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The simulation of dendritic growth in Ni-Cu alloy using the phase field model

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ABSTRACT

Purpose: The aim of this work was to develop a computer program for simulation of dendritic growth in a selected alloy using the phase field model. This model becomes very popular for modelling a variety of technological processes at the mesoscale level.

Design/methodology/approach: In the phase field model a new variable, the phase field variable is introduced, which defines the physical state of the system (liquid or solid) at each point and the governing differential equations system. The main advantage of this method is to avoid interphase tracking in contrast to the conventional method with sharp interface.

Findings: In this work an algorithm for calculation of the microstructural evolution formed during dendritic solidification is presented by application of a numerical finite difference method for solving partial differential equations.

Research limitations/implications: The presented model for dendritic solidification will be extended for modelling of phase transformations in the solid state during technological processes in metallurgy. The calculation still has to be verified using experimental methods of microstructure analysis.

Practical implications: The phase field method becomes very popular for modelling of variety of technological processes at the mesoscale. In the actual work the methodology for simulation of microstructural development during solidification is presented.

Keywords: Dendritic solidification, Phase field model, Microstructure simulation

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1. Introduction

The metallic materials are heterogeneous on the mesoscale. Their microstructure consists of grains with different chemical composition, lattice structure and orientation. The mechanical properties of structural materials depend on the size and distribution of those grains. Therefore, the knowledge of mechanisms of microstructure formation and evolution is essential, because the microstructure evolution involves a large diversity of different processes. In addition the microstructure is thermodynamically unstable and evolves in time. One of the powerful tools for modelling the microstructural evolution in the process technology and phenomena such as solidification, phase transformations in solid state, precipitate coarsening, grain growth, dislocations dynamics and diffusion in solid state, for the sake of the phase field method (PFM). In this method the microstructure considered in phase field simulations usually

consists of a number of grains. Their shape and size distribution are represented by functions that are continuous in space and time – the phase field variables (PFV). Inside the grains these variables have nearly constant values, with respect to the structure, orientation and chemical composition. The interface between two grains is defined as a narrow area where the phase field variables gradually vary between their values in neighbouring grains. This type of modelling is called a diffusive interface description in contrast to conventional method with sharp interface. The concept of diffuse interfaces was introduced into microstructure modelling about 20 years ago. A comprehensive description of the diffuse interface approach is presented in [1, 2]. Over 15 years the PFM method was extensively applied for simulations of dendritic growth [3-7]. In the phase field method used for simulation of the solidification process a new variable $\phi(x, y, z, t)$ indicates the physical state of the system at each point. It is a continuous function of spatial coordinates and time. It is constant (0 or 1) in solid and liquid and changes smoothly over a thin transition layer playing the role of the classical sharp interface. The governing partial differential equations system is applied in all points of space without distinguishing between the phases. It enables to predict the growing morphology without tracking of the phase boundaries.

Boettinger at al. [3-5] developed the phase field model for isothermal solidification of binary alloys. In this model the constant diffusivities within the solid and liquid were assumed and 2D simulations of dendritic growth into a supersaturated liquid were carried out. This model was used in several papers [6, 7].

The aim of the present paper was to use this model for analysis of the solidification progress in a Ni-Cu alloy and to check the conditions for numerous analysis of the progress of solidification.

2. Mathematical model

The Warren and Boettinger model [4] describes the progress of solidification in time, t, in a binary alloy of A and B by two partial differential equations system with two independent variables: ϕ and concentration, c:

$$\frac{1}{M_\phi}\frac{\partial \phi}{\partial t} = \bar{\varepsilon}^2\left[\nabla\cdot\left(\eta^2\nabla\phi\right)\right] + \bar{\varepsilon}^2\frac{\partial}{\partial y}\left(\eta\eta'\frac{\partial\phi}{\partial x}\right) + \bar{\varepsilon}^2\frac{\partial}{\partial x}\left(\eta\eta'\frac{\partial\phi}{\partial y}\right) - cH_B - (1-c)H_A - cor \tag{1}$$

$$\frac{\partial c}{\partial t} = \nabla\cdot D_c\left[\nabla c + \frac{V_m}{R}c(1-c)\left(H_B(\phi,T) - H_A(\phi,T)\nabla\phi\right)\right] \tag{2}$$

where V_m is the specific volume, R, T – gas constant and absolute temperature. The free energy of component H_X of element X (X=A, B) is given by equation:

$$H_X(\phi,T) = W_X g'(\phi) + 30 g(\phi) L_X\left(\frac{1}{T} - \frac{1}{T_m^X}\right) \tag{3}$$

where $g(\phi)$ is described by equation:

$$g(\phi) = \phi^2(1-\phi)^2 \tag{4}$$

Further notifications: *cor* is correction factor (described in further text), η is the anisotropy factor, T_m^X, – melting temperatures of element X, L_X, – volumetric latent heats of fusion of X, W_X – constant described by equation:

$$W_X = \frac{3\sigma_X}{\sqrt{2}T_m^X\delta_X} \tag{5}$$

$$M_\phi = cM_B + (1-c)M_A \tag{6}$$

$$M_X = \frac{\left(T_m^X\right)^2\beta_X}{\sqrt{2}L_X\delta_X} \tag{7}$$

$$\bar{\varepsilon}^2 = \frac{6\sqrt{2}\sigma_X\delta_X}{T_m^X} \tag{8}$$

where $\bar{\varepsilon}$ is a parameter related to the interface width, δ_X, and σ_X - a constant given by the surface energy of component X, β_X is a constant given by linear kinetic coefficient of component X, D_c is a constant given by the diffusivities in liquid (D_L) and solid (D_s):

$$D_c = D_s + p(\phi)\left(D_L - D_s\right) \tag{9}$$

$p(\phi)$ is given by equation:

$$p(\phi) = \phi^3\left(10 - 15\phi + 6\phi^2\right) \tag{10}$$

The effect of anisotropy in the model is given by:

$$\varepsilon = \bar{\varepsilon}\eta = \bar{\varepsilon}\left(1 + \gamma\cos\left(k\theta\right)\right) \tag{11}$$

Where γ and k are constant, and θ is given by equation:

$$\tan(\theta) = \frac{\phi_y}{\phi_x} \tag{12}$$

$$\eta' = \frac{d\eta}{d\theta} \tag{13}$$

The derivatives of θ_x and θ_y involved in equation (12) are:

$$\theta_x = \frac{\phi_x\phi_{xy} - \phi_y\phi_{xx}}{\phi_x^2 + \phi_y^2} \tag{14}$$

$$\theta_y = \frac{\phi_x\phi_{yy} - \phi_y\phi_{xy}}{\phi_x^2 + \phi_y^2} \tag{15}$$

where ϕ_x, ϕ_y, ϕ_{xx}, ϕ_{yy}, ϕ_{xy} are partial derivatives of the field variable.

3. Numerical calculations

The evolution of microstructure formed during solidification is described by the system of equations (1) and (2). The model was solved with boundary conditions applied only at the edges of a computational box. Zero Neumann boundary conditions for c and ϕ were imposed at the boundaries. The system of equations (1) and (2) was solved on a two dimensional (2D) uniform grid with the grid spacing Δx, Δy using the second order in space and the first order in time finite difference approximations to the derivatives. For solving the system of differential equations the finite difference method (FDM, explicit scheme, was used [8]. For this scheme the time step Δt must be limited for stability according to the condition:

$$\Delta t < \frac{(\Delta x^2 + \Delta y^2)}{10\, D_c} \tag{16}$$

In equation (1), both the first and the second derivatives of ϕ - ϕ_x ϕ_x ϕ_{xx} ϕ_{yy} – were calculated using central difference approximates with respect to x and y. The mixed derivative, ϕ_{xy} was calculated using the second order formulas [9] with respect to the position of the grid point in relation with the centre of the growing dendrite. In equation (2) the second derivatives, c_{xx} and c_{yy} were calculated in the same way as ϕ_{xx} ϕ_{yy} but the first derivatives, c_x and c_y were calculated using the first order one sided approximations according to the first order upwind method [9].

In order to stimulate the fluctuations at the interface of dendrite resulting from dendrite arms growth the stochastic noise was included. According to [4] the physical reasons of the noise are stochastic forces appearing in the system due to thermodynamic fluctuations near the dendrite tip. This noise was created by introducing a correction factor, *cor*, to equation (1):

$$cor = 16 g(\phi) \alpha r \left[c H_B - (1-c) H_A \right] \tag{17}$$

where r is a random number distributed in the range from -1 to +1, generated at each grid point and α is the amplifier of the fluctuations.

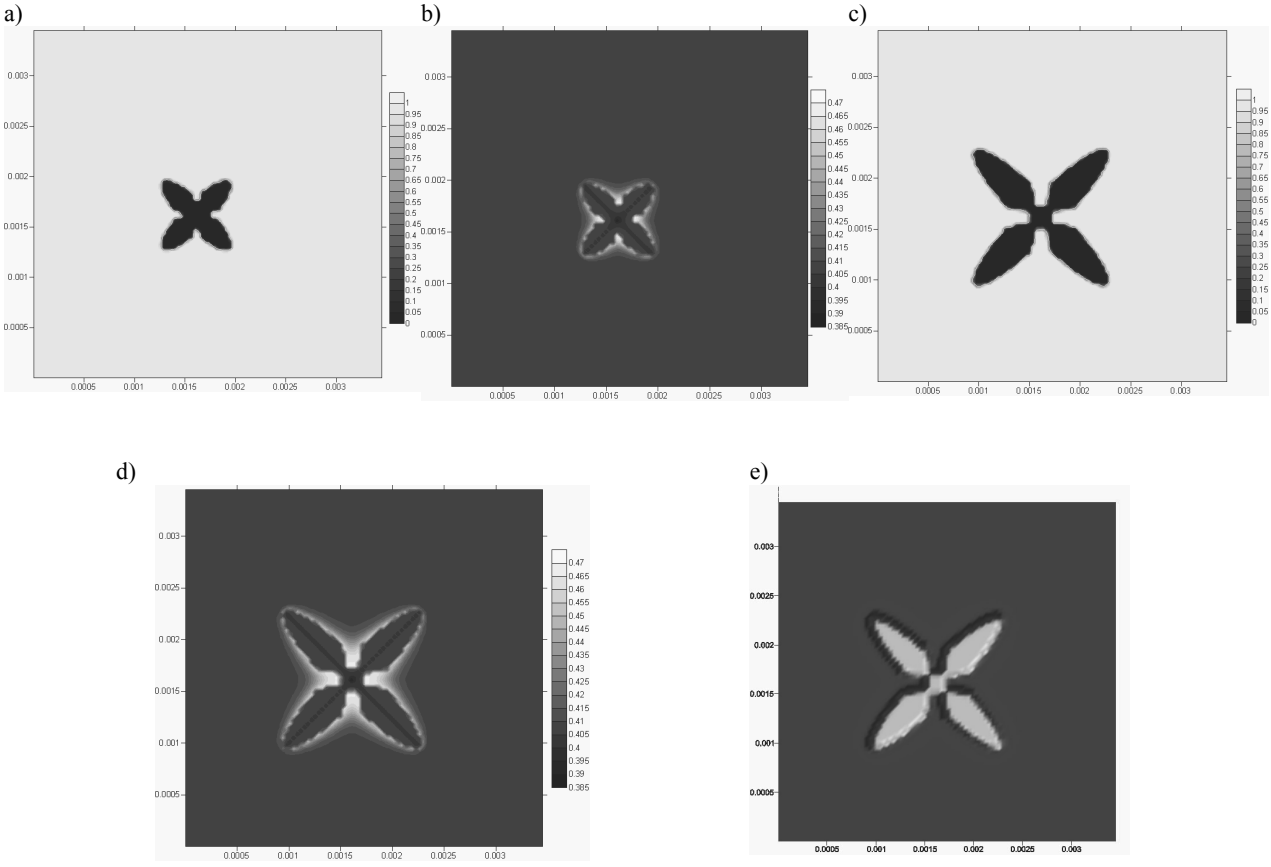

Fig. 1.The microstructure development for the case with no surface energy anisotropy (γ=0) after 0.5 (a, b) and 1 (c, d) ms of solidification a), c) - ϕ distribution, b), d) – c distribution, e) shape of dendrite

4. Physical data for calculations

The simulation of dendritic growth was performed for the nickel-copper alloy, because this binary system exhibits nearly ideal solution behaviour. In calculations it was assumed that A = Ni, *B* = Cu and following physical data were used [4]:

T_m^A=1728 K, T_m^B=1358 K, L_A=2350 J/cm^3, L_B=1758 J/cm^3, σ_A=3.7x10^{-5} J/cm^2, σ_B=2.9x10^{-5} J/cm^2. For simplification it was assumed $D_L^A=D_L^B$=10^{-5} cm^2/s, D_s=10^{-9} cm^2/s. After [4] it was assumed β_A=0.33 cm/Ks, β_B=0.39 cm/Ks and V_m=7.42 cm^3. For calculations the value of $\delta_A=\delta_B=\delta$=4.9x10^{-6} cm was taken. For simulation the alloy containing c_o=0.408 atomic fraction of Cu in Ni and T=1574 K was chosen. For this temperature, close to solidus the equilibrium concentrations in liquid, c_L and solid, c_s are: c_L=0.4668 and c_s=0.3994. This means that the initial supersaturation of liquid was Δ=0.86. The calculation of the progress of solidification was carried out using a square box size of 35 μm with grid point numbers 750x750. The initial condition was a small square area of solid (ϕ=0) in the centre of a liquid (ϕ=1) with the concentration everywhere equal c_o.

Calculations were carried out choosing anisotropy γ=0.04 (after [4]) with four fold symmetry (k=4) and a noise amplitude of α=0.4. For comparison reasons calculations neglecting the anisotropy were carried out for time interval up to 1 ms of isothermal solidifications.

5. Results of simulations

Results of microstructure development simulation during isothermal solidification are presented in Figs. 1 and 2. These figures show the phase field variable, ϕ, and copper concentration, c after different times of solidification and at different conditions in the area of 0.0035cm x 0.0035 cm. In figures presenting the ϕ distribution a line of ϕ=0.5 is drawn, which depicts the interface boundary.

In figures presenting the ϕ distribution (1a, c, 2a, c) the value of ϕ increases from 0 (solid state) to 1 (liquid). The distribution of Cu in the area of dendrite changes from 0.39 to 0.47.

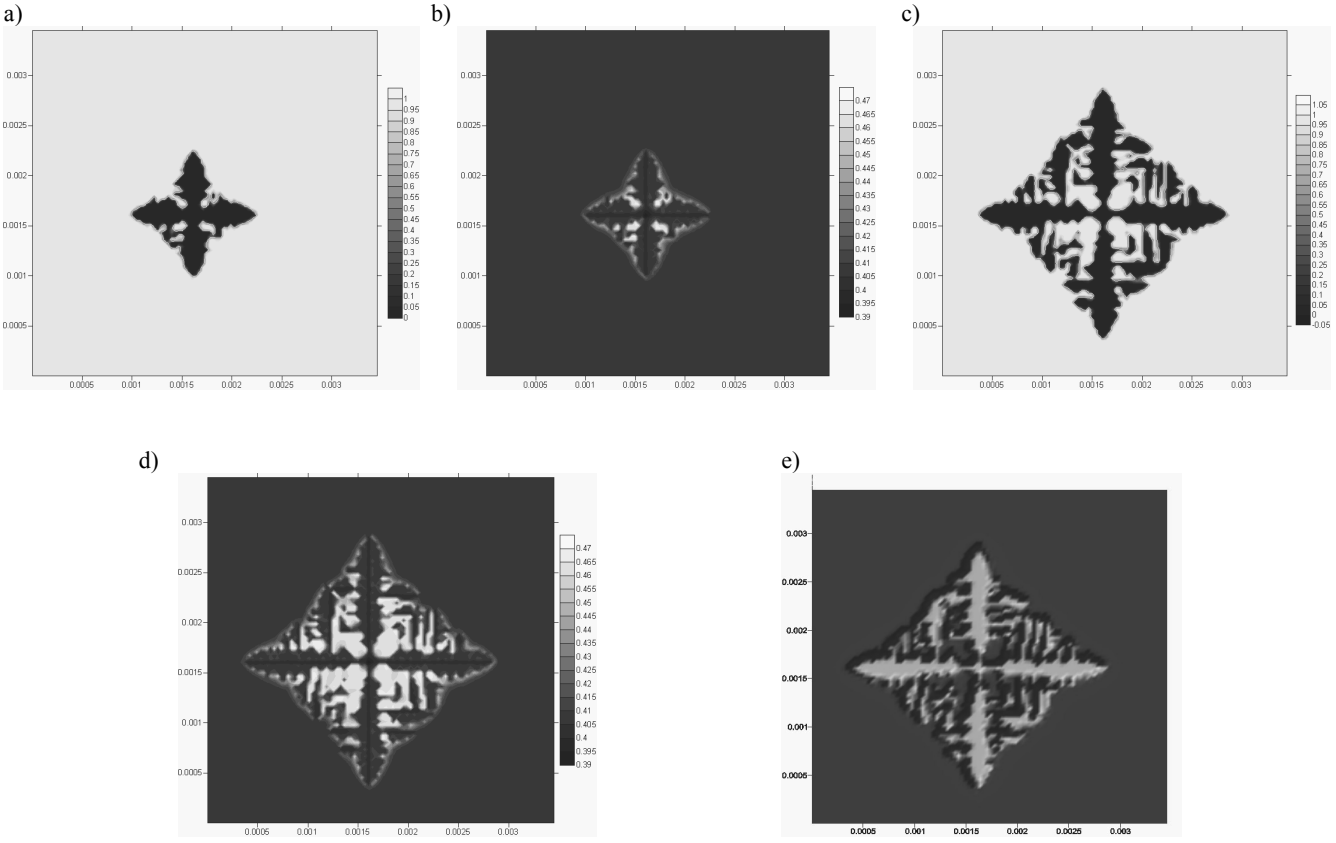

Fig. 2. The microstructure development for the case of surface energy anisotropy (γ=0.04) after 0.5 (a, b) and 1 ms (c, d) of solidification a), c) - ϕ distribution, b), d) – c distribution, e) shape of dendrite

6. Summarising remarks

The progress of dendrite growth was calculated using the finite difference method for solving the governing differential equations system (1) and (2). The simulation conditions of dendrite solidification process have a significant effect on the simulated microstructure. Calculation of dendrite growth with neglecting the anisotropy in the surface energy gives the dendrite pattern in the shape of a four leaves clover (Fig. 1). Introducing the anisotropy factor for the surface energy changes in the shape of calculated dendrite reveals dendrite arms (Fig. 2). On main arms of dendrite, the secondary branches grow perpendicularly to the axis of main arms. Results of calculations were close to the results presented in [5, 7]. Modelling the microstructure evolution using phase field method becomes more popular. The diffusive interface approach has an advantage over the conventional method with sharp interface because there is no necessity to track interfaces during the microstructure evolution. For prediction of microstructure composition and mechanical properties of engineering materials different models are applied. Examples of such models and methods used for iron alloys are presented in [10-16]. In the present paper results of the microstructural evolution obtained in the simplest case (binary Ni-Cu alloy showing ideal solution in solid state, isothermal solidification) using self developed computer program are presented as an attempt for modelling using PFM method. Further development of the program will be focused on modelling the solidification process during continuous cooling as well as microstructure evolution during phase transformations in solid state.

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References

[1] N. Moelans, B. Blanpain, P. Wollants, An introduction to phase-field modelling of microstructure evolution, Computer Coupling of Phase Diagrams and Thermochemistry 32 (2008) 268-294.

[2] I. Steinbach, Phase-field models in materials science, Modelling and Simulation in Materials Science and Engineering 17 (2009) 073001.

[3] A.A. Wheeler, W.J. Boetinger, G.B. McFadden, Phase-Field model for isothermal phase transitions in binary alloys, Physical Review 45 (1992) 7424-7438.

[4] J.A. Warren, W.J. Boettinger, Prediction of dendritic growth and microsegregation patterns in a binary alloy using the phase-field method, Acta Metallurgica et Materialia 43 (1995) 689-703.

[5] W.J. Boettinger, J.A. Warren, The phase-field method: simulation of alloy dendritic solidification during recalescence, Metallurgical and Materials Transactions A 27A (1996) 657-669.

[6] J.F. McCarthy, Phase diagram effects in phase field models of dendritic growth in binary alloys, Acta Metallurgica et Materialia 45 (1997) 4077-4091.

[7] I. Longinova, G. Amberg, J. Ågren, Phase field simulations of non-isothermal binary alloy solidification. Acta Metallurgica et Materialia 49 (2001) 573-581.

[8] C.F. Gerald, P.O. Wheatley, Applied Numerical Analysis, Addison Wesley Publishing Company, USA.

[9] T.J. Chung, Computational fluid dynamics, Cambridge University Press, 2002.

[10] H.Adrian: Thermodynamic Calculations of Carbonitride Precipitation as a Guide for Alloy Design of Microalloyed Steels; Proceedings of the International Conference "Microalloying'95", Pittsburgh, 1995, 285-307

[11] M. Glowacki, R. Kuziak, Z. Malinowski, M. Pietrzyk Modelling of heat transfer, plastic flow, and microstructural evolution during shape rolling, Journal of Materials Processing Technology 53 (1995) 159-166.

[12] B. Koczurkiewicz, The model of prediction of the microstructure austenite C-Mn steel, Archives of Materials Science and Engineering 28 (2007) 421-424.

[13] J. Trzaska, A. Jagiełło, L.A. Dobrzański, The calculation of CCT diagrams for engineering steels, Archives of Materials Science and Engineering 39/1 (2009) 13-20.

[14] D. Słota, Modelling of the optimum cooling condition in two-dimensional solidification processes, Computational Materials Science and Surface Engineering 1 (2009) 45-52

[15] B. Smoljan, D. Iljkić, S. Smokvina Hanza, F. Traven An analysis of modified Jominy-test (JMC®-test), Computational Materials Science and Surface Engineering 1 (2009) 120-124.

[16] L.A. Dobrzański, R. Honysz, Computer modelling system of the chemical composition and treatment parameters influence on mechanical properties of structural steels, Journal of Achievements in Materials and Manufacturing Engineering 35/2 (2009) 138-145.