The model of austenite structure state taking into account fluctuations of magnetic nature

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The results of magnetic state simulation of carbon steel austenite are presented in this work. Quantitative parameters of the areas of short-range magnetic order, which are presented in paramagnetic austenite matrix and are observed as potential places of α-phase nucleation, are examined. This austenite heterogeneity in steels and clean iron is confirmed by the experimental data; however, detailed quantitative study meets technical complication of such experiments. It is suggested to use the Ising model for realization of the calculation experiment. The obtained spin configurations were analyzed for determination of geometric parameters of magnetic inhomogeneities and period of their sustainable existence. Calculations were conducted within the temperature range of austenite phase existence in steel, as well as without and with taking into account presence of external magnetic field, which strengthens existing austenite heterogeneity and has the effect on conduction of phase transformations in steel. The results of simulation confirm presence of the areas of short-range magnetic order in austenite, their size is close to the existing theoretical assessments and experimental data. It is shown that temperature rise leads to decrease of dimensions, number and life period of clusters, but these parameters are still important at the temperature of martensite transformation in steel. Overlapping of external magnetic field creates the conditions for existence of large-size ferromagnetic clusters also at more high temperatures, as well as increases time of their sustainable existence. The external magnetic field provides the conditions for more intensive and multiplicative nucleation of ferromagnetic phase, similar to short-range magnetic order fluctuations in location of atoms during liquid metal cooling.
Key words: steel, austenite, magnetic state, ferromagnetic cluster, α-phase, martensite, magnetic field.
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Introduction

Experimental study of magnetic state of γ-Fe and austenite of steels [1-10] displays presence of magnetic inhomogeneities in the form of nano-metric scale areas with short-range magnetic order. Anti-ferromagnetic [1-3], ferromagnetic [4-9] and micro-magnetic [10] ordering of spins is observed in nano-clusters depending on alloy composition and conditions of studies. It is also known [11-16], that magnetic state of the initial phase has influence on scenario and products of phase transformation in steel. There are theoretical and experimental notifications [4, 5, 17-19], that nano-clusters with short-range magnetic order in austenite play the role of α-phase nuclei, e.g. in magnetic transformation.

This work is aimed on examination of such parameters of magnetic inhomogeneities in carbon steel austenite as their average size, amount, life period. Getting information on austenite magnetic state with presence of external magnetic field, which can strengthen existing austenite heterogeneity, is also one of the tasks.

It was established during study of reversed magnetic susceptibility of carbon steel with 0.8 % C [19], that superparamagnetic state, stipulated by presence of ferromagnetic nano-clusters in paramagnetic matrix, is observed within the temperature interval from 1090 K to 950 K (if the temperature is below this value, decomposition of solid solution with forming of α-phase occurs). The Curie point was determined for U8 carbon steel austenite on the base of obtained data; it corresponds ~180 K.

Unfortunately, there are no precise experimental methods for detailed examination of magnetic inhomogeneities at present time, excluding magnetic diffraction of neutrons. Thereby the technique of calculation experiment for examination of magnetic state of carbon steel austenite is used in this research.

The technique of investigations

The statements of the Ising model [20-22] were used for examination of magnetic state of austenite. Detailed description of the realized model of magnetic state of carbon steel austenite is presented in the works [23, 24] written by the authors. As a result of the models operation, statistical data massifs were obtained and the following macroscopic parameters of a system were calculated with their use: average energy <*E*>, average magnetization <*M*>, specific heat capacity *C* and magnetic susceptibility χ. Possibility of visualization of the state of spin system configuration at the required moment (cycle step) was also realized. Analysis of spin pictures using the program of quantitative image processing (QIP-1) and separately developed algorithms

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allowed to obtain the data about quantitative parameters of magnetic inhomogeneities in austenite.

Magnetic state of steel austenite with eutectoid composition was simulated via tuning of the system parameters on the base of experimental data, which were obtained for U8 steel (0.79 % C; 0.222 % Si; 0.307 % Mn; 0.016 % P; 0.0061 % S; 0.032 % Cr; < 0.01 % Ni; 0.051 % Cu) in the work [19]. Number of spins $N = 10^6$ and total number of steps $N_t = 2{\cdot}10^4$ were preset as initial parameters of the system, it was stipulated by acceptable computer processing time.

Visualization of instant spin system configuration in the selected moments was realized through presenting spins as black and white points, where white points are spins oriented in positive direction of z axis (e.g. under the effect of exchange forces and/or applied external magnetic field), and black points are spins oriented in negative direction of z axis.

Statistical calculations of the system macro-parameters (average energy, average magnetization, magnetic susceptibility and specific heat capacity) were conducted via system configurations after its reaching equilibrium state for preset temperature. Time of relaxation (number of cycles) of a static system to the equilibrium state was taken into account for this purpose. Analysis of relaxation time was conducted at each exchange of initial conditions, such as temperature, value of external magnetic field and number of spins.

Results of investigations and discussion

Parameters of ferromagnetic clusters in austenite

Let us consider heterogeneity parameters of austenite magnetic state in U10 carbon steel, which exist without external effect from magnetic field. The system simulation was conducted at the temperatures from 300 to 1,200 K. This temperature range was chosen based on the practice of steel heat treatment, when austenite phase can exist in different operations including heating and cooling.

The pictures of system spin state with resolution 1,000 x 1,000 dots were the results of this simulation. Austenite should be in paramagnetic state at these temperatures, i.e. approximate equality between black and white areas (in other words, the areas with opposite direction of spins) should be observed. The results of pictures analysis displayed domination of either white, or black areas in their summarized square; this event was equally possible in the conditions of absence of external magnetic field. Histograms of distribution of quantity of the areas with dominating direction by their dimensions were calculated. The obtained statistical data are presented on the **Fig. 1**.

The results of calculation of size of ordered areas in austenite at different temperatures testify that the average cluster size (see Fig. 1) is the average reduced diameter of the ferromagnetic ordered area. Simulated areas of short-range order have curved boundaries, while the reduced diameter characterizes the round area with the same square. It is natural, that temperature rise leads to decrease of the average cluster size with short-range order in location of spins due to strengthening temperature disordering. At the same time, temperature rise is connected with decrease of dispersion and variation coefficient of clusters sizes via degree relationship; it reduces possibility of creation of a cluster with its size large than average size at high temperatures. It should be noted that obtained sizes of clusters are close to the previously obtained experimental data and theoretical assessments [4, 5, 25].

Maximal cluster size and relationship between part of large clusters and temperature were also evaluated. Maximal cluster size means maximal reduced cluster diameter. The part of large clusters was determined via calculation of percent content of clusters with diameter exceeding 5 nm from total number of clusters at preset temperature. Starting calculation from the size 5 nm was chosen as the beginning of the last interval in distribution histogram for clusters sizes at the temperature 1200 K. Direct number of clusters at different temperatures is not a meaningful parameter due to model restrictions. Because the researched system uses relatively small, but final number of spins ($N = 10^6$). Restriction on number of spins always leads to decrease of number of clusters with enlargement of their sizes, and on the opposite, to increase of number of clusters with diminishing of their sizes; thereby the part of large clusters in the system at preset temperature is the most expressive parameter. The obtained data show that temperature rise causes reducing of a maximal cluster size and the part of large clusters via degree relationship. U8 steel at the temperature about 500 K (when martensite transformation starts during quenching) is characterizes by maximal size of fluctuations of short-range martensite order achieving ~ 7,1 nm.

Cluster life time as a parameter of cluster stability was determined. It means a number of iterations (steps) of the system, when no one of atoms containing in a cluster did not change direction of its spin. The cluster with preset size was simulated, it was presented by the area of ordered spins, which was encircled along its perimeter by spins with opposite direction. The test of each cluster spin for its overturn was conducted during one step; if at least one spin changed its direction, then number of iterations until this event was considered as life time of this cluster. 10,000 tests were conducted for each cluster size and for each examined temperature, the averaged data of these tests are presented on the **Fig. 2**.

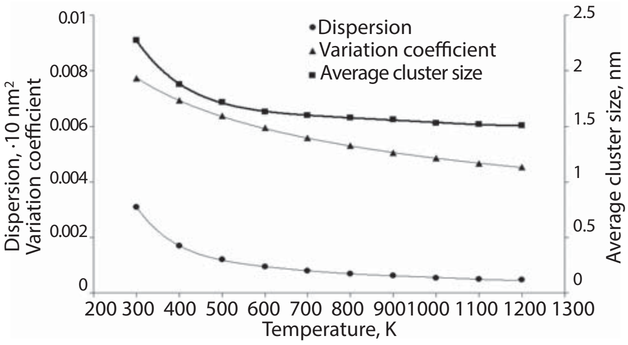

Fig. 1. Relationship between size of the areas with ferromagnetic order in austenite and temperature

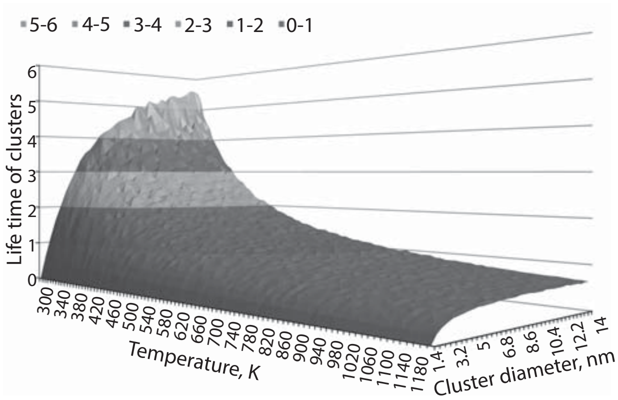

Fig. 2. Life time of clusters with different sizes depending on the temperature

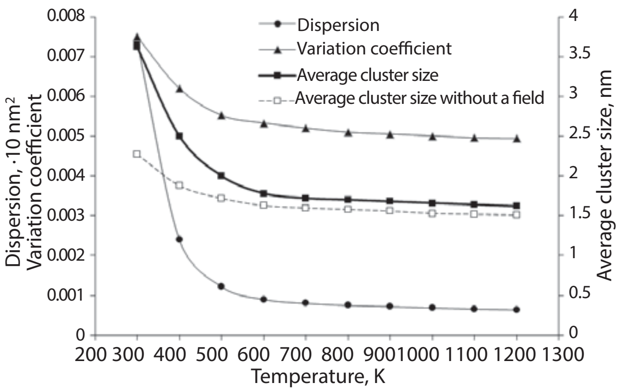

Fig. 3. Relationship between size of the areas with ferromagnetic order in austenite and temperature in the conditions of external magnetic field intensity 2.4 MA/m

Cluster life time at the room temperature strongly depends on its size. Ferromagnetic clusters consisting of larger number of atoms have larger life time. The clusters of maximal size (9.1 nm) are characterized by appr. 5 iterations, while the clusters of average size (2.3 nm) – by 1.2 iterations. As soon as temperature rises, cluster size has no serious effect on its stability. At the temperature of martensite transformation, the clusters of maximal (7.1 nm) and average (1.7 nm) size are characterized by 2 and 0.5 iterations respectively. When the temperature exceeds 800 K, the effect of cluster size on its stability is practically small. The prevailed role is played by temperature disordering, which decreases substantially life time of clusters with any size. At the temperatures above 800 K, a plateau of stable life time (~ 1 iteration) is observed for the clusters with size more than 3 nm.

The Weiss theory takes into account only the order for long distances, which is determined by difference of number of spins with two opposite directions along the whole domain, not depending on their detailed mutual location. In this case short-range order is equalized to long-range order, i.e. numbers of the closest neighbors with different orientation for each spin is proposed to be proportional to full numbers of differently directed spins in a domain. So, local magnetization of the closest neighbors for each spin is equal to magnetization calculated for a whole crystal. The results of simulation display that other picture is observed in a real crystal: parallel spins are trying to unite in single swarms under the effect of exchange forces (it was also observed experimentally [4]), like gas atoms during its condensation or forming of fluctuations in non-ideal gas.

It is seen from the obtained data, that these fluctuations are relatively high at the low temperatures. But at the high temperatures approximation, which does not take into account short-range order, is more legal. However, in this case there are also fluctuations of parallel spins in small volumes, which are caused by exchange forces and lead to local magnetization not equal to zero in the conditions of absence of resulting magnetic moment in the whole volume (i.e. in the absence of long-range order). As soon as the temperature of phase transition approximates, ferromagnetic nano-clusters in austenite begin to play the role of nuclei of ferromagnetic α-phase, especially during their overlapping on defects of a crystal lattice or instability area; these defects appear in a lattice before phase transition [17].

Influence of external magnetic field on size, amount and life timw of ferromagnetic clusters in austenite

Presence of external magnetic field provides countereffect to temperature disordering of spins. Relationship between clusters with average size and short-range order in austenite, and temperature under the effect of external magnetic field with intensity 2.4 MA/m is shown on the **Fig. 3** (the presented values of magnetic field intensity, which were recalculated from the values of 2D model using experimental data obtained on carbon steels [23] are mentioned here and later). When choosing magnetic field intensity for calculations, first of all we took into account the interests of production facilities, possibility of using such field in industrial units for heat treatment under the effect of magnetic field. In this connection the effect of permanent magnetic field with intensity 2.4 MA/m is shown, it can be easily realized in industrial-type units.

General features of these relationships is the same as without field effect, but the values of clusters sizes are larger in the conditions of external magnetic field. The most strong effect caused by magnetic field at the low temperatures: at the room temperature field overlapping provides difference in average about 1.5 nm. But with rise of the temperature, field efficiency drops: at the temperature of martensite transformation (~ 500 K) this difference made ~ 0.3 nm, while at the temperature exceeding 600 K practically permanent economical effect is reserved (~ 0.12 нм).

The effect of magnetic field is manifested in increase of the part of large clusters and maximal cluster size at the researched temperatures. At low temperature the effect of magnetic field is maximal, at room temperature difference for maximal cluster size makes ~ 5 nm, while difference in the part of large clusters makes ~ 7.2 %. When the temperature increases, the field efficiency drops: at the temperature of martensite transformation difference for maximal cluster size makes ~ 0.6 nm, while difference in the part of large clusters makes ~ 1.4 %. Consequent temperature rise leads to gradual lowering of magnetic field effect is accompanied by gradual decrease of the field effect and practically complete approximation of clusters parameters, which were obtained in calculations taking into account the field at the temperature 1200 K and without its accounting.

The data about life time of ferromagnetic clusters in austenite under the effect of external magnetic field are presented on the **Fig. 4**.

Simulation was also conducted for the fields with different intensity values (0.8, 1.6, 2.4 and 3.6 MA/m). It is shown that clusters under the effect of external magnetic field in all cases live longer, than without this field. Increase of life time with enlargement of cluster size is a general regularity, what is manifested mostly evidently at low temperatures; consequent temperature rise neutralizes the value of cluster size. Increase of magnetic field intensity leads to increase of life time for all sizes of clusters. Field efficiency is especially distinct at low temperatures. If the field intensity makes 2.4 MA/m at low temperature, then clusters of each size live in average by I iteration longer, than without magnetic field, while increase of life time in magnetic field at the temperature of martensite transformation makes 0.5 iteration in average. When the temperature exceeds 800 K, the values of life time with and without magnetic field are practically equal. However, if we take into account that maximal and average cluster size increase in the external magnetic field, then real increase of life time also will become larger. So, at the room temperature the clusters of maximal size (14 nm) are stable during about 7 iterations (compared with 5 iterations for maximal cluster size 9.1 nm without magnetic field, while the clusters of average size (3.6 nm) are stable during about 3.5 iterations (compared with 1.2 iterations for average cluster size 2.3 nm without magnetic field. As for the temperatures of martensite transformation, the maximal cluster size in magnetic field (7.7 nm) lives during 2.5 iterations (without magnetic field (7.1 nm) – 2 iterations), while the average cluster size in magnetic field (2.0 nm) lives during 1 iteration (without magnetic field (1.7 nm) – 0.5 iterations).

The value of cluster life time does not mean that cluster will terminate completely after its finishing, it shows only duration of its stable state. Further complete destruction of a cluster is quite not mandatory after overturn of one of the spins; it is more probable that a spin of parallel direction can be added during the next step again. Duration of life time characterizes cluster capacity not to lose its integrity during definite number of iterations. Each additional iteration of life time increases possibility of a cluster size increase. Potential possibility for a cluster to reach the state which is suitable for nucleation spot in austenite increases respectively, in the conditions of lower free energy in ferromagnetic phase. This means that ferromagnetic ordered clusters

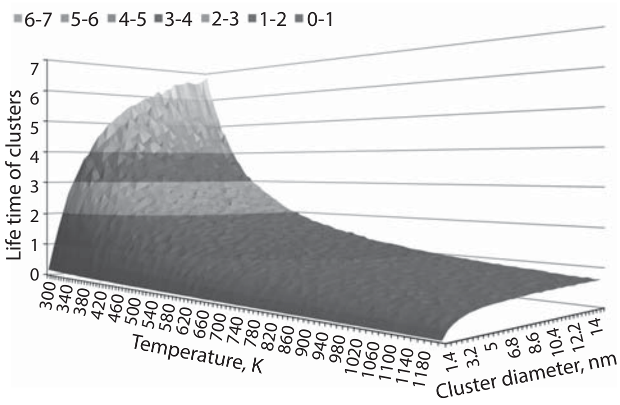

Fig. 4. Life time of clusters with different sizes depending on the temperature at magnetic field intensity 2.4 MA/m

can be compared with short-range order fluctuations in location of atoms during overcooling of liquid metal; they can reach critical size and become nucleation centers of solid phase. Based on this analogy, size and stability of appearing fluctuations have determining importance for creation of a nucleation center. The external magnetic field has the effect on parameters of ferromagnetic ordered clusters and increases possibility of nucleation centers of ferromagnetic phase. The mechanism of nuclei creation from such ferromagnetic centers is connected with magnetostriction process and. respectively, with atomic displacements, which can be overlapped on the conditions of super-plasticity and instability of crystal lattice (e.g. during of martensite transformation). The mechanism of nucleation from ferromagnetic areas in austenite under the effect of magnetic field is discussed in [17-19].

Conclusions

Thereby, the results of simulation confirm existence of the areas with short-range magnetic order in steel austenite, i.e. before martensite transformation. Martensite nuclei appear in these areas with high probability, especially during their overlapping on defects of crystal lattice and instability areas of crystal lattice, which appear before phase transition. External magnetic field can play the determining role in activation of clusters as nucleation points, because magnetostriction stresses vary the fields of elastic forces between atoms in crystal lattice, while boundaries of clusters interact with dislocations. Additionally, overlapping of the external magnetic field is the only way to manage by number and stability of ferromagnetic areas in austenite and, consequently, to manage by kinetics and scenario of phase transformation.

The obtained data testify that size and number of large clusters as well as life time of ferromagnetic ordered clusters increase after overlapping of the external magnetic field. So, size of the areas with short-range order increases during heat treatment in magnetic field, and possibility and number of nucleation points of ferromagnetic phase increases as well. Such multiplicative feature of nucleation stipulates more complete conduction of phase reaction towards forming of ferromagnetic phase. These variations in kinetics were observed previously during heat treatment in magnetic field, but they were not explained in assessment of power influence of magnetic field on phase transformation.

The results of simulation allow to take into account the existing inhomogeneities in austenite magnetic state, as well as variations in this state caused by overlapping of the external magnetic field in nucleation processes at γ-α transition. They can be used for development of practical procedures and technological equipment for aimed variation of structure and properties of steel products. Structural variations, which are connected with increase of transformation products dispersity, make it possible to realize additional increase of product strength without loss of its plasticity.

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