MODELING OF NON-STATIONARY DIFFUSION of ALLOYING ELEMENTS ON EXPOSURE OF STEEL SAMPLES TO MAGNETIC PULSES

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Abstract
The model suggested describes a nonstationary diffusion of impurities in alloyed steels under magnetic pulse action. It is established that a non-stationary diffusion of impurities is determined by structural defects that are initiated during pulse processing. On non-stationary diffusion the impurity atoms of a larger radius migrate from the grain boundary into its depth. The interaction of atoms with dislocations hinders their further movement and leads to hardening of a ferrite grain.

Keywords: Diffusion of impurities, steel, magnetic pulse action, structure, defects

Description of obtained results. Model construction and analysis.
Let us consider a ferrite grain that is a $Fe_{\alpha}(C)$ monocrystal comprised of an interstitial solid solution of carbon into α iron. The ferrite grain sizes of the investigated steels such as 45, 40X and those of the 8XΦ are in the range of 5–17 μm and 2–6 μm, respectively.
In this case in the grain there are both point defects including vacancies, interstitial atoms and impurity atoms of alloying elements and linear defects such as dislocations. The dislocation density of unprocessed, unannealed sample was 10^7–10^9 m^{-2} and that of an annealed sample 10^6–10^7 m^{-2}.
Carbon is disposed in lattice defects and atoms of alloying elements are both interstitial and substitutional atoms.
Assume that initially prior to processing the impurity atoms and defects are uniformly distributed over the grain volume [1]. Under its exposure to pulses the system that is a ferrite grain transforms into a nonequilibrium state. Here the characteristic pulse time is about 10^{-3} s (Fig. 1), which is many times smaller than the time of system relaxation [2].
The instantaneous value of a magnetic field density of an observation point that is at the distance *h* from the billet surface facing an inductor is determined by the formula [3]:

$$w = \frac{\mu\mu_0}{2} H^2(h,t), \tag{1}$$

where $H(h,t) = H_{\max}\exp(-\alpha h - \beta t)\sin(\omega t - k h)$, (2)

where μ is the medium magnetic permeability that depends on a magnetic field intensity, *H,* for a ferromagnetic sample; $\mu_0 = 4\pi 10^{-7}$ Н/м is the SI system vacuum permeability; $\omega = 2\pi/T$ is the cyclic oscillation frequency of electromagnetic field generated by an inductor in the processing zone; $\alpha = \sqrt{\mu\mu_0\omega\sigma/2}$ is the value reciprocal to a skin-layer thickness of a metal to be processed; σ is the average specific electrical conductivity of a ferrite grain; β is the attenuation coefficient and *k* is the wave number.

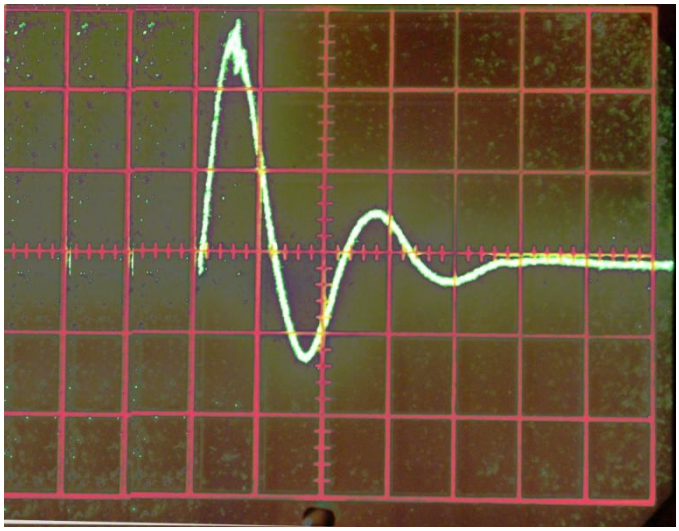

Fig. 1 *Oscillogram of a pulse shape. Time-base sweep, 50 μs/division.*

With the magnetic field intensity $H_{max} = 10^7$ A/m and pulse time $\tau = 10^{-3}$s (these parameters are determined by design features of a machine [4]), the specific resistance $\rho = 10^{-7}$ Ohm/m and the magnetic permeability of medium $\mu = 1000$ (which is characteristic of ferrite) we obtain the following numerical estimates of the process: the skin-layer thickness $\alpha^{-1} = 10^{-4}$ м and the maximum pressure exerted on a ferrite grain that is on the sample surface (at $h = 0$) $p_{max} = 10^{11}$ Pa. This value exceeds the ferrite yield strength ($\sigma_т = 5–8 \cdot 10^8$ Па) by a factor of more than 1000. Therefore, in the process of pulse treatment there occur not only dislocation displacement that results in a grain plastic deformation but also formation of additional defects such as vacancies, edge and screw dislocations.

In the general case the dynamics of a nonequilibrium system can be described by Liouville equation [5]:

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} \dot{q}_i \frac{\partial f_N}{\partial \dot{q}_i} + \sum_{i=1}^{N} \left(-\frac{\partial \Phi_i^{ext}}{\partial \dot{q}_i} - \sum_{j=1}^{N} \frac{\partial \Phi_{ij}}{\partial \dot{q}_i} \right) \frac{\partial f_N}{\partial p_i} = 0, \qquad (3)$$

where $f_N = f_N(q_1 \ldots q_N, p_1 \ldots p_N)$ is the distribution function of a total system of pairwise interacting particles placed in an external force field; q_i, p_i are the generalized coordinate and generalized momentum of *i-th* particle; $\Phi_i^{ext} = \Phi^{ext}(q_i)$ is the potential of interaction with an external field and $\Phi_{ij} = \Phi\ (q_i q_j)$ is the potential of pairwise interaction.

Due to nonstationarity of the process $\Phi_i^{ext} = \Phi_i^{ext}(t_i)$ as well as to a great number of particles contained in the system *N*, the equation (3) can not be exactly analytically solved.

To solve the equation (3) let us introduce some approximations that would allow simplifying the problem. In this connection we should note that here the potential of a pairwise interaction is a rapidly decreasing function of the distance, r_{ij} between particles [6]:

$$\Phi\ (q_i q_j) = \frac{A}{r_{ij}^6} - B \exp\left(-\frac{r_{ij}}{\rho} \right), \qquad (4)$$

where the coefficients *A* and *B* determine the potentials of attractive and repulsive forces, respectively, and depend on charges of particles and their mutual position in a crystal lattice and ρ is the characteristic length that in magnitude is equal to a lattice constant (10^{-10} m).

While the potential of interaction with an external magnetic field is determined by the expressions (1) and (2) it is a more slowly varying function of spatial coordinates and decreases with increasing the distance from the surface into the depth of the material approximately at the distance of $h = 5$ μm equal to an average grain size.

Thus, a short-range order of atomic arrangement is determined by the potential of pairwise interaction. Let us assume that in the initial state the quantity of point defects of an unprocessed sample is negligible and about 10^8 м$^{-3}$. Then considering the uniformity of defect distribution over the grain volume we would suppose that both

interstitial and substitutional impurity atoms interact only with surrounding iron atoms. They can not have direct effect on each other due to a short-range potential of pairwise interaction determined by the formula (4). Then owing to symmetry of arrangement of iron atoms in sites of volume-centered crystal lattice the resultant of forces acting on an impurity atom would be equal to zero (Fig. 2).

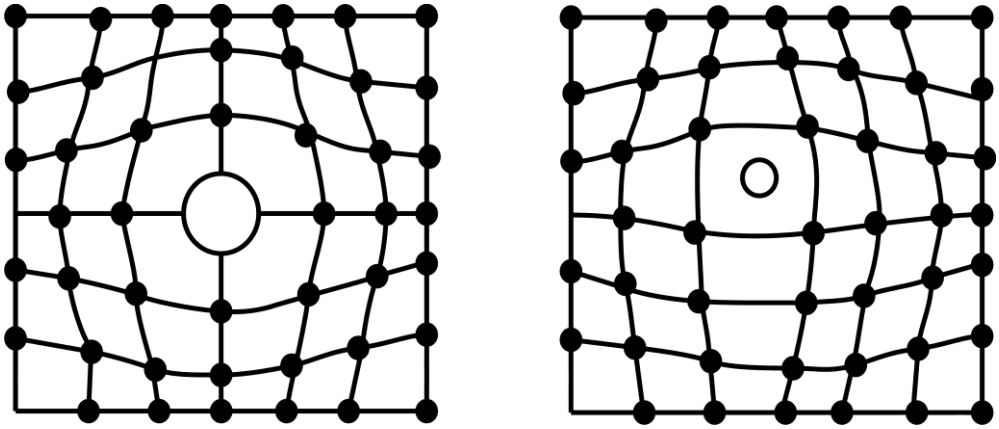

Fig. 2 *Substitutional and interstitial impurity atoms.*

In case the atomic sizes are smaller than those of iron atoms and the structure of electron shells of impurity atoms substantially differs from that of the iron atom structure the impurity is of interstitial kind. It is characteristic of carbon and boron atoms and as for atoms of metals such as tungsten, zirconium and molybdenum their presence in the form of substitutional impurities is considered energetically more favorable [7].

As noted above the pulse processing results in initiation of a great number of defects the time of which occurrence is very short and in magnitude corresponds to the pulse duration. However, in the process of formation of vacancies and edge dislocations the distance between neighboring atoms is increased which leads to decreasing the potential of a pairwise interaction by 2-3 orders. Then what concerns the impurity atoms that are in close vicinity to vacancy their possible displacement would be determined by the potential of interaction of these atoms with external field, $\Phi^{ext}(\mathrm{q}_i)$. Thus, impurity atoms and ions of the non-equilibrium system can be considered as subsystems and it is possible to introduce one-particle states for their description $f_1(\boldsymbol{q}, \boldsymbol{p})$ [5]:

$$\frac{\partial f_1}{\partial t} + \frac{\partial f_1}{\partial \mathbf{q}}\dot{\mathbf{q}} + \frac{\partial f_1}{\partial \mathbf{p}}\mathbf{F} = I_{cool}(f_1), \tag{5}$$

where $I_{cool}(f_1)$ is the collision integral determined by crystal lattice defects and F is the force acting on an impurity atom in a magnetic field.

In the vicinity of the defect the direction of force action is determined by the radius of impurity atom. In these circumstances it is energetically favorable for the atoms having the radius smaller than that of crystal lattice atoms to occupy the position near the boundary and as for those the radius of which is greater than that of atoms forming the crystal lattice their position is more energetically favorable at a considerable distance from the boundary. The relevant forces are short-range and determine the migration of impurities at the distances about ten lattice constants near the grain boundary. Let us determine the force using its projection on the axis chosen normal to the grain boundary from the expression [8]:

$$F(x) = \Theta(r_a - r_b)F_0 \exp\left(-kx\right), \tag{6}$$

where $\Theta(r_a - r_b)$ is the function that determines the sign of the projection and k is the coefficient determining the interaction between impurity atoms and a lattice defect.

The force is also determined by filling of electron shells of impurity atoms. In this respect if the total magnetic moment of an atom is equal to zero the impurity atom diffuses into the area of decreasing the magnetic field intensity. It is true for carbon and chrome atoms. As for paramagnetic atoms the diffusion is directed towards increasing the modulus of magnetic field intensity [6].

Analysis of relationship between diffusion process and values of magnetic pulse processing parameters. The experimental data indicate that diffusion of alloying elements is determined by the concentration of defects and the value of a magnetic field as well as by the pulse duration [9, 10]. The above-mentioned regularities are described within the frame of the suggested model.

In the process of pulse processing when impurity atoms move under the action of magnetic field forces the carbon and chrome atoms tend to escape from the grain volume and to move to its boundary. The near-boundary grain area is depleted of carbon and a carbide network formed around a ferrite grain leads to hardening of sample surface [11]. However, in this case the formation of a carbide network does not result in a significant increase of brittleness. This is caused by recrystallization processes that occur due to heat release. The most intensive heat release occurs at the grain boundaries owing to increase of specific resistivity [3, 11]. As a result of recrystallization the grain boundaries observed in a processing zone have ragged edges. This is indicative of a high adhesion existing between grain boundaries and carbide phase (Fig. 3).

In grains there are also volumetric defects, specifically, fragments the orientation of which differs from that of a crystal lattice of the main grain volume and this plays a significant role in formation of a fine-grained structure during pulse processing. Smaller elements of a mosaic structure such as blocks the disorientation of which is less than 1°, are not considered in this approximation. The grain sizes of Steel 45 are decreased up to the values of 2–7 μm during magnetic pulse hardening [12]. The formation of new boundaries inside a grain is associated with the processes of movement of impurities during diffusion as well as with their localization at boundary of fragments. This gives rise to the formation of areas where the concentration of impurities having dimensions that approximate the iron atom radius reaches the maximum value and this is what leads to separating of grains from each other (Fig. 3). These areas corresponding to new boundaries are not enriched in carbon.

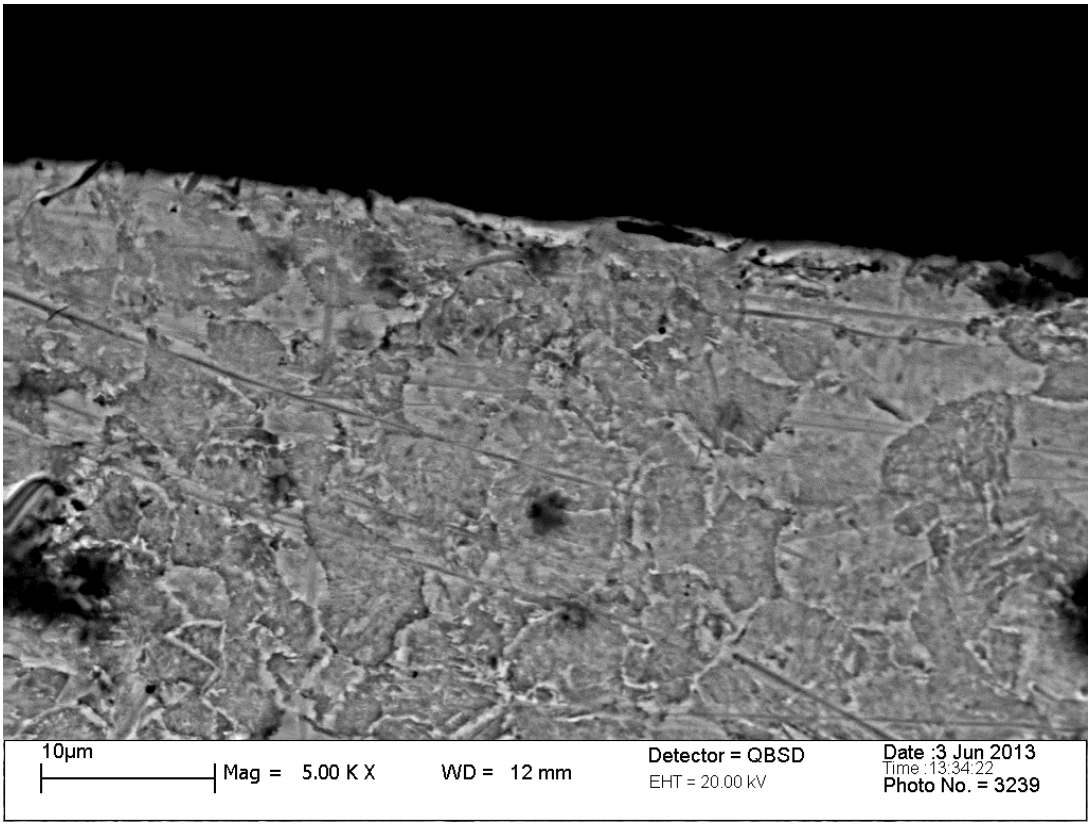

Fig. 3 *Formation of fine- grained structure on the surface of a sample made of Steel 45 during magnetic pulse hardening (2 pulses, 6 kJ)*

In the process of unsteady-state diffusion a significant role is played by the processes associated with fixation of dislocations that have been formed as a result of pulse loading by impurity atoms of greater radii (Mo, Ni and W). Their penetration/ in a rarefied area formed near an edge dislocation hinders further movement of this dislocation and results in direct hardening of the ferrite grain volume. The process also inhibits annihilation of unlike dislocations. This means that dislocations formed as a result of impulse are retained and their concentration reaches the values of 10^{15}–10^{16} м $^{-2}$. The mechanism of a hardening action is shown in Fig. 4.

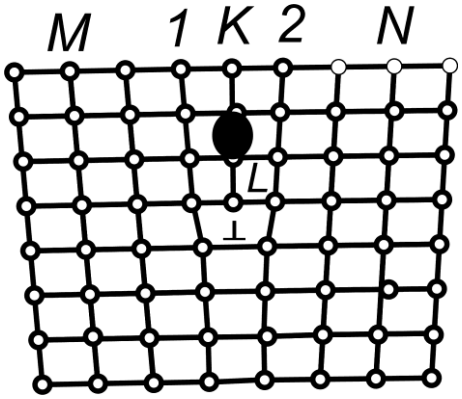

Fig. 4 *Interaction between dislocation and impurity atom.*

Conclusion

Having analyzed the relationship between hardening effects and energy pulses it is possible to deduce that the pulse energy equal to less than 2 kJ is insufficient for generation of a required quantity of defects. The significant effects are revealed in Steel 45, Steel X and Steel 8ХФ at the pulse energies of 4 kJ, 6 kJ and 6-8 kJ, respectively. The pulse energy exceeding 8 kJ gives rise to the formation of an excessive number of defects and can cause softening of a sample which is confirmed by the results described in the works [9, 10 and 12]. However, on redistribution of alloying elements the temperature of grain melting is changed which accounts for decreasing the effectiveness of subsequent pulses. Therefore, the most effective number of pulses is equal to the value of three.

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