge computing work it requires can not be realized due to chip cooling limitation and the high cost. Therefore, multi-scale modeling technique has to be the only way to overcome the difficulty to create a large market for application of modeling technology. The multi-scale modeling does not mean a single advanced model and it means to combine all effective models also including numerical modeling methods such as neural network technique and data fitting models.

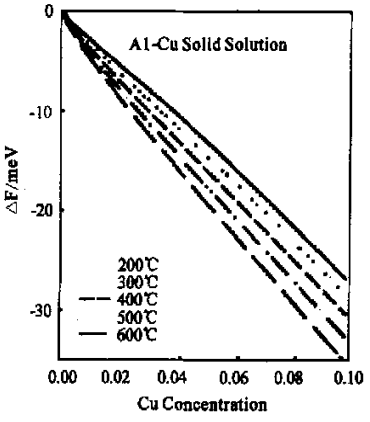

Fig. 5 Free energy of an Al-Cu solid solution, calculated from a first-principles MSCE combined with the rmodynamic integration of Monte Carlo results[10]

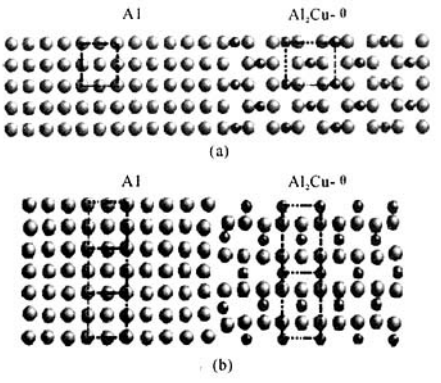

Fig. 6 Relaxed supercells used to calculate Al_2Cu/Al interfacial energies[10]

The idea of multi-scale modeling recognized presently is to build up bridges between different simulation techniques of microstructure evolution[11], and bridges between analytical and numerical models[12]. However, an extension of the multi-scale modeling is suggested to build up bridges between microstructure simulation and property predictions. Multi-scale modeling should be also extended to build up bridges between processing modeling and property prediction. For example, Fig. 8 shows the simulated tensile test curve of a 15%SiCp/Al-2618 composite with different reinforcement geometry by modified secant modulus Eshelby approach[14]. If Fig. 8 could be linked with microstructure simulation maybe by an image analyzer to read out the input data, the microstructure formation and property prediction would be achieved online simultaneously. In return, if the microstructure simulation results by phase field method could be translated into a data file that can be read by the finite element analysis code such as ANSYS, the microstructure evolution would be related to mechanical property degradation. These results will be much more significant in reference to real production in industry.

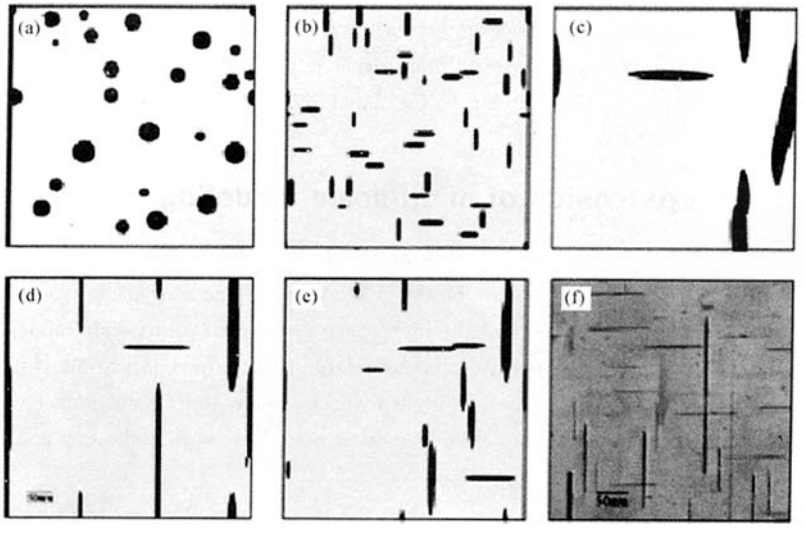

Fig. 7 Phase-field simulation using thermodynamic parameters in Fig. 5 and grain boundary energy calculated on Fig. 6 atom structure[10]
(a)Isotropic; (b)Interface only; (c)Strain only; (d)Int+train; (e)Int+strain+kinetics; (f)Experiment

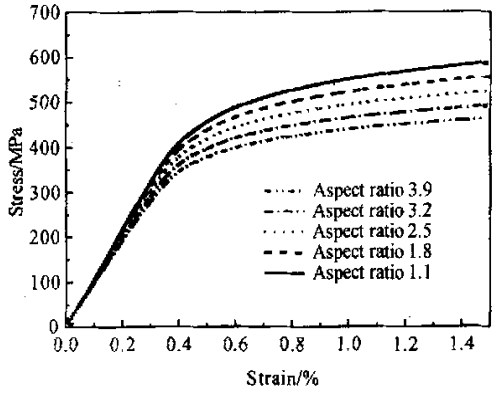

Fig. 8 Effects of particle geometry on the stress-strain curves of SiCp/Al—2618 composite predicted by a modified Eshelby secant modulus model

6 Conclusions

(1) Multi-scale modeling has caused great research attention in materials science and its rapid technique progress shows a great potential to shorten the distance between models and real components. Computational materials science is to play more and more important role in development and application of structure and function materials.

(2) Examples of one step and separate step multi-scale modeling indicate the success of the technique in solving some specific problems. However, variety of modeling applications need further development of multi-scale modeling in new flexible techniques to combine classical simulation models.

(3) The concept of multi-scale modeling should be further extended to promote more researches to build up bridges between microstructure simulation and property predictions, and between processing modeling and property prediction.

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