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METHODOLOGICAL RECOMMENDATIONS

for practical works in the discipline "RADIATION MATERIALS SCIENCE"

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Applied physics and nanomaterials: Methodological recommendations to practical classes in the educational discipline OK 03 "Radiation materials science" for students of the 1st year of study in specialty 105 Applied physics and nanomaterials.

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Methodical recommendations for practical works in the educational discipline of OK 03 "Radiation materials science" for students of the 1st year of study specialties 105 Applied physics and nanomaterials.

The material presented in the methodical recommendations highlights the basic concepts, patterns and laws of radiation damage to metals, semiconductors, radiation defects and their configuration profiles, annealing kinetics of radiation defects, radiation-stimulated processes, of radiation physics of polymers as a scientific basis for modern radiation physics technologies of modification of functional materials**.**

Keywords: radiation materials science, radiation defects, annealing kinetics of radiation-stimulated damage.

CONTENT

INTRODUCTION

Educational discipline OK 03 "Radiation materials science" for students of higher education in the 1st year of study at the third (educational and scientific) level specialties 105 Applied physics and nanomaterials according to the curriculum calculated for 3 credits totaling 90 hours. Lecture classes 24 hours (lectures – 20 hours, practical classes – 4 hours), 56 hours, and 10 hours allocated, respectively, to independent work and individual work graduate students The content of the academic discipline is divided into two according to the program content modules, the first of which is devoted to the basics of radiation physics metals and their alloys, and the second - radiation physics of polymers and semiconductors. Methodological recommendations for the discipline "Radiation materials science" cover issues of the influence of neutron, ion, and electron irradiation on the defective structure of solids and the corresponding program of practical classes. The workshop presents 2 practical works, which according to the program of the academic discipline is calculated for 4 classroom hours of work The content of practical works requires basic theoretical knowledge of the discipline "Radiation materials science" and is based on university courses of general and theoretical physics. The developed cycle of practical classes is the basis for further study of discipline OK6 "Mechanisms of aging of materials and devices".

Practical work №1

The topic of the practical work: “Modeling the cascade stage of irradiation using the program Stopping and Range of Ions in Matter (SRIM)”.

The computer providing for the practical work:

Program Stopping and Range of Ions in Matter (SRIM).

The purpose of the practical work:

To investigate the cascade (nucleation) stage of the kinetics of point defects in the process of irradiation.

5Irradiation with neutrons, ions, and electrons causes a cascade (nucleation), deterministic stages, and the Ostwald stage. The subject of this practical activity is the study of the cascade (nucleation) stage for using the program SRIM. Quantification of the amount of damage by the number of induced displacements energetic interactions of radiation particles with atoms of matter, important for a wide range of fundamental sciences and applied engineering programs ranging from semiconductor physics to nuclear energy [1]. Kinchin [2] developed the basis for the first model for calculating displacements at atom (dpa), taking into account the transfer of the kinetic energy of the particle to the atoms of the body, necessary for their displacement from the nodes of the crystal lattice (threshold energy displacement), which depends on the material. The existing international standard for quantitative determination of the specified value in irradiated materials based on more than 40 years of computer simulation of binary collisions of ions in solids [3,4]. Predicted atomic number displacements (N_d) as a function of cascade energy, or damage function, considered in this model. The damage energy per ion is determined as the total ion energy minus the energy lost to electronic interactions (ionization energy). Typical values of E_d for various materials are found in range from 20 to 100 eV [5,6]. This is essentially the Kinchin model, with an exception

of the original term of kinetic energy, which was replaced by energy damage to account for ionization effects, and a factor of 0.8 was introduced, to account for more realistic interatomic potentials. Importance of the calculated dpa parameter is that it is the starting point for calculations of almost all radiation effects in solid materials that facilitates quantitative comparisons of different materials irradiated by the same source of radiation, as well as materials irradiated in different sources irradiation, such as electron, ion and neutron irradiation [1–8]. Damage assessment is also of great importance when handling moderns materials by focused ion beams or by irradiation of nanomaterials [9,10]. However, it has been recognized for several decades that the value of dpa, which is calculated for energy cascades in pure metals, on the one hand, overestimates the number of stable defects by 3-4 times [11–14], and on the other hand, underestimates the number of displaced atoms (atoms permanently displaced from their initial position in the lattice to replace an atom in another position) [13,15,16], which occurs as a result of a cascade. Even though the initial effect occurs at the nanometric scale, it has also been estimated that he can lead to such macroscopic consequences as a 5-year understatement of the life of the nuclear reactor body under pressure, which is exposed to very high heat flux [17]. Similar trends have also been reported for intermetallic alloys [18] and ceramics [19–21].

The displacement cascade can be caused by a passing neutron or another particle with high energy (1 MeV or more). The first atom lattice, which will receive recoil energy, is called a primary shock atom. Notice how initially, when the atoms are highly excited, many of them are displaced from their nodes into lattices. However, as the cascade begins thermally equilibrate with the environment, almost all atoms restore their positions in the ideal lattice structure. The quantity of final defects formed is much smaller, and the number of atoms that

replace other atoms is much larger than predicted on the basis of simple linear cascade collision models such as the NRT-dpa model. Atomic collision processes are fundamental to many advanced materials technologies, such as electron microscopy, processing semiconductors, and nuclear energy production. Numerous experimental research and computer simulation research during of the past few decades provide a physical basis for understanding atomic-scale processes occurring during the primary moving. Existing international standard for quantification particle damage energy, Norgett-Robinson-Torrens displacement model per atom (NRT-dpa), to date has several well-known limitations. In particular, the number of radiation defects formed by energy cascades in metals, is only ∼1/3 of the NRT-dpa prediction, while the number of atoms involved in the displacement of atoms is approximately 30 times higher dpa value. Here, we provide new additional estimates of the displacement results (adjusted athermal recombination dpa, arc-dpa) and atomic functions blends that extend NRT-dpa to provide more physically realistic descriptions of the creation of the primary defect in the materials may become additional a standard measure for quantitative assessment of radiation damage. The effect of intra-cascade recombination on the formation of defects. The physical basis of the NRT-dpa model is the formation of defects at high energies enhances the recombination of defects. Simulations of binary collisions, used as the basis of the NRT-dpa 3 models were focused on the phase collision in the process of the cascade stage, did not take into account the dynamics of the cascade evolution when the speed of atoms drops to the speed of sound (~5 eV) and below, when the interaction of many bodies becomes relevant. In energetically dense cascades, local melting clearly plays a role an important role in maintaining structural defects. With increasing energy primary ejected atom, the displacement process produces more and more defects Frenkel (pairs of vacancies

and internodes), which are spatially close to others defects ~10–100 jumps per atom during the cascade cooling phase within 1–10 ps [14] can cause significant additional recombination processes as the cascading energy of atoms decreases after the collision phase from E_d to the threshold value for the migration of atoms (Em ~ 0.01–0.3 eV for their own interstitial atoms and up to ~0.5–1 eV for vacancies). Accurate modeling of these joint effects of many bodies in displacement cascades is realistically performed by using molecular dynamics method [14].

An example of a cascade stage study.

Protons were used as sources of irradiation of target samples due to their relatively large penetration depth. Experiments with proton irradiation was carried out in a recharging accelerator (tandem) laboratories of the Leach Science Center at Auburn University using of protons of 4 MeV and under a vacuum of 10^{-4} Pa. Irradiation was carried out at room temperature temperature (25°C) to separate and determine the effects of exposure and thermal aging at 500°C, respectively. However, proton irradiation caused a slight increase in the average temperature from 25°C to 50±5°C.

The proton beam was rastered over a uniformly irradiated area approximately 50 mm in diameter. Used for proton irradiation the beam current is 4 μA, which can provide a dose rate of $1.25x10^{12}$ protons cm^{-2} c^{-1}. Proton distribution and radiation-induced displacement profile, which created using the Stopping and Range of Ions in Matter (SRIM) program for protons with an energy of 4 MeV, shown in [22].

Results obtained from SRIM 2008 calculations for the proton irradiation with 4 MeV protons show the distribution of the protons during the irradiation and the displacement profile of the target after exposure.

Proton distribution and radiation-induced displacement profile, which created using the program (SRIM) for 4 MeV protons, is shown in [22]. As can be seen in [22], for a sample thickness of 50 μm, most of the protons completely penetrated the sample. Thus, an almost uniform dose throughout the thickness of the sample can be obtained with the specified irradiation. At the same time, the effect of proton implantation is minimized. Dose profile damage along the depth of the sample is shown in [22]. The dose of proton ions in the studied samples was 5 million displacements per year, which is comparable to a typical 40 years of nuclear exposure reactors of the Westinghouse type (30 mdpa) [23].

Tasks.

1. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time of commercially pure iron by iron ions with an energy of 0.25 MeV.
2. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time commercially pure iron with iron ions with an energy of 0.5 MeV.
3. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time of commercially pure iron by iron ions with an energy of 0.75 MeV.
4. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time of commercially pure iron with iron ions with an energy of 1.0 MeV.
5. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time of commercially pure iron by iron ions with an energy of 1.25 MeV.
6. Find and plot the dependence of the average radius of the cluster and

of the numerical density of clusters formed during bombardment over time of commercially pure iron with iron ions with an energy of 1.5 MeV.

8. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time of commercially pure iron by electrons with energies of 0.5, 1.0, and 1.5 MeV.

9. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters formed during bombardment over time commercially pure iron neutrons with energies of 0.5, 1.0 and 1.5 MeV.

Control questions.

1. How is the effect of neutrons on structural metals simulated?
2. How ion irradiation is used for research neutron irradiation?
3. How is electronic irradiation used for study of neutron irradiation?
4. What are the stages of the evolutionary evolution of clusters in irradiated metals?
5. What is the dependence of the radiation results on the nature of the radiation (ions, electrons, neutrons)?
6. What is the dependence of the results of irradiation on the energy of electrons?
7. What is the dependence of the irradiation results on the ion energy?
8. What is the dependence of the results of irradiation on neutron energy?
9. Was the similarity of the results of electronic, ion, and neutron irradiation?

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Practical work 2

The topic of the practical work: “Study of fluctuation and deterministic stages of point kinetics defects by the method of cluster dynamics)”.

The computer providing for the practical work:

The program for modeling the evolution of point defects using the cluster method dynamics.

The purpose of the practical work

To investigate the fluctuation and deterministic stages of point kinetics defects by the method of cluster dynamics.

The theoretical information.

The cluster dynamics method was proposed in the 1935 year by Bocker [1] in the study of phase transformations of water (evaporation and condensation). CD master equation for a closed system clusters, in which only monomers are mobile, was written in the form:

$$\frac{dC_n}{dt} = \beta_{n-1}C_{n-1} + \alpha_{n+1}C_{n+1} - (\beta_n + \alpha_n)C_n$$

where C_n is the concentration of clusters containing n monomers; αn (β n) is the coefficient emission (attachment) of a monomer from (to) a cluster of size *n* (the size of the cluster here and in the future, both the cluster size in units of length and the number of its monomers n) per unit of time. The first and second terms are on the right parts of this master equation correspond to an increase in the number of clusters size n per unit of time due to the addition of a monomer to a cluster of size (*n*-1), and monomer emissions from a cluster of size (*n*+1), respectively, a the third term is the decrease in the number of clusters of size n per unit of time account of the addition and emission of monomers from a cluster of size *n*.

Features of any system in the CD method are given by the coupling and emission coefficients, as well as additional – functions of external sources and sinks of monomers case of an open system of clusters. If the size of the clusters is not possible be neglected compared to the distance between them, then the CD method should be modified according to the approach [2] to take into account the so-called frustration effect.

Since 1997, the CD method has been fruitfully used in modeling problems processes of formation and evolution of defective structure in metals and alloys under the action of irradiation with electrons, ions, and neutrons [3], where clusters point defects and precipitates have small sizes compared to the average the distance between them. To increase the service life of a nuclear power plant it is important to foresee the possibility of the transition of the material of the reactor body to a fragile state Empirical formulas obtained for this are used for samples irradiated in research reactors. However, it seems it is important to confirm the results of these formulas for predicting the lifetime resource of reactors, investigating the physical phenomena underlying the mechanism of neutron fragility. In the case of hull reactor steels with low copper content, clusters of point defects are an important element of the defect structures. That is why it is an urgent task of physical materials science to simulate the nucleation and evolution of clusters of point defects in the specified reactor materials. The best way to do this is to simulate the processes in the case nuclear reactor from the beginning to the end of its operation. But, despite the high capabilities of modern computers, the modeling method molecular dynamics or the Monte Carlo method makes it impossible for study the behavior of the reactor during the entire period of its operation, especially given the required size of the representative volume. For now, modeling by the method of cluster dynamics based on the master equation kinetics

of clusters remains the only real possibility of researching the specified task. CD requires knowledge of material-specific parameter sets. These parameters can be obtained by atomic simulation or experimentally.

The first comprehensive analysis of thermodynamic aspects of the theoretical descriptions of phase transitions of the first kind were performed by Gibbs [4] and Van der Waals [5,6]. Gibbs' thermodynamic theory was used 60 years later after its development for the formulation of the kinetic theory of nucleation processes and growth [7–12]. The so-called classical theory of nucleation, put forward at that time with modifications is still used to interpret the experiment results of phase formation processes, starting with metastable initial one's state Van der Waals' method was, again, about 60 years after his of the first formula, reinvented by Kahn and Hilliard [10,11] for the purpose development of a theoretical model of spinodal decay. This approach is convenient a way of describing the phase transformation of processes starting with the thermodynamically unstable initial state. The state of critical clusters, and also the state of pre- and supercritical clusters can, in general, differ from the state of the final macroscopic phase. Correct determination of the state of clusters depending on their size for any arbitrary initial state. Problem arises in the description of both the nucleation and growth of clusters. For example, key problem in applying any nucleation theory to the analysis of experimental data on phase formation processes is in the specification of thermodynamic properties of the critical cluster. At high supercooling (which must be achieved to achieve a sufficiently high nucleation rate), the critical cluster has a size of the order of nanometers. For this reason, direct experimental methods of studying the properties of critical clusters cannot normally be used. Therefore, it is necessary to make certain assumptions about their properties or develop methods for their definition. Here, however, various

problems arise. of the surrounding phase is a requirement for providing an adequate description of process kinetics. However, solving this task is one of the main problems, to which no satisfactory general solution has yet been found. However, similar problems arise in almost any phase formation analysis, regardless of a specific field of application. When performing the calibration procedure of the CD model [13] used the assumption that only single vacancies and the interstitial atoms are mobile, and the energy parameters were determined from the comparison of cluster dynamics results with experiments. In the model [13] changes have been made to account for both the mobility of clusters and their presence immediately after the cascade stage. Since the predictive ability model is related to the validity of the parameters used, in this study, the energy parameters were selected not only with the use of experimental data but from the results of ab initio calculations carried out in [14-16] for α-iron. Data on the distribution of interstial loops were used by size and their numerical density in the samples after ion irradiation at a temperature of 400 °C and a dose of 0.2 dpaNRT. In [17] sought reproduce exposure to damage to thin foil using the TEM method, it is assumed that the power of absorption of point defects by boundaries grains is insignificant compared to their absorption on the surface of the sample. The parameters of pure carbon-free iron were used. However, in [17] during irradiation, implantation of carbon in the ionic can occur accelerators, which was previously observed on tomographic needles at atomic sensing [18]. In addition, a set is introduced to determine G_j in [17].additional parameters $(fn)\theta$.

CD results are used for searching correspondence between the data of small-angle neutron scattering (SANS) and PAS methods [18]. Commercially pure iron (<30 ppm carbon, the average grain size is 250 μm, the number density of dislocations

7×10^{13} m^{-2}) was irradiated with neutrons at the Callisto facility (IPS2) in the Belgian BR2 reactor (Mole, Belgium). Irradiation with the flow of neutrons ≈ 9×10^{17} n/m^2s^{-1} (E>1 MeV) was carried out at a temperature of 300 °C. This flux corresponds to a flux of 139×10^{-9} dpa/s. Neutron fluence ranged from 1.7×10^{23} to 1.3×10^{24} n/m^2 (E>1 MeV), which corresponds to the exposure range of neutrons from 0.026 to 0.19 dpa. Research using the TEM method revealed the presence of SIACs with a size from 2 to 31 nm. The average diameter and total the density of dislocation loops is about 5 nm and 0.85×10^{21} m^{-3}, 7 nm and 1.3×10^{21} m^{-3}, and 10 nm and 4×10^{21} m^{-3} for 0.051, 0.1 and 0.19 dpa, respectively. Method TEM did not detect vacancy pores under the specified irradiation conditions. However, application of the SANS method proved the presence of vacancy clusters ≈2 nm in size, the number density and volume fraction of which are 4×10^{22} m^{-3} and 0.014%, respectively. From the ratio of the general experimental of the SANS intensity to its share due to the nuclear interaction of neutrons with iron cores, the so-called A ratio of ≈1.4 was determined, which corresponds to the expected vacancy nature of scatterers in pure iron. Using the PAS method, it was observed that during exposure to VC grows with the formation of microspores. An experimental lifetime of positrons in PAS experiments corresponds to VCs with three, seven, and ten vacancies. The value of the critical size ncr is found from the condition of maximum change Gibbs energy, $G_{v(i)}(n)$ in the formation of VC (SIAC) containing *n* number monomers: for exposure doses of 0.026, 0.10 and 0.19 dpa, respectively. The value of the critical size ncr is found from the condition of maximum change Gibbs energy, $G_{v(i)}(n)$ in the formation of VC (SIAC) containing *n* number monomers:

$$n_{cr\_v} = 2\left(\frac{E_{fv} - E_{b2v}}{E_{b2v} + 3(E_{fv} - E_{b2v})\square(1-2^{-2/3}) + k_B T \ln C_{1v}}\right)^3 \quad (1)$$

$$n_{cr\_i} = \left(\frac{1}{(E_{b2i} + k_B T \ln C1_i) / \pi R_{1i} E_{eff} + 2(\sqrt{2} - 1)} \right)^2 \quad (2)$$

Here, $G_{v(i)}(n)$ is written as in [19] for spherical and flat clusters, in accordance, $\Delta\mu v\,i$ is the difference in the chemical potential of the monomer in VC (SIAC) and to the corresponding monomer in the iron matrix, $R_{nv}(i)$ is the radius of VC (SIAC) which contains n monomers, γ is specific surface energy VC, E_{eff} – energy dislocations per unit length. The values of γ and E_{eff} can be found in equation (3) [18] and equation (4), in accordance:

$$\gamma = \frac{3\sqrt[3]{2}}{8\pi R_{1v}^2} \left(E_{fv} - E_{b2v} \right) \quad (3)$$

$$E_{eff} = \alpha \mu b^2 \quad (4)$$

Here, E_{fv} is the vacancy formation energy, E_{b2v} is the bond energy of divacancies, μ is the shear modulus, α is in the range of 0.5–1.5, b is the Burgers vector. Equation (5) is derived from the equivalence principle equation detailed balance using the difference in Gibbs energy of a cluster of size (n_1) and a cluster of size n, on the one hand and the equation of the principle of detailed balance due to the binding energy of a cluster of size n, $E_{bnv(i)}$, and the concentration of single monomers, $C_{1v(i)}$, on the other hand:

$$\Delta G_{v(i)n-1} - \Delta G_{nv(i)} = E_{bnv(i)} + k_B T \ln C_{1v(i)} \quad (5)$$

Equations (6) and (7) are obtained from equations (3), (4) and (5):

$$\Delta\mu_v + 4\pi(R_{(n-1)v}^2 - R_{nv}^2)\gamma = E_{bnv} + k_B T \ln C_{1v} \quad (6)$$

$$\Delta\mu_i + 2\pi(R_{(n-1)i}^2 - R_{ni}^2)E_{eff} = E_{bnv} + k_B T \ln C_{1i} \quad (7)$$

The critical size of VC, n_{cr_v}, and SIAC, n_{cr_i}, is from the condition of the maximum change in Gibbs energy, $\Delta G_{v(i)}(n)$:

$$n_{cr\_v} = 2 \left(\frac{E_{fv} - E_{b2v}}{E_{b2v} + 3(E_{fv} - E_{b2v})\square(1 - 2^{-2/3}) + k_B T \ln C_{1v}} \right)^3 \quad (8)$$

$$n_{cr\_i} = \left(\frac{1}{(E_{b2i} + k_B T \ln C1_i)/\pi R_{1i} E_{eff} + 2(\sqrt{2}-1)} \right)^2 \quad (9)$$

Neutron irradiation leads to a significant change in $C_{1v(i)}$. So, the critical sizes n_{cr_v}, and , n_{cr_i}, change according to equations (8) and (9). Therefore, the effect of the results of the cascade stage on the long-term behavior of point clusters of defects may change with exposure time. Equations (8) and (9) were used to analyze the simulation results of the CD study [20].

The CD master equation is written in the form of the following stiff systems of differential equations for the case of neutron irradiation:

$$\frac{dC_{1v(i)}}{dt} = \eta G_{dpa}(1 - f_{vcl(icl)}) - \frac{4\pi r_{rec}(D_v + D_i)C_{1v}C_{1i}}{\Omega_{Fe}} - \rho_d Z_{v(i)} \left(1 + \frac{6\left(\rho Z_{v(i)}\right)^{-0.5}}{d} \right) D_{v(i)} \left(C_{1v(i)} - C^e_{1v(i)} \right)$$
$$- 4\beta^{v(i)}_{1v(i)} C_{1v(i)} + 4\alpha^{v(i)}_{2v(i)} C_{2v(i)} - \sum_{n=2} \beta^{v(i)}_{nv(i)} C_{nv(i)} + \sum_{n=3} \alpha^{v(i)}_{nv(i)} C_{nv(i)} + \beta^{i(v)}_{2v(i)} C_{2v(i)} - \sum_{n=2} \beta^{v(i)}_{ni(v)} C_{ni(v)} \quad (10)$$

$$\frac{dC_{2v(i)}}{dt} = G_{2V(I)} + 2\beta^{v(i)}_{1v(i)} C_{1v(i)} - 2\alpha^{v(i)}_{2v(i)} C_{2v(i)} - \beta^{v(i)}_{2v(i)} C_{2v(i)}$$
$$+ \alpha^{v(i)}_{3v(i)} C_{3v(i)} - \beta^{i(v)}_{2v(i)} C_{2v(i)} + \beta^{i(v)}_{3v(i)} C_{3v(i)} \quad (11)$$

$$\frac{dC_{nv(i)}}{dt} = G_{nV(I)} + \beta^{v(i)}_{(n-1)v(i)} C_{(n-1)v(i)} + \left(\beta^{i(v)}_{(n+1)v(i)} + \alpha^{v(i)}_{(n+1)v(i)} \right) C_{(n+1)v(i)} \quad (12)$$
$$- \left(\beta^{v(i)}_{nv(i)} + \beta^{i(v)}_{nv(i)} + \alpha^{v(i)}_{nv(i)} \right) C_{nv(i)} \quad for\ n > 2,$$

where η is the efficiency coefficient, that is, the ratio of the number of monomers point defects at the end of the cascade stage to the total number of these defects, created at the beginning of this stage, f_{vcl} (f_{icl}) is the ratio of the number of singles vacancies (interstitial atoms) that form VC (SIAC) to the total number of vacancies (interstitial atoms) at the end of the cascade stage, ρ_d is dislocation density, d is average grain size, Ω_{Fe} is atomic volume of iron, $C^e_{1v(i)}$ is the equilibrium thermal concentration of vacancies (interstitial atoms), $D_{v(i)}$ is calculated according to formula (13):

$$D_{v(i)} = D_{v(i)0} \exp\left(-\frac{E_{mv(i)}}{k_B T} \right), \quad (13)$$

where D_{i0}, D_{v0} are the pre-factors of the diffusion coefficient of a single vacancy (interstitial atom), E_{mv} (E_{mi}) is the vacancy migration energy (interstitial), $\beta^{v(I)}{}_n$ is coefficient of attachment of point defects by planes by clusters of interstitial atoms with a radius r_n, which is determined by formula (14):

$$\beta_{ni}^{v(i)} = \frac{2\pi r_{ni} D_{v(i)} C_{1v(i)}}{\Omega_{Fe}} Z_n^{v(i)} \quad (14)$$

where $Z^{v(i)}{}_n$ is a correction factor that determines vacancy capture (interstitial atoms) of the interstitial cluster is determined by formula (14), where $\beta^{v(I)}$ is the coefficient of attachment of point defects by a spherical cluster vacancies with a radius R_{nv}, calculated according to the diffusion approximation mode according to formula (15):

$$\beta_{nv}^{v(i)} = \frac{4\pi R_{nv} D_{v(i)} C_{1v(i)}}{\Omega_{Fe}} \quad (15)$$

α_{nv} i is the emission coefficient of one vacancy (interstitial atom) from the cluster vacancies (interstitial atoms), calculated according to the detailed principle equilibrium due to changes in free energy $\Delta G(n)v$ for vacancies and binding energy cluster of interstitial atoms E_{bni}:

$$\alpha_{nv}^{v} = \beta_{(n-1)v}^{v} \cdot \exp \frac{\Delta G_v(n) - \Delta G_v(n-1)}{k_B T} \quad (16)$$

$$\alpha_{ni}^{i} = \frac{\beta_{(n-1)i}^{i}}{C_{1i}} \cdot \exp\left(-\frac{E_{bni}}{k_B T}\right) \quad (17)$$

where E_{fi} is the vacancy formation energy (interstitial atom), E_{b2i} is the binding energy dimer of vacancies (interstitial atoms). The LSODA solver was used for direct integration master equation for the study of a system of point defects containing single monomers, spherical VC size from 2 to 2000 monomers, single

SIA and planar SIAC with size from 2 to 4000 SIA. The material parameters and $G_{nV(I)}$ were varied to achieve maximum correspondence of simulation results to experimental ones of TEM, SANS and PAS data [21], taking into account the experimental limitations of these methods for ferromagnetic iron.

Table 1. Material parameters for pure iron.

Vacancy formation energy, E_{fv}	1.60 eV	[3]
Binding energy of a cluster with two vacancies, E_{b20v}	0.20 eV	[3]
Vacancy migration energy, E_{mv}	1.30 eV	[3]
Pre-factor of the diffusion coefficient of singles vacancies, D_{v0}	0,1×10-3 м^2/с	[3]
Energy of interstitial atom formation, E_{fi}	4.3 eV	[3]
Binding energy of a cluster of two interstitials atoms, E_{b2i}	0.80 eV	[3]
Interstitial atom migration energy, E_{mi}	0.30 eV	[3]
Pre-factor of the interstitial atom diffusion, D_{i0}	4,0×10^{-8} м^2/с	[3]
Radius of recombination, r_{rec}	0.65×10^{-9} m	[3]
Vacancy trapping rate by the dislocation net, z_v	1	[3]
Interstitial atom trapping rate by the dislocation net, z_i	1.2	[3]
Burgers vector, b	0.20×10^{-9} m	[3]
Dislocation density, ρ_d	0.7×10^{14} m^{-2}	[20]
Average grain size, d	2,5×10^{-4} м	[20]

Table 2. Distribution of VC and SIAC by the number n of monomers at the end of the cascade stage according to (6), taking into account the difference between the values of Gdpa in (6) and in [17].

N	VC $10^{-9}\ G_{n,v}$ dpa/s	SIAC $10^{-9}\ G_{n,v}$ dpa/s
1	34.3	32
2	0.048	3.5
3	0.048	0.13
4	0.046	0.086
5	0.046	0.049
6	0	0.035
7	4.2.	0.026
8	3.3	0
>8	0	0

In the process of evolution of the population of clusters, the system undergoes the following stages:

– Fluctuation or nucleation stage at which formation occurs clusters, their growth, and decay. At the same time, the average radius of the clusters and their numerical density is increasing.

– Deterministic stage, in which there is an increase in the average radius of clusters at their constant numerical density.

– Ostwald stage, in which large clusters increase due to small clusters. At the same time, the numerical density of clusters decreases.

Tasks.

1. Find and plot the dependence of the average radius of the cluster and of the numerical density of clusters as a function of time.

2. Determine the size of the critical cluster.

3. Determine and plot the dependence of the average radius of the cluster and of the numerical density of clusters as a function of time at the fluctuation stage.

4. Determine and plot the dependence of the average radius of the cluster and of the numerical density of clusters versus time at the deterministic stage.

5. From the analysis of the received data, draw a conclusion about whether it has been achieved Ostwald stage cluster system.

Control questions.

1. What are the types of point defects in solids?

2. What stages are characteristic of the evolution of clusters in irradiated metals, semiconductors and polymers?

3. What are the limits of using the cluster dynamics method?

4. What are the main equations of cluster dynamics?

5. What are the features of the fluctuating and deterministic stages?

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6. What is the definition of a critical cluster?

7. How is the master equation of cluster dynamics integrated?

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