

Mass Transfer at Impulse Exposure to Beam of Charged Particles

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Abstracts – This article regards the processes of elements mass transfer in the surface layers of alloys at impulse electron irradiation. The work contains experimental data on elements redistribution in the surface layers. It is also proposed a model of mass transfer in alloys at electron irradiation. The model describes admixture redistribution within the field of thermoelastic wave, and in the field of temperature gradients and point defects concentration. It was conducted calculations of concentration profiles and it was also estimated the effect of different mechanisms on elements redistribution.

Elements Redistribution at Exposure to Bunch of Electrons of Microsecond Duration (Experiment)

It was performed an investigation of elements redistribution in metallic systems after exposure to heavy-current electron bunch with energy 500 keV, current density 1 kA/cm², impulse duration 2.5 μs.

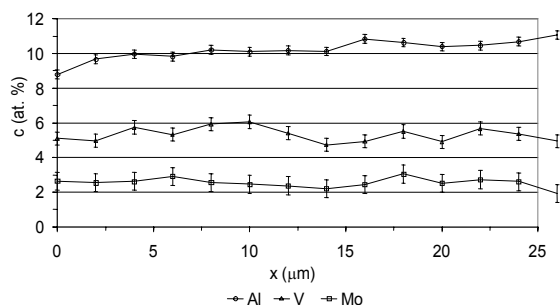


Fig. 1. BT22. Elements distribution after irradiation with electrons with $E = 500$ keV, current density 1 kA/cm², impulse duration 2.5 μs

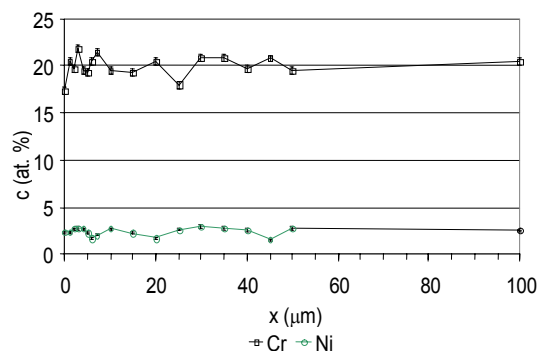


Fig. 2. Steel 12X18H10T. Elements distribution after irradiation with bunch of electrons with energy 500 keV, current density 1 kA/cm², impulse duration 2.5 μs

The results of the investigations show that the elements redistribution after irradiation is not uniform. Elements concentration local fluctuations have been observed. Thickness of the layer, in which the elements concentration is changed, is 0–50 μm (Figs. 1, 2).

Kinetic Model of Diffusion on Vacancy Mechanism at Exposure to Bunch of Charged Particles

Nonuniform heating of the sample, formation of disbalanced point defects and induction of stress wave spread in material all these effect occur at impulse irradiation. Different types of irradiation, particles energy and bunch current density may lead to induction of three types of stress fields: thermoelastic stresses, plastic deformation and a shock wave. This work regards only the thermoelastic stresses, which is, to our mind, normal when speaking on exposure to electron bunch with energy 300–500 keV, current density up to 1 kA/cm², impulse duration 1–3 μs.

The following factors are to be taken into account at formation of kinetic equation: thermal diffusion, diffusion influenced by point defect gradient and diffusion in stresses field of thermoelastic wave.

Let us consider three crystal lattice plane sections, which contain the atoms. These planes are perpendicular to the axis, along which the diffusion process is provided. There are alloy components concentration gradients, temperature gradient, vacancy concentration gradient and the pressure gradient along this axis.

It is supposed that the factors listed above are induced by some external effect, for example by irradiation.

Assume that as a result of outer effort, the crystal lattice will change its parameter. In case of stress wave transmission, the value of the lattice parameter, according to the sample depth, will be changed.

It is obvious that the number of atoms is always greater than vacancies. Therefore, the atom flux is determined by the number of vacancies. Let us consider the flux of component A in the direction of axis x . Take as the flux the component A atoms number change in plane 2 of unit area within a time unit. This change is connected with atom jumps from plane to plane. The number of component A atom jumps from plane i to plane j is calculated according to

$$n_{ij} = N_{Vj} \cdot \frac{N_{Ai}}{N_{Ai} + N_{Bi} + N_{Vi}} \Gamma_{ij} = N_{Vj} \cdot n_i \Gamma_{ij}, \quad (2)$$

where $n_i = \frac{N_{Ai}}{N_{Ai} + N_{Bi} + N_{Vi}}$ – component A atoms part in plane i .

It is acceptable to present an equation for flux J_A :

$$J_A = n_{12} + n_{23} - n_{21} - n_{32}. \quad (3)$$

Local concentration of vacancies in plane i is equal to $n_{Vi} = \frac{N_{Vi}}{b}$.

Concentrations in the neighboring planes are associated to each other with accuracy up to the terms of the first order of relatively small values using expansion in series:

$$\begin{cases} n_{V3} = n_{V2} + b_3 \frac{\partial n_V}{\partial x}; \\ n_{V1} = n_{V2} - b_1 \frac{\partial n_V}{\partial x}. \end{cases} \quad (4)$$

Put (4) to (3), marking $n_V = n_{V2}$, and obtain the following formula:

$$J_A = n_V (b_1 + b_3) \cdot [n_1 \Gamma_{12} + n_3 \Gamma_{32}] + n_2 \frac{\partial n_V}{\partial x} (b_3^2 \Gamma_{23} + b_1^2 \Gamma_{21}). \quad (5)$$

Expand in series the interplanar spacing of crystal lattice b_1 and b_2 regarding lattice parameter when non-strained b . Let us take two of the first terms of the order for expansion:

$$\begin{aligned} b_1 &= b - b \frac{\partial b}{\partial x}, \\ b_3 &= b + b \frac{\partial b}{\partial x}. \end{aligned} \quad (6)$$

Put (6) into (5), marking $\delta \Gamma = \Gamma_{12} - \Gamma_{32}$,

$$\begin{aligned} J_A &= 2nb^2 \left[\Gamma_0 \left(1 + \left(\frac{\partial b}{\partial x} \right)^2 \right) + \delta \Gamma \frac{\partial b}{\partial x} \right] \frac{\partial n_V}{\partial x} + \\ &+ b^3 \left(3 + \left(\frac{\partial b}{\partial x} \right)^2 \right) \frac{\partial \Gamma_0}{\partial x} \frac{\partial b}{\partial x} + \Gamma_{32} b^2 \left(1 - \frac{\partial b}{\partial x} \right)^2 \frac{\partial n_V}{\partial x} + \\ &+ bn_V (n_1 \Gamma_{12} - n_3 \Gamma_{32}) + b^3 \left(3 + \left(\frac{\partial b}{\partial x} \right)^2 \right). \end{aligned} \quad (7)$$

As a result of the performed mathematical transformations and change of micro parameters by diffusion factors and activation energy it was formed an equation for A component flux:

$$\begin{aligned} J_A &= D_A \left[1 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial c_A}{\partial x} + D_A c_A \frac{E_A}{kT^2} \left[2 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial T}{\partial x} + \\ &+ \frac{c_A}{c_V} D_A \left[1 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial c_V}{\partial x} + \\ &+ D_A \frac{E_A}{kT^2} b \left[\frac{c_A}{c_V} \frac{\partial c_V}{\partial x} \left(4 + \left(\frac{P}{E} \right)^2 \right) - \frac{\partial c_A}{\partial x} \right] \frac{\partial T}{\partial x} \frac{P}{E}. \end{aligned} \quad (8)$$

Consider the process of interdiffusion of two components. Crystal planes move with velocity

$$V_L = J_A + J_B. \quad (9)$$

B component flux relative to laboratory coordinate frame:

$$J'_B = J_B - c_B V_L. \quad (10)$$

Put (9) into (10):

$$J'_B = J_B - c_B J_A - c_B J_B. \quad (11)$$

Form equation for B component flux and mark as $\tilde{D} = D_B c_A + D_A c_B$:

$$\begin{aligned} J'_B &= -\tilde{D} \left[1 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial c_B}{\partial x} + \frac{c_A c_B}{kT^2} (E_B D_B - E_A D_A) \times \\ &\times \left[2 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial T}{\partial x} + \frac{c_A c_B}{c_V} (D_A - D_B) \left[1 + \left(\frac{P}{E} \right)^2 \right] \frac{\partial c_V}{\partial x}, \\ &+ \frac{Pb}{EkT^2} \left\{ \frac{c_A c_B}{c_V} \left(4 + \left(\frac{P}{E} \right)^2 \right) (E_B D_B - E_A D_A) \frac{\partial c_V}{\partial x} - \right. \\ &\left. - c_A c_B \left(\frac{E_B D_B}{c_B} + \frac{E_A D_A}{c_A} \right) \frac{\partial c_A}{\partial x} \right\}. \end{aligned} \quad (12)$$

Equation (12) is a B component flux in a binary system subject to diffusion concentrating mechanism, thermal diffusion, diffusion influenced by vacancy concentration gradient and barodiffusion.

Fist term describe concentration mechanism diffusion. Second term directed such a flux in the direction, opposite to temperature gradient, i.e. more active component is accumulated at the cold end of the sample. The third term in the right-hand member describes the process of elements redistribution, induced by heterogeneous thickness of disbalance vacancies. In this case a more active component is to move towards to the surface of the sample. The barodiffusion mechanism leads to transfer of more labile atoms towards to more stressed condition of crystal lattice.

Kinetic Model of Interstitial Diffusion at Exposure to Bunches of Charged Particles

The mass transfer of low-sized admixtures is dominantly performed per interstitial mechanism. To describe the mass transfer processes in systems with

low-sized admixtures (carbon, oxygen, nitrogen, hydrogen) at exposure to impulse bunches of electrons and ions it was obtained a kinetic equation for interstitial atoms in the temperature gradient field, and material internal stresses gradient.

At interstitial diffusion it is not needed a vacancy for atom transportation. In other respects the outcome is the same as one of kinetic equation for vacancy mechanism.

Let us examine four atomic planes of crystal lattice. There are interstitial atoms between the planes. Mark the planes of their location as Nos. 1, 2, 3. These planes are perpendicular to the axis, along which the flux of interstitial atoms is directed. There are alloy component concentration gradients, temperature gradient and stress gradient in crystal lattice, along this axis. The value of the stresses occurring in the material during irradiation is not uniform within the depth of the sample; therefore the interplanar spacing will differ.

Let us consider the flux of interstitial atoms A component in the direction of x axis. Take the change of atom number of A component in plane 2 of unit area and within a time unit. This change is due to atom jumps from plane to plane. Number of A component atom jumps from plane i to plane j is calculated using:

$$J_A = n_{12} + n_{23} - n_{21} - n_{32}. \quad (13)$$

Interplanar spacings of crystal lattice b_1 and b_2 are to be expanded in a series regarding the parameter of the lattice when it is not deformed b . Use two of the first terms in the order for expansion:

$$\begin{aligned} b_1 &= b \left(1 - \frac{\partial b}{\partial x} \right); \\ b_3 &= b \left(1 + \frac{\partial b}{\partial x} \right). \end{aligned} \quad (14)$$

The equation for A component flux (7) is as follows:

$$J_A = n_1 \Gamma_{12} + n_2 \Gamma_{12} + 2n_2 b \frac{\partial \Gamma_0}{\partial x} - n_2 \Gamma_{32} - n_3 \Gamma_{32}. \quad (15)$$

Apply the same procedure for A component concentrations in different planes, binding them to each other:

$$\begin{aligned} n_3 &= n_2 + b_3 \frac{\partial n_2}{\partial x}; \\ n_1 &= n_2 - b_1 \frac{\partial n_2}{\partial x}. \end{aligned} \quad (16)$$

Then the equation for the flux is as follows:

$$\begin{aligned} J_A &= 2c_A b^2 v_A \frac{E_A}{kT^2} e^{-\frac{E_A}{kT}} \frac{\partial T}{\partial x} + 2c_A b^2 v_A \frac{E_A}{kT^2} e^{-\frac{E_A}{kT}} \frac{\partial T}{\partial x} - \\ &- 2v_A \frac{E_A}{kT^2} e^{-\frac{E_A}{kT}} b^2 \frac{\partial c_A}{\partial x} + 2v_A \frac{E_A}{kT^2} e^{-\frac{E_A}{kT}} b^3 \frac{\partial c_A}{\partial x} \frac{\partial b}{\partial x} \frac{\partial T}{\partial x}. \end{aligned} \quad (17)$$

Express the diffusion factor using microparameters:

$$D_A = D_{0A} e^{-\frac{E_A}{kT}}. \quad (18)$$

Replace the lattice parameter change with macro-characteristics

$$\frac{\partial b}{\partial x} = \varepsilon = \frac{P}{E}, \quad (19)$$

where ε – relative deformation, P – pressure or internal stresses, E – Young's modulus.

Use equation (18, 19) and put down equation (17):

$$J_A = D_A \frac{\partial c_A}{\partial x} + D_A \frac{E_A}{kT^2} \left[2c_A + b \frac{P}{E} \frac{\partial c_A}{\partial x} \right] \frac{\partial T}{\partial x}. \quad (20)$$

Let us study the process of interdiffusion of two components. The crystal planes move with velocity

$$V_L = J_A + J_B. \quad (21)$$

The equation for the B component flux is formed similarly.

The admixture flux is difficult to be used for admixture redistribution analysis that is why we take the concentration derivative on time. Then equation (20) will be as follows:

$$\begin{aligned} \frac{\partial c_A}{\partial x} &= \frac{\partial}{\partial x} D_B \frac{\partial c_A}{\partial x} - \frac{\partial}{\partial x} c_A \left[D_B \frac{\partial c_B}{\partial x} + D_A \frac{\partial c_A}{\partial x} \right] + \\ &+ \frac{\partial}{\partial x} \frac{2c_B c_A}{kT^2} \left[\frac{D_B E_B}{c_B} - \frac{c_B D_B E_B}{c_A} - D_A E_A \right] \frac{\partial T}{\partial x} + \\ &+ \frac{\partial}{\partial x} \frac{b}{kT^2} \frac{P}{E} \left[D_B E_B - c_B (D_B E_B + D_A E_A) \right] \frac{\partial T}{\partial x}, \end{aligned} \quad (22)$$

The two first addends describe the concentration mechanism. The second addend represents a flux, induced by thermal diffusion. This flux is moves in the direction opposite to the temperature gradient, i.e. more active component is accumulated at the cold end of the sample.

The third addend in the right-hand member describes the process of elements redistribution induced by the stresses in the material. In this case the interstitial atoms will move from a more stressed region to a less stressed one.

Results of Concentration Profiles Calculation

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

Nickel and chrome concentration profiles results in iron matrix (Figs. 3, 4) are conducted according to equation (12).

Calculation results are conformed to obtained data for steel 12X18H10T, irradiated by electron bunch

with energy 500 keV, current density 1 kA/cm², impulse length 2.5 μs.

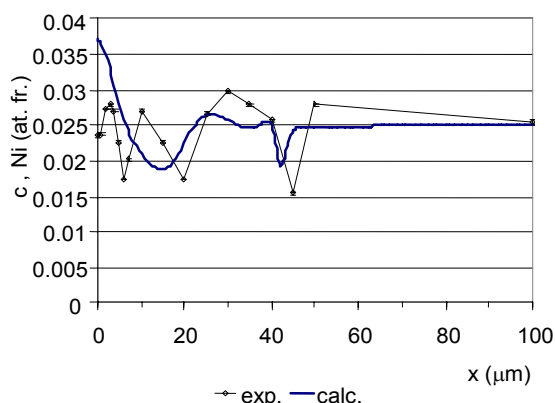


Fig. 3. Steel 12X18H10T. Nickel distribution after electrode bunch irradiation with energy 500 keV, current density 1 kA/cm², impulse length 2.5 μs

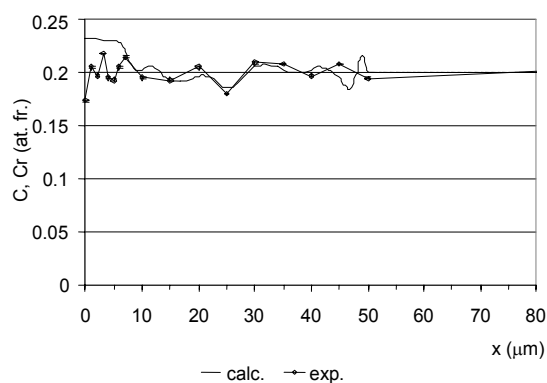


Fig. 4. Steel 12X18H10T. Chrome distribution after irradiation by electron bunch with energy 500 keV, current density 1 kA/cm², impulse length 2.5 μs

An impact analysis was carried out on the basis of calculations of each diffusion mechanism (thermodiffusion, diffusion under vacancy concentration gradient, barodiffusion) for elements redistribution. Predominant mechanism is mass transfer to stress field at irradiation by electrodes bunches with energy 300–500 keV, current density 0.5–1 kA/cm², and impulse of 2.5 μs length. However, it is necessary to create significant concentration of point defects (up to 10–2 atomic fractions) for observed mass transfer appearance according to calculations. Irradiation provides the same point defects concentration. Observed

element redistribution is possible under influence of stress fields and point defects disbalanced distribution in the aggregate.

Discussion of Result

The analysis of an equation and result of calculations demonstrate that for created mass transfer the availability of the following factors is necessary: a) availability of considerable concentration of point defects for maintenance vacancy and interstitial atom of the diffusion gear; b) of a heat of a sample for an activation of process of diffusion c) asymmetric stresses wave distributing in a stuff. Last factor is prevailing, so the flow in a field of a surge of pressure is maximum. In case of irradiation by pulse energy flows the thermoelastic pressure wave has the asymmetrical form, therefore there is a uncompensated flow of atoms conditioned spatially temporary distribution of a pressure gradient.

Conclusions

1. Element segregation in metallic systems occurs in the result of high-current electron bunch irradiation. The area, in which element segregation takes place, is 0–50 μm.

2. Kinetic diffusion models on vacancy and interstitial mechanisms were designed at high-current electrode bunch irradiation. The models take into account diffusion concentration mechanism, diffusion under vacancy concentration gradient influence, thermo diffusion, and barodiffusion.

3. The predominant mass transfer mechanism of alloy components at irradiation by electron bunch with energy 400–500 keV, current density 0.5–1 kA/cm², microsecond length is stresses wave in material.

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.