The Influence of the Thermal Stress Upon Elements Redistribution in Steels by Means of Irradiation of Charged Particles Pulse Beams

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Abstracts – The article deals with the processes of elements redistribution in surface stratums of alloys. It should be stressed that these stratums are to be subjected to pulsing of irradiation by means of beams charged. Masstransfer model in alloys using pulsing irradiation on is considered here. This model involves elements distribution in the internal stress fields, temperature gradients and point defect concentration. This article presents the calculations of concentration profiles in elements distribution. It should be emphasized that we tend to evaluate the contribution of different mechanisms in elements redistribution. This investigation allows us to obtain of alloys vs. temperature gradients and vacancy gradients concentration and also vs. internal stress if taking into account pulsing irradiation.

1. Diffusion kinetics model according to vacancy mechanism while being irradiation by charged particles beams

As a result of pulsing irradiation we can observe a nonuniform sample heating; nonequilibrium point defects formation and the appearance of stress wave being propagated in the material. If to assume different types if irradiation, particles energy and current beam density, we can obtain three types of field stress: stress such as thermoelastic stresses; plastic deformation stresses and shock wave.

The following factors should be taken into calculation when derivation a kinetic diffusion equation (1): thermodiffusion, diffusion under the impact of point defect gradient, diffusion in stress field. The diffusion kinetic equation is based on random atoms springs. Thus the diffusion kinetic equation is obtained in this case. This article [1] describes the detailed equation deduction.

The first component reflects the concentration mechanism. The second in the equation (1) describes thermal diffusion flow. It should be outlined that this flow tends to the opposite direction against temperature gradient i.e. the more mobile component is stored at the cold end of the sample. The third term in the right hand column explains the process of redistribution of elements caused clue to nonuniform of nonequilibrium vacancies.

In this case the more mobile component should move from a surface sample. The fourth component reflects barrodiffuzion mechanism, under effect of the given mechanism the more mobile atoms travel in the direction of more intense state of a crystalline lattice

$$\frac{\partial c_B}{\partial t} = -\frac{\partial}{\partial x}\left[\tilde{D}\left[1+(\frac{P}{E})^2\right] + c_A c_B \frac{P}{EkT^2}\left(\frac{E_B D_B}{c_B}+\frac{E_A D_A}{c_A}\right)\right]\frac{\partial c_\mathrm{B}}{\partial x} +$$
$$+\frac{\partial}{\partial x}\left\{\frac{c_A c_B}{kT^2}(E_B D_B - E_A D_A)\left[2+(\frac{P}{E})^2\right]\frac{\partial T}{\partial x}\right\} +$$
$$\frac{\partial}{\partial x}\left\{\frac{c_A c_B}{c_V}(D_A - D_B)\left[1+(\frac{P}{E})^2\right]\frac{\partial c_V}{\partial x}\right\} +$$
$$\frac{\partial}{\partial x}\left\{\frac{Pb}{EkT^2}\frac{c_A c_B}{c_V}(4+(\frac{P}{E})^2)(E_B D_B - E_A D_A)\frac{\partial c_V}{\partial x}\frac{\partial T}{\partial x}\right\}, \qquad (1)$$

where C_A, C_B – is atoms concentration such A и B; $\tilde{D}$ – mutual diffusion coefficient, P – Internal stress in a material, E – modulus of elasticity, k – Boltzmann constant, T – temperature, D_A, D_B – coefficient of elements diffusion, E_A, E_B – energy of diffusion activation, c_V – vacancy concentration, b – lattice parameter.

2. Numerical analyze of concentration profile

The investigation of concentration elements redistribution according to the depth sample in metallic systems carried out by means of irradiation with the help of pulse electron beam with energy 500 keV, current density 1 kA/cm^2, impulse duration 2,5 microseconds.

It was conducted the calculations of temperature in the sample by means of electron irradiation. The distribution profile of wave stress for these calculations was taken the reference documentation [2].

Nickel and chrome concentration profiles results in iron matrix (Fig.1) are conducted according to equation (1).

Calculation results are conformed to obtained data for steel 12X18H10T, irradiated by electron bunch with energy 500 keV, current density 1 kA/cm^2, impulse length 2.5 μs.

On the basis of calculations the analysis of the influence of each mechanism (such as thermodiffusion, diffusion under the vacancy concentration gradient, barrodiffusion) against elements redistribution we developed our investigation. We managed to obtain that the dominant mechanism is considered to be masstransfer in stress field by means irradiation electron beams with energy 300–500 keV, current density 0,5–1 kA/cm^2 and microsecond pulse length. Calculations analyze show that for the appearing of the masstransfer observed it is necessary to create a considerable concentration of point defects in the material (up to 10^{-2} atomic part, at.p.). Almost the same concentration of point defects is activated by irradiation. Elements redistribution observed we can obtain by effecting of stress field and nonequilibrium point defects redistribution in assemblage.

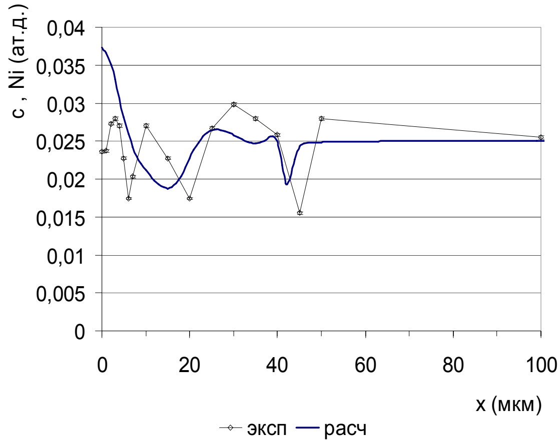

Fig. 1. Steel 12X18H10T. Nickel distribution after irradiation by electron beams with energy 500 keV, current density 1 kA/cm^2, length of impulse is 2.5 μs

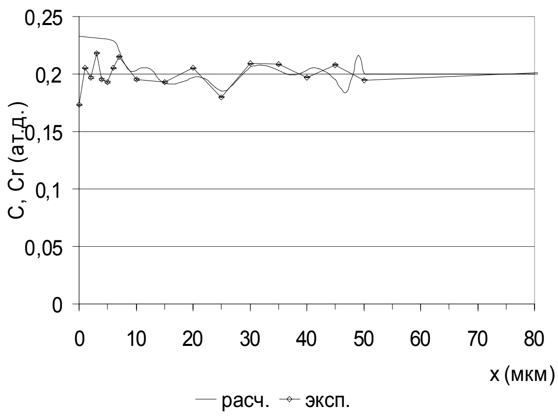

Fig. 2. Steel 12X18H10T. Chrome distribution after irradiation by electron beams with energy 500 keV, current density 1 kA/cm^2, impulse length 2.5 μs

The calculations of a doping elements flow in an iron matrix are carried out depending on major elements redistribution are made. Chrome flow induced by a temperature gradients demonstrate that when we have low values of a temperature gradient, there is a feeble impurity travel (Fig. 3). The flow makes up $3{,}46{\cdot}10^{-6}$ kg/m^{2}s at 10^4 K/m where the mean temperature of sample surface is 1000 K.

If we take low values of a temperature gradient we can notice that the mean temperature of sample surface does not effect flow increase chrome. It should be pointed out that the essential increase of impurity flow takes place at higher temperature gradient from 10^7 K/m up to 10^8 K/m. Such temperature gradients are characteristic for pulsing irradiation by ions beams. In our calculations we took the vacancy concentration gradient started equal 0, the vacancy concentration the whole depth a sample equal 10^{-4} at.p.

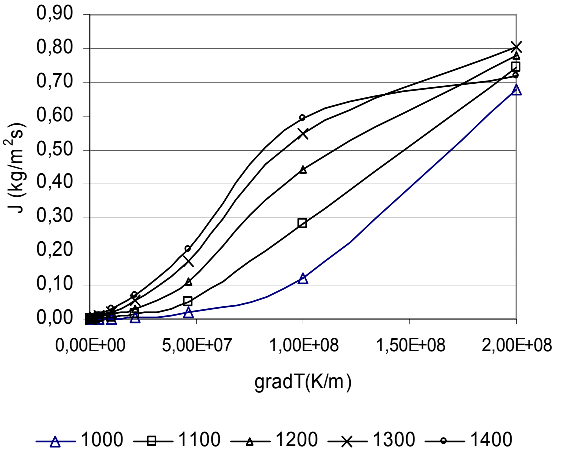

Fig. 3. Flow of a doping element in system Fe-Cr vs. temperature gradient

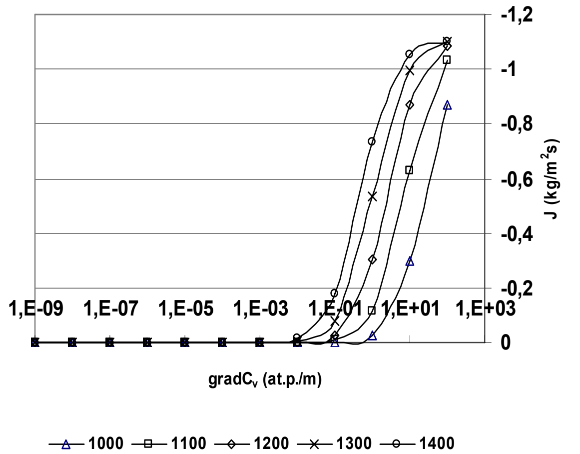

Fig. 4. Flow doping element in system Fe-V vs. vacancy concentration gradient

The second factor, which influences on upon impurity masstransfer, is associated with nonequilibrium vacancies distribution in sample depth. Vacancy concentration gradient can be charged in a range from 10^{-9} at.p/m till 10–20 at.p./m. on average.

The flow makes up $1{,}1{\cdot}10^{-5}$ kg/m^{2}s if we have low values of a vacancy concentration gradient that is 10^{-5} at.p./m and temperature 1400 K.

We can observe considerable impurity travel when the vacancy concentration gradient is more than 10^{-1} at.p./m (Fig. 4, 5). Similar dependence's are characteristic for doping elements.

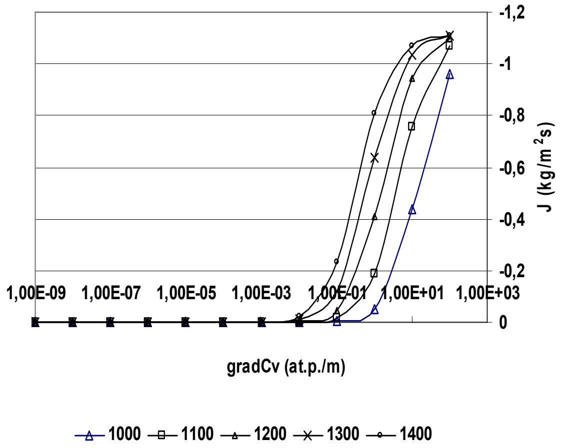

Fig. 5. The flow of doping element in system Fe-Cr vs. vacancy concentration gradient

The third factor is considered to be the internal stress with effects on mass transfer and appears in material by means pulsing irradiation. As the numerical analysis show if there are no temperature gradient and vacancy concentration gradient the flow of doping elements will be 10^{-6} kg / m^{2}s in total (sample temperature is 1000 K, vacancy concentration is 10^{-4} at. p.). I.e. the flow induced only by internal stress, does not experimentally mass transfer. But when temperature gradient is 10^3 K/m and vacancy concentration gradient is 10^{-1} at. p./m in this case impurity doping will rise up to 0,1 kg/m^{2}s.

Fig. 6 show current dependence against pressure value caused by pulse irradiation. The maximum flow which appears when using limiting pressure by means of pulse irradiation should not exceed 0,23 kg/m^{2}s. This flow is less, than the flow induced a temperature gradient and a vacancy concentration gradient.

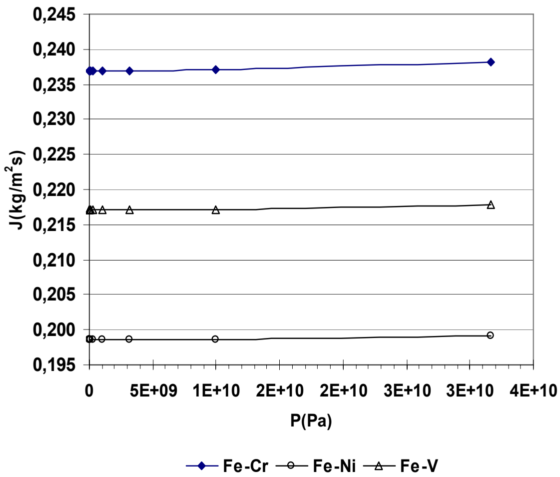

Fig. 6. The flow dependence of doping element in system on the basis of iron basis according to internal stress

The can observe the flow increase if this material has internal stress gradients (Fig. 7). As the results of computing demonstrate the flow increase is observed.

The pressure gradient is more than 10^{12} Pa/m, temperature also influence upon observed mass transfer (Fig. 7).

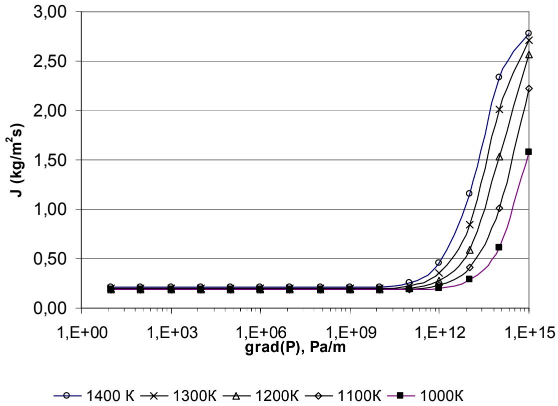

Fig. 7. Chrome flow dependence in the iron matrix vs. internal stress gradient taking into account various temperatures

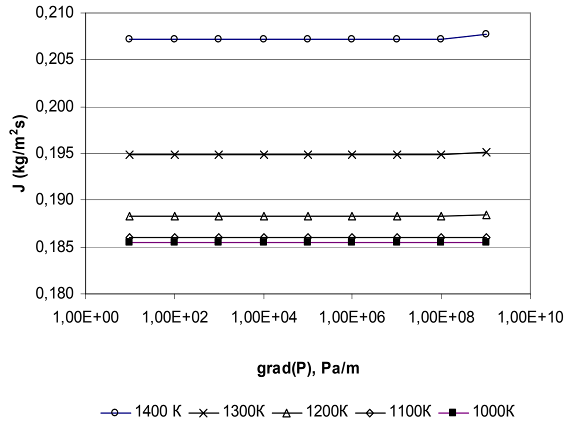

Fig. 8. Chrome flow dependence in iron matrix vs. internal stress gradient pressure (up to 10^{10} Pa/m) in accordance with various temperatures

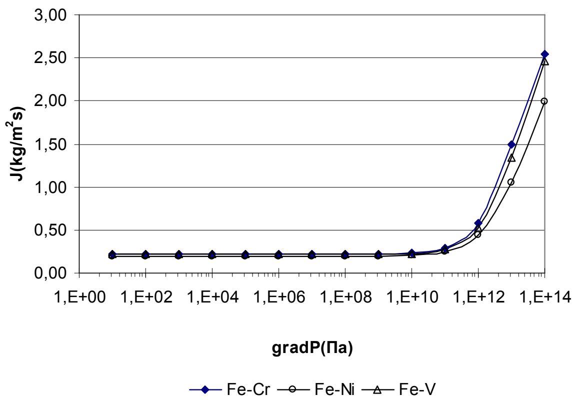

Fig. 9. Impurity flow dependence in the iron matrix vs. internal stress gradient

Dependence obtained for ferrum – chrome system can be considered for some other doping elements (Fig. 9).

Care should be taken that propagation of symmetric sine wave should not lead to masstransfer theoretically calculations according to the model indicate that the wave stress symmetric profile does not cause elements redistribution (Fig. 10).

The areas relation under stress wave profile was introduced for analyzing of the profile form influence on alloy components flow.

The areas relation was calculated concerning the part of stress wave profile with positive and negative gradients.

The computing results indicate that if increase profile asymmetric we can receive the increase of alloy components flow.

It should be emphasized that the definite mathematical dependence between wave profile and alloy components flow was discord. Hence we could suppose that stress wave of asymmetric form contribute elements distribution.

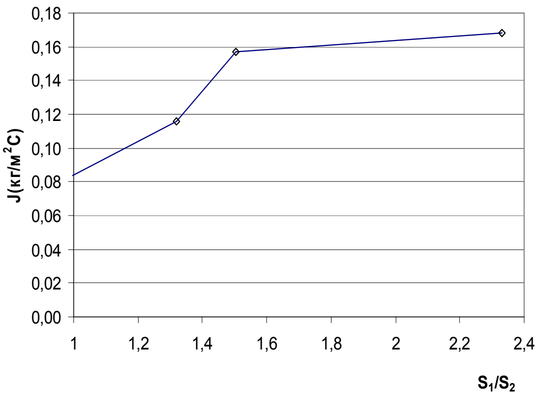

Fig. 10. The dependence of impurity flow vs. stress wave profile form propagating by means of pulse irradiation

3. Conclusion

Influence evaluation of different competitive mechanisms of mass transfer show that the maximum flow of alloys elements caused by temperature gradient under pulse irradiation by beams of charged particles is 0,8 kg/m²s, the maximum flow induced by vacancy concentration gradient is 1,1 kg/m²s. The maximum flow caused by pressure gradient which is 2,5 kg/m²s.

According to numerical analysis flow values cause by different mechanisms are close to each other. However, the flow caused by pressure gradient is maximum. The pressures gradient arising under materials irradiation plays the main role in elements distribution forming after irradiation

The equation analysis and calculations results demonstrates that the following factors should be taken into consideration to create masstransfer :

a) the presence of considerable concentration of point defects to provide vacancy and interstitial site diffusion mechanism.
b) high temperature of the sample for the diffusion process activation and as corollaries of the diffusion coefficient.
c) asymmetrical stress wave spanning out factor is in the material the last factor is predominant in the case where the flow in stress wave field is maximum. When irradiating by pulse beams flows the stress wave has an asymmetrical form therefore a noncompensated flow of atoms arises. It is stimulated by spatially time allocation pressure gradient.

References

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[2] G.A. Bleher, V.P. Krivobokov, O.V. Pashenko, *Heat-mass exchange in solid state by power beam of charged particles,* Novosibirsk. "Nauka", 1999.

[3] D.V. Postnikov, S.V. Plotnikov, V.A. Kuzminykh. "Components redistribution in alloys on the basis of iron at impulse irradiation". *12th International Conference on Radiation Physics and Chemistry of Inorganic Materials*, Tomsk, September 23–27, 2003, Russia.