АКТУАЛЬНІ ПИТАННЯ НАУКОВОГО ТА ПРАКТИЧНОГО МАТЕРІАЛОЗНАВСТВА

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STUDY OF MATHEMATICAL MODELS CHANGES IN THE STRUCTURE OF STEEL OF ENGINEERING STRUCTURES AFTER THERMAL LOADING

Abstract. *In mechanical engineering, there are a number of tasks in which it is necessary to predict the structure of steel after thermal treatment. To predict the properties and structure of steel, it is necessary to study the structural transformations in steel under thermal stress.*

The development of modern computational methods and technology makes it possible to perform highly accurate calculations of complex processes, including metal forming processes. A relevant aspect is the application of approaches that describe the structural transformations occurring in metal with sufficient accuracy. This is the basis for the use of modern numerical modelling methods and computer programs that allow calculating and predicting the structural and phase composition of the processed steels.

The article discusses modern mathematical models for predicting the evolution of steel microstructure during thermomechanical loading, analyses mathematical models for engineering structures, and presents the results of numerical modelling of the evolution of microstructure of 09G2S steel as the most common steel for freight car load-bearing systems.

The JMAK method is based on the calculation of the proportion of recrystallised grains and the average grain size through material characteristics, strain, strain rate, temperature and time. This method provides information on the processes of recrystallisation and grain growth during thermomechanical processing of the workpiece.

The paper shows the possibility of using JMatPro software to model the evolution of microstructure.

It is based on the Johnson-Mel-Avrami-Kolmogorov model during hot plastic deformation. The average size of recrystallised grains and their volume fraction in the process of dynamic recrystallisation are calculated.

The results of the thermokinetic calculation of the phase composition of steel in the equilibrium state are presented, and thermokinetic and isothermal diagrams are constructed. The obtained results can

be used to design technological processes for the production of products for various purposes based on different types of thermal deformation effects.

Key words: mechanical engineering structures, railway transport, wagon, low-carbon low-alloy steel, phase transformations, metal structure, thermokinetic diagram, reliability, mechanics, mathematical models.

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ДОСЛІДЖЕННЯ МАТЕМАТИЧНИХ МОДЕЛЕЙ ЗМІНИ СТРУКТУРИ СТАЛІ МАШИНОБУДІВНИХ КОНСТРУКЦІЙ ПІСЛЯ ТЕРМІЧНОГО НАВАНТАЖЕННЯ

Анотація. *У машинобудуванні існує низка завдань, у яких необхідно прогнозувати структуру сталі після термічного впливу. Для прогнозування властивостей і структури сталі необхідне дослідження структурних перетворень у сталі під час термічного навантаження.*

Розвиток сучасних обчислювальних методів і техніки дають змогу виконувати високоточні розрахунки складних процесів, зокрема процесів обробки металів тиском. Актуальним аспектом є застосування таких підходів, які з достатньою точністю описують структурні перетворення, що відбуваються в металі. Це є підставою для використання сучасних чисельних методів моделювання та комп'ютерних програм, що дають змогу розраховувати і прогнозувати структурно-фазовий склад оброблюваних сталей.

У статті розглянуто сучасні математичні моделі для прогнозування еволюції мікроструктури сталі в процесі термомеханічного навантаження, проаналізовані математичні моделі для машинобудівних конструкцій, представлено результати чисельного моделювання еволюції мікроструктури сталі 09Г2С як найбільш розповсюдженої сталі для несівних систем вантажних вагонів.

Метод JMAK базується на обчисленні частки рекристалізованих зерен і середнього розміру зерна через характеристики матеріалу, деформацію, швидкість деформації, температуру та час. Цей метод дає змогу отримувати інформацію про процеси рекристалізації та зростання зерен під час термомеханічної обробки заготовки.

У статті показано можливість застосування програмного забезпечення JMatPro для моделювання еволюції мікроструктури.

На основі моделі Джонсона-Мела-Аврамі-Колмогорова під час гарячої пластичної деформації. Розраховано середній розмір рекристалізованих зерен і їхню об'ємну частку в процесі динамічної рекристалізації.

Наведено результати термокінетичного розрахунку фазового складу сталі у рівноважному стані, побудовано термокінетичні та ізотермічні діаграми. Отримані результати можуть

бути використані для проектування технологічних процесів виробництва виробів різного призначення, що базуються на різних видах термодеформаційного впливу.

Ключові слова: машинобудівні конструкції, залізничний транспорт, вагон, маловуглецева низьколегована сталь, фазові перетворення, структура металу, термокінетична діаграма, надійність, механіка, математичні моделі.

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Introduction. In mechanical engineering, there are a number of problems in which it is necessary to predict the structure of steel after thermal exposure. To predict the properties and structure of steel, it is necessary to study the structural transformations in steel under thermal loading. [1].

Experimental study of structural transformations consists of constructing isothermal and thermokinetic diagrams. Experimental study has limited application. Thus, isothermal diagrams are used only for qualitative assessment of the influence of chemical composition on the process of austenite decomposition.

Thermokinetic diagrams cannot provide reliable information about the structure of steel if the thermal load regime differs from the load regimes during the experiment [2,3].

In steels under thermomechanical loading, all phase transformations known for the solid state are observed: pearlite, intermediate (bainitic) and martensitic. The possibility of occurrence of certain phase transformations and their kinetics depend on from the parameters of thermomechanical action, such as temperature, heating conditions, holding time, cooling rate, mechanical load. [4-5].

Relevance of the work. An important feature of steels is that during the transformation of supercooled austenite the transition of face-centred cubic (HCC) crystal lattice to volume-centred tetragonal (VCT) lattice can occur along with diffusive redistribution of carbon and alloying elements The transition $\gamma \rightarrow \alpha$ can be carried out by both the so-called normal (if the interfacial boundary is incoherent) and martensitic (if this boundary is incoherent) mechanisms, and martensitic (if the interface is coherent) mechanisms.

As shown by numerous experimental studies, phase transformations are the cause of the appearance of a certain set of physical and mechanical properties in a material, which largely depend on the microstructure of the material, mechanisms of its formation and change. Correct description of changes in the structure of materials makes it possible to develop new methods of obtaining materials with a given set of properties and optimise existing ones [3]. Experimental study of this issue is quite resource-intensive, therefore, the task of building models describing the state and evolution of the material structure taking into account solid-state phase transformations becomes topical during production in mechanical engineering.

The study of grain growth is of great importance for understanding and improving the properties of materials. Understanding the dynamics and mechanisms of grain growth allows to predict structural changes during the manufacturing, processing and exploitation of materials. This may favour the improvement of their strength, service life, resistance to wear and corrosion [4].

Meta and historical research. The aim of this paper is to study mathematical models of steel structure changes in machine-building structures after thermal loading. On the basis of the analysis to choose a mathematical model and apply it to the calculation of steel structure for the most common steel of bearing elements of gondola**.**

Materials and research results. A systematic study of the crystallisation process was carried out by G. Tamman, who introduced quantitative characteristics of this process: the number of new phase centres arising per unit time in a unit volume (nucleation rate of centres) and the linear growth rate of crystals from these centres [5-8]. I.L. Mirkin proposed to study the crystallisation process using two-dimensional schemes [8-12]. According to such a scheme, a certain number of nuclei of future crystals appears on the area, at the initial moment of time completely occupied by the old phase (liquid), within one second. During the next second, the nuclei grow at a certain rate, equal in all directions, and new nuclei appear on the area still occupied by the old phase. When the growing nuclei collide, growth in the corresponding area stops. The process continues until the entire available area is occupied by crystals of the new phase V over a period of time $(t_t + A_t)$

The phase field method is quite often used for modelling both diffusive and non-diffusive

(martensitic) phase transformations at the meso-level (the modelled region consists of several grains). This approach [13,14] assumes the presence of a "blurred", "diffusive" boundary between the phases in contrast to classical methods using the concept of a "sharp boundary", when the multiphase structure is described by the position of the boundary and for each region a set of differential equations is solved together with the flow equations and constitutive equations at the boundary. [15,16].

One of the methods for modelling recrystallisation kinetics are Johnson-Meil-Avrami-Kolmogorov expressions (**JMAK**) [18].

These expressions calculate the recrystallised volume fraction as a function of strain and temperature (for dynamic recrystallisation), and time and temperature (for metadynamic and static recrystallisation)

Static recrystallisation occurs after deformation, during which the resulting degree of strain is less than some critical degree of strain c. The critical strain is usually given as the fraction of peak strain p at which the yield stress reaches its maximum (the yield stress then begins to decrease due to dynamic recrystallisation, which de-strengthens the material). The value of p is determined experimentally and is usually a function of strain rate, temperature, and initial grain size, i.e., the strain rate, temperature, and initial grain size.

$$\varepsilon_p = a_1 d_o^{n_1} \dot{\varepsilon}^{m_1} \exp(Q_1/RT) + c_1 \quad (1)$$

$$\varepsilon_c = a_2 \varepsilon_p \quad (2)$$

Since static recrystallisation occurs through the formation of nucleation and their subsequent growth, a description of the relationship between the fraction of volume recrystallised and time is the kinetics of isothermal annealing of recrystallised volume and time is the kinetics of isothermal annealing, usually described by the Avrami equation:

$$X_{SRX} = 1 - exp\left[-\beta_s \left(\frac{t}{t_{0.5}}\right)^{k_s}\right] \quad (3)$$

$$t_{0.5} = a_3 d_0^{h_3} \varepsilon^{n_3} \dot{\varepsilon}^{m_3} \exp(Q_3/RT), \quad (4)$$

where t 0.5 denotes the time in which 50% recrystallisation occurs. The recrystallised grain size is a function of initial grain size, strain, strain rate and temperature:

$$d_{SRX} = a_6 d_0^{h_6} \varepsilon^{n_6} \dot{\varepsilon}^{m_6} \exp(Q_6/RT) + c_6, \quad (5)$$

if $d_{SRX} > d_0$, then $d_{SRX} = d_0$.

Metadynamic recrystallisation occurs after deformation when the degree of deformation at the end of deformation is greater than the critical degree of deformation (Fig. 1). Metadynamic recrystallisation is modelled similarly to static recrystallisation, but with a different set of material constants:

$$X_{MRX} = 1 - exp\left[-\beta_m \left(\frac{t}{t_{0.5}}\right)^{km}\right] \quad (6)$$

$$t_{0.5} = a_4 d^{h_4} \varepsilon^{n_4} \dot{\varepsilon}^{m_4} \exp(Q_4/RT) \quad (7)$$

$$d_{MRX} = a_7 d_0^{h_7} \varepsilon^{n_7} \dot{\varepsilon}^{m_7} \exp(Q_7/RT) + c_7, \quad (8)$$

if $d_{MRX} > d_0$, then $d_{MRX} = d_0$.

Mathematical modelling of microstructure parameters of 09G2S steel in the process of thermal loading using Johnson-Mel-Avrami-Kolmogorov model. The computational analysis was carried out on the basis of the JMatPro software package, which uses the CALPHAD (CALculation of PHAse Diagrams) method of thermodynamic calculation of the equilibrium state of the system [17], which is adapted to perform calculations of multi-component alloys used in industry (steel, aluminium, magnesium, heat-resistant nickel, titanium and other alloys). The mathematical modelling of phase transformation is shown in (Fig. 2).

Modelling of the material under consideration is carried out at different temperatures, according to the protocol of the real technological process. Based on the need to ensure the plastic properties of the metal for these conditions of deformation, the temperature is 800 ° C. Thermokinetic calculations of possible phases at equilibrium crystallisation of 09G2S steel (in coordinates "phase percentage from temperature") were performed in the range of temperature values from 1200 to 25°C with a step of 5°C

Fig. 3. Shows the results of modelling the phase composition of 09G2S steel at temperatures 1200 and 800°C.

As a result of modelling it was found that at 1200°C the steel has an austenitic structure with a small content of MnS (0.02%)and austenite (99.98%). During rolling, the steel strip is cooled at 1200°C, which leads to the formation of a two-phase structure due to carbon diffusion. At the rolling temperature at 800°C, a two-phase structure consisting of ferrite (55.86%), austenite (44.13%) and MnS (0.02%) is already formed.

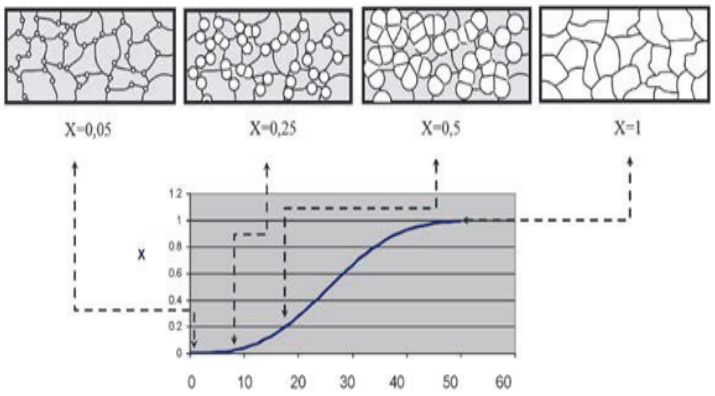

Fig. 1. Metadynamic recrystallisation in the JMAK model

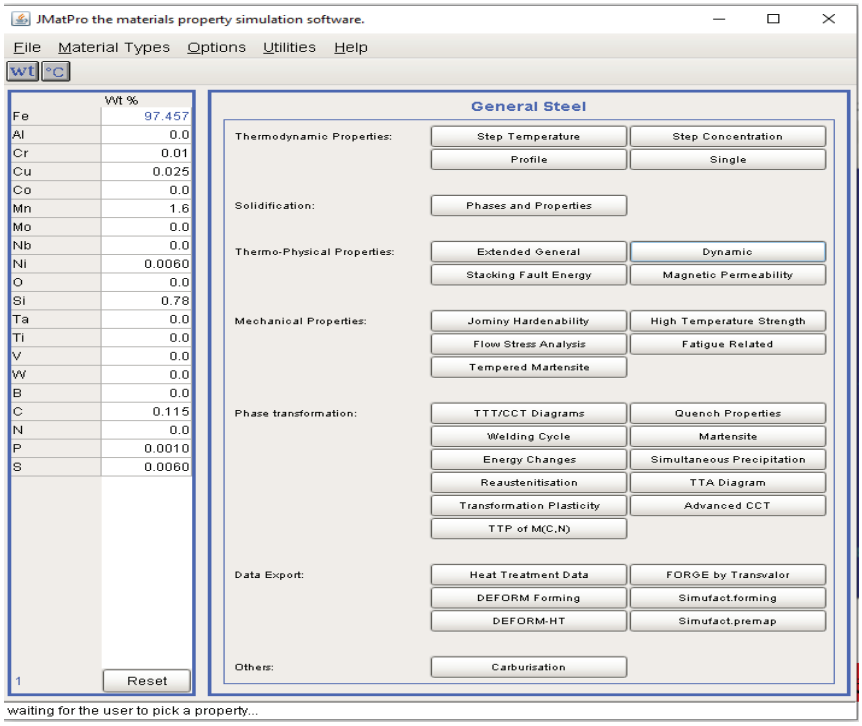

Fig. 2. Post-application of mathematical modelling of phase transformation

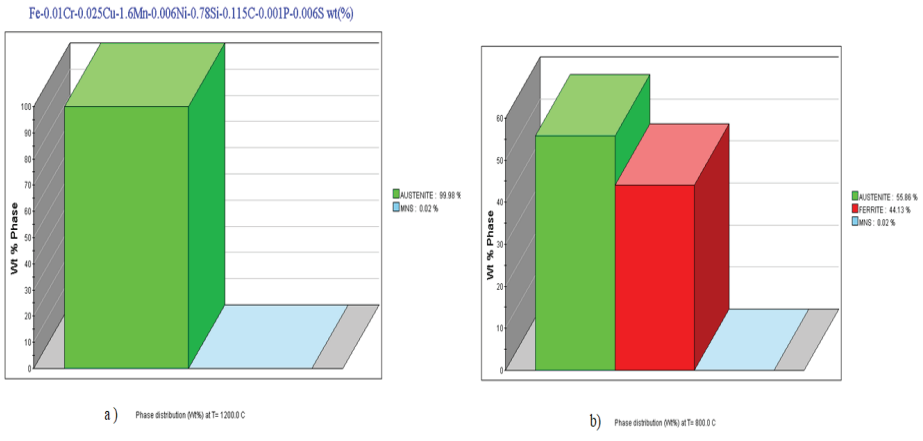

Fig. 3. Phase composition of 09G2S steel at dressing and welding temperature: a – 1200°C; b – 800°C

It is known from literature sources [20-22] that the crystallisation onset temperature of the investigated steel is below the temperature of 1200°C. At this temperature, liquid phase is present, hence the crystallisation end temperature is lower than 1200°C. The lower the phase transformation temperature, the greater the concentration difference between these phases. On cooling below 723°C, austenite decomposes into ferrite and cementite.

Fig. 4 shows the phase composition of 09G2C steel at temperatures of 600 and 20°C. It can be seen from the data obtained that at 600°C the ferrite content is 98.29% and cementite content is only 1.69% (MnS 0.02%). On further cooling to room temperature, the structure of the steel changes, the ferrite content decreases to 98.25% and the cementite content increases to 0.94% (remaining MnS).

As noted in [18-22], simultaneously with the stages of crystallisation in the temperature range from 730 to 650°C in the structure begin to develop processes called "pre-rotation phenomena". The essence of these phenomena lies in the fact that between grains there is a gradual weakening of boundary bonds, coexisting with further changes in the dislocation structure of the boundaries, their composition and thickness. As a result, at the grain boundaries and inside them there appear areas, as if prepared for the beginning of phase transformation (so-called densification or fluctuations of transformation) and having a less stressed state than the grains and their boundaries. Due to this, the grains become even more active and their temperature mobility increases.

Fig. 5 shows the results of thermokinetic calculation of the phase composition of 09G2S steel.

Phases during equilibrium crystallization of the alloy showed the results presented in (Fig. 5). According to the obtained data, it was established that the crystallization start temperature of 09G2S steel T_L = 823°C and the end temperature of recrystallization T_S = 680°C. The obtained results are consistent with the data presented in [22].

The capabilities of the JMatPro software allow constructing thermokinetic (SST) and isothermal (TTT) diagrams of the metals under study. (Fig. 6) shows the calculated diagrams of 09G2S steel, which are constructed from a temperature below the austenization temperature of 884°C. When calculating, the program takes into account that at this temperature the austenitic phase is already present.

Thus, the obtained data allowed us to determine the key phase transformations in the steel under study, as well as the temperature and rates of decomposition of austenite into the corresponding structural components. Analysis of thermokinetic calculations of possible phases during equilibrium crystallization of the alloy showed the results presented in (Fig. 6).

Conclusion. A brief review of works devoted to mathematical modelling of both diffusionless (martensitic) and diffusive phase transformations occurring in steels under thermomechanical loading has been carried out. Main conclusions on the review of mathematical models of structure change in steel of machine-building structures after thermal loading.

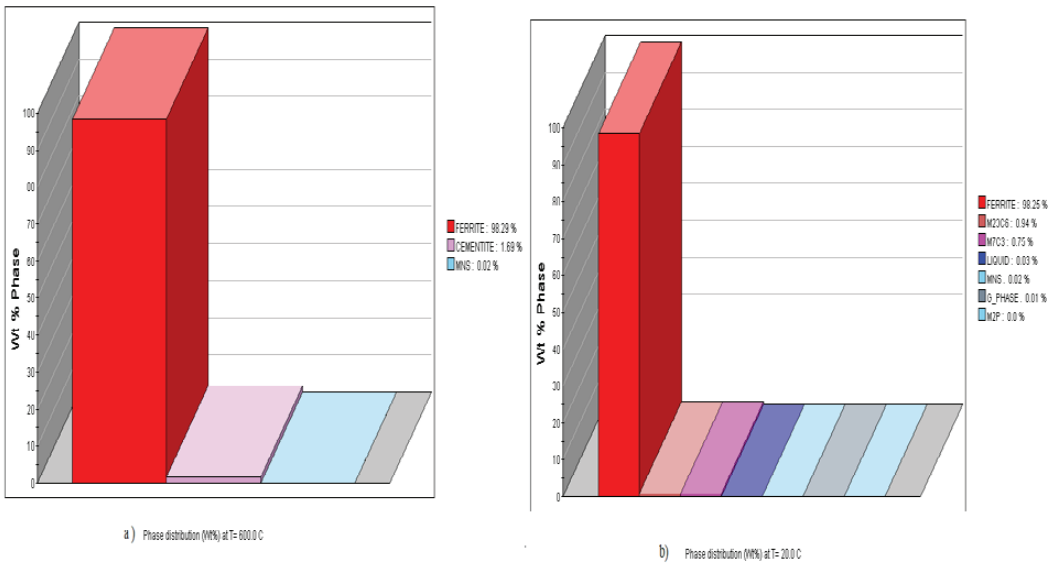

Fig. 4. Phase composition of 09G2C steel: a – 600 °C; b – 20 °C

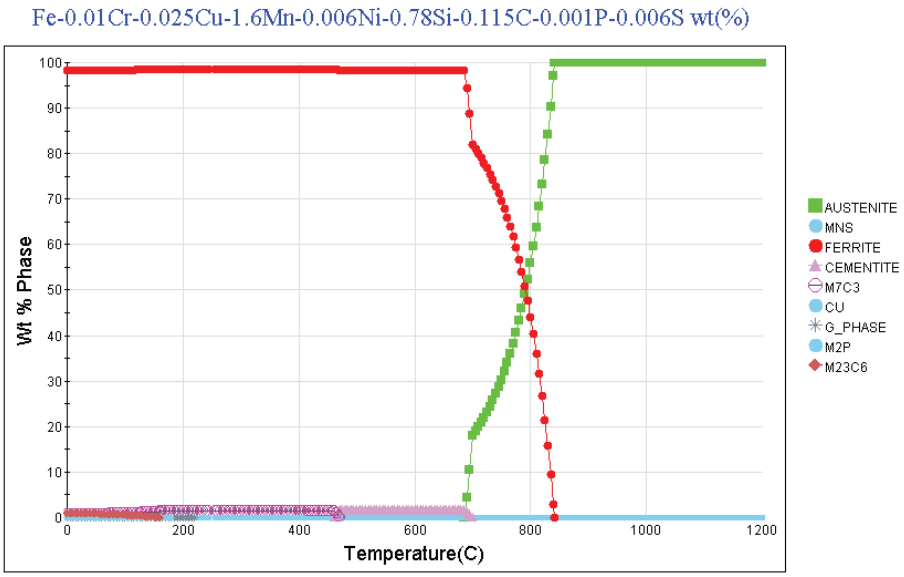

Fig. 5. Thermokinetic calculation of the phase composition of 09G2S steel in the equilibrium state

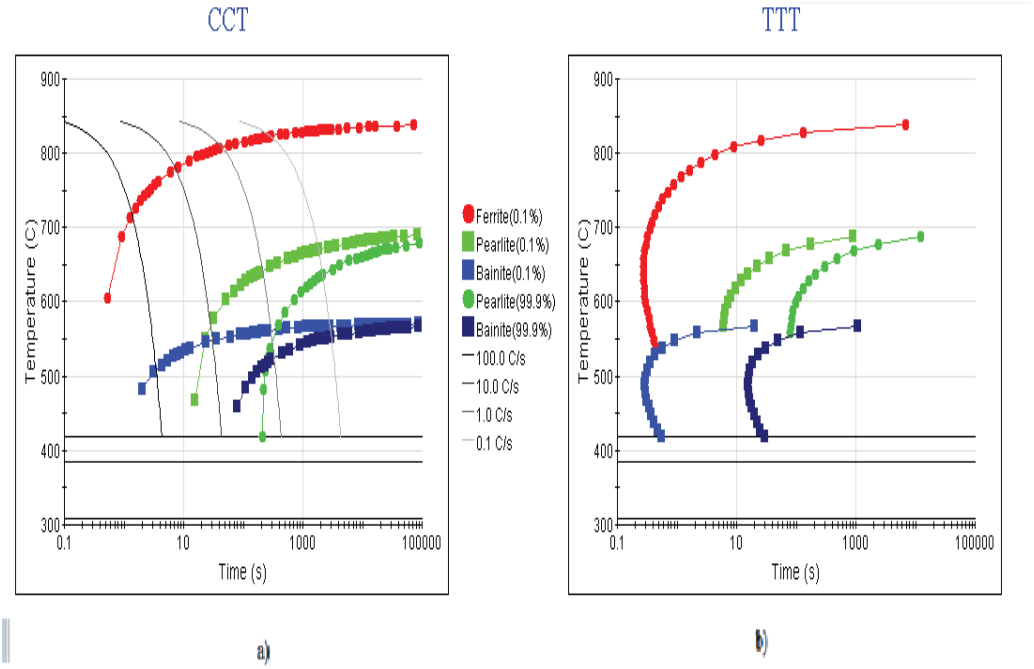

Fig. 6. Thermokinetic diagram of austenite decomposition and isothermal transformation diagram steel 09G2S: a – thermokinetic diagram; b – isothermal transformation diagram

1. The mathematical models of austenite decomposition kinetics proposed in the literature are mainly focused on decomposition under isothermal conditions. A number of these models do not take into account the stochastic nature of the process under consideration, which in turn complicates the further use of these models for the construction of thermokinetic diagrams and prediction of steel structure. The models that take into account the stochasticity of the nucleation of phase centres neglect the physics of the process and do not consider the thermodynamic parameters of the process.

2. In many papers only qualitative results of research are given, while quantitative analyses are given only in some papers.

3. digitisation of isothermal and thermokinetic diagrams using existing software products is very difficult because they do not take into account all the features of these diagrams. Therefore, it is expedient to develop a software module that performs digitisa-

tion of the diagrams under consideration taking into account their peculiarities.

4.The variety of used methods and techniques for predicting steel structures is an indirect evidence that this issue is far from being solved.Modern studies related to the modelling of structural transformations in steel do not provide an opportunity to solve the problem of quantitative description of structural transformations at any heating rates, which in turn does not allow to predict the structure of the part after thermal loading.

5. Using the Johnson-Mel-Avrami-Kolmogorov mathematical model, the evolution of the microstructure of 09G2S steel under thermomechanical action characteristic of straightening and welding is considered.The characteristics of steel microstructure under this type of hot plastic deformation are calculated: the average size of recrystallised grains and their volume fraction.

This physical and mathematical model of structure evolution allows to predict with high accuracy the structural parameters of metallic materials, which allows their successful integration into modern computational systems of calculation of industrial processes of metal processing.

The review does not pretend to be complete, since the number of works in this area is growing very intensively. The choice of sources is determined by the potential possibility of developing the considered models for a more accurate description of phase transformations under thermomechanical action and, of course, is not without subjectivity.

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