Mass Transfer in Metal Materials under High-Energy Irradiation

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Abstract – The physicomathematical model of mass transfer in metal materials under high-energy irradiation is proposed. This model is taken into account the volume and migrating grain boundary diffusion.

1. Introduction

One of the reasons of the change surface properties of materials under the action of concentrated energy flow is an atom migration. Under certain conditions of the surface treatment of metal materials the value of the efficient coefficient diffusion can prove to be on 2–3 orders more than in liquid state [1]. The unambiguous explanation of the specified phenomenon is absent in literature. In given work for interpreting of observed anomalous mass transfer is taken into account migrating grain boundary diffusion [2].

2. Mass transfer under ion implantation

In the case of continuous ion beam irradiation of metal materials (ion implantation), when migrating grain boundaries possible consider independent ("kinetics of the type B" [3]) i.e. when performing the condition $\sqrt{Dt}+Vt<d$ (where D – volume diffusion coefficient, V – average velocity of grain boundary migration, d – average size of grains, t – time of the irradiation), concentration profile along the axis y, perpendicular to irradiated surface, can be presented in the form of [3]:

$$C(y,t) = n_p c_p(y,t) + n_0 c(y,t)\big|_{V=0} + n_d c(y,t)\big|_{V\neq 0}, \quad (1)$$

where $c_p(y,t)$ describes the direct volume diffusion from irradiated surface, $c(y,t)|_{V=0}$, $c(y,t)|_{V\neq 0}$ – diffusion on sessile and migrating grain boundaries, accordingly; n_p, n_0, n_d – define the share of contribution to concentration profile of specified mechanisms.

The calculated total concentration profile of argon ions in monocrystal tungsten and measured (points) after ion bombardment with energy 15 keV and dose $7\cdot10^{19}$ ion/cm^2 are represented in Fig.1. The best possible agreement of model calculations with experiment at great depth is reached under n_p=80 %, n_0=5 %, n_d=15 % and average velocity of grain boundary migration $2.09\cdot10^{-7}$ cm/s. The intragranular diffusion coefficient relied on equal $1.5\cdot10^{-14}$ cm^2/s, the diffusion coefficient in the subboundary – $500\cdot D$, the sample temperature formed 300 K, the duration of the implantation of argon ions in tungsten – 30 minutes. The half-width of the subboundary was chose $\delta=9.75\cdot10^{-7}$ cm. Thereby as a result of migrating grain boundary diffusion implanted atoms can penetrate into irradiated material into depth much greater than the ion projected range.

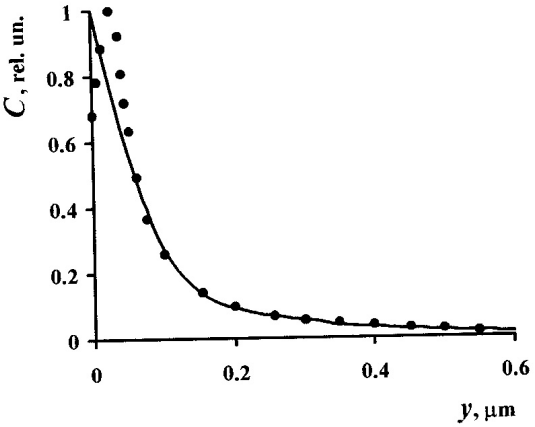


Fig. 1. Concentration profiles of argon ions in tungsten [4]

3. Mass transfer under pulsed influences

The processes of mass transfer under pulsed influence on metal systems are possible to describe as follows. On initial stage, when density extensive defects is small, but migrating grain boundaries possible consider independent ("kinetics of the type B"), impurity atoms diffuse on low-defective volume of the material under the action of the concentration, temperature and pressure gradients (volume diffusion) and insulated grain boundary diffusion. We will enter for description of these processes the two diffusion coefficients: D – volume diffusion coefficient and D_1 – grain boundary diffusion coefficient (moreover $D_1>>D$). The concentration profile of impurity atoms in grain will define by the amount of specified contributions. In the course of time in irradiated material with increase of density defects the number of points fastening grows and they become practically sessile. Herewith the fields of volume diffusion begin to be overlaying from the nearby grain boundaries so their already it is impossible consider as independent ("kinetics of the type A" [5]). For description of mass transfer in this case we will enter the efficient coeffi-

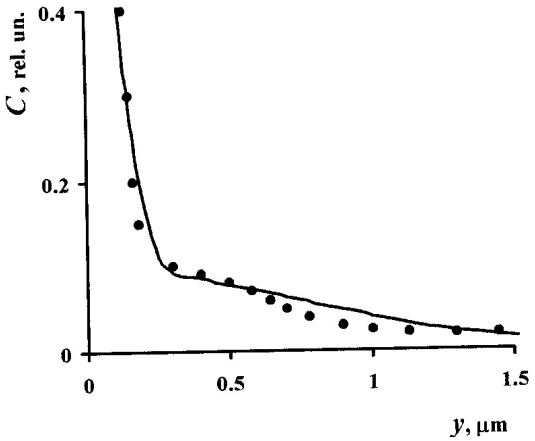
cient diffusion $D_{ef}=sD_1+(1-s)D$, where s – share of atoms of diffuse element, residing in grain boundaries (or in dislocations). Thereby, concentration profile of diffuse atoms possible to present in the form of:

$$C(y,t)=n_p c_p(y,t,D)+$$
$$+n_d c(y,t,D,D_1)+n_s c_s(y,t,D_{ef}), \quad (2)$$

where $c_p(y,t,D)$ and $c_s(y,t,D_{ef})$ – correspond the contribution of diffusion from processed surfaces on non-defective volume of the material with diffusion coefficient D and on high-defective with D_{ef}, accordingly (their type with regard to thermo- and pressure diffusion can be determined by algorithm described in work [5]); $c(y,t,D,D_1)$ – contribution of diffusion on migrating (with velocity V) grain boundaries (it is possible to neglect by contribution of diffusion on insulated grain boundaries [2]). The multipliers n_p, n_0, n_d and n_s define the contribution to concentration profile of specified mechanisms.

Under impulse action the irradiated material can be melted and be vaporized. Then it is taken into account diffusion in fluid phase with coefficient during corresponding time period. After completion of the pulsed influence the sample cools with very high velocity (for instance, order 10^9 K/s under ion irradiation) so defects in it practically does not have time to be annealed and impurity atom diffusion runs in high-defective solidified material (with diffusion coefficient D_{ef}). Consequently, under the repeated influences the generated elastic waves, getting through sample, turn out to be already not capable to bring about such restructuring as under the first influence. Contribution to the total concentration profile of the migrating extended defect diffusion decreases with increase of number of pulsed influences.

The model concentration profile of silver in copper is compared with experiment [6] in Fig. 2 under irradiation of Ag-film by thickness 0.1 μm on Cu-substrate by one pulse of the high-power carbon ion beam with energy 0,5 MeV, duration of the pulse 200 ns and density of the current 40 A/cm^2. Under such mode of the irradiation the sample is melted before depth approximately 1 μm, the boiling temperature is not reached. At modeling were used the following values of diffusion coefficient: $D=10^{-9}$ m^2/s, $D_1=3000D$, $D_l=50D$. The best possible agreement with experiment is reached at assumption that before melting $n_p=0.5$, $n_d=0.1$, $n_s=0.4$. At modeling of the frequentative pulsed influences the each newly received concentration profile is serveed by the initial distribution for the following influences. The model concentration profiles of silver in copper are got with provision for spraying the surface after 5 and 15 pulses (the migrating grain boundary diffusion under the repeated influences can be disregarding) are presented in Fig. 3. For simplification of the calculations under frequentative influences the space-temporary temperature field was described by step-like function Hevisayda $T(y,t)=T_0\theta(V_T t-y)$, where $T_0=900$ K – temperature of sample, $V_T=100$ m/s – velocity of the propagation of heat disturbances. The presented results and called calculations are showing that long range (before depths greater of thickness of the melted layer) "tails" of concentration profiles are formed to account of the migrating extended defect diffusion, basically else before of the melting of the material. The supplementary contribution to the matter transfer the thermal diffusion makes. It causes the observed after frequentative pulsed influence the irregularities of the concentration profiles.



Fis. 2. Concentration profiles of silver in copper under one-shot influence pulse of high-power carbon ion beam. The points correspond the experimental data [6]

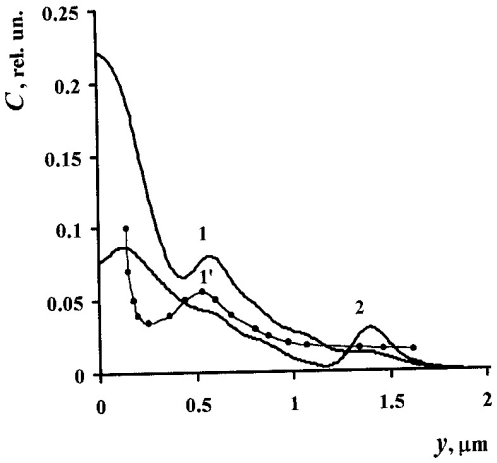


Fig. 3. Concentration profiles of silver in copper under five (the curves 1, 1') and fifteen (the curve 2) pulses of high-power carbon ion beam. The points correspond the experimental data [6]

The described model of the mass transfer can be applying not only for calculation of the atom redistribution under charged particle beam irradiation, but also under the other types of energy influence on surface of metal materials. For instance, concentration profiles of the distribution of marked iron atoms in iron sample after one-shot pulsed shock compression at room temperature are brought in Fig. 4, *a* [7].

Called on within the framework of above described model the calculations of concentration profiles well agree with experiment under the following values of diffusion coefficient: $D=5\cdot10^{-8}$ cm^2/s, $D_{ef}=350D$, $D_1=4000D$ and at suggestion that $n_p=65$ %, $n_s=28$ % $n_d=7$ %. After one-shot pulsed shock compression in the iron sample is formed many extended defects. So considering that under the repeated influences (at 300 K) extended defects were practically still and supposing that $n_p=65$ %, $n_s=35$ % the good agreement of theory with experiment is also got (Fig. 4, *b*).

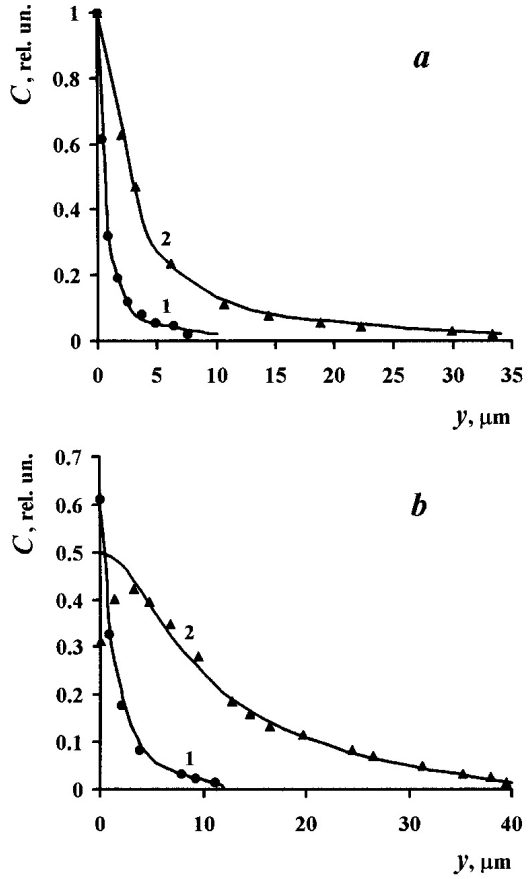


Fig. 4. Concentration profiles of the distribution of marked iron atoms in iron sample after a – one-shot, b – a three-shot pulsed shock compression at the temperature: 1 – 300 K, 2 – 973 K. Points correspond the experimental data [7]

The situation gradually changes with increasing of the temperature of the processed sample. As follows, extended defects become more mobile with growing of the temperature and are easier reforming at the process of the treatment (including repeated), as well can be partly annealed. So after three-shot influence pulsed shock compression at the temperature 973 K the depth of the penetration marked atom becomes more in contrast with one-shot influence (refer to Fig. 4, *b*), what does not exist at the temperature 300 K (Fig. 4, *a*). The calculation of concentration curves at the temperature 973 K (submitted in Fig. 4, *b*) were conducted by the following of diffusion coefficient: $D'=600D$, $D_{ef}'=17D_{ef}$, $D_1'=9D_1$ and $n_p=65$ %, $n_s=25$ % $n_d=10$ % – after the first influence, $n_p=65$ %, $n_s=30$ % $n_d=5$ % – after the second influence, $n_p=65$ %, $n_s=33$ % $n_d=2$ % – after the third influence.

Thereby, mass transfer of diffuse atoms into the great substrate depths under mechanical pulsed influences also can be realized mainly to account of the increase of their mobilities on migrating grain boundaries, dislocations and other extended defects.

4. Mass transfer in field of the shock wave

With the purpose of studies of the possibility of the entrainment of the interstitial atoms by shock wave front into metal sample in calculations of the concentration profile was taken into account the atom flow, given by shock wave. Space-temporary field of the stress in this case was described soliton pulse. The made calculations have shown that the essential effect of the entrainment of interstitial atoms by shock wave front into the metal sample can occur if the gradient of the pressure in the front is more then 10^9 GPa/m. In real materials under usually used parameter of the processing surface by pulsed ion beam such great gradients of the pressure do not exist. However under the determined pulsed mode of the irradiation (mainly, under very high density of the current 100 kA/cm^2) the generated shock waves, as well as thermoelastic stresses, really can turn out to be capable to lead away the film atoms into substrate into essential depth.

5. Conclusion

Mass transfer in metal materials under high-energy irradiation is stipulated by the increase of atom mobilities on migrating grain boundaries, dislocations and other extended defects.

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