

## PHASE TRANSFORMATIONS

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### **Mathematical Modelling of Primary Recrystallization Kinetics and Precipitation of Carbonitride Particles in Steels.**

#### **II. Recrystallization Kinetics**

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A mathematical physical based semi-empirical model and a corresponding computer program are developed for describing recrystallization process and carbonitrides particles precipitation in deformed austenite. The model is suitable for alloyed steels of a wide range of compositions. The model allows calculating a thermodynamic equilibrium for carbonitride excess phases with solid solution, the kinetics of their nucleation and growth, and their effect on recovery and recrystallization. A detailed description is given for each aspect of the model and its physical nature. Verification of the simulation results with the experimental data taken from published sources confirms the sufficient reliability of the proposed computer model for evaluative calculations. The model's features are demonstrated by an example that simulates influence of Nb content on recrystallization, recovery and nucleation, growth and Ostwald rippling of Nb and Ti carbonitride particles. The simulation shows and numerically predicts the effect of slowing down recrystallization and recovery with increasing in Nb content. That attests significance of the effect of dispersed carbonitrides on recrystallization and recovery. The simulation theoretically predicts an intensification of Ti(C, N) particles precipitation and growth with an increase in the Nb concentration. As another result, it is an increasing the dispersion and number of Nb(C, N) particles with an increase in the Nb concentration owing to more rapid transition to the Ostwald ripening stage, which is characterized by much more slowly average particle size growth than from a supersaturated solid solution.

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**Key words:** recrystallization, kinetics, austenite, steel, modelling.

Розроблено математичну фізично обґрунтовану напівемпіричну модель і відповідну комп'ютерну програму для опису процесу рекристалізації і виділення частинок карбонітридів у деформованому аустеніті. Модель параметризовано для легованих сталей широкого спектру складів. Модель дозволяє розрахувати термодинамічну рівновагу для надлишкових карбонітридних фаз у твердому розчині, кінетику їх зародження і зростання, а також їх вплив на повернення і рекристалізацію. Для кожного аспекту моделі наведено докладний опис його фізичної сутності. Перевірка результатів моделювання експериментальними даними з літературних джерел підтвердила достатню надійність запропонованої комп'ютерної моделі для оціночних розрахунків. Особливості моделі продемонстровано на прикладі моделювання впливу вмісту Nb на рекристалізацію, повернення, а також на зародження, зростання і оствальдівське дозрівання частинок карбонітридів Nb і Ti. Моделювання показало і дозволило чисельно оцінити ефект уповільнення рекристалізації і повернення у разі збільшення вмісту Nb. Це свідчить про вплив дисперсних карбонітридів на рекристалізацію і повернення. Моделювання теоретично передбачило інтенсифікацію зародження і зростання часток Ti(C, N) зі зростанням концентрації Nb. Іншим результатом є збільшення дисперсності і кількості частинок Nb(C, N) зі збільшенням концентрації Nb, внаслідок більш швидкого переходу до стадії оствальдівського дозрівання, яка характеризується набагато повільнішим зростанням середнього розміру часток, ніж у випадку їх утворення з пересиченого твердого розчину.

**Ключові слова:** рекристалізація, кінетика, аустеніт, сталь, моделювання.

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## 1. INTRODUCTION

In the previously announcement [1] (Part I) a model of carbonitride precipitation from solid solutions in deformed steels is considered. This part is primary devoted to the simulation of recovery and recrystallization processes influenced by dispersed carbonitrides particles formed against its background.

As has been formerly mentioned, physically based mathematical models are convenient tools for predicting a structure formation and properties of materials [2–4] that are able to minimize time-consuming, expense, and lengthy of experimental studies. This article proposes a physically based mathematical model that describes kinetics of primary recrystallization (after deformation) with the background of carbonitride particles evolution process. These processes influence each other, so they are simulated in aggregate. In particular, dispersed particles of carbonitrides slow down the recrystallization, at the same time, the recovery and recrystallization slow down the nucleation and

growth of the disperse carbonitride particles [5–7]. To implement the model, a special computer program in Python is written.

## 2. MATHEMATICAL MODEL

The models for thermodynamics and kinetics of carbonitride phase precipitation from a deformed solid solution are presented in the previously work (Part I) [1]. In this part only information on a model of recovery and recrystallization is given.

The recovery process consists in reducing of dislocations density in a deformed metal and reducing its strain hardening at higher temperatures.

The dislocation density can be calculated by the formula (1). The decrease in strain hardening is described by equation (1) from [11]:

$$\frac{d(\sigma - \sigma_{0.2})}{dt} = - \frac{64(\sigma - \sigma_{0.2})^2 \nu_d}{9M^3 \alpha_p^2 E} e^{-\frac{U_{rec}}{RT}} \sinh\left(\frac{\sigma - \sigma_{0.2}}{RT} V_{rec}\right), \quad (1)$$

where  $U_{rec}$ —return activation energy, J/mol;  $V_{rec}$ —activation volume of the return process, m<sup>3</sup>;  $\nu_d$ —Debye frequency ( $\nu_d = 2.0 \cdot 10^{12}$  s<sup>-1</sup>);  $E$ —Young's modulus of the material at a given temperature, Pa.

The values of the activation energy of the return process ( $U_{rec}$ ) and the activation volume of the return process ( $V_{rec}$ ) for austenite are determined in [4] ( $U_{rec} = 248100$  J/mol). The activation volume depends on temperature and can be calculated by the formula (2):

$$V_{rec} = 2900b^3 e^{-5.5 \cdot 10^{-4} T}, \quad (2)$$

where  $b$ —Burgers vector module, m;  $T$ —temperature, K.

As carbonitride particles are precipitate, the recovery process is inhibited. According to the approach adopted in [5], equation (1) should be amended to take into account the fastening of dislocations by the excess phase particles:

$$\frac{d(\sigma - \sigma_{0.2})}{dt} \left(1 - \frac{N(t)}{N_c(t)}\right) = - \frac{64(\sigma - \sigma_{0.2})^2 \nu_d}{9M^3 \alpha_p^2 E} e^{-\frac{U_{rec}}{RT}} \sinh\left(\frac{\sigma - \sigma_{0.2}}{RT} V_{rec}\right), \quad (3)$$

where  $N(t)$ —the amount of particles of the excess phase released by the time  $t$ ;  $N_c(t)$ —total number of nodes of the dislocation grid.

The values of  $N_c(t)$  can be calculated by formula (4), taking into account changes in the current dislocations density (5):

$$N_c(t) = 0.5\rho_d^{1.5}, \quad (4)$$

where  $\rho_d$ —dislocation density,

$$\rho_d = [(\sigma - \sigma_{0.2})/(\alpha_p M \mu b)]^2, \quad (5)$$

where  $\sigma$ —plastic flow stress, Pa;  $\sigma_{0.2}$ —yield strength at a given temperature, Pa;  $M$ —Taylor factor ( $M = 3.1$  [5]);  $\mu$ —shear modulus at a given temperature, Pa;  $\alpha_p$ —empirical parameter ( $\alpha_p = 0.15$  [22]).

The concept of the extended volume of recrystallized metal is introduced in [6]  $X_{ext}(t)$ , which is associated with its true value by the equation (6):

$$X(t) = 1 - e^{-X_{ext}(t)}. \quad (6)$$

According to [6], the fraction of extended recrystallized metal at a given time is determined by the formula (7):

$$X_{ext}(t) = N_{rex} \left( \int_0^t V_G^{rex}(t) dt \right)^3, \quad (7)$$

where  $N_{rex}$ —bulk density of the nuclei of recrystallized grains,  $V_G^{rex}(t)$ —grain boundary velocity.

The growth rate of recrystallized grain is determined by the product of the mobility of the boundaries and the so-called driving force (or as it is also called ‘pressure’ [5, 6]) of recrystallization (8):

$$V_G^{rex}(t) = M_{GB}^{rex} P_{rex}(t), \quad (8)$$

where  $M_{GB}^{rex}$ —grain boundary mobility,  $m^3/s \cdot H$ ;  $P_{rex}(t)$ —recrystallization driving force.

According to [12], the mobility of the boundaries of recrystallized grains  $M_{GB}^{rex}$  can be calculated by the formula (9):

$$M_{GB}^{rex} = M_0^{rex} e^{\frac{S_{GG}^{rex}}{R}} e^{-\frac{Q_{GG}^{rex}}{RT}}, \quad (9)$$

where  $M_0^{rex}$ —pre-exponential factor,  $S_{GG}^{rex}$ —change in entropy when the grain boundary shifting, J/mol·K,  $Q_{GG}^{rex}$ —activation energy of the process of displacing the grain boundary, J/mol.

It is believed [7] that both the change in entropy and the activation energy upon shifting the grain boundary are proportional to the activation energy of self-diffusion, thus:

$$Q_{GG}^{rex} = \alpha_{GG}^{rex} Q_{SD}, \quad (10)$$

$$S_{GG}^{rex} = \beta_{GG}^{rex} Q_{GG}^{rex}, \quad (11)$$

where  $Q_{SD}$ —self-diffusion activation energy, J/mol,  $\alpha_{GG}^{rex}$  and  $\beta_{GG}^{rex}$ —corresponding proportionality factors.

The numerical values of the parameters  $M_0^{rex}$ ,  $\alpha_{GG}^{rex}$  and  $\beta_{GG}^{rex}$  are determined in [7]. They are respectively equal to:

$$M_0^{rex} = 5.4 \cdot 10^{-11} \text{ m}^3/(\text{s} \cdot \text{N}), \quad \alpha_{GG}^{rex} = 0.64, \quad \beta_{GG}^{rex} = 4.33 \cdot 10^{-4} \text{ K}^{-1}.$$

The empirical formula (12) for calculating the activation energy of self-diffusion in doped austenite is proposed in [13]:

$$\begin{aligned} Q_{SD} = & 311691 - 278242(1 - \exp(-0.394y_C)) + 88752y_{Mn}^{0.31} + \\ & + 22801y_{Si} + 84864y_{Mo}^{0.65} - 38575y_{Ni}^{0.3} - 7298y_V + \\ & + 132594y_{Nb}^{0.263} + 82128y_{Ti}^{0.401}. \end{aligned} \quad (12)$$

The driving force of recrystallization  $P_{rex}(t)$ —this is actually the density of the excess energy of the deformed material. It is associated with the dislocation density [14]:

$$P_{rex}(t) = 0.5\mu b^2 \rho_d(t), \quad (13)$$

where  $\mu$ —solid solution shear modulus, Pa;  $\rho_d(t)$ —dislocation density near the grain boundary,  $\text{m}^{-1}$ .

The dislocation density at the grain boundaries is noticeably higher. The value of the boundary density of dislocations can be obtained from the average density of dislocations taking into account the fraction of the recrystallized volume according to the formula (14) from [7]:

$$\rho_d(t) = \alpha_{d1} \bar{\rho}_d (1 + \alpha_{d1}^{-1} e^{-\alpha_{d2} X(t)}), \quad (14)$$

where  $\bar{\rho}_d$ —average dislocation density,  $\text{m}^{-1}$ ;  $X(t)$ —fraction of recrystallized metal;  $\alpha_{d1}$  and  $\alpha_{d2}$ —empirical coefficients ( $\alpha_{d1} = 0.2$ ,  $\alpha_{d2} = 1.2$ ).

The influence of dispersed particles on the effective value of the recrystallization driving force is expressed by a correction called the Zener pressure [15]. So, it can be written:

$$P_{rex}^*(t) = P_{rex}(t) - P_Z(t), \quad (15)$$

where  $P_Z(t)$ —Zener pressure.

Zener pressure is calculated by the formula (16) from [15]:

$$P_Z(t) = \frac{3\gamma_{GB} f(t)}{\bar{R}(t)}, \quad (16)$$

where  $f(t)$ —volume fraction of excess phase;  $\bar{R}(t)$ —the average radius of the excess phase particles  $\text{m}^{-3}$ ;  $\gamma_{GB}$ —specific energy of recrystallized grains boundaries,  $\text{J}/\text{m}^2$ .

A value of the specific energy of the recrystallized grains boundaries

can be determined by the formula (17), obtained on the basis of data [7]:

$$\gamma_{GB} = 1.41 \cdot 10^6 e^{-0.0117T}. \quad (17)$$

According to [6, 9], the bulk density of the nuclei of recrystallized grains included in equation (7) is estimated by the formula (18):

$$N_{rex} = \frac{\alpha_{rex}^* P_{rex}^2(t=0)}{D_{\gamma 0}}, \quad (18)$$

where  $P_{rex}^2(t=0)$ —the recrystallization driving force at the initial moment, N;  $D_{\gamma 0}$ —initial austenite grain diameter, m;  $\alpha_{rex}^*$ —empirical coefficient ( $\alpha_{rex}^* = 8.6 \cdot 10^{-4} \text{ m}^2/\text{N}^2$  [7]).

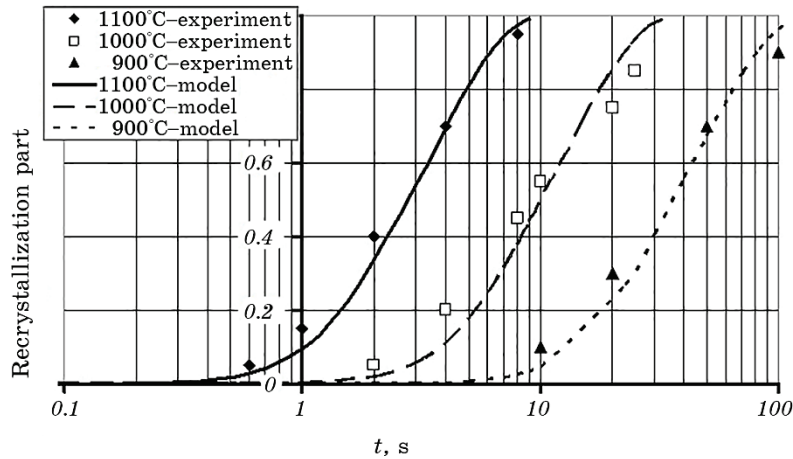
### 3. VERIFICATION OF THE DEVELOPED MODEL

To verify the proposed computer model of recrystallization during carbonitride particle formation, experimental data is used from several published sources [7–10, 16–22].

Table 1 shows the composition of the steel used in [20] to study the

**TABLE 1.** Steel composition for verification of recrystallization modelling according to [20] (% wt.) and the initial austenite grain size.

C	Si	Mn	Fe	$d_A, \mu\text{m}$
0.11	0.26	0.55	base	143



**Fig. 1.** Comparison of experimental data (points) [20] on the change in the average particle size Nb(C, N) with the results of the computer model (curves).

kinetics of deformed metal recrystallization at various temperatures. Figure 1 compares the calculated results of the recrystallization kinetics with the data from [20] for the steel with a composition shown in Table 1. The degree of deformation is 20%, the strain rate is  $3.63 \text{ s}^{-1}$ .

The verification study showed that the average deviation of the values predicted by the model from the experimental data for modelling recrystallization is about 23%.

Deviations are equally observed both up and down. This allows us to use this model to assess and analyse the nature of the influence of various factors (composition, temperature, degree of deformation) on the kinetics of recrystallization (and also precipitation—see Part I [1]) of carbonitride particles in steels. It should be mentioned that the developed computer model is not a complete alternative to experimental studies. However, it allows one to obtain quickly and with minimal costs reliable data on recrystallization kinetics and precipitation of carbonitride particles in steels sufficient for practical purposes.

#### 4. EXAMPLES OF CALCULATIONS USING THE DEVELOPED COMPUTER MODEL

To illustrate the developed program operating, calculations are performed demonstrating an effect of Nb content on kinetics of recrystallization, recovery. The steel composition for which the calculations are carried out is given in Table 2. The size of the initial austenite grain is taken to be  $100 \mu\text{m}$ .

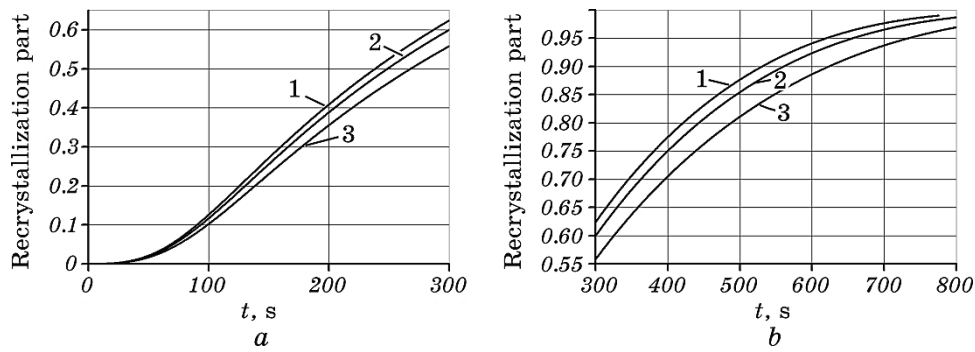
The following parameters are taken: temperature  $900^\circ\text{C}$ , deformation degree 30%, strain rate  $0.1 \text{ s}^{-1}$ .

Figure 2 shows the results of modelling an influence of Nb content in the range of 0.01–0.06% on the recrystallization kinetics of steel from Table 2. For greater clarity, the plot is divided into two parts—a period from 0 to 300 s and a period from 300 to 800 s.

As it can be seen from the results, an increase in Nb content leads to some recrystallization process slowdown. Slowing down becomes more noticeable at later stages. It is also seen that an increase in the Nb content from 0.04% to 0.06% has a stronger effect on the additional slowdown of recrystallization than an increase from 0.01% to 0.04%. This is primarily due to the fact that at high concentrations of niobium a greater number of carbonitride particles precipitate and a smaller part of dislocation nodes remain unfastened. Thus, it makes sense to

**TABLE 2.** The steel composition adopted in the simulation, % mass.

C	Si	Mn	Mo	Ti	Nb	N	Fe
0.08	0.20	1.80	0.15	0.025	0.01–0.06	0.005	base

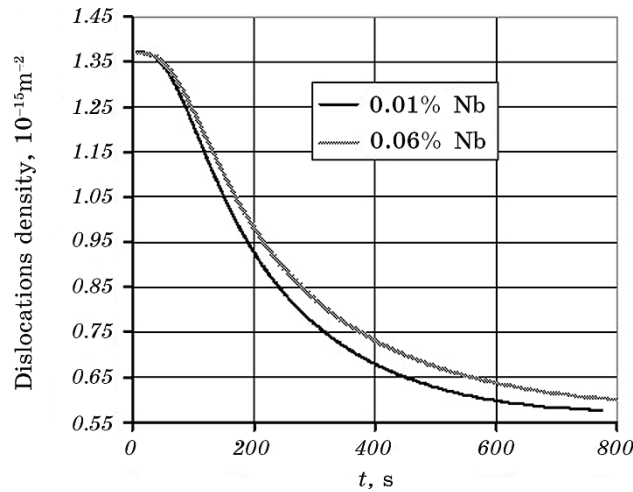


**Fig. 2.** Results of modelling of the effect of Nb content on the kinetics of low carbon steel recrystallization: 1—0.01% Nb, 2—0.04% Nb, 3—0.06% Nb.

consider the results of modelling of a decrease in the dislocation density over time and a change in the number of particles of Nb and Ti carbottitrides.

Figure 3 presents the results of modelling the effect of the Nb content in the same steel on the decrease in the dislocation density over time.

With equal initial density of dislocations, in the case of a higher Nb content, the recovery process is slower. After 600 s the curve becomes much flatter. Thus, presence of Nb as a microalloying element leads to some slowdown of the recovery process. During first seconds the difference is disparagingly small, also the process is at the incubation



**Fig. 3.** Results of modelling of the effect of Nb content on the decrease in the dislocations density in pre-deformed low-carbon steel.



stage. Then, when the number of Nb(C, N) particles becomes significant the difference appears. Mostly the effect of slowing begins to emerge after about 150–200 s. The difference is keeping at the following stage but not increase and somewhat decrease owing to decrease in quantity and increase in average size of the carbonitride particles because of Ostwald ripening (see part I [1]).

## 5. CONCLUSIONS

1. A mathematical model is developed that allows one to describe the kinetics of a deformed metal recovery and recrystallization and the effect on these processes of the simultaneous precipitation and Ostwald ripening of dispersed particles of excess phases, in particular carbonitrides, in steels microalloyed with Nb, Ti, V, Zr, and Al. The main features of our model are the ability to describe the simultaneous precipitation of carbonitrides of several elements and the thermodynamic assessment of the N and C content in these carbonitrides.

2. The results of computer simulation are compared with the published experimental data on the kinetics of recrystallization. The experimental results confirmed the reliability and practical applicability of the developed computer model for evaluative calculations.

3. A series of demonstration calculations is carried out for low-carbon structural steel microalloyed with Nb and Ti in order to demonstrate the capabilities of the developed model. In particular, in this part the effect of changes in the Nb content on the recrystallization. The effect of slowing down recrystallization and recovery with increasing in Nb content is shown, which demonstrates a result of the significant effect of dispersed carbonitrides on these processes.

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