# Role of Relaxation Processes in Microstructure Forming in Binary Alloys under Irradiated with High-Intensive Energy Flow

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**Abstract — Using the model of local non-equilibrium solidification, which takes into account space and time deviations from local thermodynamical equilibrium at the interface and bulk phases, a model for pattern formation of crystals in undercooled binary alloys is presented. Role model physical constants and parameters fast crystallization on characteristic size of the crystal structure are investigated.**

## 1. Introduction

Fast crystallization from melts due to fluxes of energetic particles, such as laser, ion or electron beams, opens up vast possibilities of obtaining new structural states of alloys that qualitatively differ from those observed after conventional metallurgical processes. It is well known that the mechanical properties to a great extent depend on the crystal structure parameter. Therefore, the study of the alloy structure under high-intensive energy flow irradiation is a topical problem of crystallization physics and materials science.

Solidification of undercooled melts can be so fast that the interface velocity is of the order of or even greater than the diffusive speed in the bulk liquid or solid. In these cases there is no local equilibrium in the bulk phases and the solute flux cannot be described by the classical mass transport theory. In the present article we consider the general model which takes into account the deviation from the local equilibrium of the diffusion field inside the phase and at the solidification front. This model incorporates the two diffusive speeds as the most decisive parameters, governing the solute concentration field in the bulk phases. The use of the hypothesis for marginal stability within the model of locally nonequitibrium solidiflcation allows the determination of the characteristic size of the grains. The experimental methods currently available do not provide a possibility of directly observing the thermal field distribution within the high-intensive energy flow action area. Therefore, we performed the numerical simulation in order estimate influence of the temperature and cuncentration gradients at the crystallization front on the grain size, since these gradients has a strong effect on structure formation.

An influence of certain model parameters and irradiation modes on the characteristic sizes of the cristal structure was also studied during the numeral experiment.

## 2. Characteristic Size of the Microstructure

According to the marginal stability hypothesis developed in Ref. [1, 2], a characteristic size d selected by crystal microstructure in solidification, is equal to the critical wavelength of interface perturbation.

Using this hypothesis in Ref. [3] was estimated the characteristic size of a structure forming during laser recrystallization taking into account time nonlocal of mass transfer. In this case the characteristic size d of the structure can be found from the relationship:

$$d = \sqrt{\frac{\Gamma/\sigma}{mG_C\xi_C - 0.5(G_L\xi_L + G_S\xi_S)}}, \quad (1)$$

where $\sigma=1/4\pi^2$ is the stability parameter which coupling microstructure size with wavelength of interface perturbation, $\Gamma$ — is a capillary constant called the Gibbs-Thompson coefficient, $m$ — the slope of the liquidus line in the kinetic phase diagram, $G_L$ and $G_S$ are the temperatures gradients on the sides of the melt and solid phase, respectively.

The stability functions $\xi$ have the form:

$$\xi_L = 1 - 1/\sqrt{1+1/P_T^2},$$

$$\xi_S = 1 + 1/\sqrt{1+1/P_T^2},$$

$$\xi_C = 1 + 2k/\sqrt{1 - 2k - \frac{(1+(1-\gamma_1^2)}{\sigma P_C^2}}, \quad (2)$$

and depend on the thermal $P_T = Vd/2a$ and concentration $P_C = Vd/2D$ Peclet numbers ($a = \lambda/c_P$ is the thermal diffusivity).

The slope of the liquidus line in the kinetic phase diagram in view of the relaxation effect is found from the relationship [3]:

$$m(V) = \frac{m_e}{1-k_e}\left(1 - k + \ln\left(\frac{k}{k_e}\right) + (1-k)^2\gamma_1\right), \quad (3)$$

where $m_e$ is the slope of the liquidus in the equilibrium phase diagram of the pseudobinary alloy.

One can see from the (1) microstructure size dependent not only on temperatures gradients on the sides of the melt $G_L$ and solid phase $G_S$, but also on interfacial impurity concentration gradient $G_C$.

In order to obtain microstructure size in the zero-order approximation taking into account both time and space nonlocal of mass transfer solution of generalization diffusion equation

$$\frac{\partial c}{\partial t} + \tau_1 \frac{\partial^2 c}{\partial t^2} = D \frac{\partial^2 c}{\partial x^2} + \tau_2 \frac{\partial^3 c}{\partial t \partial x^2} \qquad (4)$$

for description solidification is used [4, 5]. Eq. 4 is the mathematical model combining the diffusive dissipative mode and the propagative wave mode of mass transport under local nonequilibrium conditions. In such a case, Eq. 4 describes mass transport processes under non-Fickian diffusion.

In this case the degree of local nonequilibrium is estimated by the relation of the interface velocity V and the diffusion speed: $V_{D1}=(D/\tau_1)^{1/2}$ (is the rate of propagation of concentration perturbations, which characterize time nonlocal), and $V_{D2}=(D/\tau_2)^{1/2}$ (is the rate of smoothing concentration gradien, characterize space nonlocal), which are parameter of the process of diffusion. Here $D$ is the diffusion coefficient, and $\tau_1$ and $\tau_2$ — is the time of relaxation of diffusion flux and gradient of concentration to its steady-state value, respectively, $\gamma_1=V/V_{D1}$, $\gamma_2=V/V_{D2}$.

We consider directional solidification of a binary alloy at constant velocity V in the x direction. For the sake of simplicity assume that there is no convection in the melt, that diffusion can be neglected in the crystal, and that the material parameters is independent of temperature.

In that case expression for the liquid solute $c_L$ in coordinate system moving with the planar interface $\xi=x-Vt$, are obtained for the steady-state regime of solidification as follows [7]:

$$c_L = c_0 \left( 1 + \frac{(k-1)\exp(-\beta V \xi / D_L)}{(1-k+\beta(1-\gamma_1^2)+\gamma_2^2\beta^2)} \right), \qquad (5)$$

where

$$\beta = \frac{\sqrt{(1-\gamma_1^2)^2 + 4\gamma_2^2} - (1-\gamma_1^2)}{(2\gamma_2^2)}, \qquad (6)$$

$C_0$ is the impurity concentration away from the crystallization front ($\xi\rightarrow\infty$) (equal the initial concentration), $D_L$ is diffusion coefficient in the melt.

Using the (5) one can obtain the local nonequilibrium interfacial impurity concentration gradient in the form:

$$G_c = -\frac{(1-k(V))VC_0}{k(V)D^*}, \qquad (7)$$

where

$$D^* = D_L / \beta \qquad (8)$$

is local nonequilibrium diffusion coefficien;

$$k(V) = \frac{k_e - \gamma_1\beta}{1-\gamma_1\beta} \qquad (9)$$

is the coefficient of nonequilibrium solute partitioning [7], where $k_e$ is the coefficient of equilibrium distribution of a solute defined by the ratio of equilibrium concentration of solute in the solid and liquid phases.

The system of Eqs. (1−3), and (6−9) allows one to obtain microstructure size in the zero order of magnitude.

### 3. Analysis of Results

Using the set of equations (1−3) taking into account (6−9) we investigated role model physical constants and parameters fast crystallization on characteristic sizes of the crystal structure. Calculations were carried out for a structural steel [3], whose the thermophysical properties are summarized in Table 1.

Table 1. Physical parameters of system

| Partition coefficient | $k_e$ | 0.35 |
|---|---|---|
| Liquidus slope | $m_e$, at. % | −14 |
| Diffusion coefficient | $D$, m²/s | $2 \cdot 10^{-8}$ |
| Diffusion speed | $V_{D1}$, m/s | 17 |
| Concentration | $C_0$, at. % | 2.29 |
| Rate of solidification front | $V_s$, m/s | 0.5 |
| Gibbs-Thompson coefficient | $\Gamma$, Km | $1.9 \cdot 10^{-7}$ |
| Heat conductivity | $\lambda$, W/Km | 35 |
| Specific heat at constant pressure | $C_p$, J/Km³ | $5.74 \cdot 10^6$ |

The main governing factors structure forming during recrystallization is interfacial temperatures gradients and interfacial impurity concentration gradient.

In Fig. 1. the dependence of the microstructure size on the magnitude of temperatures gradients for different value of space nonlocal parameter is represented. Microstructure size is increasing with increasing of the temperature gradient. This dependence account for stabilizing action gradient of the temperature on solidification front, which lead to sizes of the structure increase.
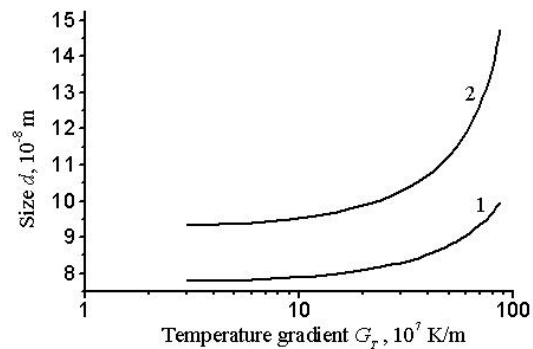


Fig. 1. Dependence of the microstructure size on the magnitude of temperatures gradients for different value of space nonlocal parameter: $1 - \gamma_2=0,1$; $2 - \gamma_2=1$

As show in Fig. 2, similar influence produce not only temperature gradient, but also surface tension. An increase the concentration gradient brings about reduction of the microstructure sizes (increase was produced by increasing to initial concentration of impurity $C_0$) (Fig. 3.) Probably, this is connected with that that when increase the concentrations gra-

dient ahead solidification front increases value of the concentration undercooling, that brings about reduction of the critical size of the crystal nucleus.
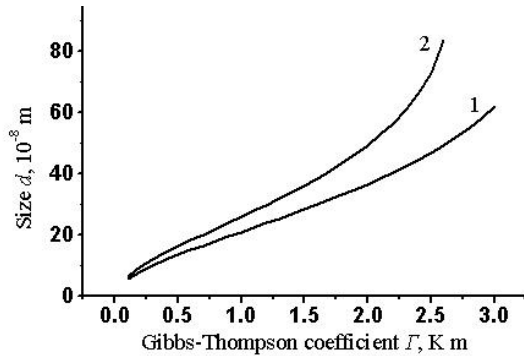


Fig. 2. Dependence of the microstructure size on the Gibbs-Thompson coefficient for different value of space nonlocal parameter: $1 - \gamma_2=0,1; 2 - \gamma_2=1$
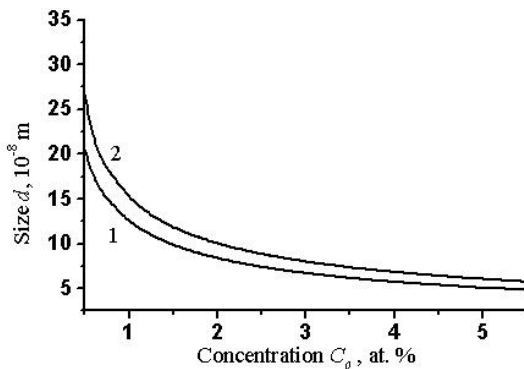


Fig.3. Dependence of the microstructure size on the initial concentration for different value of space nonlocal parameter: $1 - \gamma_2=0,1; 2 - \gamma_2=1$

Hence, possible draw a conclusion that concentrations gradient causes the destabilization action on planar solidification front, but gradient of the temperature, and surface tension, opposite, stabilize the planar front.

One can see from the (4) concentration gradient is determined not only composition of alloys but also solidification conditions.

In order to understand how space and time nonlocal influence on the microstructure size, role of relaxation process one on impurity concentration gradient is investigated.

Within the local equilibrium limit $\gamma_1 \ll 1$ and $\gamma_2 \ll 1$, (i.e., when the interface velocity is much smaller than the diffusion speeds), solution (5) transforms into solution obtained, for example, in ref. [7] for the case of the local equilibrium solute diffusion. In this case accumulation of impurity with diffusion layer $D_L/V$ ahead of the solidifying front is arise. Taking into account only time non local of mass transfer ($\gamma_2 \ll 1$) lead to increasing of interfacial concentration gradient as a result of decreasing diffusion layer up to $D_L(1-\gamma_1^2)/V$ [8] on the crystallization front. On the assumption of $\gamma_1 \geq 1$ diffusion layer reduce up to zero, i.e. under such solidification conditions concentration gradient is equal zero.

Additional taking into account space non local ($\gamma_2 \neq 0$) lead to decreasing of interfacial concentration gradient when $\gamma_1 \leq 1$, but when $\gamma_1 \geq 1$ in melt remain zone in which goes the impurity segregation from solid phase in melt that gives not zero value of the concentration gradient.

With growing of the contribution space nonlocal effect (with growing $\gamma_2$) increase width diffusion layer ahead of the solidifying front that reduces the concentration gradient. So, take into account space nonlocal lead to reduction of the concentration gradient that, in one's turn, leads to increase microstructure size as this is well seen from Fig. 1−3.

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