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MODELLING OF PHASE TRANSFORMATIONS IN STRUCTURAL STEELS

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Abstract. An analytical dependence of the influence of alloying elements on the equilibrium temperature of vanadium nitride in austenite is established for the main alloying elements based on an analysis of state diagrams, which describe an actual process with an error of 0.9%.

As a result of the process analysis is theoretically justified and experimentally confirmed that the precipitation of the secondary phases from the supersaturated solution kinetics is controlled by the thermodynamic activity, diffusion mobility and solubility of the components forming the secondary phase in the solid solution, the deviation degree of the system from the equilibrium state, where the equilibrium state is the formation temperature and dissolution of the secondary phase.

The established quantitative regularity shows that the precipitation kinetics of the vanadium nitrides in austenite with a probability of 99.9% and an error of 7.1% is reliably described by the thermodynamic activity of nitrogen and vanadium, the deviation degree of the system from the equilibrium state, and the process time. In this case, the correlation coefficient between experimental and theoretical data is 0.915.

An analysis of the obtained analytical equations shows that the influence of the chemical composition on the content of the carbide and nitride-vanadium phases in the solid solution is significant. The elements are arranged according to the degree of increasing influence in the following sequence: the content of vanadium nitrides in austenite increases Si and decreases Mn, C, Cr.

As a result of studying the process of converting austenite to ferrite and perlite, martensite, and bainite, it was found that the nonequilibrium critical points of phase transformations are controlled by the equilibrium temperature of austenite and ferrite, the content of secondary phases in them, the diffusion mobility of carbon in austenite, the degree of alloying, and the grain size of austenite and in the case of diffusion transformations by the heating and cooling rate. Quantitative influence laws are determined, which describe the real process with a probability of 95% and an error from 2.3% to 7.1%.

Key words: structural steel, chemical composition, heat treatment, austenite, ferrite, perlite, martensite, bainite, phase transformations.

Introduction

The structure formation of structural low- and medium-alloyed steels can be carried out by diffusion pearlitic, diffusionless martensitic, mixed bainitic transformations and decomposition of a supersaturated solid solution. Quantitative transformation characteristics are determined by the laws of nucleation of new phase centers and their growth.

Formulation of problem

It is necessary to study the effect of alloying on the thermodynamic and kinetic parameters of the dissolution and precipitation of secondary phases in austenite and the austenite transformation to perlite, martensite and bainite for solve this problem.

Analysis of recent research results

Alloying elements and modifiers can affect the change to the ferrite center nucleation rate of during pearlite transformation and the perlite growth rate [1, 2].

This occurs as a result of changes of the austenite stability to super cooling, the specific energy of the interface, the activation energy of diffusion, and the degree of imperfection of the matrix crystal structure.

In case of the martensitic transformation, the influence of alloying elements and modifiers on the rate of nucleation of martensite centers is associated with changes of the austenite stability to supercooling, its chemical and structural homogeneity, mainly [3-5].

Bainitic transformation occurs in the temperature range of low diffusion coefficients, the rate of nucleation and growth of perlite. Partial carbon redistribution occurs in austenite, diffusionless $\gamma \rightarrow \alpha_m$ transformation and precipitation of the carbide phase under these temperature conditions. Alloying elements insignificantly affect to the activation energy of crystal growth of the α_b - phase, but alloying elements have a significant effect to the bainitic transformation rate.

The kinetics of the solid solution decomposition of a martensitic and bainitic structure, the secondary phase dispersion and interparticle distances depend with the temperature and the influence of alloying and modifying elements to the crystal lattice of a stable phase, the element chemical affinity and their diffusion mobility.

Alloying elements affect the change of parameters such as austenite grain size, its resistance to supercooling, element chemical interaction, their solubility and diffusion mobility in a solid solution, and the defective crystal structure of the matrix.

A lot of research is devoted to the study of the influence of alloying elements, modifiers and impurities on the structure formation process [1-3]. However, the bulk of research covers dual and triple alloying systems. This eliminates the quantitative analytical forecasting of the influence of alloying elements, modifiers and impurities on the structure formation process and structure characteristics in multicomponent industrial structural steels.

The complex formation of a favorable ratio of a high level of strength and plastic steel properties with a minimum consumption of alloying elements can be achieved only when the regimes of its modification and heat treatment will ensure dispersion of all structural elements at all stages of casting formation.

Purpose of research

The article presents a method for solving the problem of eliminating the oscillations of the load on the articulated suspension during the simultaneous movement of the two links of the boom system, namely the lifting of the handle and reducing the departure of the telescopic section.

Results of research

The formation of microstructural features in steels, containing 0.2 to 0.4 wt.% carbon; 1 to 3% silicon, manganese and chromium; 0.005-0.035% nitrogen, up to 30% of vanadium are predicted according to the following scheme. The equilibrium content of nitrogen and vanadium, in a solid solution during the austenization is determined by their solubility, the latter depends on the chemical composition of steel and the heat treatment temperature. Using general principles of phases equilibrium in a ternary phase diagrams, the unknown parameters of interaction of alloying elements in austenite, the austenization temperatures, t_{VN} is given by the following relationship:

$$t_{VN} = \frac{(-9473 + 2436[V] + 8950[N] + 932[C] + 160[Mn] - 67[Si] + 419[Cr] + 1610[Al] - 535[Ni] + 411[Ce] + 2659[Mo])}{(lg[V] + lg[N] - 3.97 + 1.5[V] + 5.44[N] + 0.06[Si] + 0.13[Cr] + 0.06[Mn] + 0.83[Al] + 0.2[Ca] + 0.41[C] - 0.03[Ni] + 1.45[Mo])}, \quad (1)$$

Steel 20KhGSAFL taking as the base. It was determined the effectiveness of the influence of elements on the change in the equilibrium temperature of dissolution (formation) of vanadium nitrides (Fig. 1).
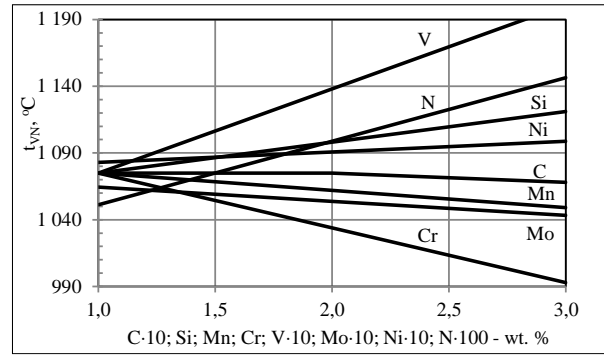
Fig. 1. The influence of element contents on the equilibrium temperature of dissolution (formation) of vanadium nitrides.

It can be seen that Si, V, N, Ni increase, and C, Mn, Cr, Ce, Al, Mo, decrease the equilibrium temperature of vanadium nitride dissolution (formation).

It is revealed that at the austenization temperature of the structural steel, the approximation of anomalous phase equilibrium is valid. Phase analysis shows that at the $\alpha \rightarrow \gamma$ transformation significant change in the solubility limit of nitrogen and vanadium and in the diffusion mobility occurs.

The base is - steel containing (wt.%) 0.2C, 1Si, 1Mn, 1Cr, 0.015N, 0.1V.

As a result the content of nitrogen and vanadium in the solid solution to exceeds its equilibrium value up to 1100 °C. As a result during austenization vanadium nitride precipitates instead of the dissolution of the respective elements. It is established experimentally, that kinetics of this process is determined by the influence of alloying elements on the coefficients of thermodynamic activity of nitrogen (f_N) and vanadium (f_V). The other influencing factors are the difference of the austenization temperature from the equilibrium temperature of vanadium nitrides in austenite (Δt) and the time of the process (τ)

$$q_{VNa} = (3.63 + 0.0556 \cdot \tau - 4.36 \cdot (f_N) \cdot (f_V) + +0.176 \cdot \Delta t) \cdot q_{st} /100,$$

$R = 0.915; \delta = 7.1\%; F_p = 11.3 > F_T = 3.7, (2)$

where q_{VNa}, q_{st} is the content of vanadium nitrides in weight fraction in austenite and its stoichiometric value in the steel, respectively; R- is the multiple correlation coefficient; δ - the average relative error of approximation; F_p, F_T are the estimated and tabulated values of the Fischer's criterion.

The experimental results and calculations show that the vanadium nitrides quantity in austenite depends from the alloying element content in steel, temperature and austenitization time (Fig. 2).

It can be seen that silicon increases, and manganese, carbon, and chromium decrease the vanadium nitrides quantity in austenite. It should be noted that the vanadium nitrides quantity in austenite increases with increasing austenitization time.

The influence of the alloying elements is essentially distinguished not only by their values but also by their "sign". In this case the influence is multivariant-not only the equilibrium solubility is changed, but the solubility at the $\alpha \rightarrow \gamma$ transformation and the rate at which the system approaches to the equilibrium state are changed as well. To

find the required content of nitrogen in a solid solution for stabilization and nitrogen content in the nitride phase at the austenization a study was conducted. The study discussed the influence of chemical composition, nitride phase content and temperature upon the austenite grain stabilization. The effect of chemical composition, nitride and carbide phase content, austenite grain size and cooling rate on the thermokinetic parameters of ferrito-pearlite, bainite and martensite transformations are discussed. The influence of above-mentioned factors on secondary structure characteristics and properties of steel were also investigated.
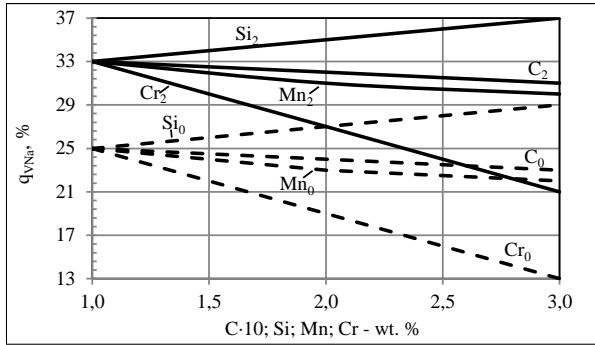
Fig. 2. The influence of element contents on the vanadium nitrides quantity in austenite.

The base is - steel containing (wt.%) 0.2C, 1Si, 1Mn, lCr, 0.015N, 0.1V.

Indexes 0 and 2 - the initial moment of austenitization and after 2 hours exposure, respectively.

The statistical analysis of dilatometry results of steels, containing up to 0.4% C, 3% of Si, Mn, Cr each, 0.03% N and 0.2% V at cooling rates, (V_{cool}) within 20-40 °C/minutes were studied. The relationship below established dependencies of the start temperatures, t_{ar3}, finishing temperature, t_{ar1}, and the duration of diffusion dissolution, τ, of austenite phase:

$$t_{ar3} = 1220 - 208.3 \cdot C + 66 \cdot Si - 174.7 \cdot Mn - 36.72 \cdot Cr +$$
$$+ 51 \cdot V_a - 10610 \cdot N_a - 3.39 \cdot V_{cool} + 82 \cdot q_{VNa} - 2.34 \cdot D_{aust} -$$
$$-0.1436 \cdot t_r, \qquad (3)$$

$R = 0.933; \delta = 2.3\%; F_c = 24.2 > F_T = 2.4;$

$$t_{ar1} = 1030 - 117.5 \cdot C + 72.06 \cdot Si - 192.2 \cdot Mn - 47.14 \cdot Cr -$$
$$- 654 \cdot V_a - 3472 \cdot N_a - 2.94 \cdot V_{cool} + 916 \cdot q_{VNa} - 2.827 \cdot D_{aust} -$$
$$-0.0293 \cdot t_r, \qquad (4)$$

$R = 0.924; \delta = 2.7\%; F_c = 21 > F_T = 2.4;$

$$\tau = -7.55 + 0.75 \cdot C - 3.71 \cdot Si + 4.06 \cdot Mn + 0.46 \cdot Cr +$$
$$+ 79.4 \cdot V_a - 607.6 \cdot N_a - 0.041 \cdot V_{cool} - 101.7 \cdot q_{VNa} +$$
$$0.086 \cdot D_{aust} + 0.01 \cdot t_r, \qquad (5)$$

$R = 0.883; \delta = 14.4\%; F_c = 12.42 > F, 0.05 = 2.4$

where: C, Si, Mn, Cr, V_a, N_a, q_{VNa} are the content of carbon, manganese, silicon, chromium, vanadium, nitrogen and vanadium nitride phase in austenite in wt.%, respectively; D_{aust} - the size of austenite grain, μm; t_r - the temperature balance of austenite and ferrite, °C.

As it follows from equations (3)-(5) the complex optimization of the vanadium, nitrogen contents and the austenitization temperature regime is one of the necessary conditions for dispersion of the ferrite - pearlitic structure of carbon and low-alloy steels containing nitrogen and vanadium.

The influence of element contents on the start and finishing temperatures and the duration of diffusion dissolution of austenite phase is shown in Fig. 3.

a

b

c
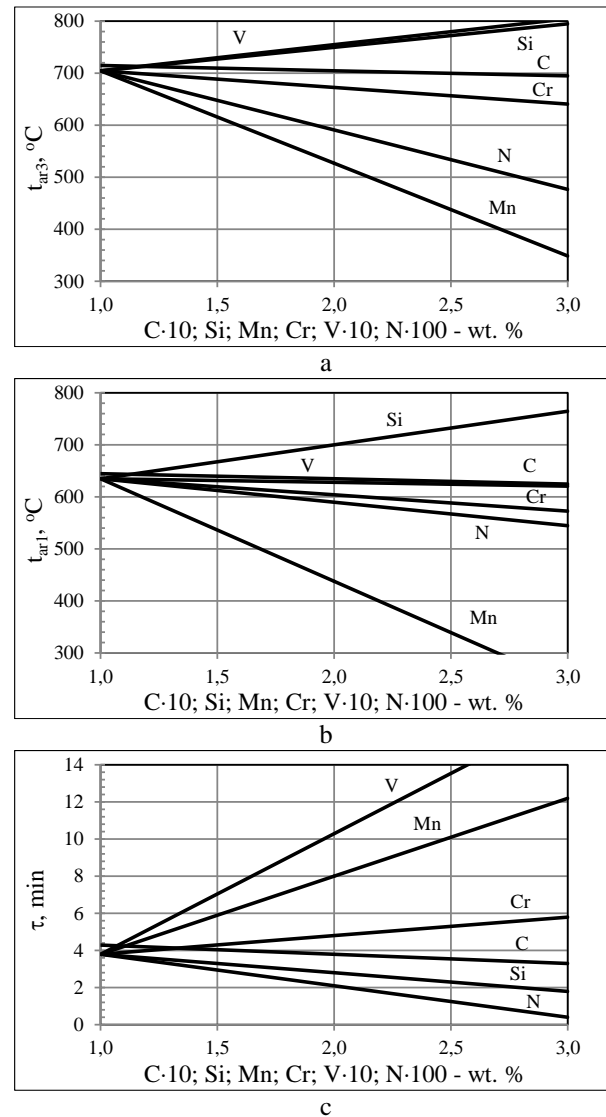
Fig. 3. The influence of element contents on the start (a) and finishing (b) temperatures and the duration of diffusion dissolution (c) of austenite phase.

The base is - steel containing (wt.%) 0.2C, 1Si, 1Mn, lCr, 0.01N, 0.1V.

The data given in fig. 3 show that increasing the carbon, chromium, nitrogen and manganese content in the steel leads to a decrease of start temperature decomposition of austenite into ferrite and pearlite (Fig. 3a) and of silicon and vanadium - to its growth.

Elements effect on the end temperature of ferrite-pearlite transformation (Fig. 3b) according to another regularity. Carbon has almost no effect, chromium, nitrogen and manganese are lowered, silicon is increased, and vanadium has an ambiguous effect on the position of the t_{ar1} point. Such an effect of the elements can be explained by their change of the ratio of the thermodynamic and kinetic factors of the process, which characterize the rate of nucleation and growth of new phases during the diffusion decomposition of austenite.

A austenite diffusion decomposition time changing of correlates with a changing of the carbon thermodynamic

activity by chemical elements. The transformation time is increased by elements that lower the carbon activity, and decrease elements that increase the carbon activity. This indicates that the process kinetics of the austenite transformation to ferrite and perlite is determined by the thermodynamic activity of carbon and the development of the process of carbide formation, mainly. Chrome, manganese and vanadium increase, and nitrogen, silicon and carbon decrease the conversion time as a result (Fig. 3 c)

The influence of the above considered factors, the martensite start temperatures, t_{sm} and bainite start temperature, t_{sb}, is also equally important. The following dependencies have been established:

$$t_{sm} = 439 - 58 \cdot C - 37 \cdot Mn - 8 \cdot Cr - 2578 \cdot N_a - 0.21 \cdot D_a, \quad (6)$$
$$R = 0.904; \delta = 8.7\%; F_c = 178 > F_t = 4.1.$$

$$t_{sb} = 940 - 97.4 \cdot C - 25.1 \cdot Mn - 972 \cdot N_a + 11.9 \cdot \ln D_C, \quad (7)$$
$$R = 0.987; \delta = 2.3\%; F_c = 192 > F_t = 4.4,$$

where: D_c - the carbon diffusion coefficient in austenite at the temperature interval of the bainite transformation which may shift with the chemical composition.

From the equations 6 and 7 it follows that during the supercooling of austenite in the region of bainitic and martensitic transformations in structural steels with permissible nitrogen and vanadium content, the nitrogen content present in the solid solution renders influence on the process. The analysis of the equations 6 and 7 shows, that depending on the content of vanadium, nitrogen and the temperature of the austenitization, the concentration of nitrogen in a solid solution and the bainite and martensite transformations start temperatures can be changed significantly. In case of the bainite structure the decrease in the transformation start is accompanied by a regular reduction in the diffusion mobility of carbon atoms.

The influence of element contents on start temperatures of the martensite and bainite transformations is shown in Fig. 4, 5.
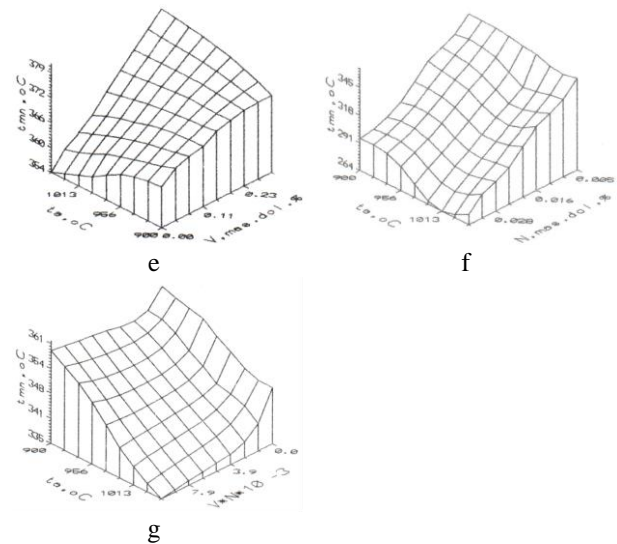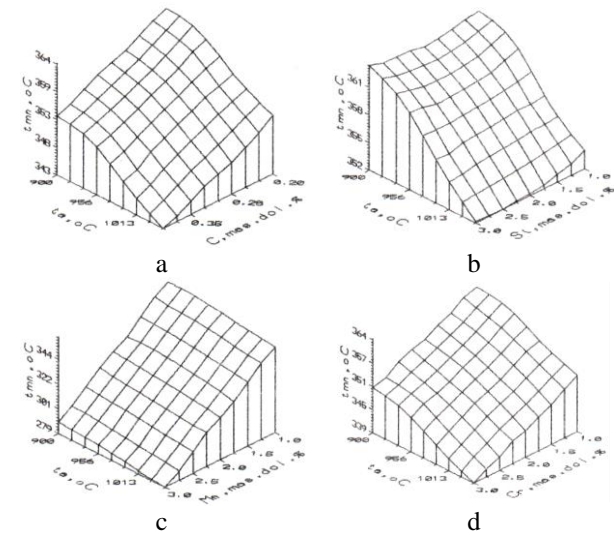
Fig. 4. The influence of the carbon (a), silicon (b), manganese (c), chromium (d), vanadium (e), nitrogen (f), vanadium and nitrogen (g) on start temperature of the martensite transformation.

The base steel contains (wt.%) 0.2C, 1Si, 1Mn, lCr.
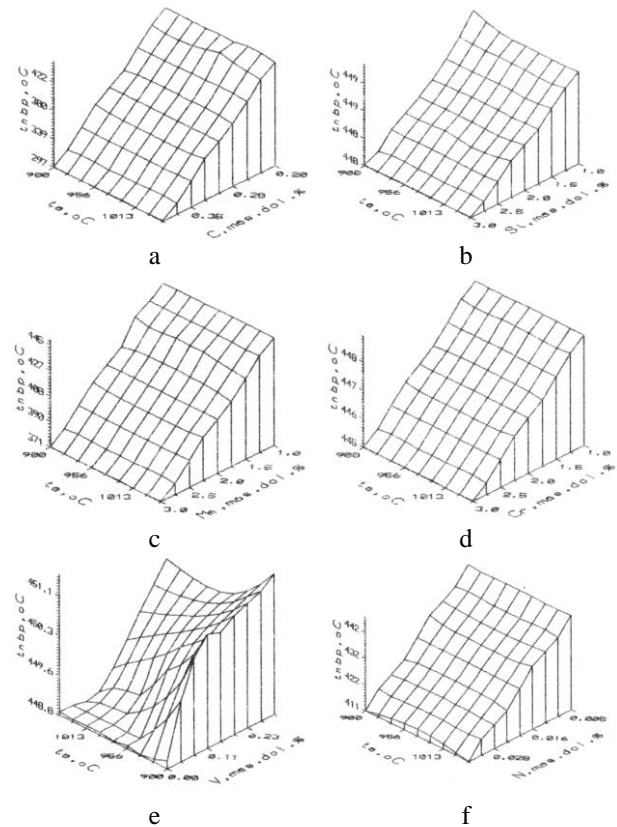
Fig. 5. The influence of the carbon (a), silicon (b), manganese (c), chromium (d), vanadium (e), nitrogen (f) on start temperature of the bainite transformation.

The base steel contains (wt.%) 0.2C, 1Si, 1Mn, lCr.

Analysis of the data shown in Fig. 4 shows that carbon, chromium, manganese and nitrogen are reduced, silicon has practically no effect, and vanadium raises the temperature t_{sm}. The element effectiveness depends on their content in steel and the austenitization temperature

and can vary not only quantitatively, but also qualitatively. So if in steel 20KhGSL nitrogen and vanadium content increases, temperature t_{sm} decreases during austenitization from 1050 °C, and it increases at austenitization from 900 °C.

The element influence explains by simultaneously two parameters: thermodynamic (equilibrium temperature of austenite and martensite and kinetic (austenite grain size).

C, Mn, Cr reduce, and Si, V do not affect to the equilibrium temperature of austenite and martensite. When in steel silicon, manganese, and nitrogen content increase it leads to growth and, therefore, should lower, and carbon, chromium, and vanadium to disperse austenite grains, which should increase the temperature of the start of martensitic transformation.

The study results show that when the direction of influence of these factors coincides, for example, in the case of steel alloying by manganese, temperature t_{sm} decreases. If the direction of influence does not coincide, for example, when steel alloying by chromium, the efficiency of lowering the temperature t_{sm} decreases. So if in steel the manganese content increases from 1 to 3% it leads to a decreasing t_{sm} on 74-75 °C, then a similar alloying by chromium on 13-15 °C.

Taking 20KhGSL steel as the base, we determined the effectiveness of the influence of alloying elements on the start temperature of bainitic transformation t_{sb} at various austenitizing heating temperatures (Fig. 5).

It can be seen that C, Si, Mn, Cr, N lower the temperature t_{sb} of structural steels and, in terms of the specific influence efficiency, they can be arranged in the following sequence: Si, Cr, Mn, C, N.

Vanadium has practically no effect on the changing of temperature t_{sb}. Joint nitrogen and vanadium steel alloying leads to an extreme changing of the start temperature of bainite formation. The effectiveness of the effect of co-alloying with nitrogen and vanadium depends of the austenitization temperature of the steel.

For example, alloying steel 20KhGSAFL by nitrogen and vanadium in quantity up to $V \cdot N = (3-4) \cdot 10^{-3}$ % of the mass fraction leads to a decrease during cooling after heating to 900 °C, and at more additions to an increase of t_{sb} temperature, then after heating to 1050 °C, it observes of t_{sb} decreases in the studied range of nitrogen and vanadium content in steel.

Conclusions

1. An analytical dependence of the influence of alloying elements on the equilibrium temperature of vanadium nitride in austenite is established for the main alloying elements based on an analysis of state diagrams, which describe an actual process with an error of 0.9%.

2. As a result of the process analysis is theoretically justified and experimentally confirmed that the precipitation of the secondary phases from the supersaturated solution kinetics is controlled by the thermodynamic activity, diffusion mobility and solubility of the components forming the secondary phase in the solid solution, the deviation degree of the system from the equilibrium state, where the equilibrium state is the

formation temperature and dissolution of the secondary phase.

3. The established quantitative regularity shows that the precipitation kinetics of the vanadium nitrides in austenite with a probability of 99.9% and an error of 7.1% is reliably described by the thermodynamic activity of nitrogen and vanadium, the deviation degree of the system from the equilibrium state, and the process time. In this case, the correlation coefficient between experimental and theoretical data is 0.915.

4. An analysis of the obtained analytical equations shows that the influence of the chemical composition on the content of the carbide and nitride-vanadium phases in the solid solution is significant. The elements are arranged according to the degree of increasing influence in the following sequence: the content of vanadium nitrides in austenite increases Si and decreases Mn, C, Cr.

5. As a result of studying the process of converting austenite to ferrite and perlite, martensite, and bainite, it was found that the nonequilibrium critical points of phase transformations are controlled by the equilibrium temperature of austenite and ferrite, the content of secondary phases in them, the diffusion mobility of carbon in austenite, the degree of alloying, and the grain size of austenite and in the case of diffusion transformations by the heating and cooling rate. Quantitative influence laws are determined, which describe the real process with a probability of 95% and an error from 2.3% to 7.1%.

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МОДЕЛЮВАННЯ ФАЗОВИХ ПЕРЕТВОРЕНЬ В КОНСТРУКЦІЙНИХ СТАЛЯХ
Є. Г. Афтанділянц

Анотація. На основі аналізу діаграм стану для основних легуючих елементів встановлено аналітичну залежність впливу легуючих елементів на температуру рівноваги нітридів ванадію в аустеніті, яка з похибкою 0,9% описує реальний процес. В результаті аналізу процесу виділення вторинних фаз з пересиченні розчину теоретично обґрунтовано і експериментально підтверджено, що кінетика процесу контролюється термодинамічної активністю, дифузійної рухливістю і розчинністю в твердому розчині компонентів, що утворюють вторинну фазу, а також ступенем відхилення системи від стану рівноваги, де за стан рівноваги приймається температура утворення і розчинення вторинної фази. Встановлена кількісна закономірність показує, що кінетика виділення нітридів ванадію в аустеніті з ймовірністю 99,9% і похибкою 7,1% достовірно описується термодинамічної активністю азоту і ванадію, ступенем відхилення системи від стану рівноваги і часом процесу. При цьому коефіцієнт кореляції між експериментальними і теоретичними даними становить 0,915. Аналізом отриманих аналітичних рівнянь показано, що вплив хімічного складу на вміст карбідної і нітрідванадієвої фаз в твердому розчині істотно. За ступенем зростаючого впливу елементи розташовуються в наступній послідовності: вміст нітридів ванадію в аустеніте збільшує Si і зменшують Mn, C, Cr. В результаті дослідження процесу перетворення аустеніту в ферит і перліт, мартенсит, бейнит встановлено, що нерівноважні критичні точки фазових перетворень контролюються температурою рівноваги аустеніту і фериту, вмістом в них вторинних фаз, дифузійної рухливістю вуглецю в аустеніті, ступенем легування і розміром зерна аустеніту і в разі дифузійних перетворень швидкістю нагріву і охолодження. Визначено кількісні закономірності такого впливу, які з ймовірністю 95% і похибкою від 2,3% до 7,1% описують реальний процес.

Ключові слова: конструкційна сталь, хімічний склад, термічна обробка, аустеніт, ферит, перліт, мартенсит, бейніт, фазові перетворення.

МОДЕЛИРОВАНИЕ ФАЗОВЫХ ПРЕВРАЩЕНИЙ В КОНСТРУКЦИОННЫХ СТАЛЯХ
Е. Г. Афтандилянц

Аннотация. На основе анализа диаграмм состояния для основных легирующих элементов установлена аналитическая зависимость влияния легирующих элементов на температуру равновесия нитридов ванадия в аустените, которая с погрешностью 0,9% описывают реальный процесс.

В результате анализа процесса выделения вторичных фаз из пересыщенного раствора теоретически обосновано и экспериментально подтверждено, что кинетика процесса контролируется термодинамической активностью, диффузионной подвижностью и растворимостью в твердом растворе компонентов, образующих вторичную фазу, а также степенью отклонения системы от состояния равновесия, где за состояние равновесия принимается температура образования и растворения вторичной фазы.

Установленная количественная закономерность показывает, что кинетика выделения нитридов ванадия в аустените с вероятностью 99,9% и погрешностью 7,1% достоверно описывается термодинамической активностью азота и ванадия, степенью отклонения системы от состояния равновесия и временем процесса. При этом коэффициент корреляции между экспериментальными и теоретическими данными составляет соответственно 0,915.

Анализом полученных аналитических уравнений показано, что влияние химического состава на содержание карбидной и нитридванадиевой фаз в твердом растворе существенно. По степени возрастающего влияния элементы располагаются в следующей последовательности: содержание нитридов ванадия в аустените увеличивает Si и уменьшают Mn, C, Cr.

В результате исследования процесса превращения аустенита в феррит и перлит, мартенсит, бейнит установлено, что неравновесные критические точки фазовых превращений контролируются температурой равновесия аустенита и феррита, содержанием в них вторичных фаз, диффузионной подвижностью углерода в аустените, степенью легирования и размером зерна аустенита и в случае диффузионных превращений скоростью нагрева и охлаждения. Определены количественные закономерности такого влияния, которые с вероятностью 95% и погрешностью от 2,3% до 7,1% описывают реальный процесс.

Ключевые слова: конструкционная сталь, химический состав, термическая обработка, аустенит, феррит, перлит, мартенсит, бейнит, фазовые превращения.

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