

01 Phase transformations in single-component multiphase systems: phase-field approach

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The problems of constructing a multiphase model of the phase field for the processes of phase transitions of the first kind are considered. Based on the Gibbs energy of the complete system expressed in terms of antisymmetrized combinations of phase fields, it is shown that the equations of dissipative dynamics of a locally nonequilibrium system follow from the condition of its monotonic decrease, preserving the normalization of the sum of variables by one and the following properties of the previously known two-phase model.

Keywords: multiphase systems, phase transformations, locally nonequilibrium processes, dissipative systems with constraints.

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Introduction

Modelling of processes of microstructure formation at phase transitions is important for the development of new technologies [1]. The phase field method is among the most efficient and reliable approaches in microstructure modelling [2]. The most well-studied are two-phase models [3–6], which make it possible to describe grain interaction or growth of dendrite structures in materials. These models have covered the way from phenomenological ideas of a diffuse interface [7–11] to thermodynamically consistent [12–14] models. The situation in multiphase systems [15–21] is more complex, because the origination of new phases on the interface of two phases cannot be reduced to equations [3–6] or [12–14]. The main problem is the presence of a holonomic constraint [22] for the phase order parameters (called phase fields).

Indeed, the dynamics of a system with N phases in isotropic materials is described by a vector with N components φ_α ($\alpha = 1 \dots N$), which correspond to each phase. Phase field φ_α unambiguously characterizes (except the diffuse interface between phases) the presence of the α phase a given point of space and time. We adopt the value $\varphi_\alpha = 1$ for the equilibrium phase, while inside the other phases $\varphi_\alpha = 0$. The phase field across the diffuse interface changes quickly but continuously, which presupposes fulfillment of the correlation

$$\sum_{\alpha=1}^N \varphi_\alpha = 1, \quad (1)$$

which prevents from considering φ_α as independent variables. Anisotropy, inherent in crystalline phases, leads to additional degrees of freedom [21] (phase fields that control the growth direction) with their correlation of kind (1).

An explicit resolution of correlation (1) by isolation of the dependent phase is not satisfactory either from the thermodynamic viewpoint or from the pragmatic viewpoint of numerical modeling. Implicit use of correlations in variational problems has been known for a long time. The universal approaches in such problems are the methods of Lagrange multipliers [23] and penalty functions [24]. But the application of dissipative systems in relaxation dynamics nowadays is absolutely unreasonable. Nevertheless, Lagrange multipliers [23] were actively used in [15–21].

Another approach, related to selection of independent non-redundant variables and dynamic equations which satisfy correlation (1), has been suggested in [16]. Despite the achievements [15–21], the currently used multiphase models [10,11], while being a development of model [16], have no with the description of two-phase systems [2–5], in particular, the conditions of thermodynamic stability of phases (4) according to Kessler [25] are not met in them, due to which the equilibrium state, as distinct from two-phase models, is a quasi-periodic function. Therefore, despite the large number of performed calculations, the task of a consistent description of phase transformations in multiphase systems is still far from completion.

The aim of this paper is to obtain a phase field model for phase transformations in multicomponent systems in non-redundant variables. The described model has been consistent with previously known two-phase models, e.g. [26]. The principle of pairwise interaction of phases was used for coordination. The principle of pairwise interaction assumes that a multiphase model on the phase interface must degenerate till interaction of each of the possible phase pairs, while preventing the origination of new ones. Since the dynamics of phase transformations in single-component systems is determined solely by the difference

of Gibbs potentials, which is a simpler case as compared to solutions, a single-component system is used to better understand the ways for implementing this approach. We have obtained a model possessing the required behavior, based on the Steinbach variables [16] in an isotropic model of a phase field and the demand for monotonic decrease of Gibbs potential in the course of relaxation. The latter is checked both analytically and numerically, based on the simulation of solidification of hafnium melt (Hf), which leads to competitive growth of two solid phases from the melt.

1. Multiphase description based on the paired principle

Let us reformulate the multiphase model [10,11] in independent variables of antisymmetric combinations of phase fields [16], while retaining the common structure of the two-phase model [26]. For derivation, we demand monotonic decrease of the total Gibbs potential of the entire system [27], which attains a minimum in the equilibrium state. To do so, we will express it in terms of antisymmetric variables. Let us consider different physical contributions to the Gibbs energy of a multiphase single-component system.

1.1. Contribution of the surface

In the case of multiphase systems, we choose antisymmetric combinations as independent quantities due to the redundancy of variables φ_α [16]

$$\psi_{\alpha\beta} = \varphi_\alpha - \varphi_\beta.$$

Density of the diffuse interface is written as the sum for independent pairs of indices (α, β) :

$$\varepsilon_k = \frac{1}{8} \sum_{\alpha, \beta=1}^N \sigma_{\alpha\beta} (\nabla \psi_{\alpha\beta})^2, \quad (2)$$

where $\sigma_{\alpha\beta}$ is related to the surface energy of the phase interface (α, β) . Multiplier 1/8 appears in expression (2) due to the degree and symmetry $\sigma_{\alpha\beta} = \sigma_{\beta\alpha}$.

1.2. Potential barrier between phases

According to Steinbach [16], let us substitute the well-known double-well-potential, see [26]:

$$\varepsilon_p = \frac{1}{2} W g(\varphi) \equiv \frac{1}{2} W \varphi^2 (1 - \varphi)^2 \quad (3)$$

by a convex polynomial of a lower order, also expressing it in terms of an antisymmetric combination. A formal generalization for the multiphase case gives

$$\varepsilon_p = \frac{1}{2} \sum_{\alpha, \beta=1}^N W_{\alpha\beta} \psi_{\alpha\beta}^2, \quad (4)$$

where $W_{\alpha\beta}$, as before, defines the magnitude of the energy barrier between phases (α, β) .

1.3. Equilibrium thermodynamic contribution

Let us present the equilibrium thermodynamic contribution of a multiphase system of a single-component system [26]:

$$\varepsilon_e = \sum_{\alpha=1}^N \varphi_\alpha G_\alpha(T) \quad (5)$$

in terms of combinations

$$\varepsilon_e = \sum_{\alpha, \beta=1}^N \psi_{\alpha\beta} \Delta G^{\alpha\beta}, \quad (6)$$

where $\Delta G^{\alpha\beta} = G^\alpha(T) - G^\beta(T)$.

1.4. Locally nonequilibrium processes

To describe the rapid phase transformations, nonequilibrium kinetic contribution is added to the bulk density of Gibbs energy

$$\varepsilon_k = \frac{1}{2} \Gamma \sum_{\alpha=1}^N \dot{\varphi}_\alpha^2, \quad (7)$$

which considers the decreased volume of the system phase space in nonequilibrium processes [27]. Parameter Γ will be determined later.

1.5. Time derivative of Gibbs energy

Aggregating the energy densities (2), (4), (6), (7), we obtain the total energy of the multiphase system

$$G(t) = \int \sum_{\alpha, \beta=1}^N \left[\frac{1}{2} \Gamma \dot{\varphi}_\alpha \dot{\varphi}_\beta \delta_{\alpha\beta} + \frac{1}{8} \sigma_{\alpha\beta} (\nabla \psi_{\alpha\beta})^2 - \frac{1}{2} W_{\alpha\beta} \psi_{\alpha\beta}^2 + 3 \psi_{\alpha\beta} \Delta G^{\alpha\beta} \right] d\Omega. \quad (8)$$

The corresponding time derivative is equal to

$$\frac{dG(t)}{dt} = \int \sum_{\alpha=1}^N \dot{\varphi}_\alpha \sum_{\beta=1}^N \left[\Gamma \ddot{\varphi}_\beta \delta_{\alpha\beta} - \frac{1}{2} \sigma_{\alpha\beta} \nabla^2 \psi_{\alpha\beta} - 2 W_{\alpha\beta} \psi_{\alpha\beta} + 6 \Delta G^{\alpha\beta} \right] d\Omega \leq 0 \quad (9)$$

and formally considers the contribution to a change of the α -phase from all possible system phases. However, the real number of coexistent phases near the equilibrium must be limited due to minimization of surface energy. Based on this, we will use the principle of paired phase interaction.

1.6. Paired principle

This principle will mean the condition that $dG(t)/dt \leq 0$ must be satisfied only with account of the phases which are in direct contact with each other inside the diffuse

interface. In other words, we insert the squared projection operator $\hat{P}_\alpha \hat{P}_\beta \geq 0$ in expression (9); it takes into account the presence of both α and β phases inside the diffuse interface

$$\frac{dG(t)}{dt} = \int \sum_{\alpha=1}^N \dot{\phi}_\alpha \sum_{\beta=1}^N \hat{P}_\alpha \hat{P}_\beta \left[\Gamma \ddot{\phi}_\beta \delta_{\alpha\beta} - \frac{1}{2} \sigma_{\alpha\beta} \nabla^2 \psi_{\alpha\beta} - 2W_{\alpha\beta} \psi_{\alpha\beta} + 6\Delta G^{\alpha\beta} \right] d\Omega \leq 0. \quad (10)$$

Particular selection of projection operators in each term is not unambiguous, but must retain the fixed sign of expression (10). Comparison with the two-phase problem makes it possible to adopt

$$\hat{P}_\alpha \hat{P}_\beta = \varphi_\alpha \varphi_\beta \quad (11)$$

for contributions of potential barriers and thermodynamic potentials. At the same time, to retain the simplest shape of the interface, for the kinetic construction we restrict ourselves to a product of Heaviside functions:

$$\hat{P}_\alpha \hat{P}_\beta = \theta(|\nabla \varphi_\alpha(x)|) \theta(|\nabla \varphi_\beta(x)|), \quad (12)$$

where $\theta(a) = 1$ at $a \geq 0$ and $\theta(a) = 0$ at $a < 0$. Assuming that

$$\theta_\alpha \equiv \theta(|\nabla \varphi_\alpha(x)|),$$

we rewrite (10) as follows:

$$\frac{dG(t)}{dt} = \int \sum_{\alpha} \dot{\phi}_\alpha \sum_{\beta} \left[\Gamma \ddot{\phi}_\beta \delta_{\alpha\beta} - \frac{1}{2} \sigma_{\alpha\beta} \theta_\alpha \theta_\beta \nabla^2 \psi_{\alpha\beta} - 2W_{\alpha\beta} \varphi_\alpha \varphi_\beta \psi_{\alpha\beta} + 6\varphi_\alpha \varphi_\beta \Delta G^{\alpha\beta} \right] d\Omega \leq 0, \quad (13)$$

from here, equations of the multiphase model phase field follow:

$$\tau \ddot{\phi}_\alpha + \dot{\phi}_\alpha = M_0 \sum_{\beta \neq \alpha} \left[\frac{1}{2} \sigma_{\alpha\beta} \theta_\alpha \theta_\beta \nabla^2 (\varphi_\alpha - \varphi_\beta) - 2W_{\alpha\beta} \varphi_\alpha \varphi_\beta (\varphi_\beta - \varphi_\alpha) - 6\varphi_\alpha \varphi_\beta \Delta G^{\alpha\beta} \right], \quad (14)$$

where $\tau = \Gamma M_0$ is the characteristic relaxation time. Quantity M_0 is phase field mobility, which is usually a function of temperature. M_0 is determined from solidification kinetics experiments [29], while the equilibrium conditions are sufficient for determination of the other parameters [26].

It can be easily seen that the sum of equations (14) is identically equal to zero, therefore if the sum of phases at the initial moment is equal to unity in compliance with (1), it will also remain such at subsequent time moments. It should be noted that this is possible only on condition of equal mobilities M_0 and equal relaxation times τ for all phases.

In the limit case, when only two phases are in contact, conventionally φ_1 and φ_2 , we have

$$W_{12} = W_{21} = W_0, \quad \sigma_{12} = \sigma_{21} = \sigma_0, \quad \varphi_1 = \varphi, \quad \varphi_2 = 1 - \varphi.$$

Two equations are obtained in this case

$$\tau \ddot{\phi}_1 + \dot{\phi}_1 = \tau \ddot{\phi} + \dot{\phi} = M_0 [\sigma_0 \nabla^2 \varphi - 2W_0 \varphi (1 - \varphi) (1 - 2\varphi) - 6\varphi (1 - \varphi) \Delta G^{(12)}],$$

$$\tau \ddot{\phi}_2 + \dot{\phi}_2 = -(\tau \ddot{\phi} + \dot{\phi}) = M_0 [-\sigma_0 \nabla^2 \varphi + 2W_0 \varphi (1 - \varphi) \times (1 - 2\varphi) - 6\varphi (1 - \varphi) \Delta G^{(21)}], \quad (15)$$

which coincide up to a sign.

2. Gibbs potentials

Let us consider the dynamics of phase formation in pure hafnium. Hafnium has three stable (at different temperatures) phases and its behavior allows for demonstrating the capabilities of a multiphase model. Analytical expressions for Gibbs potentials as temperature functions were taken from [28]. The curves of the lowest-energy Gibbs potentials are shown in Fig. 1. They show that a (metastable) HCP_A3 phase and a stable BCC_A2 phase can originate, in addition to the liquid phase, in the melt upon temperature decrease to $T = 2000$ K.

3. Numerical algorithm

Since the main aim of this paper is to derive equations that describe the phase transformation processes in pure (single-component) multiphase systems (14), a comparison with the experiment is outside the scope of this paper. The results of the numerical calculations are also given below mainly for illustration: to show that ratio (1) in case of a

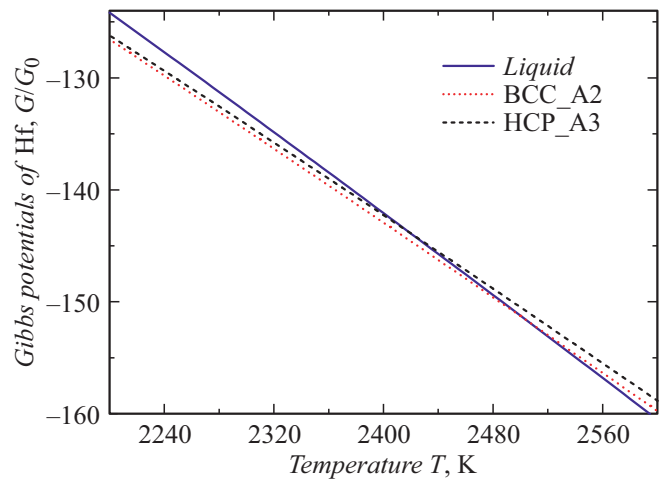


Figure 1. Molar Gibbs potentials of the Liquid, BCC_A2, HCP_A3 phases for pure hafnium [28].

numerical solution of equations (14) will always be carried out during modeling of the process of structure formation.

By writing equations (14) for the three phases, we have a system of equations

$$\begin{aligned}
 \tau \ddot{\varphi}_1 + \dot{\varphi}_1 &= M_0 \left[\sigma_{12} \vartheta_1 \vartheta_2 \nabla^2 (\varphi_1 - \varphi_2) + \sigma_{13} \vartheta_1 \vartheta_3 \nabla^2 (\varphi_1 - \varphi_3) \right. \\
 &\quad - 2\varphi_1 (W_{12}\varphi_2(\varphi_1 - \varphi_2) + W_{13}\varphi_3(\varphi_1 - \varphi_3)) \\
 &\quad \left. - 6\varphi_1 (\varphi_2 \Delta G^{(12)} + \varphi_3 \Delta G^{(13)}) \right], \\
 \tau \ddot{\varphi}_2 + \dot{\varphi}_2 &= M_0 \left[\sigma_{21} \vartheta_2 \vartheta_1 \nabla^2 (\varphi_2 - \varphi_1) + \sigma_{23} \vartheta_2 \vartheta_3 \nabla^2 (\varphi_2 - \varphi_3) \right. \\
 &\quad - 2\varphi_2 (W_{21}\varphi_1(\varphi_2 - \varphi_1) + W_{23}\varphi_3(\varphi_2 - \varphi_3)) \\
 &\quad \left. - 6\varphi_2 (\varphi_1 \Delta G^{(21)} + \varphi_3 \Delta G^{(23)}) \right], \\
 \tau \ddot{\varphi}_3 + \dot{\varphi}_3 &= M_0 \left[\sigma_{31} \vartheta_3 \vartheta_1 \nabla^2 (\varphi_3 - \varphi_1) + \sigma_{32} \vartheta_3 \vartheta_2 \nabla^2 (\varphi_3 - \varphi_2) \right. \\
 &\quad - 2\varphi_3 (W_{31}\varphi_1(\varphi_3 - \varphi_1) + W_{32}\varphi_2(\varphi_3 - \varphi_2)) \\
 &\quad \left. - 6\varphi_3 (\varphi_1 \Delta G^{(31)} + \varphi_2 \Delta G^{(32)}) \right]. \quad (16)
 \end{aligned}$$

To simplify the numerical calculation, we will further assume that a local nonequilibrium is absent: $\tau = 0$, while barrier magnitudes and surface energy on all boundaries are equal:

$$\begin{aligned}
 W_{12} &= W_{13} = W_{23} = W_0, \\
 \sigma_{12} &= \sigma_{13} = \sigma_{23} = \sigma_0.
 \end{aligned}$$

By choosing time and space scales, we have the following after a transition to dimensionless variables

$$\begin{aligned}
 \dot{\varphi}_1 &= \vartheta_1 \vartheta_2 \nabla^2 (\varphi_1 - \varphi_2) + \vartheta_1 \vartheta_3 \nabla^2 (\varphi_1 - \varphi_3) \\
 &\quad - 2\varphi_1 (\varphi_2(\varphi_1 - \varphi_2) + \varphi_3(\varphi_1 - \varphi_3)) \\
 &\quad - 6\varphi_1 (\varphi_2 \bar{\Delta G}^{(12)} + \varphi_3 \bar{\Delta G}^{(13)}), \\
 \dot{\varphi}_2 &= \vartheta_2 \vartheta_1 \nabla^2 (\varphi_2 - \varphi_1) + \vartheta_2 \vartheta_3 \nabla^2 (\varphi_2 - \varphi_3) \\
 &\quad - 2\varphi_2 (\varphi_1(\varphi_2 - \varphi_1) + \varphi_3(\varphi_2 - \varphi_3)) \\
 &\quad - 6\varphi_2 (\varphi_1 \bar{\Delta G}^{(21)} + \varphi_3 \bar{\Delta G}^{(23)}), \\
 \dot{\varphi}_3 &= \vartheta_3 \vartheta_1 \nabla^2 (\varphi_3 - \varphi_1) + \vartheta_3 \vartheta_2 \nabla^2 (\varphi_3 - \varphi_2) \\
 &\quad - 2\varphi_3 (W_{31}\varphi_1(\varphi_3 - \varphi_1) + W_{32}\varphi_2(\varphi_3 - \varphi_2)) \\
 &\quad - 6\varphi_3 (\varphi_1 \bar{\Delta G}^{(31)} + \varphi_2 \bar{\Delta G}^{(32)}), \quad (17)
 \end{aligned}$$

where $\bar{\Delta G}^{(\alpha\beta)}$ are dimensionless differences of Gibbs potentials. The last equations are written in the vector form as

$$\dot{\boldsymbol{\varphi}} = \hat{L}(\boldsymbol{\varphi}), \quad (18)$$

which will be modelled using the finite difference method. For the explicit scheme, we have $\hat{L}$:

$$\boldsymbol{\varphi}^{(n+1)} = \boldsymbol{\varphi}^{(n)} + \Delta t \hat{L}(\boldsymbol{\varphi}^{(n)}). \quad (19)$$

Given the non-linearity of the right member of problem (19), calculation must be performed with a small time grid step, therefore we did not consider the implicit methods and the corresponding stability conditions. Stability of explicit scheme (19) was checked empirically by selecting an increment. The explicit scheme for the one-dimensional setting is stable on a lattice sized $N \approx 1000-2000$ at $\Delta t \leq 0.325\Delta x^2$. For the two-dimensional setting (on the lattice $N \approx 500 \times 500$) — the solution is stable at $\Delta t \leq 0.145\Delta x^2$ where Δx is the spatial grid step.

4. Directional solidification problem

Let us consider the dynamics of phase formation in hafnium for the directional solidification problem. A combination of the Liquid and HCP_A3 phases is used as the initial condition in the directional solidification problem (Fig. 2, a).

The given phases are initially not in equilibrium, therefore the phase interface starts moving. During motion of the Liquid–HCP_A3 phase interface (Fig. 2, b), an instability originates which causes a distortion of the liquid phase profile and formation of a „nucleus“ of the BCC_A2 phase. In Fig. 2, b is the formation of a new phase. Then (Fig. 3, a) the formation of a complete stable BCC_A2 phase is shown (the phase field for the BCC_A2 phase reaches the unity), inside which the Liquid, HCP_A3 phases gradually stop contacting each other. Fig. 3, b shows displacement of the metastable phases by the stable BCC_A2 phase. Since the difference of the Gibbs potentials between the liquid and the stable solid phase is higher than between the solid phases, the interface motion speed is significantly higher than the phase interface motion speed for the solid phases.

Since the right member of expression (29) was calculated using the known values of $\boldsymbol{\varphi}^{(n)}$, for which condition (1) is met, the said condition was identically met on the next time increment. Construction of implicit methods for solving the multiphase system equations still remains a topical unsolved problem.

5. Two-dimensional modeling

Modeling was done on a square lattice sized $N \approx 500 \times 500$. An isotropic model is under consideration. The initial condition corresponds to the (pseudo) random location of the spherical nuclei of the HCP_A3 phase (its phase field is shown by red color (in the online version)) inside the hafnium liquid phase (phase field is shown by blue color (in the online version)) at $T = 2000$ K (Fig. 4). Both above-mentioned phases are metastable at the given temperature, therefore fluctuations of the value of a phase field of approximately 10^{-8} , which corresponds to the BCC_A2 phase, have been assigned in the vicinity of each spherical nucleus.

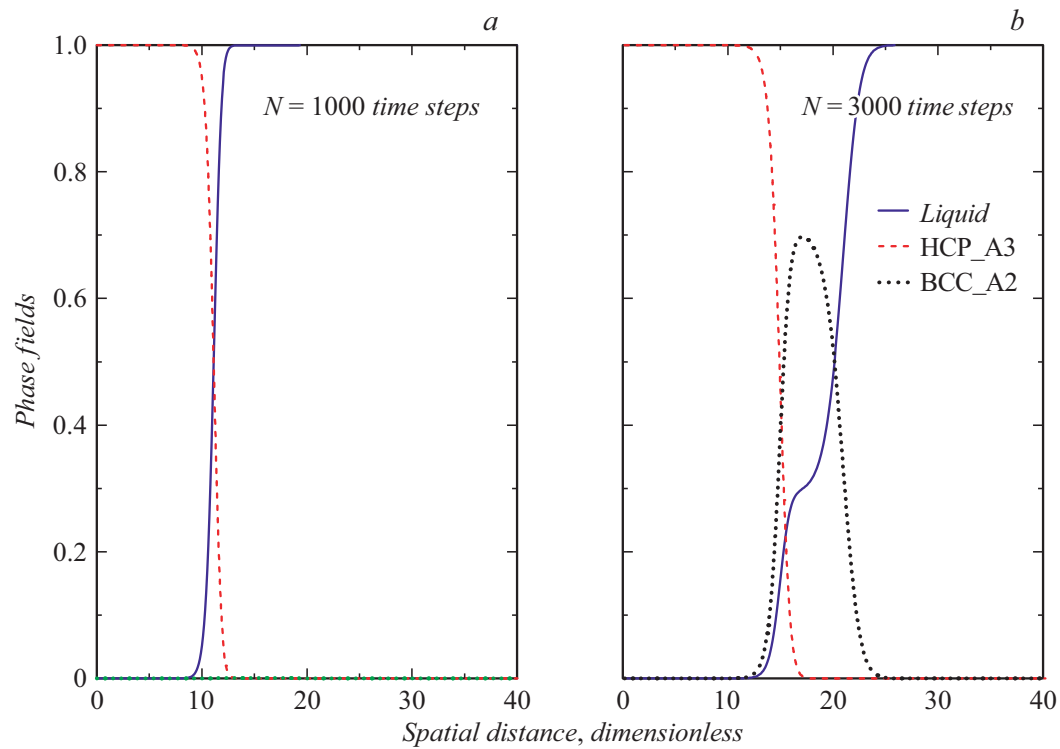


Figure 2. Process of BCC_A2 phase origination on the interface between the Liquid and HCP_A3 phases for pure hafnium at $T = 2000$ K.

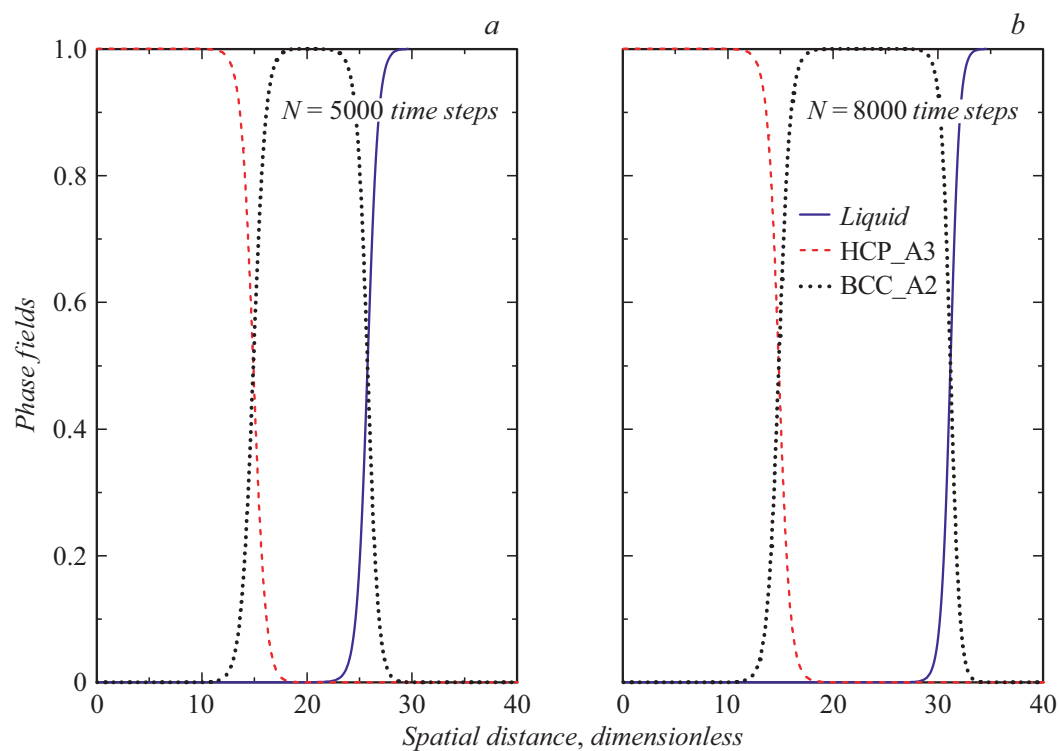


Figure 3. Formation of a stable BCC_A2 phase on the interface of metastable phases for pure hafnium at $T = 2000$ K (evolution from left to right).

Slow motion of the interface of the BCC_A2 phase inside the liquid phase provokes instability and growth of the BCC_A2 phase field (green color (in the online version)) on the interface between the Liquid and HCP_A3 phases (Fig. 5, 6). Then the BCC_A2 phase substitutes the Liquid phase and gradually displaces the HCP_A3 phase (Fig. 7).

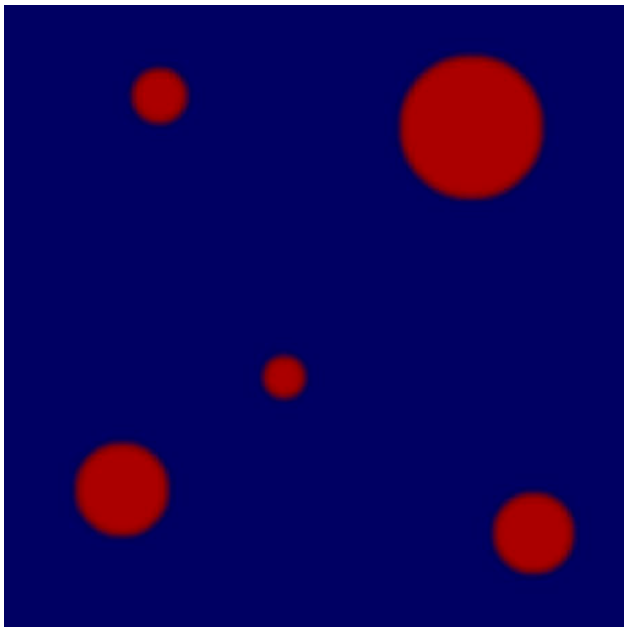


Figure 4. Initial state: nuclei of the HCP_A3 phase (red circles (in the online version)) inside the Liquid phase (blue background (in the online version)) for hafnium at $T = 2000$ K.

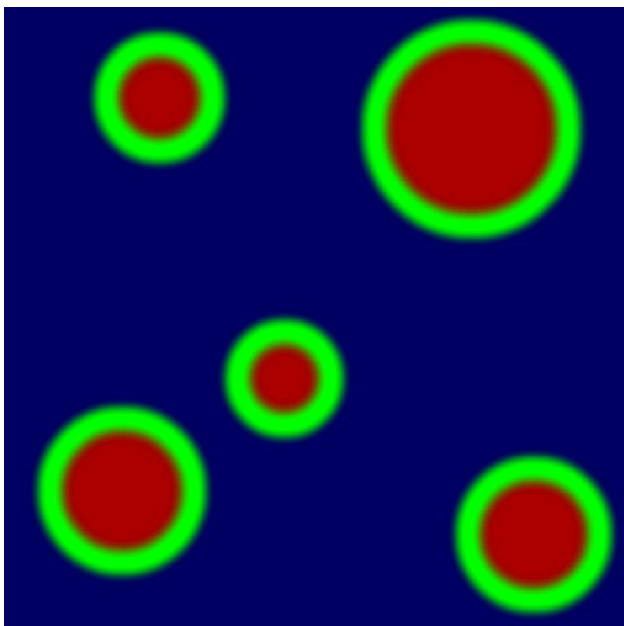


Figure 5. Origination of BCC_A2 phase (green (in the online version)) on the interface between the Liquid and HCP_A3 phases for hafnium at $T = 2000$ K.

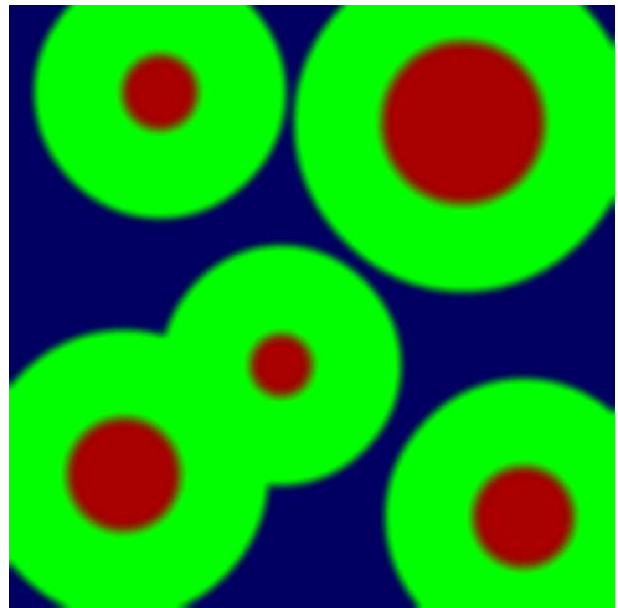


Figure 6. Growth of the BCC_A2 phase on the interface between the Liquid and HCP_A3 phases for hafnium at $T = 2000$ K.

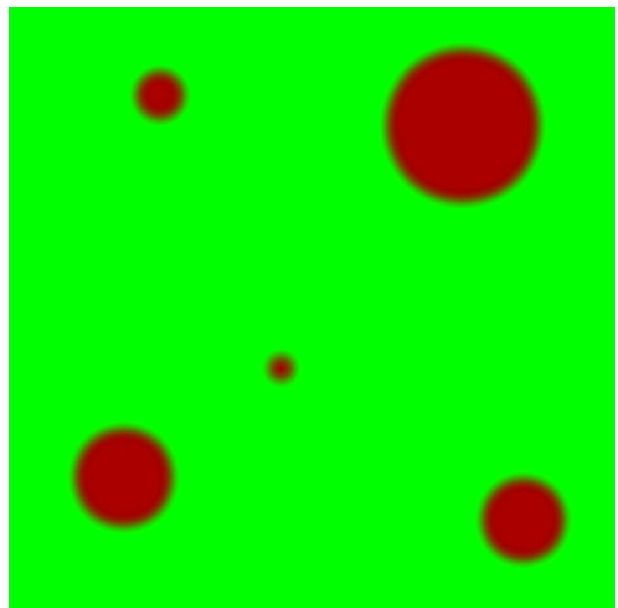


Figure 7. The BCC_A2 phase replaced the Liquid phase and gradually displaces the HCP_A3 phase for hafnium at $T = 2000$ K.

Conclusion

The paper presents derivation of a multiphase locally nonequilibrium model of phase transformations in single-component systems. The advantage of the presented model is the fulfilled principle of matching with the previously known two-phase field of a phase field [26] and the absence of necessity for evident tracking of correlation (1) in numerical calculations.

Fulfillment of the matching principle guarantees correct physical behavior on phase interfaces and existence of thermodynamic steady states in the system, which differentiates the model from the previously suggested approaches.

Absence of the need for evident tracking of correlation (1) in numerical modeling of phase transitions within the framework of this approach makes it possible to consider the equations of all phase fields as independent ones. The latter considerably simplifies the technology of modeling of structure formation processes in multiphase systems, since it enables a separate solution of phase field equations. Modeling include a check of the condition of phase sum normalization, which was met at any time moment of the calculation. The modeling results match the expected behavior of a nonequilibrium system and confirm applicability of the presented model.

The suggested approach can be generalized for the case of solutions and is a basis for subsequent development of the phase field method in the material science.

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Conflict of interest

The author declares that he has no conflict of interest.

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