Formation and evolution of radiation defects under low-temperature neutron irradiation

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Abstract

In studies of processes occurring in materials under neutron irradiation, temperature, radiation damage rate, and displacement dose are typically employed as characteristic parameters. However, these parameters alone are insufficient for describing microstructure evolution, which depends on both the quantity of generated point defects and their spatial configuration. Therefore, the present study proposes a consistent framework for describing the formation and evolution of radiation defects under low-temperature neutron irradiation. The distinguishing feature of this approach is the utilization of a statistical model for defect migration. For describing the cross sections of neutron-atom interactions (as a function of neutron energy), analytical fitting procedures are implemented, enabling calculations without requiring expensive high-performance computing systems. This methodology was applied to characterize the evolution of radiation defects in chromium (as a prototype BCC structure) subjected to low-temperature neutron irradiation in the IVV-2M reactor. The calculated results exhibit good agreement with experimental data on the number of vacancies accumulated in the sample during irradiation, as obtained from dilatometer measurements. The developed approach is anticipated to be broadly applicable for describing defect formation and evolution in both pure metals and alloys under irradiation across a wider temperature range and in reactors with various neutron spectra.

Full Text

Formation and Evolution of Radiation Defects Under Low-Temperature Neutron Irradiation

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Abstract

In studies of processes occurring in materials under neutron irradiation, temperature, the rate of radiation damage, and the damaging dose are conventionally used as characteristic parameters. However, these characteristics are insufficient for describing microstructure evolution since it depends on both the number of generated point defects and their spatial configuration. Consequently, the current study proposes a consistent approach for describing the formation and evolution of radiation defects under low-temperature neutron irradiation. The distinctive feature of this approach is the use of a statistical model of defect migration. For describing the cross sections of interactions between neutrons (depending on their energies) and atoms, a fitting procedure for analytic expressions is performed, enabling calculations without requiring expensive high-performance computing systems. This approach was applied to describe the evolution of radiation defects in chromium (as a BCC structure prototype) exposed to low-temperature neutron irradiation in the IVV-2M reactor. The calculated results show good agreement with experimental data regarding the number of vacancies accumulated in the sample during irradiation, as obtained through dilatometric measurements. The developed approach is expected to be universally applicable for describing defect formation and evolution in both pure metals and alloys under irradiation across a wider temperature range in reactors with various neutron spectra.

Keywords: Low-temperature neutron irradiation; neutron energy spectrum; primary knock-on atom spectrum; point defects; point defect complexes; interstitial atom migration energies.

1. Introduction

Temperature, the rate of irradiation damage, and the damaging dose are conventionally used as characteristic parameters in studies of processes occurring in materials under neutron irradiation. Since the evolution of point defects generated during irradiation depends on both their number and cluster configuration, the irradiation damage rate alone is insufficient to describe the evolution of point defect assemblies. More detailed information about the spatial distribution of developing defects is also required. Three stages are typically distinguished in describing the generation and evolution of point defects under neutron irradiation \cite{1–3}: (i) a dynamic stage characterized by the non-equilibrium state of the system in the region of energy transfer from neutrons to atoms; (ii) a kinetic stage when the system is in a metastable (quasi-stationary) state in the local region of cascade formation; and (iii) a thermodynamic (diffusion) stage when defects leave the cascade region and subsequently migrate throughout the crystal, resulting in microstructure evolution. The resulting structural variations depend on both the characteristics of neutron energy transfer to atoms and the redistribution of energy among them, as well as on the mobility of point defects and their interaction with the microstructure [**?**, **?**]. The latter characteristics are obtained primarily from computer simulations, often using molecular dynamics methods that are insufficiently verified against experimental data \cite{6–8}. Instead, comparisons with earlier calculations by other authors are performed, which are assumed to "verify" the approach. The greater the uncertainty of the characteristics used in subsequent diffusion process calculations, the less reliable the predictive estimates for microstructure evolution become.

One approach to obtaining more reliable data is neutron irradiation at temperatures where both types of point defects lack thermal mobility—namely, cryogenic neutron irradiation. Such investigations were conducted using the IVV-2M reactor during 1987–1998 [**?**, **?**] when studying the radiation resistance of materials for the ITER superconducting magnetic system. However, this technology was later abandoned and subsequently lost.

Currently, the IVV-2M reactor enables low-temperature neutron irradiation under which interstitials are mobile while vacancies have almost no ability to migrate throughout the crystal [**?**]. This type of study simplifies the description of point defect evolution under irradiation and the interpretation of experimental data.

The goals of the current study are: (1) to develop a computational approach for the formation and evolution of point defect complexes in metals based on an alternative stochastic model of defect migration for low-temperature neutron irradiation conditions, as an alternative to molecular dynamics methods \cite{12–14}; (2) to perform low-temperature neutron irradiation of Cr as a representative of BCC structures and describe the evolution of radiation defects using the proposed scheme; (3) to conduct post-irradiation electron microscopy and dilatometric studies to experimentally evaluate the number of vacancies accumulated in the sample during irradiation using a specialized procedure; and (4) to verify the calculated characteristics of point defects and their complexes accumulated in Cr under irradiation in the IVV-2M reactor based on experimental data from post-reactor studies.

2. Materials and Methods

Irradiation was performed in the IVV-2M reactor using a specialized cell 6-14 where, according to preliminary thermometric experiments, the temperature did not exceed 45 °C. To characterize the neutron spectrum, a set of indium detectors was used. Based on the specific activities obtained during the experiment, the fluence of neutrons in different energy ranges was calculated using a certified precision program implementing the Monte-Carlo MCU-PTR procedure (certificate No. 498 dated December 14, 2020). The results are presented in Table 1

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2.1 Estimation of Primary Damage at the Dynamic Stage

The calculations performed in this study involve several physical quantities and designations, which are explained in Table 2 .

Estimation of primary damage at the dynamic stage was performed using the procedure described in [**?**, **?**, **?**]. First, the neutron energy spectrum was determined based on experimental results from neutron detectors using a spectrum calculation program. The energy range division was specified in this program and is represented by a 26-group standard structure in the current study. The neutron cross-section for interaction conditions was determined as the probability per unit area for a neutron with energy E_n to interact with nuclei in the irradiated material. These characteristics were taken from the ENDF/B-VII.1 Incident-Neutron Data [**?**]. If the energy transferred to an atom exceeds the threshold for Frenkel pair formation, a primary knock-on atom is created. Different amounts of energy can be transferred during collision depending on the relative orientation of neutron and atom positions. Since this process is stochastic, averaging over all possible collisions is required to determine the residual energy of the primary knock-on atom.

Consider the elastic collision of a neutron and a nucleus. In the elastic model, the momentum of the incident neutron can be decomposed into a component along the line connecting the centers and a perpendicular component that does not transfer momentum to the atom, as shown in Fig. 1 [Figure 1: see original paper]. The averaging procedure is carried out first over the angle of rotation in the plane, and then the obtained value undergoes averaging over all possible directions of neutron incidence relative to the atom. Based on momentum and energy conservation laws, the mean value of energy E_a transferred to an atom during elastic collision was obtained:

$$E_a = \alpha E_n$$

where $\alpha = \frac{4m_n m_a}{(m_n+m_a)^2}$ is the coefficient of kinetic energy transfer from neutron to atom, and m_n and m_a are the neutron and atom masses, respectively.

The transfer of neutron energy and momentum to atoms depends on the elastic interaction cross-section. Under this probability implementation, the neutron transfers to the atom energy that can be averaged over various spatial configurations of neutron-atom collisions and evaluated by Expr. 1. When this energy exceeds the threshold for Frenkel pair formation, a primary knock-on atom appears.

The build-up rate of primary knock-on atom formation with neutron flux density in the energy range from E_n to $E_n + dE_n$ is calculated by the expression:

$$\frac{dN_{pka}}{dt} = \sigma(E_n)\phi(E_n)n_a dE_n$$

where n_a is the number of atoms per unit volume.

Since analytic expressions for the dependence of neutron flux density on neutron-atom interaction cross-section could not be established for the entire energy range, the former was divided into intervals where analytic dependencies of neutron flux density ϕ_i and cross-sections σ_j were found.

The build-up rate of primary knock-on atom formation was estimated by the following expression:

$$\frac{dN_{pka}}{dt} = \sum_{i,j} \sigma_j \phi_i n_a$$

where i and j are interval numbers.

Each primary knock-on atom generates a certain number of displaced atoms. In the energy range of primary knock-on atoms from E_{pka} to $E_{pka} + dE_{pka}$, the number of Frenkel pairs is one when $E_{pka} < 2.5$ keV, while at higher energies this amount is proportional to $E_{pka}^{2/3}$, which is associated with partial energy transfer to the electronic subsystem \cite{1–5}.

Hence, taking into account Expr. 1, the build-up rate of point defect generation by neutrons from energy range ij at the dynamic stage is:

$$\frac{dN_{dp}}{dt} = \sum_{i,j} \nu(E_{pka})\sigma_j \phi_i n_a$$

where $\nu(E_{pka})$ is the number of Frenkel pairs created by a primary knock-on atom.

Expr. 4 was adjusted to account for the fact that at energies of primary knock-on atoms above a certain threshold energy E_{pka}^i, some secondary atoms receive sufficient energy to produce new subcascades. The cascade breaks into subcascades. The energy range for primary knock-on atoms in the current study, as in [**?**], was divided into 25 keV intervals. The energy distribution in the first interval was assumed to be proportional to E_{pka}^1. Each primary knock-on atom with energy exceeding 25 keV creates a number of subcascades equal to:

$$N_{sub} = \frac{E_{pka}}{25 \text{ keV}}$$

2.2 Evolution of the Displacement Cascade at the Kinetic Stage

Selection of analytical approximations is required to perform calculations for the functions included in Expr. 2–4. The evolution of defects at the kinetic stage depends strongly on the cascade region area and the concentration of point defects created at the dynamic stage. Since atom displacement during Frenkel pair formation occurs at distances exceeding the spontaneous recombination radius, a primary knock-on atom with energy E_{pka} creates N_{FP} point defect pairs. The number of jumps equals the number of point defects formed.

In the displacement cascade description, Frenkel pair formation is considered a stochastic process. In this case, the interstitial atom moves away from the vacancy remaining at the collision site of the primary knock-on atom with a lattice atom to a distance greater than the spontaneous recombination radius. The generated point defects are located randomly within this diameter. The process of point defect formation is spatially heterogeneous.

Under elastic collision of the primary knock-on atom with kinetic momentum p, flying past an impacted atom at distance b from its center, the transferred kinetic momentum can be found as:

$$\Delta p_z = \frac{2pb}{r_a}$$

and in the perpendicular direction:

$$\Delta p_x = \frac{pb}{r_a}$$

where r_a is the atomic radius.

Averaging over b from 0 to $2r_a$ results in:

$$\langle \Delta p_z \rangle = \frac{p}{2}$$

Further, we assume that the probability of flying over in a certain direction is proportional to the momentum transferred in that direction. A line along which the momentum of a primary knock-on atom is directed was chosen as the z-axis. Knock-on atom jumps provide orientation either along the z-axis (in the positive direction only), or in one of the orthogonal x or y directions. Taking into account normalization conditions:

$$w_z + 2w_x = 1$$

the probability of performing a jump along the z-axis is:

$$w_z = \frac{\langle \Delta p_z \rangle}{\langle \Delta p_z \rangle + 2\langle \Delta p_x \rangle}$$

and that for x and y directions:

$$w_x = w_y = \frac{1 - w_z}{2}$$

Statistical thermodynamics indicates that for jump probability w in prescribed directions during N jumps, the distance from the initial point is:

$$R = a\sqrt{Nw(1-w)}$$

where a is the distance to the closest lattice site (in the crystallographic direction $[\frac{1}{2}\frac{1}{2}\frac{1}{2}]$), and $l = a \times N$ is the jump distance under Frenkel pair formation conditions. This distance must exceed the spontaneous recombination radius, which is accepted to be $1.2a \times \sqrt{N}$. As a result, the cascade area exhibits an ellipse-like shape elongated in the direction of primary knock-on atom movement. The length of the semi-axis along the primary knock-on atom momentum is:

$$L_z = aNw_z$$

and that for the lateral direction:

$$L_x = a\sqrt{Nw_x}$$

where N is the number of jumps in the cascade, equal to the number of Frenkel pairs at the dynamic stage.

The volume of the elliptic cascade area is defined as:

$$V_{cascade} = \frac{4}{3}\pi L_z L_x^2$$

which is equivalent to a sphere with an effective diameter:

$$d_{eff} = 2\left(\frac{3V_{cascade}}{4\pi}\right)^{1/3}$$

Hence, the cascade area in subsequent calculations is considered spherical with diameter d_{eff}.

According to Table 3 , Frenkel pair recombination in the BCC crystal lattice occurs when the distance between vacancy and interstitial is less than five coordination shells. The sixth coordination shell, consisting of 6 sites, is located at a distance exceeding the spontaneous recombination radius. Thus, a Frenkel pair forms when the interstitial atom moves beyond the fifth coordination shell.

Cascade distributions by generated defects were obtained using the primary knock-on atom spectrum. Typically, the size of the area occupied by the cascade formed at the kinetic stage is calculated using molecular dynamics approaches. We employed the statistical migration model \cite{12–14}, where the Frenkel pair formation process is treated as random, with the maximum distance of the formed pair from the collision point with the primary knock-on atom calculated by d_{eff}. Generated point defects are randomly located in the region of effective diameter d_{eff}. The relative concentration of point defects in the cascade can be identified using data about the region size and the number of Frenkel pairs inside:

$$c_{i(v)} = \frac{N_{FP}}{V_{cascade}} \times W$$

where W is the volume per atom (here $W = a^3/2$).

To describe subcascade evolution at the kinetic stage, concepts of spontaneous recombination processes and formation of complexes of identical point defects were applied. According to these concepts, the processes occur under the influence of elastic fields when defects are found at distances not exceeding critical values. The radius of spontaneous recombination, as well as the spontaneous formation of di-interstitials and di-vacancies, is associated with elastic fields created by point defects in the crystal lattice. During recombination and complex formation, the energy gain is:

- $\Delta E_{rec} = E_i + E_v$ for Frenkel pair recombination
- $\Delta E_{ii} = 2E_i - E_{ii}$ for di-interstitial formation
- $\Delta E_{vv} = 2E_v - E_{vv}$ for di-vacancy formation

where E_i and E_v are the formation energies of interstitials and vacancies, respectively; E_{ii} is the energy for di-interstitials; and E_{vv} is the energy for di-vacancies.

According to [**?**], the spontaneous recombination radius was assumed to be equal to two nearest-neighbor distances. When estimating radii for spontaneous generation of di-interstitial complexes and di-vacancies, it was assumed that the interstitial formation energy has twice the value of that for vacancies. Thus, the radius for spontaneous formation of di-interstitials was taken as $1.7a$, and that for di-vacancies as $1.2a$.

If the interstitial concentration in the cascade area is c_i, the probability of finding no interstitial site in a position close to a vacancy equals $1 - c_i$. The probability that the interstitial will be found neither in the first nor second positions is $(1 - c_i)^2$. The recombination region in BCC materials includes five coordination shells located at distances equal to or less than the spontaneous recombination radius. Further calculations for other coordination shell positions given in Table

3 reveal the probability of finding no interstitial in the region of spontaneous recombination:

$$w_{rec} = 1 - (1 - c_i)^{s_{rm}}$$

where c_i is the interstitial concentration in the cascade region at the dynamic stage, and s_{rm} is the number of sites in surrounding coordination shells involved in the vacancy recombination region. Consequently, the recombination probability is:

$$P_{rec} = 1 - w_{rec}$$

According to the accepted values of radii for spontaneous formation of interstitial and vacancy complexes, the radius for spontaneous formation of interstitial atom pairs equals the radius of the corresponding coordination shell. If an interstitial occurs in a region containing another interstitial (and the recombination area contains no vacancy), then a complex of two interstitials forms. The same applies to vacancies, but their spontaneous capture radius is assumed equal to that of the second coordination shell, as shown in Table 3. Thus, the probability that an interstitial at the kinetic stage does not recombine and does not form a bound state (remains single), w_{ik}, is defined by:

$$w_{ik} = 1 - P_{rec} - P_{ii}$$

where P_{ii} is the probability of di-interstitial formation. Similarly, for a vacancy, taking into account the radius size for the region of spontaneous capture:

$$w_{vk} = 1 - P_{rec} - P_{vv}$$

where P_{vv} is the probability of di-vacancy formation, and s_{vv} is the number of sites in surrounding coordination shells involved in the region of spontaneous generation of di-vacancies.

Expressions 21 and 22 permit evaluation of the number of single interstitials and vacancies remaining at the end of the kinetic stage. The probability to produce any interstitial complex P_{ick} is defined by:

$$P_{ick} = 1 - w_{ik}$$

and that for vacancy complexes P_{vck}:

$$P_{vck} = 1 - w_{vk}$$

Similarly, taking into account probabilities of various mutual positions of point defects, expressions can be obtained to calculate the generation probability for more complex defects.

The calculated generation rate for point defects at the dynamic stage according to Expr. 4, combined with recombination probabilities and point defect complex formation probabilities according to Expr. 19–24, allows evaluation of the accumulation rate for single point defects at the kinetic stage of subcascade formation:

$$\frac{dN_{i(v)k}}{dt} = \sum_{i,j} \nu(E_{pka})\sigma_j \phi_i n_a w_{i(v)k}$$

where $w_{i(v)k}$ is defined in accordance with Expr. 21 and Expr. 22.

Similarly, the number of point defects contained in complexes can be evaluated using $P_{i(v)ck}$ instead of $w_{i(v)k}$:

$$\frac{dN_{i(v)ck}}{dt} = \sum_{i,j} \nu(E_{pka})\sigma_j \phi_i n_a P_{i(v)ck}$$

where $P_{i(v)ck}$ is the generation probability for point defect complexes calculated using Expr. 23 and Expr. 24.

Along with spontaneous processes, migration of interstitial sites occurs. The latter process allows interstitials to leave the cascade region and enter the matrix, with a possibility to recombine with vacancies along this path. It was shown that during the kinetic stage of irradiation, only a tiny number of interstitial jumps occurs, so nearly all remain within the cascade region.

2.3 Displacement Cascade Evolution at the Diffusion Stage

Since the majority of interstitial sites have not left the cascade region by the end of the kinetic stage, they continue to escape during the thermodynamic (diffusion) stage. While migrating through the vacancy-enriched cascade region, interstitial sites can either recombine with vacancies (reducing their number) or escape into the matrix. When an interstitial site is located at distance r from the cascade center, it must move radially outward to leave the cascade region, as shown in Fig. 2 [Figure 2: see original paper]. The number of interstitial sites found in a spherical layer of thickness dr is:

$$dN = 4\pi r^2 c_i(r) dr$$

Averaging over distance from the cascade region center yields the average radial distance:

$$\langle r\rangle = \frac{\int_0^{R_c} r \cdot 4\pi r^2 c_i(r)dr}{\int_0^{R_c} 4\pi r^2 c_i(r)dr}$$

Hence, the average number of jumps required for an interstitial site to escape the cascade region is:

$$N_{jump} = \frac{\langle r\rangle}{a}$$

where the subscript "t" indicates that this number of jumps occurs at the thermodynamic (diffusion) stage.

The probability for an interstitial site to encounter a vacancy at the first jump is defined by c_v, and the probability to miss the vacancy is $1 - c_v$. The probability for an interstitial site to leave the cascade region without on-the-way recombination is:

$$w_{esc} = (1 - c_v)^{N_{jump}}$$

while the probability of recombination during migration before leaving the cascade region is:

$$P_{rec,t} = 1 - w_{esc}$$

Vacancy concentration in the cluster after spontaneous processes at the kinetic stage is defined by:

$$c_{v,k} = c_{v,0} \times w_{vk}$$

and that after the thermodynamic stage:

$$c_{v,t} = c_{v,k} \times w_{esc}$$

Substituting w_{esc} from Expr. 32, assuming $c_v \ll 1$, gives:

$$c_{v,t} \approx c_{v,k} \exp(-c_v N_{jump})$$

Thus, the expression for point defect accumulation at the thermodynamic stage takes the form:

$$\frac{dN_{i(v)t}}{dt} = \sum_{i,j} \nu(E_{pka})\sigma_j\phi_i n_a w_{i(v)k} w_{esc}$$

The proposed technique allows estimation of displacement cascade evolution at the dynamic, kinetic, and thermodynamic (diffusion) stages.

3. Results and Discussion

The methodology described above was applied to characterize defect evolution in displacement cascades in Cr under low-temperature irradiation in IVV-2M. For calculations, an energy-dependent interaction cross-section between neutrons and atoms, shown in Fig. 3 [Figure 3: see original paper], was utilized (based on data from [**?**]).

Conventionally, calculating the rate of point defect generation uses a discrete representation with small energy steps, requiring operation with large data tables and engaging information-intensive high-speed tools (for instance, [**?**]). For the present calculations, an analytical dependence of the elastic interaction cross-section between neutrons and Cr atoms, $\sigma(E_s)$, on neutron energy was selected.

To select analytical approximations for primary knock-on atoms capable of forming Frenkel pairs, the neutron energy range was split into sub-ranges j, where the computer fitting criterion R^2 is close to 1. For analytical description, a polynomial model was used:

$$\sigma_j(E_n) = \sum_{k=0}^{m} a_{jk} E_n^k$$

The subdivision of the neutron energy spectrum into intervals and polynomial coefficients from Expr. 35 are given in Table 4 .

For instance, Figs. 4 and 5 demonstrate graphical views of elastic interaction cross-sections for neutrons and atoms and fitting lines for intervals $j = 1$ and $j = 2$.

To evaluate the accumulation rate of primary damage according to Expr. 25, an analytical approximation was applied for the dependence of neutron flux density on energy, $\phi(E_n)$, to satisfy:

$$\phi_i = F_i \cdot f(E_n)$$

where F_i is the neutron flux in energy group i, and $f(E_n)$ is a fitting function.

To construct an expression for neutron flux density, the dependence was obtained and a fitting model for the function was selected. Since selecting such a function across the entire neutron energy range is rather complicated, the range was divided into four intervals, as shown in Fig. 6 [Figure 6: see original paper].

Neutron flux density in specific intervals was approximated by the function:

$$\phi_i(E_n) = \exp\left(\sum_{k=0}^{n} b_{ik}(\ln E_n)^k\right)$$

where i is the interval number in the range subdivision for fitting the neutron flux density function, and b_{ik} are coefficients describing the differential density. The dependence of neutron flux density on average interval energy, energy intervals, and coefficients from Expr. 37 are shown in Fig. 6.

To enable calculation of defect generation rates at the dynamic stage (with respect to results in Table 4 and Fig. 6), the overall neutron energy range was divided into 10 intervals where the number of generated point defect pairs was estimated by:

$$N_{dp} = \int_{E_{min}}^{E_{max}} \nu(E_{pka})\sigma(E_n)\phi(E_n)n_a dE_n$$

Table 5 shows neutron energy interval ranges ij and corresponding analytical expressions for indefinite integrals.

The energy threshold for Frenkel pair formation in Cr was accepted to be 40 eV [**?**]. The dependence of point defect generation rate in cascades at the dynamic stage on average neutron energy, calculated by Expr. 4, is shown in Fig. 7 [Figure 7: see original paper].

The total generation rate of point defects at the dynamic stage was obtained to be 1.2×10^{-6} dpa/s. The main contribution to point defect generation comes from neutrons in the spectrum energy range from 0.2 to 12.8 MeV.

For calculating defect evolution in displacement cascades at the kinetic stage using Expr. 21, Expr. 22, and Expr. 25, the number of sites contributing to recombination (s_{rm}) when point defects occur, or forming complexes of identical defects (s_{iim}, s_{vvm}), must be estimated. The parameters of coordination spheres enabling this estimation are given in Table 3, yielding:

$$s_{rm} = 42, \quad s_{iim} = 8, \quad s_{vvm} = 6$$

The obtained dependence of accumulation rates for vacancies and interstitial sites on average neutron energy at the kinetic stage is shown in Fig. 8 [Figure 8: see original paper].

The number of interstitial sites at the thermodynamic stage that recombine when leaving the cascade region, with respect to expressions for interaction probability of point defects leaving the cascade region (Expr. 32 and Expr. 33), is defined by Expr. 34. Using Expr. 40, the vacancy accumulation dependence (see Fig. 9 [Figure 9: see original paper]) in the cascade region at the thermodynamic stage on average neutron energy can be obtained. Similar values at the kinetic stage are provided for comparison.

According to performed calculations, the relative number of accumulated vacancies in clusters during irradiation for 179 hours is 2.3×10^{-5}. With respect to elastic distortions, since vacancy presence enlarges the volume by $0.85 \times W$ (W being the volume per atom), one remaining vacancy in the isotropic case reduces linear dimensions by $0.15 \times W^{1/3}$. Dilatometric measurements produce differential dilatograms (the elongation difference between irradiated and unirradiated samples during heating) that allow verification of the performed calculations for generation and evolution of point defects in Cr under low-temperature neutron irradiation. The experimental differential dilatogram is shown in Fig. 10 [Figure 10: see original paper]. The dashed line indicates the relative variation of elongation expected when the calculated amount of accumulated vacancies leaves the sample. The comparison reveals that the measured dimensional variation is larger than estimated from the calculated amount of generated vacancies. This can be associated with vacancies causing a volume decrease of 0.85 atomic volumes when they leave the sample. If vacancies are absorbed by internal sinks (dislocations, grain boundaries, etc.), the volume variations appear lower.

4. Conclusion

The evolution of displacement cascades at dynamic, kinetic, and thermodynamic stages under low-temperature neutron irradiation was investigated. The following results were obtained:

- A calculation method for point defect formation and evolution in metals was developed. Its peculiarity is the application of a statistical defect migration model at kinetic and thermodynamic stages, combined with analytical tools for primary damage at the dynamic stage based on literature data.
- A fitting procedure was proposed for analytical expressions describing the dependence of neutron-atom interaction cross-sections on neutron energy.
- Application of the alternative stochastic defect migration statistical model, instead of molecular dynamics approaches, was shown to reliably provide analytical description of displacement cascade evolution at the kinetic stage while significantly simplifying calculations.
- Cr irradiation was performed in the IVV-2M reactor at 40–45 °C for 179 hours, followed by dilatometric measurements. The obtained results, combined with pre-irradiation studies, enabled assessment of vacancy concentration accumulated during irradiation.
- Generation and accumulation rates for vacancies were calculated using the developed approach, and verification against dilatometric measurements of dimensional variations caused by vacancy release during heating was performed. Calculated results and experimental data showed satisfactory agreement.

The combination in one study of calculation method development for defect accumulation, experimental determination of vacancy concentration developed under irradiation, and results verification makes the study complete. The developed approach can be applied to describe generation and evolution of defects not only in pure metals but also in alloys under irradiation in reactors with various neutron energies at different temperatures.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Authorship Contribution

Kozlov A.V.: Conceptualization, Data curation, Formal analysis, Methodology, Software, Validation, Writing - original draft.
Glushkova N.V.: Project administration, Methodology, Formal analysis.
Kozlov K.A.: Data curation, Visualization, Writing - review & editing.
Ladeyschikov K.M.: Investigation, Methodology, Visualization.
Panchenko V.L.: Investigation, Methodology.
Shabelnikov E.V.: Validation.
Zyryanova A.A.: Supervision, Investigation, Visualization.

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Note: Figure translations are in progress. See original paper for figures.