

# Kinetic Melting and Crystallization Stages of Strongly Superheated and Supercooled Metals<sup>1</sup>

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**Abstract**—The heterogeneous melting/crystallization of metals with different crystallographic lattices in conditions where the phase front propagates on overheated/supercooled media was modeled in the context of the molecular dynamics approach. In order to obtain the temperature dependence of the kinetic velocity in analytical form, the results of atomistic modeling were approximated by the function obtained from the kinetic representations. For the first time, stationary temperature dependences of kinetic velocity  $v(T_{s\ell})$  for the limit values of superheated/supercooled copper and iron were built.

**Keywords:** atomistic modeling, kinetic velocity, superheated/supercooled states, melting/crystallization, molecular dynamics

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## 1. INTRODUCTION

Melting of a solid body and solidification of a liquid are a common phenomena in nature. There are two mechanisms of melting/crystallization of metals: heterogeneous (also called surface or front) and homogenous (volumetric). In the first case, in classical thermodynamics [1], the melting of solids and solidification of liquids are related to the phase transformations of the first kind running at a certain (equilibrium) temperature  $T_m$ , which corresponds to the equality of the Gibbs free energy of the solid and liquid states. Heterogeneous melting/crystallization mechanisms correspond to the motion of a continuous medium with the surface of a strong discontinuity on which the thermophysical and thermodynamic characteristics have changed abruptly. A homogeneous melting mechanism is characterized by the start of a new phase (liquid) in a volume of superheated crystal, and in this study it will not be considered.

In the case of fast phase transitions, typical for the pulsed influence of a concentrated energy flow [2], the characteristic propagation velocity of the phase fronts are in the range  $(10-10^2 \text{ m/s}) \leq v_{s\ell} \leq u_{\text{sound}}$ , and for the correct description of the phase transformations, it is necessary to use a complete set of continuum equations for mass, momentum, and energy flows. At the same time for the correct formulation of the heterogeneous melting/solidification processes, using relations that express the conservation laws at the interface  $\Gamma_{s\ell}(t)$  is no longer enough, as some additional kinetic relations are required. The most important kinetic characteristic of heterogeneous phase transformations is the mobility of the interface defined by the velocity  $v_{s\ell} = v(T_{s\ell})$  depending on the magnitude of superheating/supercooling of the surface of interface  $\Delta T = T_{s\ell} - T_m$  [3]. In the definition of the temperature dependence of  $v_{s\ell}(\Delta T)$ , several directions are known [4, 5], based on the thermodynamic, kinetic, and molecular-dynamics approach with the use of continual and atomistic models and their combinations.

In this paper, based on the simulation of molecular dynamics, we considered the possibility of these approaches to define the kinetics of the melting and solidification of metals in highly superheated and supercooled states in a wide temperature range.

<sup>1</sup> The article was translated by the authors.

## 2. THE KINETICS OF MELTING AND SOLIDIFICATION OF STRONGLY SUPERHEATED/SUPERCOOLED METALS

We briefly describe the main approaches to solve problems for determining the kinetic speed  $v_{s\ell}(\Delta T)$  depending on the magnitude of superheating/supercooling of the surface of interface  $\Delta T$  on the example of metals with different crystallographic gratings—copper and iron.

### 2.1. Thermodynamic Approach

Thermodynamics are a macroscopic theory, in which from an energy point of view, we consider the properties of macroscopic bodies in a state of equilibrium. This allows us to make conclusions on thermodynamics to have a great deal in common. In equilibrium thermodynamics one way to describe the equilibrium processes is the theory of thermodynamic potentials [1]. The method of thermodynamic potentials is based on the possibility of introducing for equilibrium processes functions whose total differentials describe the change in the state of a thermodynamic system. Typically, achieving an equilibrium state of a system is characterized by the Gibbs potential, which in this case takes the minimum value and becomes the constant  $dG = 0$ . This allows using the condition of the minimum of the Gibbs potential for describing equilibrium states in which  $T = \text{const}$  and  $p = \text{const}$ .

If the components of a thermodynamic system are not in equilibrium with each other, then there are thermodynamic flows through their interface. At the same time, the process of converting material from one aggregate state to another will take place, i.e., a phase transformation. Considering the processes in the system to be quasi-static and the flows to be infinitely small, we can use the methods of equilibrium thermodynamics to describe such a nonequilibrium system. In this case, an infinitely small difference in the thermodynamic parameters of the various parts of the system is assumed. The classic version of Stefan's problem [6, 7] is based on this assumption.

The driving force of phase transitions of the 1st kind is determined by the free energy difference between the two phases at the interface  $\Gamma(t)$  (or the superheating/supercooling value  $\Delta T$ ). Considering that in the process of the phase transitions of the 1st kind at the interface a number of quantities undergo abrupt changes; in the thermodynamic equations, we replace the differential symbol by the difference between the corresponding value  $dF \approx \Delta F$  at the equilibrium temperature of phase transition  $T_{\text{eq}}$  and the excess of Gibbs free energy for the two phases at the interface can be written in two forms:

$$\Delta G = (\varepsilon_1 - \varepsilon_2) + p_{\text{eq}}(V_1 - V_2) - T_{\text{eq}}(S_1 - S_2) = \Delta\varepsilon + p_{\text{eq}}\Delta V - T_{\text{eq}}\Delta S, \quad (1)$$

$$\Delta G = V\Delta p - S\Delta T, \quad (2)$$

where  $\Delta p = p - p_{\text{eq}}$ ,  $\Delta T = T - T_{\text{eq}}$ ,  $\Delta\varepsilon = \varepsilon_1 - \varepsilon_2$ ,  $\Delta V = V_1 - V_2$ ,  $\Delta S = S_1 - S_2$ , and  $T_{\text{eq}}$  and  $p_{\text{eq}}$  are the equilibrium temperature and pressure, respectively. In the case of melting  $T_{\text{eq}} = T_m$  and  $p_{\text{eq}} = p(T_m)$ , and in the case of evaporation,  $T_{\text{eq}} = T_b$  and  $p_{\text{eq}} = p_{\text{sat}}(T_b)$ , where  $T_b$  is the equilibrium boiling temperature in normal conditions and  $p_{\text{sat}}$  is the pressure of the saturated vapor.

At equilibrium  $\Delta G = 0$ , Eq. (1) takes the form:

$$\Delta\varepsilon + p_{\text{eq}}\Delta V - T_{\text{eq}}\Delta S = \Delta H - T_{\text{eq}}\Delta S = 0,$$

where the difference in enthalpy  $\Delta H = \Delta\varepsilon + p_{\text{eq}}\Delta V$  is known as the equilibrium latent heat of transition

$$L_{\text{eq}} = \Delta H = T_{\text{eq}}\Delta S. \quad (3)$$

At constant pressure,  $P = \text{const}$ , and from Eq. (2) it follows that the free energy difference is linearly proportional to supercooling (superheating):

$$\Delta G = -\Delta S \cdot \Delta T = L\Delta T/T_{\text{eq}}. \quad (4)$$

Subsequently, setting the free-energy  $\Delta G$  difference equal to the speed of the phase transformation, we find that the rate of conversion in the thermodynamic approach at constant pressure for small deviations from equilibrium is linearly proportional to superheating (supercooling)  $\Delta T$

$$v \approx \mu\Delta T, \quad (5)$$

where  $\Delta T = T_{s\ell} - T_m$ ,  $\mu$ —is the constant of proportionality between the normal velocity of the boundary and its supercooling. Equation (5) coincides in appearance with the well-known equation for determining the linear speed of crystal growth obtained on the basis of classical molecular-kinetics models in which the constant of proportionality  $\mu$  is called the kinetic coefficient [8, 9]. The main application of Eq. (5) and its different modifications [10, 11] was found in the description of melting/solidification processes,

where the coefficient  $\mu$  is the main parameter characterizing the mobility of the crystal-melt boundary. Comparison with the experimental data showed that Eq. (5) gives good agreement mainly at small supercooling [12, 13], i.e., in the vicinity of the temperature  $T_m$ . Despite the importance of this characteristic, there are only a few successful experiments on measuring the kinetic coefficient in metals and alloys [14, 15]. The main difficulties of the experimental determination related to the substantial complexity of measuring the supercooling of a melt on a solidification front.

Thus, the kinetic coefficient  $\mu$  determined from the thermodynamic approximation, closely describes the behavior of the front near the equilibrium melting point  $T_m$ , where the temperature dependence of the velocity is mainly controlled by the difference in the free energies of the crystal and the liquid phase. However, the melting/solidification kinetics away from the equilibrium melting temperature differ greatly from the kinetics in the vicinity  $T_m$ , due to the strong temperature dependence of the thermodynamic driving forces and atomic mobility.

Since thermodynamics do not consider the internal structure of bodies, a number of thermodynamics conclusions and their provisions are not sufficiently accurate and physically demonstrative. Being in constant motion, the structural particles of matter are displayed in the main provisions of molecular kinetics theory, in which all processes are considered at the atomic or molecular level, and the particles have a Maxwellian velocity distribution.

## 2.2. Kinetic Approach

The kinetic approach is based on the phenomenological theory of Wilson-Frenkel [16, 17] and some of its generalizations [12, 18, 19]. One of the directions based on the mechanism of the diffusion restriction of the velocity of the crystallization/melting front, using the assumption of the necessity to overcome the atoms' (molecules) diffusion barrier in the transition from the liquid to the solid phase [16, 17]. The second one uses as a restriction [20, 21] the frequency of the thermal collisions of atoms with the interphase boundary.

The velocity of the crystallization/melting front  $v_{s\ell} = v(T_{s\ell})$  with the diffusion restriction expressed by the equation of type [12]

$$v(T_{s\ell}) = \frac{D_0 a}{\lambda^2} f_0 \exp\left(-\frac{Q}{k_B T_{s\ell}}\right) \left[ \exp\left(\frac{L_m}{k_B T_m} \frac{T_{s\ell} - T_m}{T_{s\ell}}\right) - 1 \right] = C^{\text{WF}} \frac{D}{a} \left[ \exp\left(\frac{L_m}{k_B T_m} \frac{T_{s\ell} - T_m}{T_{s\ell}}\right) - 1 \right], \quad (6)$$

where  $C^{\text{WF}} = \frac{a^2}{\lambda^2} f_0$ ,  $a$  is the interatomic distance, and  $\lambda$  is the mean free path of the atoms in this process ([22] is assumed, i.e., that it is proportional to the lattice parameter,  $a$ ,  $\lambda < a$ ),  $f_0$  is the efficiency factor (the constant is of the order of unity  $f_0 < 1$ ) characterizing the part of the collisions of atoms of the liquid with the solid leading to crystallization,  $Q$  is the activation energy for diffusion movement in the liquid,  $k_B$  is the Boltzmann constant,  $k_B T$  is the average thermal energy for one atom, and  $D_0$  is the pre-exponential factor on which the velocity of the process depends.

Equation (6) was used to study the kinetics of the melting/crystallization of silicon in a relatively small vicinity of the temperature  $T_m$  [23]. The results were compared with the results of simulating molecular dynamics with the Stillinger-Weber interaction potential [24] and the experimental data. The comparison showed an acceptable match. However, for pure metals, molecular dynamics simulation of the crystallization kinetics [20] with the Lennard-Johnson potential [25] showed that at high supercooling, where the diffusion coefficient  $D$  is very small, the velocity of the new phase growth in monoatomic metals was much higher than the interface velocity determined from Eq. (6).

This defect was eliminated by modifying the Wilson-Frenkel model (6) through the introduction of a factor limiting the solidification velocity and the collision frequency of atoms of the liquid phase with the faces of the crystal [21] instead of their diffusion. This resulted in the so-called BGJ (Broughton, Gilmer, Jackson) model in which the diffusion term was replaced by the average thermal velocity of the atoms

$$v_T = \sqrt{3k_B T_{s\ell} / m}$$

$$v(T_{s\ell}) = \frac{a}{\lambda} f_0 v_T \left[ \exp\left(\frac{L_m}{k_B T_m} \frac{T_{s\ell} - T_m}{T_{s\ell}}\right) - 1 \right] = C^{\text{BGJ}} \sqrt{\frac{3k_B T_{s\ell}}{m}} \left[ \exp\left(\frac{L_m}{k_B T_m} \frac{T_{s\ell} - T_m}{T_{s\ell}}\right) - 1 \right], \quad (7)$$

where  $C^{\text{BGJ}} = \frac{a}{\lambda} f_0$  is a dimensionless coefficient and  $m$  is the atomic mass.

The obtained dependence (7) was used to study the kinetics of melting/crystallization of sodium [26] in the vicinity of the temperature  $T_m$ . The results were compared with the results of molecular dynamics simulation with the potential of Lennard-Johnson and the experimental data. With an appropriate choice of fitting coefficients, quite a satisfactory agreement between the results was achieved.

Within the kinetic approach, it is easy to formulate an analytical view of the kinetic coefficient  $\mu$  [11, 13]

$$\mu = C^{\text{WF}} \frac{D}{a} \frac{L_m}{k_B T_m^2}, \quad (8)$$

$$\mu = C^{\text{BGJ}} \sqrt{\frac{3k_B T_m}{m}} \frac{L_m}{k_B T_m^2}. \quad (9)$$

It is not difficult to see that Eqs. (8) and (9) represent the first term in the expansion of Eqs. (6) and (7) in the vicinity of the equilibrium temperature  $T_m$ . Equations (8) and (9) are widely used in studies mostly of solidification kinetics [27–29].

These approaches to determine the melting and crystallization kinetics have two major drawbacks:

(a) equations (6)–(9) contain the coefficients  $C^{\text{WF}}$  and  $C^{\text{BGJ}}$  containing the quantities  $\lambda$  and  $f_0$  for which there is no strict definition. Their presence is taken into account in the form of fitting parameters and methods for their selection are unknown when entering deep into the metastable region of superheated and supercooled states;

(b) a narrow temperature range (vicinity of the equilibrium temperature  $T_m$ ) of superheated and supercooled states in which the adequacy of the results is guaranteed.

### 2.3. Molecular Dynamics Approach

At present, most of the current information on the understanding of the physics of melting/crystallization kinetics is obtained from the results of molecular dynamics modeling (MDM) [11–13, 20, 23, 26–34].

The representation of physical processes at the atomistic level with the subsequent MDM allows us to take a fresh look at the properties of interphase boundaries (interfaces) of the crystal-melt related to the melting and crystallization of highly superheated/supercooled microstructures.

With the help of MDM, observations of the formation of metastable phases and studies of the kinetics of fast phase transitions present interesting new possibilities, including in the field of the mathematical description of heterogeneous melting/crystallization processes in continuum approximation [5, 35]. Theoretical consideration of the heterogeneous mechanisms in the phase transformations of the first kind leads to various variants of Stefan's problem [2, 36], which in mathematical physics means a wide class of problems with moving boundaries, described by equations of a parabolic or elliptic type. The basis of continuum models, with the help of which the most complete description of phase transformations is realized, are the equations of mass, momentum, and energy flows. Heterogeneous phase transitions of the first kind (melting/crystallization) are treated here as the motion of a continuous medium with a strong discontinuity surface (a front of zero thickness), on which the requirements for executing the conservation laws and extracting some additional information on nonequilibrium singularities of phase transitions of the first kind are imposed. For melting/crystallization processes, this information is determined by the temperature dependence of the kinetic velocity  $v(T_{s\ell})$  determined in the range of the maximum permissible values of superheating/supercooling.

Taking advantage of the possibilities of computer molecular dynamics modeling, let us consider the process of heterogeneous melting/crystallization of metals under the conditions of the propagation of an interphase front over a superheated/supercooled medium.

## 3. MODEL AND MODELING RESULTS

The molecular dynamics approach is based on a model representation of a polyatomic molecular system in which all the atoms are represented by material points whose motion is described in the classical case by Newton's equations. Thus, there are  $N$  point particles, each of which has the following properties:

- a mass, radius vector, and velocity, respectively  $m_i$ ,  $\mathbf{r}_i$ , and  $\mathbf{v}_i$ , where  $i = 1, \dots, N$ ;
- interacts with the rest by means of forces  $\mathbf{F}_i = -\frac{\partial U(\mathbf{r}_1 \dots \mathbf{r}_N)}{\partial \mathbf{r}_i}$ , where  $U(\mathbf{r}_1 \dots \mathbf{r}_N)$  is the potential interaction energy of a system of  $N$  particles;

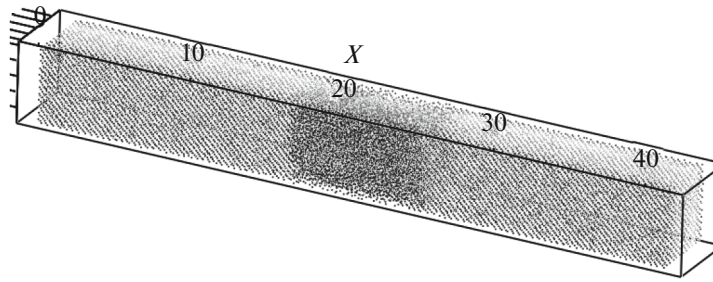


Fig. 1. Computational domain  $5 \times 5 \times 41$  nm, (57600 particles).

—interacts with external fields by force  $\mathbf{F}_i^{\text{ext}}$ .

The evolution of this model is described by a system of  $2N$  ordinary differential equations of motion:

$$\begin{cases} m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i + \mathbf{F}_i^{\text{ext}}, \\ \frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \end{cases} \quad (10)$$

$i = 1, \dots, N.$

To integrate the system of equations (10), knowledge of the coordinates and velocities  $(\mathbf{r}_i, \mathbf{v}_i)|_{t=0}$  at the initial instant of time  $t = 0$  of all  $N$  particles is required.

Thus, the mathematical model consists of a system of differential equations, their difference analog (difference scheme), interatomic interaction potential, and specifically defined initial and boundary conditions.

As the object of research, metals with different crystallographic lattices were selected: copper with the fcc lattice and iron with bcc lattice. For both metals, the temperature dependences of the stationary kinetic velocity of melting/crystallization were determined in the crystallographic plane (100) in the range of the maximum permissible values of superheating/supercooling.

The computational domain of  $5 \times 5 \times 41$  nm in the form of a parallelepiped is filled with 57600 particles (Fig. 1). MD calculations are performed using various multiparticle EAM potentials: for copper [37, 38] and for iron [39] with parametrization [40]. In all three spatial directions, periodic boundary conditions are imposed on the boundaries of the computational domain. At the start, the plane interface between the solid and liquid phases is created, and then its speed is measured directly, depending on the temperature. The particles form a layered structure containing two phases in contact with each other: crystalline and liquid. At the initial stage, to study the melting process, the liquid phase occupies approximately 18% of the computational domain volume; and to study the crystallization process,  $\sim 80\%$ . Figure 1 shows the initial state of the computational domain for modeling the heterogeneous melting process of metal. The liquid layer in the middle part of the computational domain is highlighted in a dark color.

By means of a thermostat, a fixed temperature value is established and maintained throughout the computational domain during the entire numerical experiment. At the same time, a constant value of the external pressure is maintained by the barostat. It should be noted that the thermostat that was used tried to keep the temperature at each point of the computational domain, including at the melting/crystallization fronts, not the average temperature over the entire volume. Thus, the inverse effect on the local temperature of the emission/absorption process of the latent heat of melting at the fronts was excluded.

As a result, the process of heterogeneous melting/crystallization quickly reaches a steady state and the change in the amount of the new phase occurs almost linearly. The position of the melting/crystallization fronts is tracked automatically by monitoring the parameter of the order.

The melting/crystallization kinetics were investigated by setting up a series of computational experiments for supercooling the liquid and overheating the solid phase with respect to the equilibrium melting temperature  $T_m$  in the temperature range:  $0.6T_m - 1.2T_m$ , at zero external pressure. Going beyond the specified temperature range in the case of overheating is restricted the loss of mechanical stability of the crystal and the formation of packaging errors on the crystallographic plane in the case of overcooling.

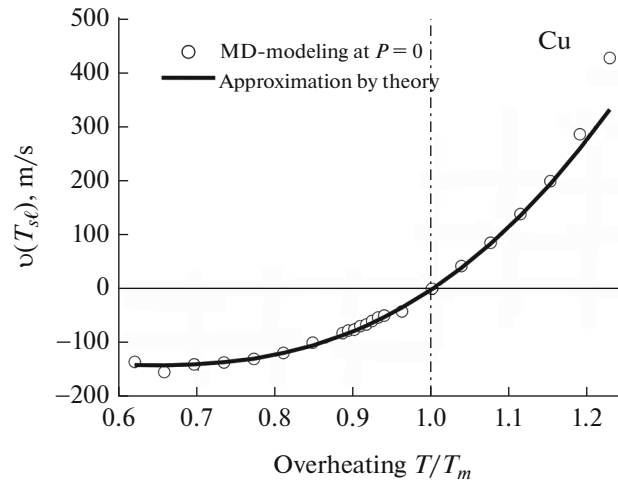


Fig. 2. Dependence of melting/crystallization front velocity on superheating/supercooling value for copper.

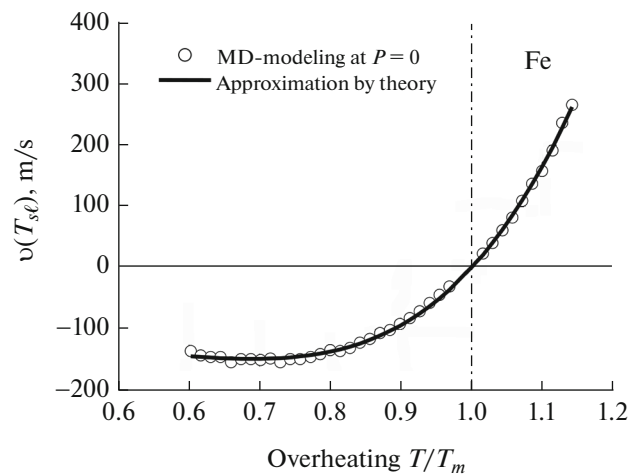


Fig. 3. Dependence of melting/crystallization front velocity on superheating/ supercooling value for iron.

The result of the molecular dynamics simulation was the production of a discrete set of phase front velocity values  $v(T_{s\ell})$ , indicated in Figs. 2 and 3 by markers, in the range of the limiting values of superheating and supercooling for Cu and Fe.

The next step was to compare the results of the molecular dynamics simulation with the results of the kinetic BGJ model [20] (Eq. (7)). Equation (7) contains two thermophysical parameters: the values of the equilibrium melting temperature  $T_m$  and the latent heat of melting  $L_m$ . Since these values in the molecular dynamics approach may differ slightly from the real ones (because of the imperfection of the used interaction potentials), for the purity of comparing the two curves in Eq. (7) the  $T_m$  and  $L_m$  values, which were determined by MDM using the techniques described in [30] with the same potentials [37–40], were used.

The results of the calculations are given in Table 1.

Table 1

Metal	Pressure, [kBar]	$T_m$ , [K]	$L_m$ , [kJ/mole]
Cu	0	1315	11.48
Fe	0	1775	15.57

**Table 2**

	Cu		Fe	
	$\alpha$	$\beta$	$\alpha$	$\beta$
$P = 0$	0.45	4.91	0.365	6.34

Using Eq. (17) as the approximating function, the discrete set  $\nu(T_{s\ell})$  was approximated by equation

$$\nu(T_{s\ell}) = \alpha \sqrt{\frac{3k_B}{m} T_{s\ell}} \left[ \exp\left( \beta \frac{L_m}{k_B T_m} \cdot \frac{T_{s\ell} - T_m}{T_{s\ell}} \right) - 1 \right], \quad (11)$$

where  $\alpha$  and  $\beta$  are approximation parameters and  $\alpha = C^{\text{BGJ}}$ , i.e., the unknown  $C^{\text{BGJ}}$  coefficients in the BGJ model are automatically determined from MDM. By introducing additional parameters  $\beta$  into the exponential index the necessary accuracy of temperature dependence  $\nu(T_{s\ell})$  is reached over a wide temperature range.

The best agreement, with the error not exceeding several percent over the entire temperature range, was achieved with the approximating coefficient values presented in Table 2.

In Figs. 2 and 3, the solid lines show the approximations of the simulation results using formula (2).

#### 4. CONCLUSIONS

The use of the equilibrium theory of thermodynamic potentials to describe phase transformations (nonequilibrium processes) allows us to take into account only a shallow entry into the metastable superheated/supercooled region and to investigate the phase transformations near the equilibrium line. The drawbacks of the thermodynamic approach are also that the constant  $\mu$ , as judged by its dimensionality [ $\text{cm s}^{-1} \text{K}^{-1}$ ], does not have a clear physical meaning and is selected experimentally for each material separately.

The main disadvantage of the kinetic approach is the presence of two poorly determined quantities, which make it difficult to use in a wide temperature range.

The problem of determining the kinetic velocity of heterogeneous melting/crystallization can be solved using a molecular dynamics approach that uses the atomistic representation of phase transformation processes. Its application allows us to obtain the following results:

- On the basis of MDM, a simple method is proposed for constructing the most important kinetic characteristic of the heterogeneous mechanism of melting/crystallization of metals: the velocity of the phase front's motion  $\nu(T_{s\ell})$ .
- For the first time, a steady-state temperature dependence of the heterogeneous melting/crystallization velocity  $\nu(T_{s\ell})$  for a wide temperature range limited by the limiting superheating/supercooling values of the phases has been constructed for copper and iron crystals. The constructed dependence contains two approximation coefficients independent of temperature and determined in advance from the molecular dynamics simulation.
- On the example of metals with different crystallographic lattices (copper and iron), it is shown that the proposed method makes it possible to construct temperature dependences of the kinetic velocity  $\nu(T_{s\ell})$  for a wide class of metals.

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