

Phase field modelling on the growth dynamics of double voids of different sizes during czochralski silicon crystal growth

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Abstract. To investigate their dynamics and interaction mechanisms, the growth process of the two voids with different sizes during Czochralski silicon crystal growth were simulated by use of an established phase field model and its corresponding program code. On the basis of the several phase field numerical simulation cases, the evolution laws of the double voids were acquired as follows: the phase field model is capable to simulate the growth process of double voids with different sizes; there are two modes of their growth, that is, either mutual integration or competitive growth; the exact moment of their fusion can be also captured, and it is τ of 7.078 (simulation time step of 14156) for the initial vacancy concentration of 0.02 and the initial space between two void centers of $44\Delta x$.

1. Introduction

In the past decades, along with the development of computer technology, the simulation research on microdefect evolution in Czochralski silicon crystal develops so rapidly that numerical modelling becomes one of the important research approaches to understanding microdefect dynamics thoroughly as well as predicting the microdefect size and distribution. Phase field modelling is a burgeoning numerical simulation method to be usually applied to microstructure evolution in materials in recent years. Unlike traditional sharp interface model, phase field model is capable of modelling the evolution process of microstructures without real-time tracking of the interface movement. Thus, it is widely used in the simulation research of the material microstructure evolution at mesoscopic level.

For the sake of investigating the dynamics of microdefect evolution and capturing the essential features of the formation and growth of the grown-in microdefects, different theoretically analytical models and simulation tools were developed [1-3]. In recent years, researchers [4-5] in the field of nuclear materials are carrying out relative researches about the void-type microdefect evolution in irradiated materials using phase field modelling, which provides us the inspiration of applying phase field modelling on the microdefect evolution in single crystal growth.

The growth dynamics of double voids of different sizes during CZ silicon crystal growth are concerned using phase field modelling in this paper, which is the follow-up work and extension of our previous study [6], in which phase field simulations of the growth dynamics of double voids of the same size during CZ silicon crystal growth were reported. Based on the constructed phase field model, the phase field modelling experiments for the growth dynamics of double voids of different sizes were



conducted to illustrate the evolution mechanism of the concerned voids and study the influence laws of relative factors.

2. Simulation model and conditions

2.1. Phase field model

The simulation system concerned is consisted of two phases, the matrix phase containing vacancies of supersaturated concentration and the void phase. The vacancy concentration field, c_v , and order parameter field, ϕ , were introduced as phase variables to describe the vacancy diffusion and void evolution, where \mathbf{r} is spatial position and t is time. In the matrix phase, ϕ is 0. While in the void phase, both c_v and ϕ are set to be 1. The total free energy functional of the system includes the chemical free energy and gradient energy as follows:

$$E = N \int_V (F(c_v, \phi, T) + wg(\phi) + k_v |\nabla c_v|^2 + k_\phi |\nabla \phi|^2) dV \quad (1)$$

where N is the number of the lattice sites per unit volume of the crystal; $F(c_v, \phi, T)$ is the total chemical free energy; T is the absolute temperature; $g(\phi)$ is a double-well function related to phase transition barrier; w is a positive constant; $\kappa_v |\nabla c_v|^2$ and $\kappa_\phi |\nabla \phi|^2$ represent the interfacial energy contributed by the gradients of composition and chemical ordering, repetitively, where κ_v and κ_ϕ are gradient energy coefficients. The total chemical free energy and the double-well function are:

$$F(c_v, \phi, T) = (1 - h(\phi))f_m(c_v, T) + h(\phi)f_v(c_v) \quad (2)$$

$$g(\phi) = \phi^2 - 2\phi^3 + \phi^4 \quad (3)$$

where $h(\phi)$ is a interpolating function; $f_m(c_v, T)$ and $f_v(c_v)$ are chemical free energy of matrix phase and void phase, repetitively:

$$h(\phi) = 3\phi^2 - 2\phi^3 \quad (4)$$

$$f_m(c_v, T) = (E_{f,v} - k_B T \ln(c_{v,0}))c_v + k_B T (c_v \ln(c_v) + (1 - c_v) \ln(1 - c_v)) \quad (5)$$

$$f_v(c_v) = (c_v - 1)^2 \quad (6)$$

where $E_{f,v}$ is the vacancy formation energy; k_B is the Boltzmann constant; $c_{v,0}$ is the pre-exponential factor of the thermal equilibrium vacancy concentration in the matrix, $c_{v,e} = c_{v,0} \exp(-E_{f,v}/k_B T)$.

The process of vacancy diffusion and void evolution were described by Cahn-Hilliard conservative field equation [7] and Allen-Cahn non-conservative field equation [8], repetitively:

$$\frac{\partial c_v}{\partial t} = \nabla \cdot M_v \nabla \left(\frac{1}{N} \frac{\delta E(c_v, \phi, T)}{\delta c_v} \right) \quad (7)$$

$$\frac{\partial \phi}{\partial t} = -L \left(\frac{\delta E(c_v, \phi, T)}{\delta \phi} \right) \quad (8)$$

where $M_v = D_v c_v / k_B T$ is the vacancy mobility with D_v being the vacancy diffusivity; L is the free surface mobility.

2.2. Initial conditions and parameters

The two-dimensional simulation region was divided into isometric grids of $256\Delta x \times 256\Delta x$, where Δx was grid length. There were two isolated voids with the radiuses of $10\Delta x$ and $30\Delta x$, respectively, at the center of the solution domain, surrounded by the matrix containing uniform vacancies of supersaturated concentration, and the initial temperature was set to be 1385K. In the simulation, periodic boundary condition was applied. The simulation parameters were listed in Table 1, and the physical meanings can be referred in the Reference [6].

Table 1. The parameters used in the phase-field simulation.

Parameters	Value
$E_{f,v}$ [eV]	4
$\Delta\tau$	5.0×10^{-4}
q [$K \cdot \Delta\tau^{-1}$]	0.5
\tilde{D}_v	2
\tilde{L}	100
κ_v [$eV \cdot l^{*2}$]	1
κ_ϕ [$eV \cdot l^{*2}$]	1
w	1
$c_{v,0}$	10^{11}

3. Results and Discussion

Figure 1 shows the evolution of order variable field for the initial vacancy concentration, $c_{v,i}$, of 0.02 and the initial space between two void centers of $50\Delta x$ at $\tau = 0, 50, 100, 150$, respectively. With the pulling of the silicon single crystal and the cooling of the simulation system, the supersaturated vacancy in the matrix enhances the instability of this thermodynamic system, which prompts the vacancy's inward diffusion to void and void growth. As seen in Figure 1, the two voids grow discretely in the whole simulation. The left void grows into an irregular one with edges and corners, while the right void grows into an oval shape one. The irregular left void can be interpreted by the nine-point method applied on the calculation of Laplace operator, and the oval-shaped right void attributes to the more affluent vacancies in its upper and lower matrix, compared with the vacancies in the matrix of the two voids gap which are absorbed by the bigger left void.

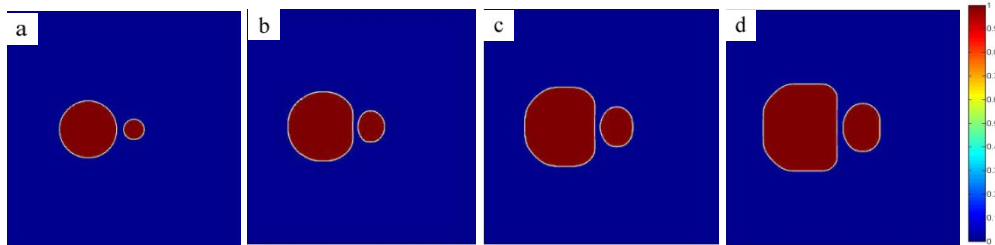


Figure 1. The evolution of ϕ field for $c_{v,i} = 0.02$ and the initial space between two void centers of $50\Delta x$ (a) $\tau = 0$; (b) $\tau = 50$; (c) $\tau = 100$; (d) $\tau = 150$.

Figure 2 shows the evolution process of order variable field for the initial vacancy concentration, $c_{v,i}$, of 0.02 and the initial space between two void centers of $44\Delta x$ at $\tau = 0, 50, 100, 150$, respectively. Unlike the independent growth mode shown in Figure 1, the initial isolated voids in Figure 2 merge together at some moment and grow into an irregular void sequentially. The two processes demonstrate that the initial space between void centers affects the growth modes of the double voids, that is, either mutual integration or competitive growth.

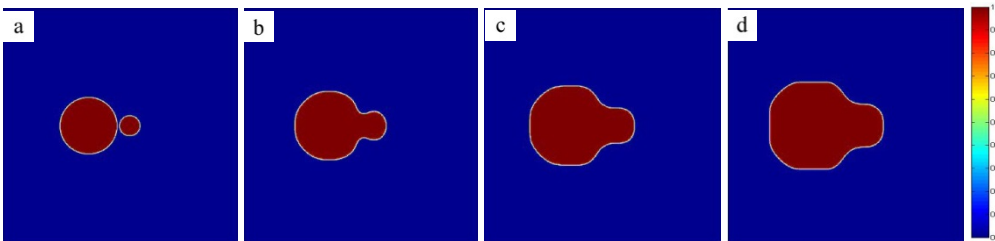


Figure 2. The evolution of ϕ field for $c_{v,i} = 0.02$ and the initial space between two void centers of $44\Delta x$ (a) $\tau = 0$; (b) $\tau = 50$; (c) $\tau = 100$; (d) $\tau = 150$.

To capture the exact fusion moment of the two voids, a result- processing program was written and their fusion process for the initial vacancy concentration, $c_{v,i}$, of 0.02 and the initial space between two void centers of $44\Delta x$ is simulated in Figure 3. The exact moment of fusion, τ_e , is 7.078 in the phase field simulation, which corresponds to simulation the time step of 14156. From this moment, the two isolated voids merge into a void, and the single void will go on its growth by absorbing vacancies in the matrix until the simulation system reaches thermodynamic equilibrium state, where the vacancy concentration in the matrix is equilibrium concentration at some temperature.

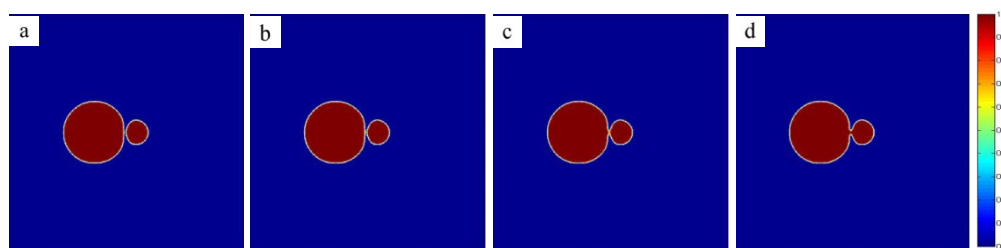


Figure 3. The fusion process of voids for $c_{v,i} = 0.02$ and the initial space between two void centers of $44\Delta x$ (a) $\tau = 6.5$; (b) $\tau = 6.75$; (c) $\tau = 7.0$; (d) $\tau = 7.078$.

4. Conclusion

The growth dynamics of double voids of different sizes were studied by using an established phase field model and related program codes for simulating the evolution behavior of void growth during Czochralski silicon single crystal growth. Series of simulation cases aimed to illustrating the growth dynamic laws of the double voids of different sizes were conducted. The results show that the phase field model can simulate the growth process of the two voids, and the initial space between the two void centers has a significant effect on their growth modes, and the related program codes have also the ability to capture the process and exact moment of void fusion.

Acknowledgments

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