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On modeling the martensite nucleation on ferromagnetic clusters

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Introduction. The study of the austenite magnetic state in steels has provided the mechanism of the external magnetic field impact on steel under the hardening process. Previous studies have established a positive practical effect of heat treatment in a magnetic field. The work objectives were to create a computer model of the magnetic state of carbon steel austenite; to conduct computational experiments with a system of spins at various values of temperature and external magnetic field.

Materials and Methods. The positions of the Ising model were used. The canonical ensemble of spins was modeled by the Monte Carlo method using the Metropolis algorithm.

Results. The algorithm was implemented with the initial parameters selected through experimental data on the magnetic state of austenite. The inhomogeneity of this state without exposure to a magnetic field was studied. Data on the sizes of ferromagnetic clusters in austenite at various temperatures were obtained. It has been noted that the presence of an external magnetic field counteracts the temperature disordering of spins. Data on an increase in the size of ferromagnetic clusters under growing magnetic field strength were obtained.

Discussion and Conclusions. A two-dimensional computer model of the spin state of austenite of carbon steel has been developed. The computational experiments with various parameters of the model have shown that there is a short-range order in the arrangement of spins above the Curie temperature. With a rise of the temperature of the system, the sizes of ordered regions decrease; but when an external magnetic field is applied, they increase.

Keywords: quenching, steel, magnetic field, martensite, martensitic transformation, austenite.

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Introduction. The magnetic state of austenite in steels and the effect that an external constant magnetic field can exert on it is considered. Previous studies have shown that heat treatment in a magnetic field has positive practical value [1–4]; therefore, it appears important to study the mechanisms of such an effect. C. Zener [5] pointed out the need to take into account the role of magnetic transformations when considering martensitic transitions in iron-based alloys. In calculating the thermodynamic characteristics of the martensitic transformation, he used two parameters – the magnetic and non-magnetic components of the change in the free energy of pure iron.

A number of researchers [6–8] found a deviation of the temperature dependence of the inverse magnetic susceptibility from the linear Curie – Weiss law in the paramagnetic region of some steels. In this case, the curve was satisfactorily described by the Langevin function for superparamagnetics. This change in the magnetic properties of austenite in steels is associated with spontaneous fluctuations of the long-range ferromagnetic order.

The experiments [9, 10] proved the existence of short-range order of spins (the so-called “swarms”) above the Curie temperature using magnetic neutron diffraction.

A constant magnetic field during quenching cooling affects regions with an ordered arrangement of spins in austenite and their interaction. As a result, the nucleation of martensitic crystals on ferromagnetic clusters is initiated.

Materials and Methods. At the moment, there is only one accurate and detailed method for experimental studies of "swarms" of spins – magnetic neutron diffraction. In this paper, the magnetic state of austenite of carbon steel is studied through a computational experiment. The positions of the Ising model [11–13] are applied. Using the Monte Carlo method [14–16], a canonical ensemble[1] of spins was modeled, the use of which provides simulating the behavior of the spin system at a constant temperature. To obtain an arbitrary non-uniform probability distribution, the Metropolis algorithm is used [17] – a special case of the sampling procedure by significance when some possible samples are dropped.

The Ising model is used to simulate phase transitions in magnetic substances or binary alloys. This lattice model takes into account interactions between the nearest nodes. Spins are represented by the magnetic moments of atoms in the lattice sites, which interact with each other and with an external magnetic field (if any).

The Ising model is based on the following simplifications:

- kinetic energy of lattice sites is not considered;
- when calculating the energy of interaction of spins, only the nearest neighbors are taken into account;
- only two possible spin states are provided (positive ↑ or negative ↓ direction along z axis).

As shown in [18], the study of the classical two-dimensional Ising model reveals common behavior patterns of magnetic systems near the phase transition temperature, even despite the simplifications.

Using the Ising model, such macroscopic system characteristics as the average energy$\langle E\rangle$, average magnetization$\langle M\rangle$, specific heat C and magnetic susceptibility χ were studied. When calculating the average values for all system configurations, the period until the system reached a relaxation state, which was excluded from the calculations, was taken into account[2].

Research Results. Let us describe the total energy of the system of two-dimensional spins in the Ising model taking into account the possible magnetic field h:

$$E = -J\sum_{\langle i,j\rangle}^{N} s_i s_j - h\sum_{i=1}^{N} s_i.$$

Here, J is the exchange coupling constant, which characterizes the strength of interaction of neighboring spins; N is the number of all spins; $\langle i,j\rangle$ means summation over all the nearest pairs of spins. The number s_i is associated with each i-th lattice site. It characterizes the direction of the magnetic moment and can take the values either +1 (if the spin is oriented in the positive direction of the z axis), or –1 (if the spin is oriented in the negative direction of the z axis).

If the value of the exchange interaction constant is greater than zero, then the unidirectional state of two neighboring spins is energetically more favorable, i.e., the state with the lowest total energy is ferromagnetic. Otherwise, it will be more preferable that the neighboring spins are antiparallel with each other (antiferromagnetic state).

The application of an external magnetic field along the z axis adds or subtracts additional internal energy of the spins according to their direction along the z axis.

In further discussions on the thermodynamic characteristics of the system, the energies J and h will be measured in temperature units. This is convenient when considering the interaction between spins, because when heated, the communication system between them weakens.

We find the relation between the specific heat C and the system energy fluctuation in the canonical ensemble:

$$C = \frac{1}{T^2}(\langle E\rangle^2 - \langle E^2\rangle).$$

[1] The canonical ensemble is a statistical ensemble corresponding to a special physical system. It exchanges energy with the environment (thermostat) being in thermal balance with it, but does not exchange matter since it is separated from the thermostat by a membrane that is impermeable to particles. For a brief description of such a system, two parameters are used: number of particles N and average energy E [13].

[2] Further in the text, when it comes to system configurations, the configurations after the system reaches relaxation state are implied.

The magnetization M of the system was calculated by adding all the values of s_{ij} in this configuration. Then, the average magnetization $\langle M \rangle$ over all system configurations was calculated

Magnetic susceptibility χ at a given temperature:

$$\chi = \frac{1}{T}(\langle M^2 \rangle - \langle M \rangle^2).$$

Possible configurations of the spin system will be determined by the values of 2^N spin numbers s. Using the Metropolis algorithm, spin configurations S with probability $w(S)$ can be generated, and then the sought quantities over all configurations can be averaged. The configurations that differ among themselves by one spin flip were considered. The decision on the flip of one or another spin (i.e., on the adoption of a trial configuration Sp) depended on the ratio of weight functions:

$$r = \frac{w(S_p)}{w(S)} = e^{-\frac{E_{Sp}}{T}} \cdot e^{\frac{E_S}{T}},$$

where E_s and E_{Sp} are energies of the systems with spin configurations S and S_p, respectively.

Spin s_{ij} flipped over and a new configuration was adopted if $r > 1$ or $r < 1$, but greater than a random number generated due to the uniform distribution over the interval from 0 to 1. Otherwise, the spin remained unchanged. At one Monte Carlo step, a number of flip attempts equal to the number of spins of the system N is made.

For the two-dimensional case, toroidal boundary conditions were chosen: the lattice is represented by a ring in which spins located on the right boundary of the original square lattice interact with spins located on the left boundary. A similar ring interaction is provided for the upper and lower boundaries. This provides the same number of interactions for all spins. The interaction of any spin with neighbors can be considered as the interaction with one spin whose value is equal to the sum of the values of four neighboring spins (it can be 0, ± 2, or ± 4). In the two-dimensional case, the minimum possible value of the energy change when the considered (central) spin is overturned is 4J.

Algorithm and initial parameters for the implementation of the model of the magnetic state of austenite. The algorithm structure and the basic functions developed under its implementation are performed in a mathematical package taking into account the recommendations [19].

The model was implemented through sequential performing the following operations.

1. Setting the initial conditions: the number of spins of the system N, the exchange interaction constant J, the intensity of the external magnetic field h, temperature T, the number of steps of the Monte Carlo method N_t (analogue of time).

2. Performing the function that creates the initial configuration of the system considering the given N, J, h.

3. Calculation of the instantaneous system configurations for each step N_t considering N, J, h and the initial state of the system.

4. Visualization of:

- instantaneous system configurations at points of interest,

- the dependence of the instantaneous energy of the system on time,

- the dependence of the instantaneous magnetization of the system on time.

Through observing spin configurations, the current magnetic state of the system can be evaluated. A study of these time dependences provides estimating the required relaxation time of the system τ for considering it in subsequent calculations.

5. Calculation of the average energy of the system$\langle E \rangle$, he specific heat$C$, the magnetic susceptibility χ and the average magnetization$\langle M \rangle$.

6. Calculation of parameters characterizing the sizes of ferromagnetically ordered regions: average size, maximum size, minimum size, root-mean-square size deviation. (The calculation is based on a set of spin configurations.)

The algorithm was implemented at the initial parameters selected due to experimental data on the magnetic state of austenite [8, 20]. The temperature of the Curie point of iron-carbon austenite of U8 steel is ~ 180 K, i.e., if it

were possible to keep the austenite lattice to this temperature, then below the Curie point, austenite would obtain ferromagnetic properties. The exchange interaction constant of the two-dimensional model was selected so that the system experienced a magnetic phase transition at a given temperature. The value of the exchange interaction constant for the two-dimensional case does not coincide with the real value of this constant for the iron-carbon alloy. However, in the framework of the two-dimensional model, the following parameters were selected: $N = 625$, $J = 0.78$, $h = 0$, $N_t = 2500$. Due to this, under modeling in the temperature range including the region of the Curie point of austenite, effects have been observed that are completely analogous to the effects of a real system experiencing a phase magnetic transition from the paramagnetic state to the ferromagnetic state, namely:

— maxima of the specific heat and magnetic susceptibility at the Curie point,

— sharp decrease in the average magnetization during the phase transition,

— discrepancy between the magnetization curve and the specific heat and magnetic susceptibility curves upon transition to the ferromagnetic state (Fig. 1).

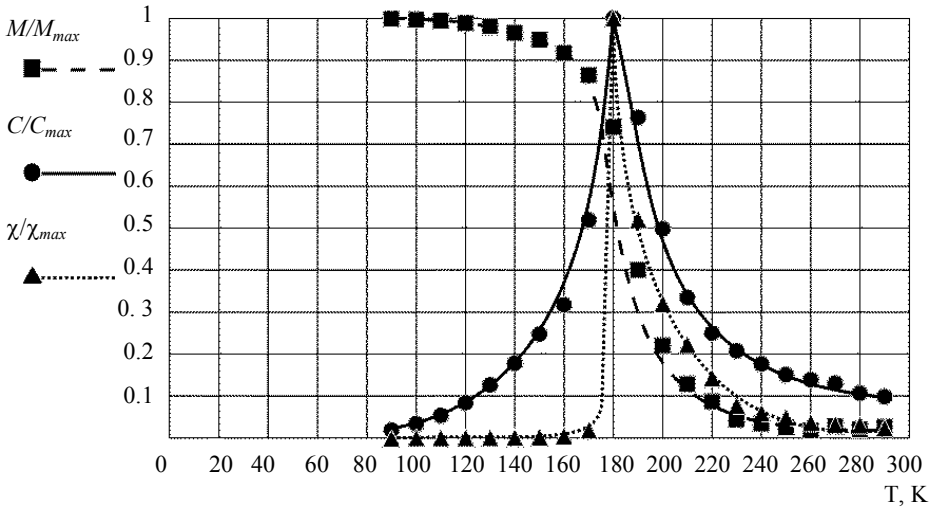


Fig. 1. Behavior of steel U8 properties near the ferromagnetic Curie point of austenite according to the results of computational experiments

Fig. 1 shows that the magnetization does not drop to zero at the Curie point. The remains of the "anomalies" above the Curie point were repeatedly observed experimentally [6–10, 19]. L. D. Landau [12] and other researchers [6, 8, 9, 19] attributed this to fluctuations of order at $T > \Theta$. Fluctuations of spontaneous magnetization should be most pronounced near the Curie point, because they tend to infinity at the Curie point itself.

Fig. 2 schematically shows the temperature dependence of the short-range order parameter σ from [19].

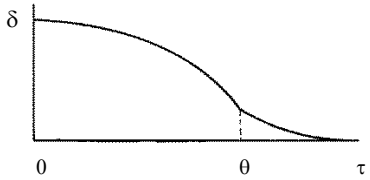


Fig. 2. Temperature dependence of the short-range magnetic order parameter [19]

Near the Curie temperature, σ decreases sharply, and at $T > \Theta$, it asymptotically tends to zero. From the point of view of short-range order, this "unsharpness" of the Curie temperature predetermines the following phenomenon: all anomalies of ferromagnetics have a steep maximum at the Curie point, however, at $T > \Theta$ they should not immediately go to zero, but only gradually decrease in accordance with the gradual destruction of order at close distances.

As shown in [19], the exchange interaction energy often determines the forces that are noticeably acting precisely at close distances. Therefore, the thermodynamically-equilibrium state of a ferromagnetic should be determined by the short-range order between spins. This is a special case of the general problem of the cooperative behavior of interacting atoms (for example, during a first-order phase transition).

Ferromagnetism is largely a quantum phenomenon [15]. Nevertheless, even within the framework of the classical statistical approach, the theory considering order at close distances is certainly useful in illustrative and qualitative terms [15, 19].

L. S. Stilbans took into account the "magnetic order" at close distances in the Ising scheme [21] and theoretically explained the "remnants" of the heat capacity anomaly at temperatures above the Curie point. The abnormal heat capacity is due to the necessity of destroying the order at short distances, which is partially conserved above the Curie point.

This method was developed by S. V. Vonsovsky [22–24]. He theoretically showed the differences between the ferromagnetic and paramagnetic Curie points. The results of his work prove that the paramagnetic susceptibility near the Curie point is finite, and does not tend to infinity, as follows from the theory without considering short-range order.

Such a great interest in the simplified Ising model is explained by the fact that it provides solving the fundamental difficulties arising in the theoretical interpretation of second-order phase transitions.

Analysis of regions with short-range ferromagnetic order in austenite using a computational experiment. In this section, we study the inhomogeneity of the austenite magnetic state without external exposure to a magnetic field.

To visualize the system instantaneous spin configuration at selected moments, the spins are represented by white and black squares. White squares are spins oriented in the positive direction of the z axis (for example, under the impact of exchange forces and (or) an applied external magnetic field). Black squares are spins oriented in the negative direction of the z axis (Fig. 3).

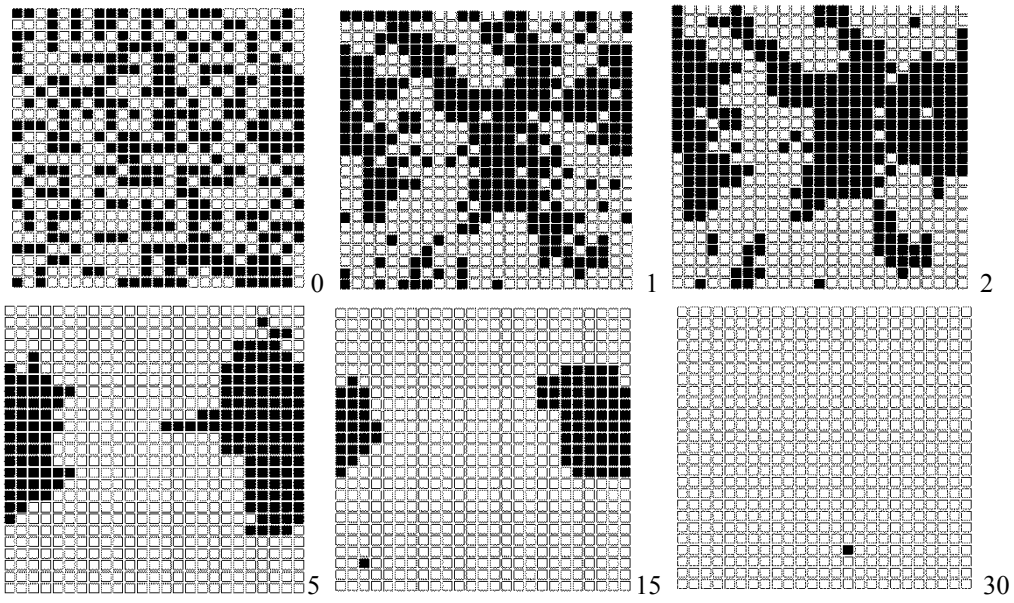


Fig. 3. System instantaneous configurations at selected moments (T = 100 K, h = 0)

Fig. 3 shows the system visualization at a temperature of 100 K (i.e., below the Curie point) without the action of a magnetic field at different moments. The following is an interpretation of these configurations.

- At time moment 0, the system is in the initial state, which is initiated using a random value generator (fully disordered state).

- At time 0, the system is in the initial state, which is initiated using a random value generator (fully disordered state).

- The transition to moment 1 means that each spin of the system (N = 625) was considered to make a decision on its revolution according to the conditions described above.

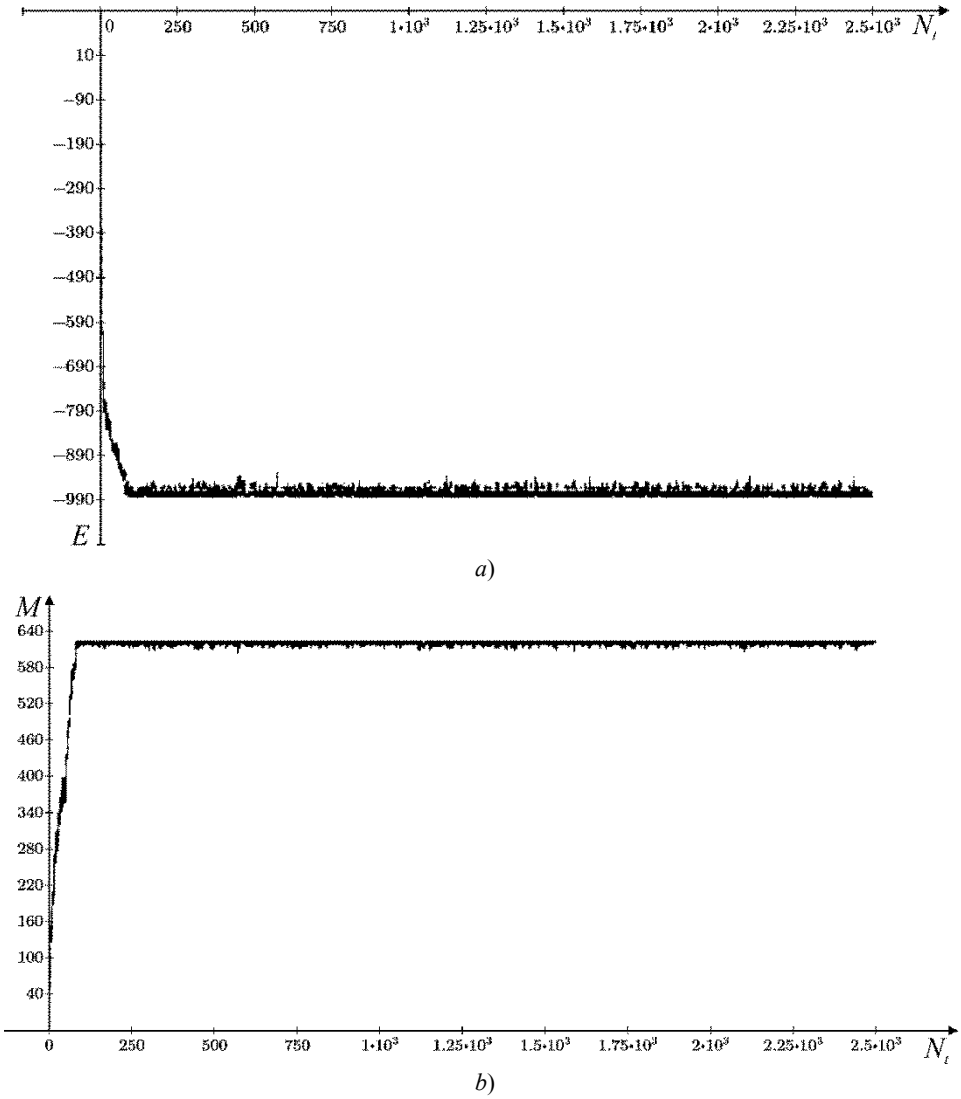
- By the third step, each spin was examined three times for a flip.

- Subsequent moments show that the system tends to a state with a ferromagnetic order.

- At the 30th step, a completely ordered state is recorded (with the exception of one spin). A similar picture (with small fluctuations of 1–3 spins) is observed at all subsequent moments. The total number of steps is N_t = 2500. Consequently, the system has come to a stable state (that is, the relaxation stage has been completed before the 30th step).

It should be noted that the described picture is characteristic of the current generation of the model with given conditions. When generating the model, a random number generator is used, therefore, the results of the recounting will differ in details, but qualitatively, the model always behaves in a similar way under the same initial conditions.

Consider the graphs of the instantaneous values of energy (Fig. 4 *a*) and magnetic moment (Fig. 4 *b*) of the system versus time.



a)

b)

Fig. 4. Dependence of the instantaneous values of the system total energy (*a*) and magnetic moment (*b*) on time

Fig. 4 shows that the system quickly tends to an equilibrium state (relaxation process). After the transition of the system to the equilibrium state, only small fluctuations are noted. Upon reaching equilibrium for a given temperature, macro parameters (average energy, magnetization, magnetic susceptibility, specific heat) were statistically calculated from the system configurations. For this, the ratio of the relaxation time of the static system to the equilibrium state was estimated from the corresponding graphs. The initial system configurations were cut off for 400 steps (16% of the total calculation time), that, on the safe side, blocked the relaxation stage of the system, which did not exceed 150 steps (see Fig. 4).

When hardening U8 steel, the martensitic transformation starts at a temperature of ~ 500 K. It is interesting to study the model behavior near this temperature, because under quenching in a magnetic field, the field action initiating the phase transition is manifested here. Naturally, at this temperature, the paramagnetic state of austenite will be stable, as the model showed that. However, in the spin state of austenite, nanoscale regions with short-range order in the arrangement of spins are observed [9]; they play a significant role under the impact of an external magnetic field [8] (the

effect of the field is manifested in the influence on the size and stability of such regions, but they exist without an external field).

To obtain the most reliable statistical data on ferromagnetically ordered regions in austenite, a system was simulated with the maximum possible (according to the technical limitations of the RAM and processor speed) number (N = 10000) of spins at temperatures from 100 to 500 K. Other initial conditions remained the same.

Fig. 5 presents the results of measuring ordered regions in austenite. The size was determined by the number of atoms per horizontal and vertical sections of the ordered region: $\bar{L}$ is average size, *Max* is maximum, *Min* is minimum, σ is root-mean-square deviation.

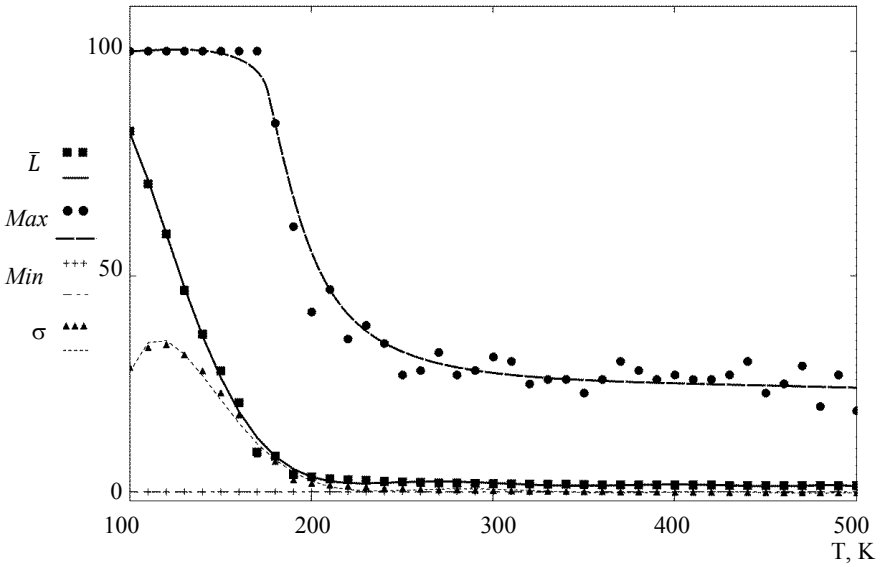


Fig. 5. Temperature dependence of area sizes with ferromagnetic order in austenite

According to the data obtained, fluctuations of the short-range magnetic order in U8 steel are preserved up to temperatures of about 500 K, when martensitic transformation starts under the steel quenching. In this case, the maximum sizes of such regions in austenite at a temperature of 500 K can reach 20 atoms in the cross section (~ 7.2 nm). The maximum size at temperatures in the region of the Curie point and below is limited by the model conditions and does not exceed 100 atoms (i.e., the maximum transverse size of the modeled region). The observed oscillations on the curve of the maximum cluster size are associated with the use of a random number generator in the model.

The Weiss theory considers only the order at long distances [19], which is determined by the difference in the number of spins oppositely directed throughout the domain, regardless of their detailed relative position. It turns out that the short-range order is simply equated to the long-range order, i.e., the numbers of the nearest neighbors of different orientations for any spin are assumed to be proportional to the total numbers of multidirectional spins in the domain. Thus, the local magnetization of the nearest neighbors at each spin is equal to the magnetization calculated over the entire crystal. A different picture is observed in a real crystal: parallel spins under the action of exchange forces tend to unite into separate "swarms" [9, 19] like gas atoms during its condensation or the formation of fluctuations in a non-ideal gas. As can be seen from Fig. 5, at low temperatures, these fluctuations are very large. At high temperatures, a more reasonable approximation does not consider the short range order. However, in this case, there are still fluctuations of parallel spins in small volumes caused by the exchange forces and leading to nonzero local magnetization in the absence of the resulting magnetic moment in the entire volume (i.e., in the absence of long-range order).

Thus, the model predicts the existence of regions with short-range magnetic order in the austenite of U8 steel before the martensitic transformation. In these areas, with a high degree of probability, martensite nuclei arise. Clusters with ferromagnetic ordering can overlap defects in the crystal lattice and instability regions of the crystal lattice [4] that occur before the phase transition. In this case, the probability of martensite nucleation is especially high.

Adding an external magnetic field to the austenite magnetic state model. The presence of an external magnetic field counteracts the temperature disordering of spins. Fig. 6 shows the dependences of the cluster parameters in

austenite with short-range order (the parameters are the same as in Fig. 5) on the external magnetic field strength for U8 steel at a temperature of 500 K.

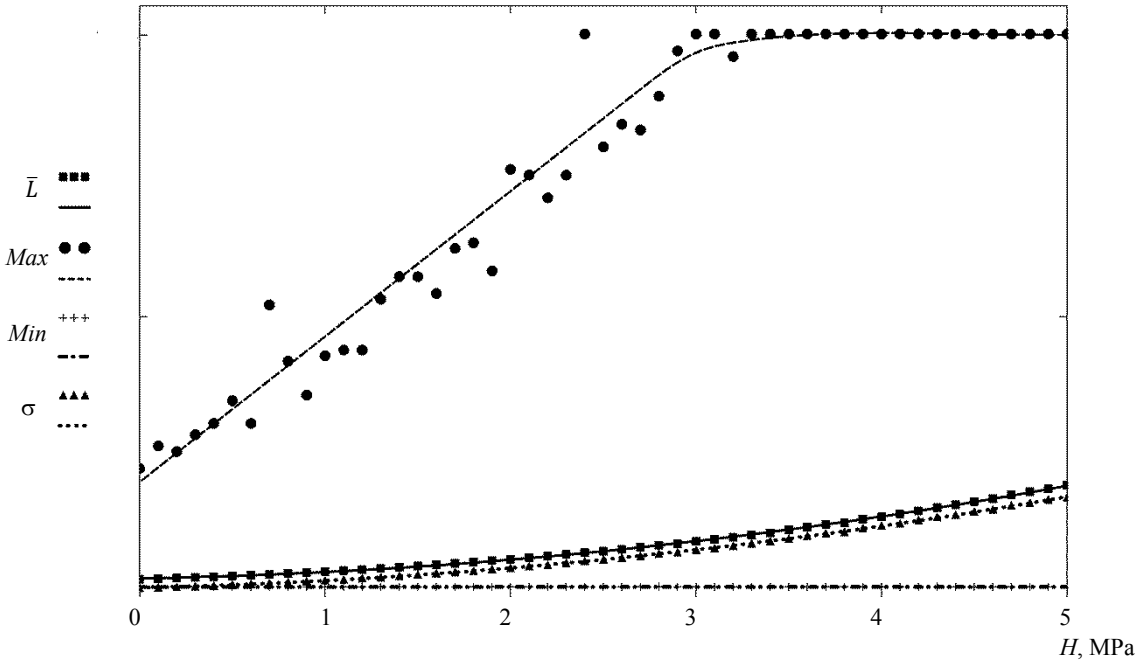


Fig. 6. Dependence of sizes of regions with ferromagnetic order in austenite on strength of external magnetic field at a temperature of 500 K

As can be seen from Fig. 6, with increasing magnetic field strength, cluster sizes grow up to the state of complete magnetic ordering at high magnetic field strength. Thus, under quenching in a magnetic field, regions with short-range order expand. Moreover, the probability of martensite nucleation is higher, and the number of nucleation sites is greater.

Discussion and Conclusions. A two-dimensional computer model of the spin state of austenite of U8 carbon steel is developed. The computational experiments with various parameters of the model have shown that there is a short-range order in the arrangement of spins above the Curie temperature. With an increase in the temperature of the system, the sizes of ordered regions decrease; however, even at the temperature of the onset of martensitic transformation (500 K), short-range fluctuations with a maximum size of ~ 7 nm are possible. When an external magnetic field is applied and its intensity is enhanced, the sizes of clusters with ferromagnetic ordering increase. Using the presented model in future research, it is supposed to study in more detail the impact of the magnetic field on the characteristics of the swarm of spins, their number, lifetime and interaction features.

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Claimed contributorship

Yu.V. Dolgachev: basic concept formulation, research objectives and tasks setting, computational analysis, text preparation, formulation of conclusions. V.N. Pustovoit: academic advising, research results analysis, the text revision, correction of the conclusions. I.O. Filonenko: implementation of the model algorithm in the programming environment, preparation of calculations. I.V. Ivankov: simulation modification and model adjustment in the programming environment, participation in the preparation of calculations.

All authors have read and approved the final manuscript.