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Modeling of Phase Transitions Kinetics in Systems With Two Interacting Order Parameters

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Abstract. We present common 1D model of first order phase transition based on coupled solution of order parameters evolution and heat transfer equations. Such a model may be used for simulation of phase transitions in multiferroics or magnetostructural phase transitions, for example. First order phase transition process has been described by Landau-Khalatnikov-like equation with the thermodynamic potential of 2-3-4 and 2-4-6 types.

Introduction

In recent years new effects of electromagnetic waves generation under nonequilibrium processes in phase field models attract great attention of researchers in field of phase transitions simulation. Recently, the phase field methods have been used for modeling and predicting morphological and microstructural evolution in crystalline and amorphous materials [1]. Phase field modeling has been successfully applied for solidification problems [2], modeling of materials defects and deformations [3], precipitate growth and coarsening [4], solid-state phase transformations [5], martensitic phase transition modeling [6], etc. Phase field method is a phenomenological one, and evolution equations of phase field variables may be derived based on general thermodynamics and kinetics principles.

Phase transitions in many materials may be triggered by both temperature and external field. For temperature-driven phase transition kinetics heat transfer process is essential. It is well known that near phase transition heat capacity of the material increases. This leads to the slowing down of heat transfer into the material near phase boundary. By the other hand, one may have different possibilities of the sample heating in different experiments. Different heating regimes may also lead to some features in phase transition process.

Here, we present general 1D model of temperature-driven first order phase transition in systems with two interacting order parameters based on coupled self-consistent system of phase field evolution and heat transfer equations solution. Such a model may be applied for simulation of different phase transitions, for example, phase transitions in multiferroics or magnetostructural ones.

Model

Phase transition process in a system with two scalar order parameters η_1 and η_2 may be described by Landau-Khalatnikov-like equations:

$$\partial\eta_i/\partial t = -\gamma_i \, \delta\Phi/\delta\eta_i , \quad i = 1, 2, \tag{1}$$

where Φ is thermodynamic potential (or Ginzburg-Landau functional), γ_i are kinetic coefficients, which should be defined from experimental data. For describing of first order phase transition the thermodynamic potential of two types may be used. The first one is 2-3-4 potential:

$$\Phi = \int \varphi \mathbf{dr} = \int \left[\sum_{i=1,2} \left(\frac{a_i}{2} \eta_i^2 + \frac{b_i}{3} \eta_i^3 + \frac{c_i}{4} \eta_i^4 + \frac{D_i}{2} \left[\nabla \eta_i \right]^2 \right) + \frac{f}{2} \eta_1^2 \eta_2^2 \right] \mathbf{dr} . \quad (2)$$

The second one is 2-4-6 potential:

$$\Phi = \int \varphi \mathbf{dr} = \int \left[\sum_{i=1,2} \left(\frac{A_i}{2} \eta_i^2 + \frac{B_i}{4} \eta_i^4 + \frac{C_i}{6} \eta_i^6 + \frac{D_i}{2} \left[\nabla \eta_i \right]^2 \right) + \frac{f}{2} \eta_1^2 \eta_2^2 \right] \mathbf{dr} . \quad (3)$$

In both cases, a, b, c, A, B, C, and D are phenomenological parameters.

We will assume, that temperature dependence is essential only for parameters a_i and A_i and has a form $(a, A)_i = \alpha_i(T-T_{0i})$, where α_i is a constant, T_{0i} is critical temperature.

Equation (1) with potential (2) should be solved with heat transfer equation:

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \Delta T + Q. \quad (4)$$

In (4) ρ is the density of material, c_p is a heat capacity, λ is a heat transfer constant, T is the temperature, Q is heat sources distribution. Heat sources distribution is caused by energy releasing/absorption by the system at phase transition and may be expressed in the form

$$Q = -\sum_{i=1,2} \frac{\partial \eta_i}{\partial t} \left(\frac{\delta \Phi}{\delta \eta_i} + T \frac{\delta S}{\delta \eta_i} \right), \quad (5)$$

where S is entropy of the system

$$S = \int \left(-\frac{\partial \varphi}{\partial T} \right)_{\eta_i, p} \mathbf{dr} . \quad (6)$$

Choosing particular type of thermodynamic potential Φ, and boundary/initial conditions, we will obtain self-consistent problem.

This system of equations should be solved with some initial and boundary conditions. We will consider the following conditions:

$$T(x,0) = T_{start}; \quad \eta_1(x,0) = \eta_{1+}(T_{start}); \quad \eta_2(x,0) = \eta_{2+}(T_{start});$$

$$T(0,t) = T_{start} + \left[T_{cr} + \Delta T - T_{start} \right] exp\left(\frac{\left[t - t_0 \right]^2}{\Delta t^2} \right); \quad (7)$$

$$\left. \frac{\partial T(x,t)}{\partial x} \right|_{x=L} = 0; \left. \frac{\partial \eta_i(x,t)}{\partial x} \right|_{x=0} = \left. \frac{\partial \eta_i(x,t)}{\partial x} \right|_{x=L} = 0$$

Chosen border conditions correspond to the case of linear heating/cooling of left sample side. Temperature of the left boundary has a Gaussian-like time dependence. Maximum temperature of heated sample side is $T_{cr} + \Delta T$. Such temperature will be reached at moment t_0. Characteristic duration of the heating/cooling process is Δt. This situation is quite unreal due to the fact that we cannot to control temperature, but only heat flow. We will use such border condition for simplicity of results understanding. Initial condition corresponds to the ordered state of the sample. Heating should lead to order-disorder phase transition.

For numerical modeling we will use the following values of parameters for 2-3-4 model: $\alpha_1 = 5\ 10^8$ erg/K cm^3, $b_1 = -10^{12}$ erg/cm^3, $c_1 = 6\ 10^{12}$ erg/cm^3, $T_{01} = 300$ K, $\gamma_1 = 0.5\ 10^{-8}$ (erg s)$^{-1}$, $D_1 = 10^4$ erg/cm, $\alpha_2 = 5.2\ 10^8$ erg/K cm^3, $b_2 = -0.99\ 10^{12}$ erg/cm^3, $c_2 = 6.1\ 10^{12}$ erg/cm^3, $T_{02} = 200$ K, $\gamma_2 = 0.57\ 10^{-8}$ (erg s)$^{-1}$, $D_2 = 1.1\ 10^5$ erg/cm. In case of 2-4-6 model parameters will be following: $\alpha_1 = 2.6\ 10^8$ erg/K cm^3, $b_1 = -5\ 10^9$ erg/cm^3, $c_1 = 8\ 10^{11}$ erg/cm^3, $T_{01} = 350$ K, $\gamma_1 = 0.5\ 10^{-8}$ (erg s)$^{-1}$, $D_1 = 10^4$ erg/cm, $\alpha_2 = 3\ 10^7$ erg/K cm^3, $b_2 = -2\ 10^{10}$ erg/cm^3, $c_2 = 10^{11}$ erg/cm^3, $T_{02} = 200$ K, $\gamma_2 = 0.57\ 10^{-8}$ (erg s)$^{-1}$, $D_2 = 1.1\ 10^5$ erg/cm. For both models $\rho = 10$ g/cm^3, $c_p = 10^7$ erg/(K cm^3), $\lambda = 5\ 10^7$ erg s/(K cm). Length of the sample $L = 1$ cm. The scheme of problem is shown on Fig. 1.

Fig. 1. Geometry of the problem. The sample is placed at $0 < x < L$. Left side of the sample (at $x = 0$) is heated/cooled; at the right side ($x = L$) heat fow is equal to zero.

Results and Discussion

We will investigate what effect will have the interaction between order parameters on phase transition kinetics. For simulation we will use the following heating/cooling parameters: $T_{start} = 190\,K$, $\Delta T = 100\,K$, $t_0 = 2\,s$, $\Delta t = 2\,s$. This situation corresponds to heating of left boundary of the sample from 190 to 290 K and cooling back to 190 K per 2 s. For chosen material parameters at such process the part of the sample will be heated to temperature more than critical one for the second order parameter. The results of simulation are shown on Fig. 2.

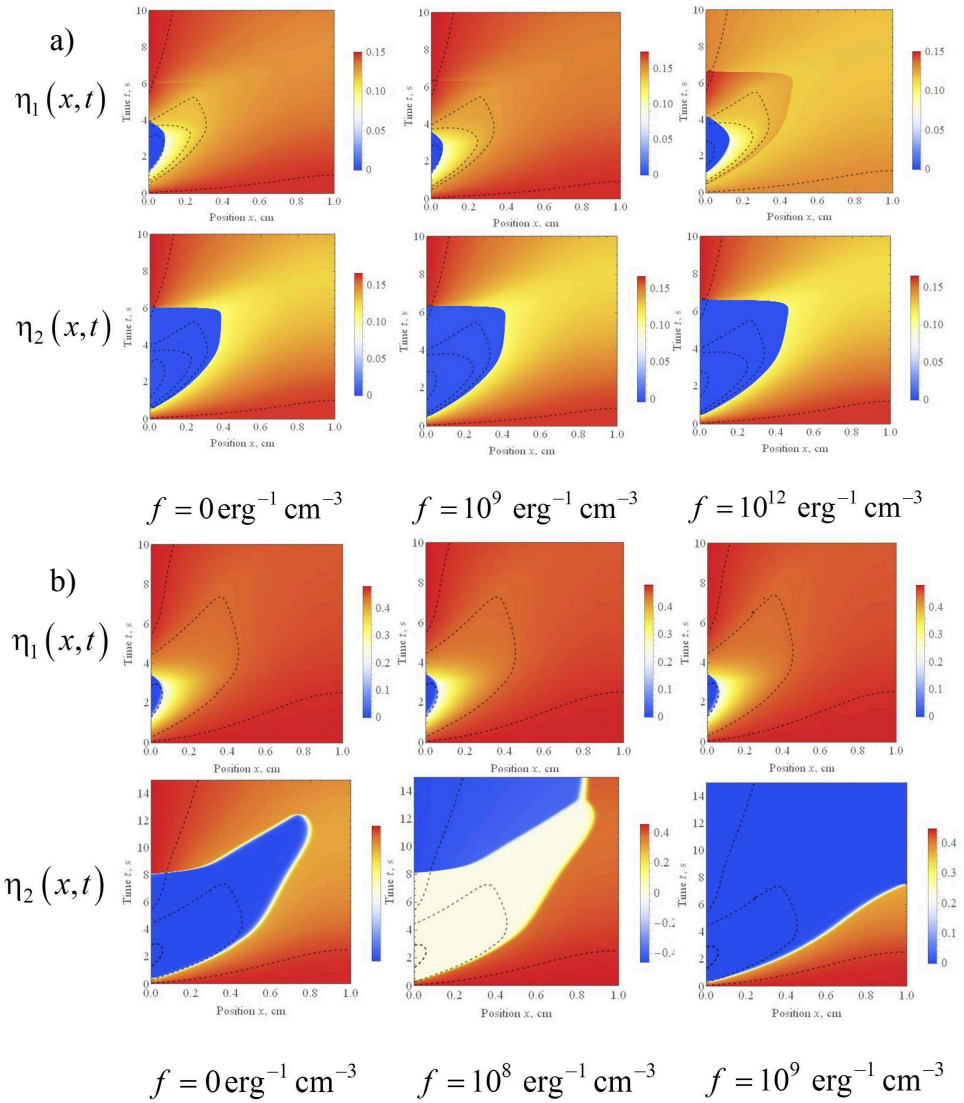

Fig. 2. Time-space distribution of order parameters: a) model 2-3-4, b) model 2-4-6.

One can see that in 2-3-4 model increasing of interaction parameter f has almost no effect on behavior of the second order parameter. Phase transition associated with the first order parameter

occurs in greater part of the sample when *f* increases. Increasing of interaction leads also to decrease in the first order parameter value at the ground state. In the sample part where the second order parameter disappears the first order parameter has greater values.

For 2-4-6 model the situation differs. Behavior of the first order parameter is almost insensitive to the change in interaction between subsystems. The second order parameter at small enough interaction goes to another stable state. At some interaction parameter values, coexisting of two ordered phases with the opposite signs of order parameters becomes possible. Withal, time-space area of disordered state arises. Further increasing of interaction leads to impossibility of the second order parameter switching.

Summary

We have proposed and investigated the model of first order phase transition kinetics in systems with two interacting order parameters based on the order parameters Landau-Khalatnikov-like evolution equations and heat transfer equation. Investigation showed the possibility of phase transition kinetics describing by the proposed model. The model show believable results, and may be used for describing of many real phase transitions: magnetostructural, phase transitions in multiferroics, etc. Our model may be easily generalized on the case of many component order parameters.

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