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Determination of kinetic parameters of a phase-field model by a neural-network method

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The inverse problem of restoring the kinetic parameters of the phase-field model of pure iron crystallization in an isothermal setting is considered herein. A neural network method is proposed that estimates the mobility and relaxation time parameters of the phase field based on the dependence of the front velocity on supercooling. The training is executed through an iterative cycle that aligns with the underlying physics of the process. The demonstration is made of the reproduction of target velocity curves for reference data from molecular dynamics. The proposed method has the potential to reduce the labor intensity of calibrating models that are transferable to related materials and other physical problem formulations.

Keywords: phase-field method, neural network, pure element, parameter optimization.

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Modeling of phase transitions in real materials is accompanied by uncertainty of kinetic parameters that determine the dynamics of the interface. In the phase-field approach [1] such parameters as mobility of the phase field and the relaxation time are not produced directly from the basic principles and require selection using experimental or reference data. Besides, the computational cost of phase-field calculations significantly limits the use of the classic iteration methods.

Under these conditions the key objective becomes definition of physically agreed values of kinetic parameters suitable for subsequent analysis of other system characteristics. The promising tool to solve such an inverse problem are the neuron networks capable of detecting nonlinear links between the model parameters and the observed dependences. This paper uses a fully connected neuron network to determine the kinetic parameters of a phase-field model of pure iron crystallization based on molecular dynamic data in isothermal setup under the condition of the limited computational resources.

The phase field method introduces an order parameter $\varphi(\mathbf{r}, t)$, which describes the phase state of the point: inside the phases the value φ is constant, and in the interphase area it changes smoothly, shaping a diffuse boundary. Usually $\varphi = 1$ is adopted for a solid phase (S) and $\varphi = 0$ for a liquid phase (L) [1].

The functionality of the total entropy of the system at constant pressure and phase densities [2] is

$$S = -\int\limits_V \left[\frac{\partial g(\varphi, T)}{\partial T} + \frac{1}{2T_m}\left(\sigma^2\left(\nabla\varphi\right)^2 + \gamma\dot{\varphi}^2\right)\right] dV,$$

where the equilibrium density of Gibbs energy $g(\varphi, T)$ is shown in the form of interpolation by phases with an interphase „double-well" potential

$$g(T, \varphi) = p(\varphi)g^S(T) + \big(1 - p(\varphi)\big)g^L(T) + Wg(\varphi),$$

where $g^S(T)$ and $g^L(T)$ — specific Gibbs' energies of solid and liquid phases; $p(\varphi) = \varphi^2(3 - 2\varphi)$ — an interpolation polynomial describing a volume phase fraction; $g(\varphi) = \varphi^2(1 - \varphi)^2$ — a potential with two minima at $\varphi = 0,\ 1$; W — height of a potential barrier between phases [3]. Coefficients σ and γ characterize accordingly the surface energy and kinetic properties of the interface. For brevity sake further the function arguments are omitted.

To produce a system of relaxation equations of the phase transition, let us determine the speed of change of full entropy, using the enthalpy bulk density conservation law

$$\frac{\partial h}{\partial t} = -\nabla \cdot \mathbf{J}_T, \qquad h = g - T\frac{\partial g}{\partial T},$$

and request the positive certainty of entropy generation in the considered volume

$$\frac{dS}{dt} \geqslant 0.$$

The system of equations is produced from the principles of non-equilibrium thermodynamics [4]. The paper uses a simplified isothermal setup without heat transfer and geometric effects, where the model is reduced to a single equation of the phase field

$$\tau_\varphi\ddot{\varphi} + \dot{\varphi} = M_\varphi\left[\sigma^2\nabla^2\varphi - \frac{T_m}{T}\left(Wg' + \Delta g p'\right)\right], \qquad (1)$$

where τ_φ — relaxation time of the phase field, M_φ — phase field mobility, $\Delta g = g^S - g^L$. A dash in p' and g' means

derivatives with respect to φ. In the isothermal setup all the parameters of equation (1), including a thermodynamic source Δg, are accepted as constant. The mobility of the phase field M_φ usually depends on temperature and selected in the form of the Arrhenius dependence

$$M_\varphi(T) = M_0 \exp\left(-\frac{E_0}{T}\right).$$

If you study the conditions of equilibrium and the limit cases of the phase field equation [3], you can get the expressions for σ and W via the interface parameters

$$\sigma^2 = 3\chi\delta, \qquad W = \frac{6\chi}{\delta}, \tag{2}$$

where δ — width of diffuse boundary, χ — specific surface energy.

To exclude the effect of interface curvature, let us consider the motion of the flat front in a unidimensional setup. Let us convert equation (1) into a dimensionless form, redetermining the coordinate and the time in the form of a product of a dimension parameter and a dimensionless value: $x = \delta\xi$ and $t = t_0\tau$. With account of expressions (2) we get

$$\bar{\tau}_\varphi \ddot{\varphi} + \dot{\varphi} = \bar{M}_\varphi \left[\nabla^2\varphi - \frac{T_m}{T}\left(2g' + p'\,\overline{\Delta g}\right)\right], \tag{3}$$

where the dimension parameter of time and dimensionless parameters are defined as

$$t_0 = \frac{\delta}{3M_\varphi^0\chi}, \qquad \overline{\Delta g} = \frac{\delta}{3\chi}\Delta g,$$

$$\bar{\tau}_\varphi = \frac{\tau_\varphi}{t_0}, \qquad \bar{M}_\varphi = \frac{M_\varphi}{M_\varphi^0}.$$

Mobility M_φ in the isothermal setup is deemed to be constant, but maintains temperature dependence; the time scale t_0 is fixed by selection of $M_\varphi^0 = M_\varphi(T_m)$. Thermodynamic potentials for pure iron are taken from paper [5], the melting temperature is $T_m = 1811$ K.

The key parameter in the obtained equation is a combination $\delta/(3\chi)$, which combines the characteristics of the interface. Values χ for many systems are well-known, and the width of the diffuse boundary δ is a parameter specific for phase-field models that reflects the thickness of the transition region between the long-range and short-range order; usually $\delta \sim 10^{-9}$ m. To reduce the uncertainty, let us introduce $a = \delta/(3\chi)$; typically $a \approx 10^{-9}$ m^3/J (for example, at $\chi = 0.333$ J/m^2 and $\delta = 10^{-9}$ m).

To solve equation (3), a gradient-stable scheme is used [6], which is implemented by the sweep method. The calculations were made in the area $\xi \in [20; 120]$ with steps $\Delta\xi = 0.1$ and $\Delta\tau = 0.1$. The front position was determined using value $\varphi = 0.5$; upon achievement of $\xi = 100$ the region would move cyclically. The established speed was calculated by averaging using the last 200 steps with the total number of iterations $N_\tau = 10\,000$.

Further a problem of defining the kinetic parameters of the phase-field model is considered using the known dependence of the front speed on the supercooling under the conditions of the limited computing resources. The purpose is to detect a set of parameters

$$\mathbf{P}_{exp} = \{M_0, E_0, \tau_\varphi\},$$

providing for the physically agreed reproduction of the reference dependence of front speed $\mathbf{V}_{exp}$ at the fixed number of algorithm iterations equal to 20. The reference data are „quasi-experimental" results of molecular-dynamic modeling [7].

To determine the parameters, a neuron network is used – a three-layer fully connected perceptron with the architecture of 16-48-3. The front speeds $\mathbf{V} = \{V(\Delta T_1), V(\Delta T_2), \dots\}$ obtained as a result of computational modeling are supplied to the network input, and the output data are the model parameters $\mathbf{P}$. The input and hidden layers applied the function of activation tanh, the training was done with Adam algorithm using a meansquare error (MSE); the criterion to stop training was a total error of $\leqslant 10^{-3}$. All input and output values were normalized linearly in the range of $[-1; 1]$.

The initial approximation $\mathbf{P}_0$ was determined from the limit of the sharp boundary [2], where phase-field model is reduced to analytical dependence. In this paper the expression is used with account of ratios (2) and with the condition $\tau_\varphi = 0$, the front speed is expressed as

$$v = -\frac{3}{2}\delta M_\varphi(T_0)\sqrt{\frac{T_m}{T_0}}\Delta g(T_0).$$

Comparing estimated speeds v_i with the data of molecular-dynamic modeling $\tilde{v}_i$, the initial values of parameters M_0 and E_0 were defined from the minimization of the residual functionality

$$r = \sum_i \left(1 - \frac{v_i}{\tilde{v}_i}\right)^2. \tag{4}$$

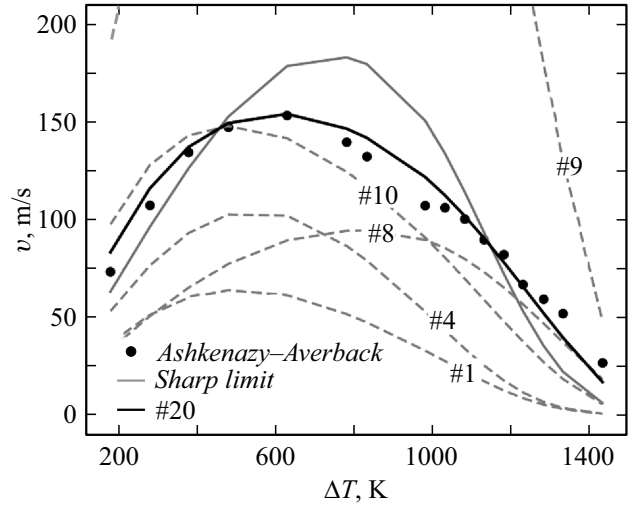
The training is done in iteration manner: at step j the network is trained using the accumulated set of pairs $\{(\mathbf{V}_k, \mathbf{P}_k)\}_{k=0}^{j}$. Then $\mathbf{V}_{exp}$ speed vector is supplied to the input of the network, and the network predicts new approximation of the parameters

$$\mathbf{P}_{j+1} = Neural\ Network\,(\mathbf{V}_{exp}).$$

Using $\mathbf{P}_{j+1}$, the numerical solution to the phase field equation is provided, and speeds

$$\mathbf{V}_{j+1} = Phase\ Field\,(\mathbf{P}_{j+1}),$$

are calculated, and afterwards the pair $(\mathbf{V}_{j+1}, \mathbf{P}_{j+1})$ is added to the training sample, and the network is retrained. Such approach makes it possible to use the phase-field model as



Dependence of crystallization front speed v on supercooling ΔT. Points — data of molecular dynamics [7]; grey solid line — calculation within the sharp boundary; dashed lines — results of modeling at different iterations of neuron network training, black solid line — curve corresponding to the final stage of parameter confirmation and characterized by the least residual.

an „arbiter", who assesses the correctness of the current approximation of the parameters without a direct feedback with the neuron network. To improve the stability at the first iterations prior to the prediction $\mathbf{P}_{j+1}$, a pseudo-random disturbance of low amplitude is introduced into the network weights, which is aimed at expanding the area of searching for the parameters and preventing the premature stabilization at the non-physical local solutions; then it is disconnected. The resulting set of parameters is selected as a solution with the least residual achieved at the stage of the parameters confirmation. In this paper ten stabilizing (with disturbance in the weights) and ten confirming iterations were conducted.

The figure shows a wide spread of curves $v(\Delta T)$ for the first iterations, the training sample is being formed. By the tenth iteration, the shape and the maximum of the curve with data are matched [7]. At subsequent steps the algorithm confirms all incoming parameters.

Table 1. Values of model and residual parameters for some iterations of neuron network training

Iteration	M_0, $m^3/(J \cdot s)$	E_0, K	τ_φ, 10^{-12} s	Residual r
Sharp boundary	589.4	2620.0	0.0	1.6940
1	694.8	3688.1	9.3	8.7991
4	1040.0	3796.2	2.2	6.2628
8	177.2	1650.8	6.1	1.8602
9	1327.6	2088.5	0.8	89.0104
10	1249.1	2928.0	9.5	2.1976
18	630.9	2148.4	7.3	0.2727
19	631.1	2146.0	7.3	0.2696
20	631.2	2143.4	7.4	0.2680

Table 2. Values of model and residual parameters at different specified values of parameter $a = \delta/(3\chi)$

a, 10^{-9} m^3/J	M_0, $m^3/(J \cdot s)$	E_0, K	τ_φ, 10^{-12} s	Residual r
0.8	583.1	2000.5	10.4	0.0958
1.0	631.2	2143.4	7.4	0.2696
1.2	526.4	1901.2	7.9	0.0997
1.5	564.0	1943.7	7.3	0.1657
2.0	475.0	1822.2	7.1	0.1160

Table 1 provides the values of the parameters corresponding to the iterations shown in the figure, and also the data for the last three steps of the algorithm; additionally the values of the residual (4) used as a comparison criterion are specified. At the initial stage there is a considerable spread of the parameters related to the formation of the training sample. In the considered example at the stage of confirmation the residual fades monotonically; such behavior is not a guaranteed property of the method, the surge of the residual in the iteration #9 reflects the non-monotonic nature of the stabilization stage.

Table 2 shows the parameters of the phase-field model at different values of the coefficient a, specifying the connection between the width of the diffuse boundary and the surface energy. From the data you can see that the change a leads to variation M_0, E_0 and τ_φ, which reflects the sensitivity of the model to the characteristics of the interface. The minimum value of the residual was found for a, equal to $0.8 \cdot 10^{-9}$ m^3/J.

The paper proposed an approach to the definition of the kinetic parameters of the phase-field model of pure iron crystallization using a neuron network in a combination with computational modeling under the conditions of the limited computing resources. The iteration interaction of the neuron network with the phase-field model makes it possible to select the values of parameters M_0, E_0 and τ_φ, providing for the reproduction of the front speed dependence on supercooling obtained in molecular-dynamic modeling.

The analysis of the results sensitivity to parameter $a = \delta/(3\chi)$ shows that the proposed algorithm remains operable at different characteristics of the interface, leading to agreed sets of kinetic parameters. Transfer of the algorithm to other materials and phase-field models will not require the change in its principal scheme and reduces to replacement of the used thermodynamic and reference data with subsequent retraining for a specific system. The proposed approach may be used for primary calibration of the phase-field models in the study of the phase transitions in different setups.

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Conflict of interest

The authors declare that they have no conflict of interest.

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