CV-07

Modeling of First Order Phase Transition Kinetics.

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Phase field models attract great attention of researchers in field of phase transitions simulation. So, 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.

Heat transfer process is essential for the phase transition kinetics. 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, scientists 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 common 1D model of first order phase transition based on coupled solution of phase field evolution and heat transfer equations. Such a model may be used for simulation of magnetic phase transitions, for example.

First order phase transition process may be described by Landau-Khalatnikov-like equation with the thermodynamic potential of 2-3-4 type: $\partial\eta/\partial t = -\gamma\times\delta\Phi/\delta\eta$, $\Phi = \int\phi\boldsymbol{dr} = \int(a\eta^2/2 + b\eta^3/3 + c\eta^4/4 + D[\nabla\eta]^2/2)\boldsymbol{dr}$, where η is a phase field variable (or order parameter), Φ is a thermodynamic potential (or Ginzburg-Landau functional), γ is a kinetic coefficient, which should be defined from experimental data. Constants a, b, c, and D are a phenomenological parameters. We will assume, that temperature dependence is essential only for parameter a and has a form $a = \alpha(T-T_0)$, where α is a parameter, T_0 is a critical temperature. It is well known that for such thermodynamic potential there are three equilibrium values of the order parameter. Non-zero order parameters are possible at $T < T_{cr}$, true temperature of phase transition is T^*.

Heat equation is $\rho c_p \partial T/\partial t = \lambda\triangle T + Q$, $Q = -\partial\eta/\partial t(\delta\Phi/\delta\eta + T\delta S/\delta\eta)$, $S = -\int(\partial\phi/\partial T)\boldsymbol{dr}$. Here, ρ is a density of material, c_p is a heat capacity, λ is a heat transfer constant, T is a temperature, Q is a heat sources distribution, S is entropy.

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

$T(x, 0) = T_{\text{start}}$, $T(0, t) = T_{\text{start}} + [T_{cr}+\Delta T-T_{\text{start}}]\times\text{tri}(k[t-t_0])$, $\partial T/\partial x|_{x=L} = 0$, $\eta(x, 0) = \eta_+(T_{\text{start}})$, $\partial\eta/\partial x|_{x=L} = \partial\eta/\partial x|_{x=0} = 0$

Here, $\text{tri}(t) = \max(1-|t|, 0)$ is a triangular function.

For numerical modeling we will use the following values of parameters: $\alpha = 5\ 10^8$ erg/K cm^3, $b = -10^{12}$ erg/cm^3, $c = 6\ 10^{12}$ erg/cm^3, $T_0 = 200$ K, $\gamma = 0.5\ 10^{-8}$ (erg s)$^{-1}$, $D = 10^4$ erg/cm, $\rho = 10$ g/cm^3, $c_p = 10^7$ erg/(K cm^3), $\lambda = 5\ 10^7$ erg s/(K cm), $T_{cr} = 283$ K, $T^* = 274$ K, $L = 1$ cm. Results of modeling are shown on figs. 1 and 2.

We have demonstrated the model of first order phase transition based on coupled solution of phase field evolution and heat transfer equations. Time and space distributions of the order parameter and temperature have been obtained for different heat regimes. Position and speed of the interphase boundary have been calculated.

This work was particularly supported by grants of RFBR # 13-07-00462, 15-07-08806 and RSF # 14-22-00279.

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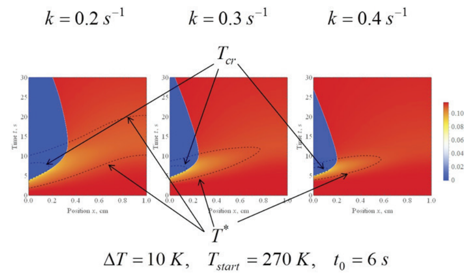
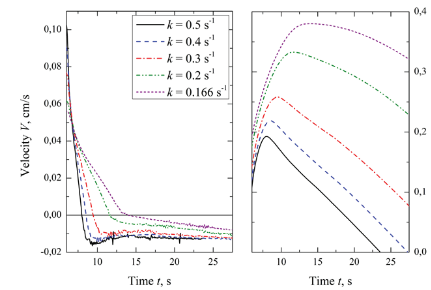


Time and space distribution of the order parameter



Position and speed of interphase boundary