

Phase-field modelling of dendritic growth behaviour towards the cooling / heating of pure nickel.

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We are interested in modelling the dendritic growth occurring during the solidification process of a pure material and especially to see the effect of the cooling / heating on the growth behaviour of this dendrite.

For this purpose we use a phase-field model. The obtained partial differential equations are solved numerically by a finite difference method. In order to appreciate the shape of the resulting dendrites we expose some figures obtained from simulations in 2D.

Key words: Simulation, dendritic growth, phase-field models, finite difference method.

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I. INTRODUCTION.

Dendritic growth is a challenging area of research and is a subject of many articles published in the last decade. Understanding the way and the circumstances in which dendrites grow up will make the materials engineers able to reach the desired properties of the manufactured materials in the future.

Many models have been investigated in order to understand dendritic growth, for example M. Plapp and J.-F. Gouyet [1,2] have used a mean-field lattice gas model to derive microscopic equations governing this growth, while J. A. Warren et al [3,4] and A. A. Wheeler et al [5] have treated this problem using phenomenological equations derived from phase-field models.

These approaches have attracted much interest in the last years because of their success to produce dendrites similar to real ones and have been improved to be able to treat other phase transitions [6].

In the phase-field models a variable $\Phi(x, t)$ called order-parameter is added. This order-parameter acts as an indicator function determining the location of the phases, in the case of solidification $\Phi(x, t)$ takes for example the values 0 in the solid-phase and 1 in the liquid-phase. From a classical point of view the solid and liquid phases are separated by a sharp interface of which the explicit tracking has posed a serious problem to those who have tried to treat dendritic growth by Stefan problem [7]. In the phase-field models this problem has been solved by abandoning the notion of sharp interface and considering the existence of a diffuse interface for which $0 < \Phi(x, t) < 1$.

In the present work we investigate the effect of the cooling / heating on the morphology of a growing dendrite. P. K. Galenko and M. D. Krivilyov [8,9]

have already investigated the effect of varying undercooling and recently D. Danilov and B. Nestler [10] have investigated the effect of the alloy composition. For this reason we first model the growth of a dendrite occurring during the solidification process by cooling pure nickel melt, we secondly see the effect of the heating on the structure of this dendrite and thirdly we cool again the nickel. Finally, we compare the shape of the final obtained dendrite with the one grown without undergoing heating.

As far as our work is concerned, we use a thermodynamically consistent phase-field method to model nickel dendritic growth. Basing on the work of C. Andersson [11] we solve the partial differential equations governing the evolution in time of the order-parameter and temperature by an explicit scheme. In the second section we give a brief description of the thermodynamically consistent phase-field method used. In the third section we present the numerical calculation and we include anisotropy. In the fourth section we show the resulting dendrites.

II. PHASE-FIELD MODEL.

There are many phase-field models, however, since we are interested in modelling a non-isothermal dendritic growth we prefer to use a thermodynamically consistent phase-field model which is derived from the entropy functional of the system, see the work of O. Penrose and P. C. Fife [12]. The derivation in great detail of this model was published by S. L. Wang, R. F. Sekerka et al [13].

• The order-parameter $A(x, t)$ is defined as:

$$\phi(x, t) = 0 \quad x \in (\text{Solid-phase}) \quad (1.a)$$

$$0 < \phi(x, t) < 1 \quad x \in (\text{Interface}) \quad (1.b)$$

$$\phi(x, t) = 1 \quad x \in (\text{Liquid-phase}) \quad (1.c)$$

• The entropy functional S and the internal energy functional E of any given subvolume $V \subset \Omega$ (Ω is the volume of the system) are:

$$S = \int_V \left[s(e, \phi) - \frac{\delta^2}{2} |\nabla \phi|^2 \right] dV, 2.a \quad (1)$$

$$E = \int_V \epsilon(T, \phi) dV, 2.b \quad (2)$$

where s is the entropy density and e is the internal energy density.

The term

$$\int_V \left[-\frac{\delta^2}{2} |\nabla \phi|^2 \right] dV$$

is added in order to take into account the contributions of the diffuse interface.

• The temperature T and the order-parameter Φ evolve in such a manner that the energy is conserved and the entropy increases. Near the melting temperature TM ($|T - TM| \ll TM$) the derived equations of evolution in time are of the form:

$$\tau \frac{\partial \phi}{\partial t} = \frac{L}{T_M^2} (T - T_M) p'(\phi) - \frac{1}{4a} g'(\phi) + \delta^2 \Delta \phi, 3.a \quad (3)$$

$$\frac{\partial}{\partial t} \left(T + \frac{L}{c} p(\phi) \right) = D \Delta T, 3.b \quad (4)$$

where τ is a positive parameter, L is the latent heat of fusion, a is the inverse depth of the potential [13], c is the heat capacity and D the thermal diffusivity. The functions $g(\Phi)$ and $p(\Phi)$ are chosen as in [11]:

$$g(\phi) = \phi^2(1 - \phi)^2, 4.a \quad (5)$$

$$p(\phi) = \phi^3(6\phi^2 - 15\phi + 10), 4.b \quad (6)$$

The parameters a , τ and δ are related to the interface thickness and to the surface tension.

III. NUMERICAL CALCULATION.

In order to solve numerically the evolution equations of the order-parameter and temperature it would be desirable to write them in a dimensionless form:

$$\frac{\epsilon^2}{m} \frac{\partial \phi}{\partial t} = \epsilon \alpha d u p'(\phi) - \frac{1}{4} g'(\phi) + \epsilon^2 \Delta \phi, 5.a \quad (7)$$

$$\frac{\partial}{\partial t} \left(u + \frac{1}{d} p(\phi) \right) = \Delta u, 5.b \quad (8)$$

where u is the dimensionless temperature, ϵ is the interface thickness, d is the undercooling, α is the inverse capillary length and m the interfacial mobility.

• In the equation governing the evolution in time of the order-parameter Φ the $\Delta \Phi$ has replaced the ordinary Laplacian operator ∇^2 in order to include anisotropy. In 2D it takes the form:

$$\Delta \phi = -\frac{\partial}{\partial x} (\eta(\theta) \eta'(\theta) \frac{\partial}{\partial y}) + \frac{\partial}{\partial y} (\eta(\theta) \eta'(\theta) \frac{\partial}{\partial x}) + \nabla \cdot (\eta^2(\theta) \nabla). \quad (6)$$

where $\eta(\theta) = 1 + \gamma \cos(k\theta)$, γ is the relative strength of the anisotropy, k the number of symmetry axes and $\theta = \arctan(\frac{\partial \phi / \partial y}{\partial \phi / \partial x}) - \theta_0$, θ is the angle between a referential direction and the local direction of solidification (we choose $\theta_0 = 0$).

We solve in 2D the obtained dimensionless evolution equations using a finite difference method. Since we are interested just in a qualitative description of dendritic growth we solve the both partial differential equations using an explicit scheme. In our case choosing $\Delta x = \Delta y = 0.02$ the time step Δt has to fulfil the following condition:

$$\Delta t \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) < \frac{1}{2}. \quad (7)$$

Numerical resolution in the case of pure nickel solidification is performed considering:

• Initial conditions corresponding to a circular seed of radius 0.02:

$$\phi(x, y, 0) = \frac{1}{2} \left[\tanh \left(\frac{\sqrt{x^2 + y^2} - 0.02}{2\sqrt{2}\epsilon} \right) + 1 \right], 8.a \quad (9)$$

$$u(x, y, 0) = -18, 8.b \quad (10)$$

• Zero Neumann conditions on all boundaries.

• The dimensionless physical parameters corresponding to pure nickel:

$$\epsilon = 0.005 \quad d = 0.95$$

$$\alpha = 400 \quad m = 0.05$$

$$\gamma = 0.015 \quad k = 4$$

We choose the value of d as 0.95 for modelling the cooling of nickel and as -0.95 in the case of heating.

IV. COMPUTATIONAL RESULTS AND VISUALIZATION.

• Growth of nickel dendrite starting from a circular initial seed of radius 0.02 at time levels $t = 0.1998$ (Fig. 1-a) and 0.333 (Fig. 1-b). In the plots the grey area represents the solid-phase while the white area represents the liquid-phase.

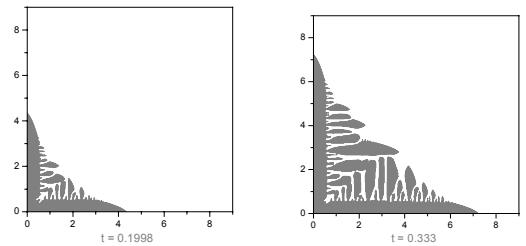


Fig. 1: Nickel dendritic growth at time levels: a) $t = 0.1998$ and b) $t = 0.333$.

- The effect of the heating on the structure of the dendrite. This part of modelling is performed taken the dendrite at time level $t = 0.1998$ (Fig. 1-a) and a temperature $T > T_M$ for which the solid-phase is stable as new initial conditions in order to model heating of the nickel.

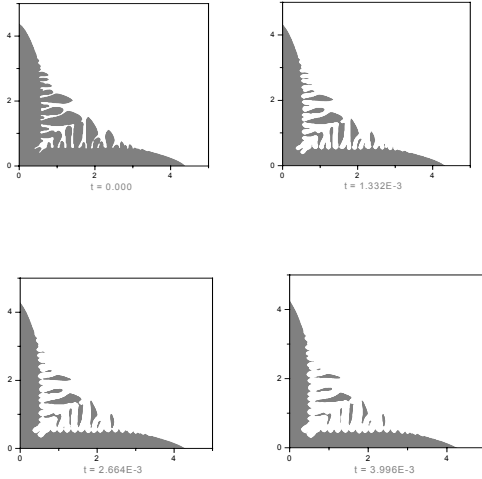


Fig. 2: Heating at time levels: a) $t = 0.000$, b) $t = 1.332E - 3$, c) $t = 2.664E - 3$ and d) $t = 3.996E - 3$.

We can notice how the side-branches separate completely from the mainbranch through the time and we can also notice the disappearance of the side-branches that have small size. All these events occur during a short time ($\Delta t = 3.996.10^{-3}$) compared with the time needed by the dendrite to grow up.

- Growth of nickel dendrite at time levels $t = 0.0666$ (Fig. 3-a) and 0.1332 (Fig. 3-b) after undergoing heating. Modelling of cooling is performed by taking the dendrite at time level $t = 3.996.10^{-3}$ (Fig. 2-d) and a temperature $T < T_M$ as new initial conditions.

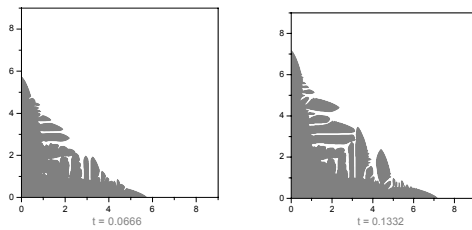


Fig. 3: Growth of nickel dendrite at time levels: a) $t = 0.0666$ and b) $t = 0.1332$ after it has undergone heating .

Comparing the resulting dendrite (Fig. 3-b) with the one grown without undergoing heating (Fig. 1-b) we realize the impact of heating on the morphology of the dendrite. The size of the solidified area in Fig. 3-b is larger than the one in Fig. 1-b, emphasizing that the cooling time in both cases is 0.333 , this can be explained by the fact that the dendrite in Fig. 1-b is generated just by a single small seed while the dendrite in Fig. 3-b is generated by the remainder of the main-branch and by the small separated side-branches that have acted as many seeds.

V CONCLUSION.

We have modelled nickel dendrite using a thermodynamically-consistent phase-field model. In particular, the numerical computation of the derived equations has allowed us to describe the effect of heating on the structure of the nickel dendrite and also to appreciate the effect of the cooling / heating on the morphology of a growing dendrite.

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