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Method for Determining the Diffusion and Drift Components of Anomalous Mass Transfer in Metals under External Influences

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Within the framework of this investigation based on experimental data, the approach to determine the process parameters of anomalous mass transfer in solid state using isotopic technique under external influences is developed. This approach is used to determine the process parameters of mass transfer in high-entropy alloys (HEA) AlFeNiCoCuCr and steel S235 (analogue of steel 3) after electric-spark alloying and subsequent impact treatment. Radioactive ^{60}Co isotope is used as indicator of mass transfer process. As shown in this work using the developed method, the predominant mechanism of mass transfer in condition of electric-spark alloying and mechanical impact is the directed movement of atoms carried away by mobile dislocations in S235 and HEA. Calculating the mean and root-mean-square displacements of atoms, the force acting on each atom and the mobility of ^{60}Co atoms in S235 under mechanical-impact processing are determined. As shown, the Einstein–Smoluchowski equation may be used to determine the atoms mobility under external influences and the process of anomalous mass transfer, if D_T to replace by D_{ef} .

Key words: anomalous mass transfer, radioactive ^{60}Co isotope, atoms mobility, external influence, high-entropy alloys, steel S235.

В рамках даного дослідження на основі експериментальних даних розроб-

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лено підхід для визначення параметрів процесу аномального масоперенесення у твердих тілах з використанням методу радіоактивних ізотопів за умов зовнішніх впливів. Даний підхід використано для визначення параметрів процесу масоперенесення у високоентропійних стопах (ВЕС) AlFeNiCoCuCr і криці S235 (аналог криці 3) після електроіскрового легування та подальшого ударного оброблення. Як індикатор масоперенесення, використовували радіоактивний ізотоп ^{60}Co . За допомогою розробленої в даній роботі методики показано, що переважним механізмом масоперенесення в умовах електроіскрового легування та механічного удару в S235 і ВЕС є спрямований рух атомів, що захоплюються рухомими дислокаціями. Розрахунком середнього та середньоквадратичного зміщень атомів визначено силу, що діє на кожен атом, і рухливість атомів ^{60}Co в S235 в умовах механічного ударного впливу. Показано також, що рівняння Айнштайна–Смолуховського можна використовувати для визначення рухливості атомів в умовах зовнішніх впливів і процесу аномального масоперенесення, якщо зробити заміну D_T на D_{ef} .

Ключові слова: аномальне масоперенесення, радіоактивний ізотоп ^{60}Co , рухливість атомів, зовнішній вплив, високоентропійні стопи, криця S235.

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1. INTRODUCTION

The study of the diffusion mechanism features, mass transfer and structural changes under external influences is one of the main fundamental problems in solid-state physics. In scientific works [1, 2], the theoretical approaches to determining the diffusion parameters and anomalous diffusion are described.

1.1. Definition of Anomalous Mass Transfer and Anomalous Diffusion

The phenomenon of tracer atoms penetration to macroscopic depths (tens and hundreds of microns) in solids in an extremely short time compared to ordinary diffusion, called ‘anomalous mass transfer’, was discovered in the study of processes occurring in metals under pulsed vacuum welding conditions [3–5]. The mass transfer was called ‘anomalous’ due to the fact that under conditions of high-speed plastic deformation of crystalline solids (deformation rate $\varepsilon' > 1 \text{ s}^{-1}$), the migration rate of self and impurity atoms in them exceeds by several orders of magnitude the rate of stationary diffusion mass transfer and diffusion in the liquid phase [4]. The term ‘accelerated non-stationary mass transfer’ is also used for this phenomenon. Usually, diffusion obeys the central limit theorem [6], which implies that the sum of random jumps of atoms will approach a stable distribution that has the same shape as a normal distribution (according to Gauss):

$$\rho_N(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}. \quad (1)$$

There is a term ‘anomalous diffusion’ when the probability distribution profile (which has a normal Gaussian form) according to the central limit theorem is violated, as well as the usual laws of Brownian motion following from this theorem [1, 6]. The anomalous diffusion behaviour manifest in Eq. (2) is intimately connected with the breakdown of the central limit theorem (3), caused by either broad distributions or long-range correlations. Anomalous diffusion is found in a wide diversity of systems, its hallmark being the non-linear growth of the mean squared displacement in the course of time [2]:

$$\langle x^2(t) \rangle \sim D_\alpha t^\alpha, [D_\alpha] = \text{cm}^2 \text{s}^{-\alpha}, \quad (2)$$

$$\langle x^2(t) \rangle \sim D_1 t, [D_1] = \text{cm}^2 \text{s}^{-1}. \quad (3)$$

According to the value of the anomalous diffusion exponent α , defined in Eq. (2), one usually distinguishes several domains of anomalous transport, as shown in Fig. 1.

The Cauchy distribution has no moments (they are infinite), but it is a stable distribution:

$$\rho_c(x) = \frac{1}{\pi} \frac{1}{x^2 + 1}. \quad (4)$$

It does have a well-defined full width half maximum. The Cauchy distribution is also known as a Lorenz distribution. Therefore, there is no first moment (mean) even though the function is symmetrical about $x=0$. Likewise, the variance is infinite. This distribution has tails (Fig. 2).

The consequences of violating the central limit theorem are that tails dominate eventually in a sum of randomly generated variables. The

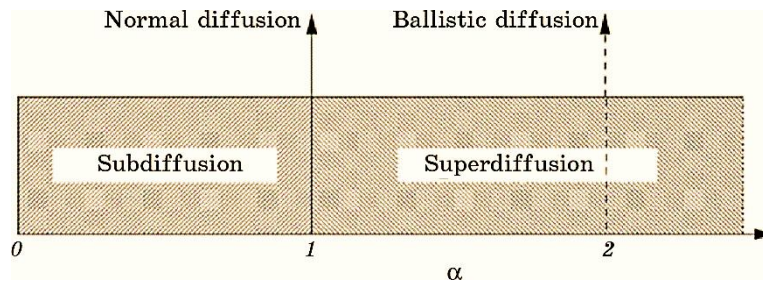


Fig. 1. Different domains of anomalous diffusion, defined through the mean squared displacement, equation (2), parametrized by the anomalous diffusion exponent α : subdiffusion for $0 < \alpha < 1$, normal Brownian diffusion $\alpha = 1$, superdiffusion for $\alpha > 1$. Another special case is ballistic motion $\alpha = 2$ [2].

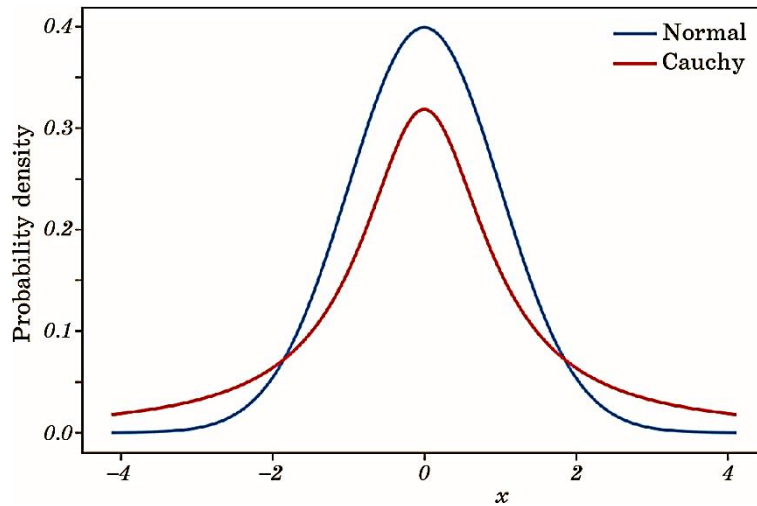


Fig. 2. A comparison of the shape of the normal (1) and Cauchy distributions (4) [6].

standard deviation of a distribution of random walkers increases limitless. A random walker obeys something like a Cauchy distribution if every once in a while, the walker takes a big jump. Moreover, every once in a longer time, the walker takes even bigger jump and so on in a self-similar (fractal) or power law form. This parameter leads to superdiffusion.

If jumps are made, on the contrary, from time to time, with stops, which each time become even longer in time, then, this leads to the phenomenon of subdiffusion (Fig. 3) and is related to a phenomena called intermittency that is sometimes seen in chaotic dynamical systems [2].

That way, the graphical representation $\rho(x, t)$ for the subdiffusive case $\alpha = 1/2$ is obtained, which is displayed in Fig. 3. In comparison to the standard Gaussian result, shown in Fig. 4, the pronounced cusps of the subdiffusive propagator are distinct.

1.2. Formulation of the Problem

The currently existing theoretical approaches consider the effect of the length of the atom jump and the duration of stops and are based on the dependence of the concentration distribution on time. In contrast, the experiment contains data on the distribution of concentration as function from depth.

In this paper, it is proposed a method for determining the parameters of diffusion and mass transfer based on experimental data on the distribution of concentration over depth, which does not require studying the time dependence. In addition, the method makes it possible to

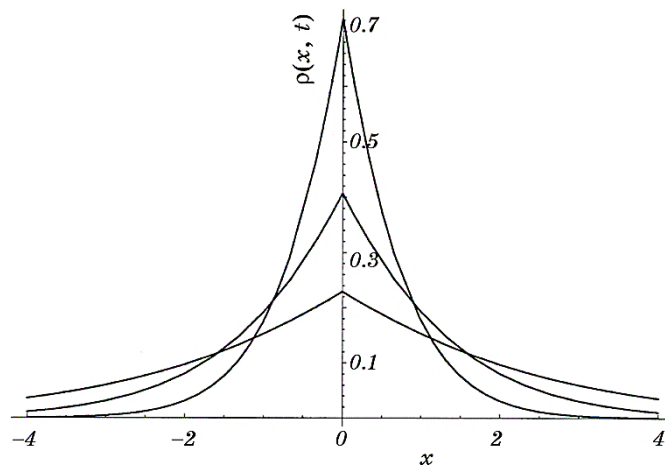


Fig. 3. $\rho(x, t) = (4D_\alpha t^\alpha)^{-1/2} \sum_{n=0}^{\infty} (-1)^n (n! \Gamma(1 - \alpha(n + 1) / 2))^{-1} (x^2 / D_\alpha t^\alpha)^{n/2}$ as a form of the probability distribution function for subdiffusion with the parametric exponent of anomalous diffusion $\alpha = 1/2$, drawn for the consecutive times $t = 0.1, 1, 10$. The graph is characterized by the cusp shape [2].

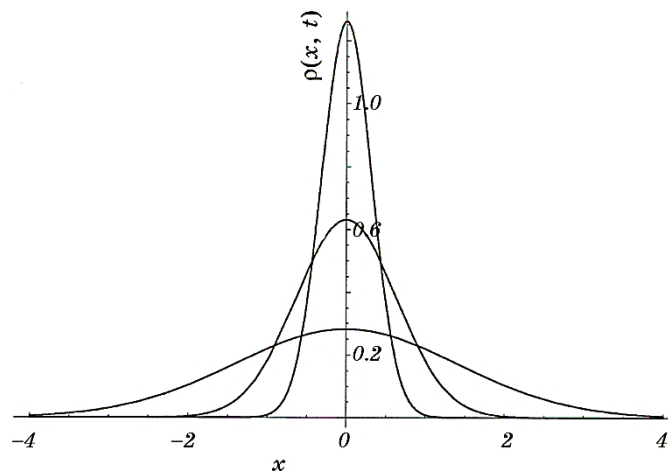


Fig. 4. Form of the probability distribution function $\rho_N(x, t)$ for Brownian diffusion $\alpha = 1$ for the times $t = 0.05, 0.2, 1$. The much smoother shape close to the origin sets this solution apart from the subdiffusive counterpart drawn in Fig. 3 [2].

determine the contribution of the driving force due to external action, and thereby distinguish the diffusion component and the drift contribution to the total mass transfer.

To achieve this purpose, the following tasks were solved in the work.

1. A method for calculating the effective diffusion coefficient (mass transfer) is proposed, taking into account the diffusion component and directional motion under the action of a driving force.
2. The diffusion coefficients and the average rate of atomic migration for different materials are compared.
3. The contribution of each of the different types of influences to the mass transfer process during complex processing is highlighted.
4. On the basis of the data obtained, conclusions were drawn about the mechanisms of mass transfer.

2. EXPERIMENTAL AND THEORETICAL DETAILS

2.1. Description of Materials

The following materials were selected as research materials: widely used S235 steel (analogue of steel 3) with a b.c.c. structure and a challenging high-entropy alloy (HEA) AlFeNiCoCuCr with a mainly b.c.c. structure, the diffusion processes in which are noticeably lower compared to diffusion in its components [7].

The samples were a steel cylinder 10 mm high and 10 mm in diameter with an electrolytically deposited layer of the radioactive ^{60}Co isotope 0.3–0.5 μm thickness. A layer of high-entropy AlFeNiCoCuCr alloy 30 μm thick was deposited onto the isotope layer by electrospark alloying (ESA) under the following conditions: current strength $I = 2.2$ A, processing time $\tau = 120$ s and 180 s, respectively. The operating frequency was 50 Hz. The standard industrial plant ‘ELTRON-22’ was used for the formation of electrospark coatings.

The next type of external influence on the samples was impact treatment with a load of $m = 10.5$ kg falling from a height $h = 1$ m.

To obtain the concentration distribution of ^{60}Co isotope, the autoradiography and layer-by-layer removal techniques were used [8, 9].

3. RESULTS AND DISCUSSION

3.1. Diffusion and Mass Transfer Parameters in S235 and HEA after Electric-Spark Alloying

To determine the time t , the diffusion calculation takes into account the electric-spark alloying (ESA) processing frequency, which is 50 Hz. The duration of one contact of the tip of the electrode with the treated surface is of 0.01 s and 0.01 s cooling between touches. The radius of the spot formed by the transferred drop of cathode material on the surface of S235 is of 0.35 mm. Taking into account the thermal

conductivity of steel b , the depth of the heated layer is $z = 2(bt)^{1/2} = 0.5$ mm. Using these data, it is possible to estimate that the cooling time of sample surface to $0.7T_{\text{melt}}$ is of $\cong 0.015$ s. It takes about 30–50 pulses to form one spot. The time between pulses can be neglected from the point of view of the influence on the temperature since the heated volume in the intervals between pulses does not have time to cool below $0.7T_{\text{melt}}$ before the next pulse. Thus, the exposure time of a thermal pulse for the formation of one spot during ESA is

$$t = \tau / N = 1.2 \text{ s.} \quad (5)$$

where N is equal to 100, the number of spots with an alloying substance on the surface of the sample, τ is equal to 120 s, the overall time of processing the surface of the sample.

The application of the random walks theory to the diffusion of ^{60}Co atoms as a result of ESA leads to equations analogous to the first and second Fick's laws, who adapted the heat conduction equations derived by Fourier [10]. If we take into account that the source of the diffusing substance consists of a finite amount of impurity, then, the solution of the second Fick equation has the form

$$C(x, t) = \frac{Q_0}{\sqrt{\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right); \quad (6)$$

from the experimental data, a graph of the dependence of $\ln C(x, t)$ on x^2 was plotted, and according to formula

$$\ln C(x, t) = \ln \frac{Q_0}{\sqrt{\pi Dt}} - \frac{x^2}{4Dt}, \quad (7)$$

a straight line was obtained: the ratio

$$\frac{1}{x^2} \ln \left(\frac{C}{C_0} \right) = \text{const.} \quad (8)$$

This explains the bulk nature of diffusion, which prevails over grain boundary diffusion. At the same time, the exponent '2' at x indicates that the application of the second Fick's law is justified in this case due to the fact that the contribution to the total flux from the drift tends to '0'. The exponent at x , which would differ from '2', would indicate that the process of atoms transfer under pulsed impacts occurs under the action of a significant driving force, which is comparable in magnitude to $k_B T$ [5]:

$$\text{tg} \alpha = -\frac{1}{4Dt}. \quad (9)$$

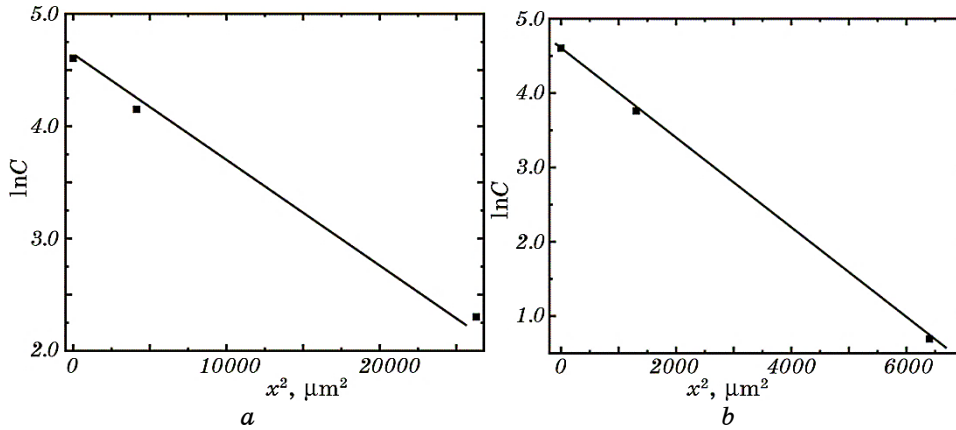


Fig. 5. Dependence graph according to $\ln C = x^2$: S235 after ESA (a), for HEA after ESA (b).

Knowing $\text{tg}\alpha$ from Figure 5 and diffusion time t , the mass transfer coefficients D_M after ESA were found. For S235, $D_M = 4.3 \cdot 10^{-8} \text{ m}^2/\text{s}$, and for HEA, $D_M = 3.1 \cdot 10^{-9} \text{ m}^2/\text{s}$.

The diffusion coefficient is 14 times higher in S235, than in HEA, which is consistent with the idea that the driving force of mass transfer is dislocations that move the radioactive isotope through the mechanism of capture and transfer of an interstitial atom [11, 12]. In HEA, due to the presence of atoms of different sizes in the composition, elastic displacements will occur during the movement of a dislocation and an additional 'friction' force will arise. The local Burgers vector \mathbf{b} varies both in magnitude and in direction [13]. Thus, mass transfer is going slower in HEA, than in S235.

3.2. Diffusion and Mass Transfer Parameters in S235 and HEA under Impact Deformation

Determination of the diffusion time t as a result of impact (2.3 ms) at sample S235 + HEA after ESA processing was carried out by the occurrence of an electromotive force (EMF) from the electrical-signal oscillogram according to the method described in Ref. [14], since the estimated diffusion time corresponds to the plastic deformation time (Fig. 6).

As follows from the oscillograms of electrical signals in Fig. 6, the plastic deformation time is 2 ms. During this time, diffusion proceeds predominantly by the interstitial mechanism, which is realized while the dislocations are moving intensively [15, 16]. The role of vacancies in the process of plastic deformation is low due to the high activation energy and due to the low mobility of vacancies [17]. Therefore, the

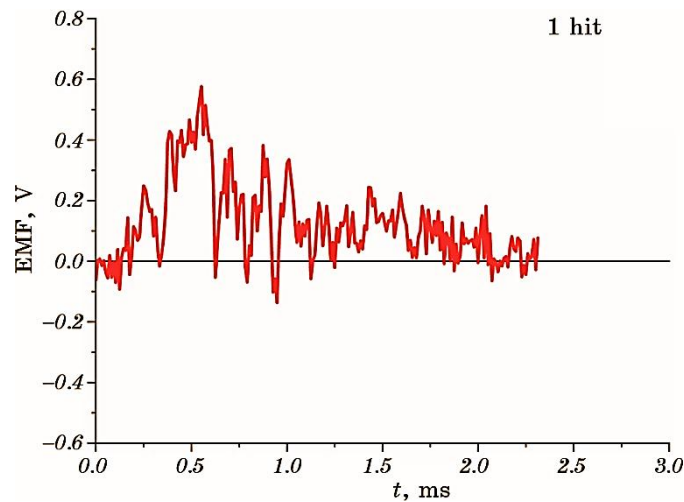


Fig. 6. Dependence graph of the electrical signals from loading time at sample S235 + HEA after ESA processing.

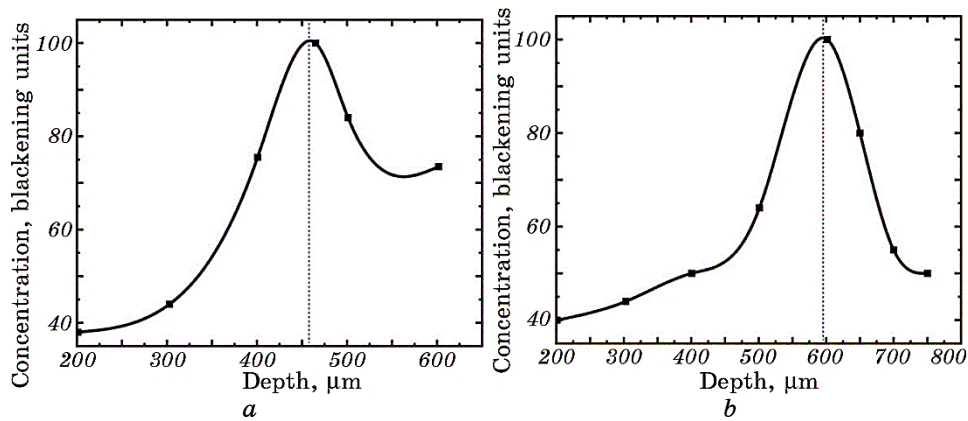


Fig. 7. Normalized concentration distribution of ^{60}Co isotope in depth in S235 (to the left of the maximum) and in HEA (to the right): after ESA (*a*), after complex processing (*b*).

contribution of vacancies to mass transfer by the random walk mechanism at 300 K can be neglected.

The impact load contribution to the mass transfer process in S235 and HEA during complex processing (ESA with next impact processing) is separated out.

As a result of the directed impact load, the dependence of ^{60}Co concentration on depth changed (Fig. 7): the concentration maximum of the radioactive tracer shifted to the right, which can be explained by

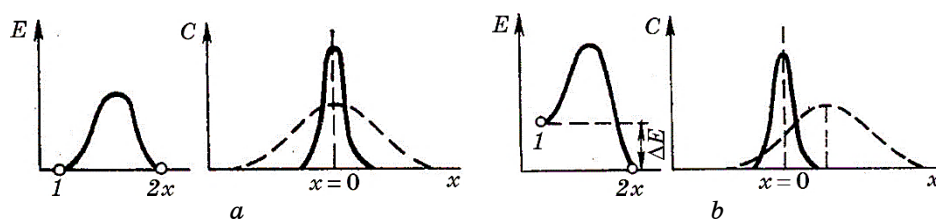


Fig. 8. Energy diagrams of potential barriers and corresponding concentration curves: without external forces (a), with external forces [18] (b).

the appearance of an external force, which leads to a symmetry breakdown of the potential barrier for atoms (Fig. 8, b). The probability of atoms transition in the direction of the force is more than in the opposite direction. Therefore, the symmetry of the concentration curve is broken; its maximum is shifted [18].

Since the total amount of the diffusing substance did not change due to the impact, but the concentration distribution over the depth (x coordinate) changed, in order to distinguish the contribution to the mass transfer of the impact load, the following was done:

1. The position of the maximum (100%) was found, which was taken as the 0-reference point by co-ordinate (Fig. 7, b),
2. Depths were found, at which concentrations of 90%, 80%, etc. are observed for each of the graphs in Fig. 7, b,
3. The subtraction from the data of the graph in Fig. 7, b of the data from Fig. 7, a was carried out according to the corresponding x coordinate found.

In this way, a displacement of x points was obtained, which correspond to the same relative concentrations before and after the impact, which is the result of the impact. This procedure was applied to each of the branches in the graphs of Fig. 7, which characterize the penetration of the diffusant into S235 and into HEA. The subtraction result characterizes the role of mass transfer in the impact process, is shown in Fig. 9. Thus, from the mass transfer under complex processing (ESA with next impact processing), the contribution of impact treatment was separated out.

When the contribution of drift to the total mass transfer is significant, the resulting distribution of concentrations may differ significantly from that predicted by the theory of diffusion by the mechanism of random walks. Dependence (5) of the natural logarithm of the C/C_0 concentration on the square of the depth x^2 , as in the case of diffusion for random walk mechanism, at ESA is not fulfilled, and the values fall on a straight line with power exponents for x : where $n = 1.5$ and $n = 1$ for S235 and HEA, respectively (Fig. 10). That is, the concentration distribution is described by the dependence $C(x)/C_0 = \exp(-ax^n)$ [19].

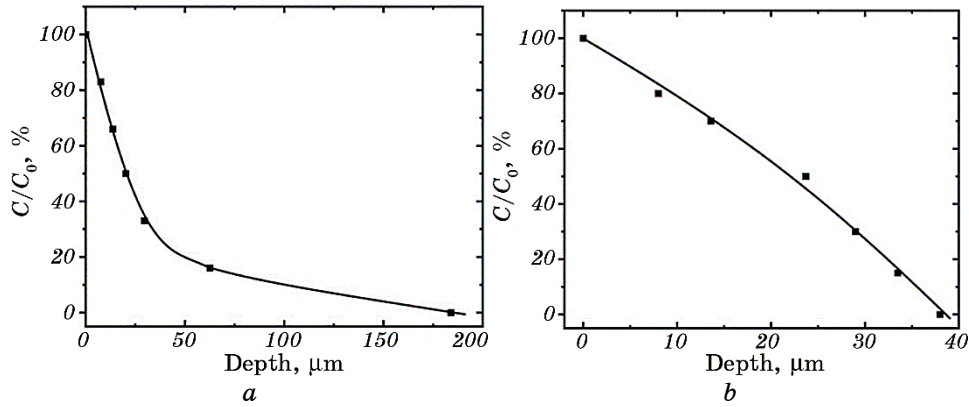


Fig. 9. Distribution of ^{60}Co concentration in depth in S235 (a) and HEA (b) under impact processing.

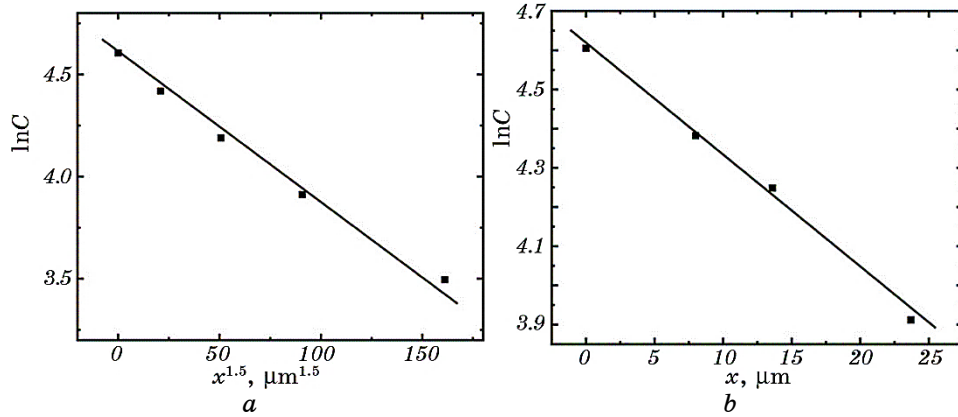


Fig. 10. The graphs of dependence $C(x)/C_0 = \exp(-ax^n)$: S235, $n = 1.5$ (a) and HEA, $n = 1$ (b) after impact processing.

This indicates an anomalous mass transfer and the unsuitability of the Fick’s second law application.

According to formulas (9), (10), it can be found the mean and mean-square shifts as the first and second normalized statistical moments. The sources [1,2] show the possibility of using these moments to describe and find diffusion parameters, including anomalous ones, by the mechanism of random walks.

In this paper, for the first time, the graphical method of finding such statistical moments and determining the parameters of anomalous mass transfer on the basis of experimental data on the distribution of concentration is proposed. From the processed experimental

data (Fig. 9) of concentration distribution, the general (due to both diffusion and drift) mean and root-mean-square displacement for the ^{60}Co penetration into S235 and HEA is found out:

$$\langle x \rangle = \frac{\int (C / C_0) x dx}{\int (C / C_0) dx}, \quad (10)$$

$$\langle x^2 \rangle = \frac{\int (C / C_0) x^2 dx}{\int (C / C_0) dx}. \quad (11)$$

To find $\langle x \rangle$ by the formula (10), the task was solved graphically (Fig. 11). In a similar way, when plotting the concentration distribution, but depending on x^2 , $\langle x^2 \rangle$ was found using the formula (11).

To find $\langle x \rangle$ by the formula (10), it is used the data approximation from Fig. 9, *a* for S235 by the rectangles' method with a variable subinterval. The same way $\langle x \rangle$ was found by the formula (10) for HEA (the graphs are similar both for S235 and HEA) using the data approximation from Fig. 9, *b* (Table 1).

To describe mass transfer and comparison with diffusion by the ran-

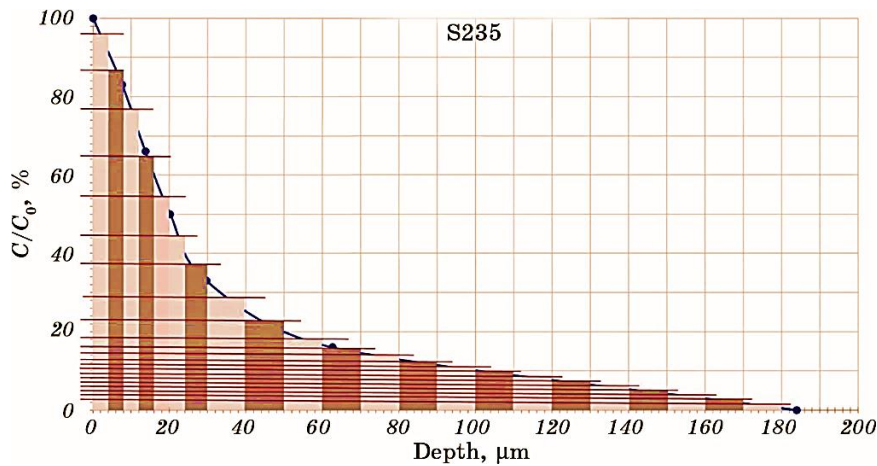


Fig. 11. An example of data approximation from Fig. 9, *a* by the rectangles' method with a variable subinterval to find $\langle x \rangle$ by the formula (10).

TABLE 1. The results of determining $\langle x \rangle$ and $\langle x^2 \rangle$ by the formulas (10), (11).

Value	S235	HEA
$\langle x \rangle$, μm	44.9	11
$\langle x^2 \rangle$, μm^2	9674.4	460.2

TABLE 2. The values of mass transfer parameters under impact processing.

Value	S235	HEA
$\langle v \rangle$, m/s	0.0225	0.0055
D_{ef} , m ² /s	$1.9 \cdot 10^{-6}$	$8.5 \cdot 10^{-8}$

dom walk mechanism, the effective diffusion coefficient is used [2]:

$$D_{\text{ef}} = \frac{\langle x^2 \rangle - \langle x \rangle^2}{2t}. \quad (12)$$

The average velocity of the directed motion of atoms is found by the formula

$$\langle v \rangle = \langle x \rangle / t. \quad (13)$$

As a result, the following values of mass transfer parameters under impact processing were obtained (Table 2).

The self-diffusion coefficient in iron by the interstitial mechanism is $3.6 \cdot 10^{-13}$ m²/s by the molecular-dynamics method at 300 K [20], which is 7 orders of magnitude lower than the calculated effective mass transfer coefficient for S235 ($1.9 \cdot 10^{-6}$ m²/s) under impact processing. Therefore, it can be concluded that the main foundation to the anomalous mass transfer under impact processing is contributed by the directional drift of particles, which is described by the second term in the general flux equation (14).

The flux equation assumes the sum of directed motion with random walks about its trajectory and has the form [18]

$$J = -D \frac{\partial C}{\partial x} + \langle v \rangle C, \quad (14)$$

where J is the flux of atoms, and x is the co-ordinate, which for a one-dimensional process is equal to the distance from the origin.

As a result of impact processing, the effective diffusion coefficient (mass transfer) is 22 times higher in S235, than in HEA (see Table 2). This can be explained by the fact that the additional ‘friction’ force, which has arisen due to the incommensurability of its own atoms in the HEA, complicates directional mass transfer process because of the dislocations glide [11, 13].

3.3. Determination of Driving Forces and Mobility of Atoms in the Process of Mass Transfer under Impact Processing

The average value of the resultant force $\langle F \rangle$ is a result of the impact,

which consists of the average normal response force $\langle N \rangle$ and the force of gravity on sample at perpendicular impact. Then, $\langle F \rangle$ is found by formula

$$\langle N \rangle = \langle F \rangle + mg. \quad (15)$$

When falling a block of mass 10.5 kg from a height 1 m, the kick-back is equal to 17 cm; then,

$$\langle F \rangle = \Delta p / \Delta t. \quad (16)$$

The velocity of the body at the moment of falling, *i.e.*, the maximum speed

$$v = \sqrt{2hg} = 4.5 \text{ m/s}. \quad (17)$$

As a result of the calculations, $\langle F \rangle = 42.5 \cdot 10^3 \text{ N}$, $\langle N \rangle = 4.2 \cdot 10^4 \text{ N}$.

Our estimates show that about 50% of the energy is spent on elastic deformation, damping pad in the basement of equipment, heating the sample, and on elastic compression of a hardened steel spacer plate. Therefore, in further calculations, a normal response force value will be used as a twice less: $2 \cdot 10^4 \text{ N}$.

Using the obtained data, the normal stresses, σ_0 , in the cross-section are calculated according to the formula

$$\sigma_0 = \langle N \rangle / A_0 = 2.5 \cdot 10^2 \text{ N/mm}^2. \quad (18)$$

The tangential stress that leads to dislocation glide was calculated [21]:

$$\tau = \sigma_0 \cos \varphi \cos \lambda = \sigma_0 / 2 = 1.25 \cdot 10^2 \text{ N/mm}^2. \quad (19)$$

From the data on the dependence of dislocation glide speed on tangential stress [22], it follows that the dislocation velocity is about 10^4 cm/s . Based on these data, the dislocation density ρ leading to mass transfer was estimated by the Taylor–Orowan equation [23]: $1.1 \cdot 10^5 \text{ cm}^{-2}$.

From the second relation of the Einstein–Smoluchowski equation founding the force acting on each atom [2],

$$\langle x(t) \rangle = \frac{1}{2} \frac{F \langle x^2(t) \rangle}{k_B T}. \quad (20)$$

As a result, the driving force F for S235 at 300 K temperature, which is of $3.8 \cdot 10^{-17} \text{ N}$, and for HEA is of $1.96 \cdot 10^{-16} \text{ N}$, is determined. The average displacement and average quadratic displacement for S235 and

HEA were calculated above (see Table 1).

The authors of Ref. [24] showed that the HEA coating applied by ESA to stainless steel consists of zones of interdroplet spaces having a nanoscale structure (2.5–15 nm) with a b.c.c. crystal lattice and areas of droplet fall having a grain structure. AlCuCoFeNiCr in the cast state contains of three phases: two with an f.c.c. lattice and one with a b.c.c. lattice. Lattice parameter is as follows: $a_{f.c.c.(1)} = 0.3625$ nm (1%), $a_{f.c.c.(2)} = 0.3593$ nm (26%), $a_{b.c.c.} = 0.2879$ nm (73%) (in parentheses, it is indicated the percentage content of the corresponding phase). To calculate the work A of force acting on each atom by formula (21), the used lattice spacing for a b.c.c. iron crystal is equal to 0.286 nm, since the volume fraction of a b.c.c. phase is significantly larger for case of AlCuCoFeNiCr:

$$A = FS = Fa / \sqrt{2} . \quad (21)$$

The calculations found that $A_{S235} = 7.7 \cdot 10^{-27}$ J, $A_{HEA} = 4 \cdot 10^{-26}$ J.

The work of force directed action on the atoms is not enough to make atom a jump to the neighbouring position, because the magnitude of the work of force is significantly less than the thermal oscillations energy $k_B T$ ($4.11 \cdot 10^{-21}$ J). Nevertheless, in our case, the transfer of radioactive tracers to new positions is observed. This indicates that mass transfer under external influences is realized due to mobile dislocations, rather than direct diffusion jumps of atoms.

Let us estimate the mobility of atoms in the process of anomalous mass transfer for S235 and HEA. Some authors use the concept of diffusion mobility as a synonym for the diffusion coefficient, although they have different dimensions. Mobility of atoms depends on strength and velocity according to the formula

$$\mu = \langle v \rangle / F ; \quad (22)$$

the founded $\langle v \rangle$ for S235 and HEA are presented in Table 2.

The calculations found that the mobility of ^{60}Co atoms in S235 is equal to $5.9 \cdot 10^{14}$ m/(s·N), and for HEA, it is of $2.7 \cdot 10^{13}$ m/(s·N).

On the other hand, diffusion mobility is related to the diffusion coefficient according to the Einstein–Smoluchowski equation:

$$\mu = D_T / (k_B T) . \quad (23)$$

If, in formula (22), D_T is replaced by D_{ef} (see Table 2), then, the following mobility values are obtained: $4.6 \cdot 10^{14}$ m/(s·N) for S235 and $2.07 \cdot 10^{13}$ m/(s·N) for HEA. This is consistent with the results of the calculation by the previous formula (21). Therefore, the well-known Einstein–Smoluchowski equation for determining mobility can be used

for the process analysis of the anomalous mass transfer under external influences, if to replace D_T by D_{ef} .

4. CONCLUSIONS

1. For the first time, on the basis of experimental data, a method for determining the parameters of anomalous mass transfer with separation of the diffusion component and drift under driving force is proposed. The method is based on determining the exponent of the power n at x when plotting the concentration dependence of the following form: $(\ln(C/C_0))/x^n = \text{const}$. Based on the numerical value of the exponent n , a conclusion about the mass transfer mechanism and the selection of appropriate formulas for finding the parameters of mass transfer: D , D_{ef} , $\langle v \rangle$, μ , F is made.

2. As shown using our method, the predominant mechanism of mass transfer under the ESA and mechanical impact conditions in S235 and HEA is the directed motion of atoms, which are entrained by mobile dislocations, since the drift component of the flux equation is significantly larger than the diffusion component by the mechanism of random walks. This is also confirmed by estimates of the work of force due to the atoms' movement, the value of which ($A_{S235} = 7.7 \cdot 10^{-27}$ J, $A_{HEA} = 4 \cdot 10^{-26}$ J) is much less than the energy of thermal vibrations $k_B T$ ($4.11 \cdot 10^{-21}$ J).

3. It is shown that the effective diffusion coefficient (mass transfer) as a result of external influences (mechanical impact and ESA) is tens of times higher in S235 than in HEA, which is consistent with the dislocation mechanism of mass transfer. This coincides with the conclusions of the authors of Ref. [13] that the additional 'friction' force, which has arisen due to the incommensurability of its own atoms in the HEA, complicates directional mass transfer process because of the dislocations glide.

4. For the first time, based on the mean and root-mean-square displacements of atoms obtained from the experimental concentration profiles, the force acting on each atom and the mobility of ^{60}Co atoms in iron under mechanical impact processing are determined.

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