Driven Diffusion of Radiation Defects in α-Uranium by Temperature/Stress Gradients: Molecular Dynamics Insights into Anisotropy and Directional Migration

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Abstract

The anisotropic diffusion of irradiation defects in α-uranium (α-U) has been investigated using classical and nonequilibrium molecular dynamics methods, with the aim of better understanding the complex response of the microstructure to irradiation damage, which depends on temperature and internal stress. Our results show that (i) both vacancy and self-interstitial atoms exhibit significant anisotropic diffusion characteristics at elevated temperatures, arising from their unique diffusion mechanisms. The difference in anisotropic diffusion rates between the two species strongly supports the previously proposed hypothesis of the irradiation growth mechanism. (ii) When a temperature gradient exists, the additional driving force introduced by the gradient accelerates the diffusion of vacancy and interstitial atoms, causing both to move directionally toward the high temperature region. Kinetic modeling suggests that the direction of this driving force is primarily determined by the sign of the 'heat of transport Q' and the direction of the temperature gradient together. (iii) The stress gradient field similarly promotes the anisotropic diffusion of vacancies and interstitial atoms. Additionally, the stability and migration behavior of defects change with the stress state, leading to species separation under stress gradients. We showed that the stress effect can be well predicted by the continuum model based on the formation volume tensor of point defects. (iv) A change in the sign of the migrating volume tensor alters the monotonicity of the migration barrier with respect to stress. This study provides valuable new insights into the complex irradiation damage behavior of α-U and, for the first time, reveals how the gradient environment within the reactor interacts with irradiation defects.

Full Text

Preamble

Driven Diffusion of Radiation Defects in α-Uranium by Temperature/Stress Gradients: Molecular Dynamics Insights into Anisotropy and Directional Migration

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The anisotropic diffusion of irradiation defects in α-uranium (α-U) has been investigated using classical and nonequilibrium molecular dynamics methods, with the aim of better understanding the complex response of the microstructure to irradiation damage, which depends on temperature and internal stress. Our results show that (i) both vacancy and self-interstitial atoms exhibit significant anisotropic diffusion characteristics at elevated temperatures, arising from their unique diffusion mechanisms. The difference in anisotropic diffusion rates between the two species strongly supports the previously proposed hypothesis of the irradiation growth mechanism. (ii) When a temperature gradient exists, the additional driving force introduced by the gradient accelerates the diffusion of vacancy and interstitial atoms, causing both to move directionally toward the high-temperature region. Kinetic modeling suggests that the direction of this driving force is primarily determined by the sign of the 'heat of transport Q' and the direction of the temperature gradient together. (iii) The stress gradient field similarly promotes the anisotropic diffusion of vacancies and interstitial atoms. Additionally, the stability and migration behavior of defects change with the stress state, leading to species separation under stress gradients. We showed that the stress effect can be well predicted by the continuum model based on the formation volume tensor of point defects. (iv) A change in the sign of the migrating volume tensor alters the monotonicity of the migration barrier with respect to stress. This study provides valuable new insights into the complex irradiation damage behavior of α-U and, for the first time, reveals how the gradient environment within the reactor interacts with irradiation defects.

Keywords: Molecular dynamics simulation, Driven diffusion, Irradiation defects

INTRODUCTION

As a solid-state uranium allotrope at low temperatures (< 940 K), the orthorhombic α-U is important in both engineering considerations and basic science. Understanding the effects of irradiation damage to α-U is critical for modeling the behavior of U-based metallic fuels, as it is a key component of certain metallic fuels used in fast reactors (e.g., U-Zr, U-Pu-Zr, U-Mo). The α-U consists of corrugated atomic sheets in a highly asymmetric face-centered orthorhombic crystal structure [?]. As a result, both the parallel and perpendicular corrugated planes exhibit unique physical properties, such as thermal expansion [?] and elastic constants [?]. Its high anisotropy and temperature-dependent response to irradiation offer new insights into understanding irradiation effects in metals.

In the late 1940s and early 1950s, significant efforts were made to develop an understanding of the anisotropic thermal expansion [?, ?] and radiation creep [?] of α-uranium. Another behavior of significant interest is the anisotropic irradiated growth [?]. Loomis et al. [?] measured the irradiation growth rate of single-crystal α-U samples, and their work determined that the single-crystal samples grew in the [010] direction, contracted in the [100] direction, and remained constant in the [001] direction, with the total volume of the crystals conserved during irradiation growth. In polycrystalline α-U, irradiation growth can cause tearing along grain boundaries and the formation of crystallographically aligned pores [?, ?, ?], leading to significant volume changes in the fuel. These porosities are believed to result from the interaction of lattice defects and stresses induced by radiation and temperature gradients [?]. The mechanism of irradiated growth in α-U is currently unclear. Seigle and Opinsky [?] suggested that the dimensional instability of irradiated α-U materials may be driven by the anisotropic diffusion of SIAs and vacancies along the [010] and [100] crystal directions. They assume that lattice defects generated during irradiation can anisotropically diffuse to and be eliminated at grain boundaries and free surfaces. In this process, interstitial atoms cause lattice expansion, while vacancies lead to lattice contraction at the grain boundaries. If diffusion is sufficient and the fluxes remain imbalanced, macroscopic growth can be observed. Another proposed mechanism for irradiated growth is driven by an anisotropic arrangement of interstitial and vacancy loops. This hypothesis is based on the first thin-film transmission electron microscopy measurements conducted by Hudson et al. [?], which observed the formation of dislocation loops in α-U after neutron irradiation, although the nature of these loops remains unclear. Generally, the evolution of microstructures under irradiation conditions is governed by the migration of isolated defects and clusters of small defects. Whether arising from the net diffusive flux of point defects or the anisotropic condensation of vacancy and interstitial defects into planar clusters, the dominant mechanism of α-U irradiation growth behavior is closely linked to the anisotropic diffusion of point defects. Therefore, understanding the behavior of irradiated defect motion at high temperatures can provide valuable insights into the α-U irradiation growth mechanism and the evolution of cavity structures. It is also crucial to employ advanced characterization and simulation techniques to study the atomic-level behavior of point defect diffusion.

Due to the inherent challenges of conducting experimental studies, computational simulation techniques are widely used in design and development within the nuclear field. Several studies on the fundamental properties of point defects in α-U, based on density functional theory (DFT) and molecular dynamics (MD) methods, have been conducted. Beeler et al. [?] reported the defect formation energies of α-U at temperatures ranging from 100 K to 800 K using ab initio molecular dynamics (AIMD) and investigated the lattice strains induced by point defects. Their findings indicated that strains caused by isolated point defects are unlikely to be the primary cause of the significant irradiation-induced dimensional changes observed in the experiments. Huang et al. [?] calculated the formation energies and migration barriers of intrinsic point defects in α-U using the DFT method. Their results show that the migration of point defects in α-U is highly anisotropic and confirm that the self-diffusion phenomenon is dominated by the vacancy mechanism. Later, Wang et al. [?] investigated the diffusion of mono- and dimeric defects in α-U under high-temperature conditions using the MD method. They demonstrated that the diffusion of vacancies and di-vacancies exhibited strong anisotropy, while interstitials and di-interstitials were nearly isotropic. These studies provide valuable insights into the fundamental properties of point defects in α-U. Nevertheless, further investigation into the collective behavior of point defects is still necessary. Recently, a mean field cluster dynamics (CD) model was developed by Mazumder et al. [?] to predict the size and distribution of dislocation loops in α-U, which was then compared with the experimental results of Hudson et al. [?]. Their findings show that diffusion parameters, particularly the migration barrier, are sensitive to the size and number of dislocation loops.

In reactors, the fuel is subjected to harsh environments, such as irradiation, high heat loads, and thermal shocks. The coupling of radial temperature gradients with thermal stresses due to anisotropic expansion results in a complex microstructural evolution in α-U. Recent modeling studies have shown that temperature changes of 50 to 100 K are enough to generate stresses on the order of hundreds of MPa, which can initiate plastic flow or cracking [?]. Irradiation growth-induced stresses can also lead to internal stresses of hundreds of MPa, even at very low levels of burnup [?]. Thermal and stress gradients act as additional driving forces that can influence the evolution of the structure [?]. When the gradients are sufficiently large, they can even drive the migration of grain boundaries and voids [?]. Given this, it is natural to associate the diffusive behavior of irradiated defects in α-U with the fact that they are likely influenced by temperature and stress inhomogeneities. Additionally, the formation and growth of various types of porosity observed experimentally [?] (such as small aligned or non-aligned pores, massive cavities, and jagged cavities along grain boundaries) may involve the directional aggregation of vacancies within the material, in addition to the effects of internal stress. The common explanation for porosity in metals is the localized accumulation of an excess concentration of vacancies, which then condense to form macroscopic voids. Pores are typically observed to develop within and at the interfaces of grains with different orientations. This may depend on several factors, such as the surface tension or creep strength of the material, as well as the presence of suitable nucleation sites for the precipitation of vacancies. Grain boundaries are typically regions of stress concentration and can therefore act as defect sinks, leading to the aggregation of vacancies. It is thus crucial to study the effects of temperature and stress inhomogeneities on the behavior of irradiated defects in α-U. However, no study has been conducted on the diffusion behavior of irradiated defects in gradient fields, either through experimental or computational methods.

This work systematically investigates the diffusion behavior of self-interstitial atom (SIA) and vacancy in single-crystal α-U under equilibrium temperature fields, temperature gradient fields, and stress gradient fields using the MD method. The irradiation response of polycrystalline α-U is influenced by the interaction between single-crystal behavior and grain boundaries, and is thus closely correlated with single-crystal properties. First, we investigated the diffusion behavior of vacancy and SIA at different temperatures, both of which were found to be highly anisotropic. Next, temperature and stress gradients were applied along each of the three axes (X, Y, and Z) to examine how the gradient fields affect the diffusion behavior of the defects. We found that the presence of these gradients leads to an accelerated diffusion rate and directional migration of the defects. The physical origin of the additional driving force is also explored. Finally, we discuss possible explanations for the experimentally observed phenomena and the general understanding of irradiation effects in α-U, and summarize the main findings.

II. METHODS

In this work, all simulations are performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [**?**]. A recently developed modified embedded-atom method (MEAM) potential, labeled MEAM_1 in the literature [**?**], has been used to characterize the interactions of uranium. Comprehensive test results demonstrate that this potential accurately describes the lattice constants, elastic constants, point defect properties, and surface energy of α-uranium. More importantly, it reliably captures the anisotropic diffusion behavior of point defects, thereby ensuring the credibility of subsequent simulations.

The simulation of defect diffusion in the equilibrium temperature field is performed in an orthogonal simulation box of a 12 × 12 × 12 α-uranium supercell containing 6912 atoms. Periodic boundary conditions were applied to all three directions. During the simulation, the perfect crystal was first equilibrated by relaxing for 100 ps in the isothermal-isobaric (NPT) ensemble with a timestep of 2 fs at a given temperature and zero pressure. The system was investigated over the temperature range of 400 K to 900 K with an interval of 100 K. Subsequently, a vacancy or interstitial was created by removing or adding an atom and allowed to evolve continuously under the NPT ensemble for 50 ns. Each simulation result was analyzed using OVITO software [**?**] to examine the defect diffusion trajectory. The α-U crystal structure is shown in Fig. 1 [Figure 1: see original paper], with the lattice parameters measured by Barrett [**?**] as a0 = 2.84 Å, b0 = 5.87 Å, c0 = 4.94 Å, and an offset fraction y = 0.102. Considering the anisotropic diffusion resulting from the asymmetry of the crystal structure, the defect diffusivity was measured as the total diffusion coefficient (Dtotal) and three principal tensor components (DX , DY , DZ). In this work, the Cartesian axes X, Y, and Z are oriented along the [100], [010], and [001] crystal directions, respectively. The diffusion coefficient of a defect in a specific direction can be obtained by tracking the mean square displacement (MSD) over the time length of the simulation as $\sum_{j=1}^{N} \Delta r_{i,j}^2$ where $\Delta r_{i,j}^2$ is the displacement of the jth atom in the system along direction i(i x, y, z), N is the total number of atoms in the system. Since the diffusion tensor is diagonal in orthorhombic crystal systems, the total defect diffusivity, expressed as the trace of the tensor, is Dtotal = DX +DY +DZ [**?**]. The MSD data processing employed a statistical ensemble averaging method [**?**] for smoothing, where individual trajectories were systematically decomposed into discrete independent segments of equal duration, followed by ensemble averaging to achieve enhanced statistical reliability. Each temperature condition was repeated 20 times to ensure statistically reliable results.

The effect of stress gradients on defect behavior cannot be ignored. In this study, a non-equilibrium molecular dynamics (NEMD) approach [**?**, **?**] was used to investigate how stress gradients with varying directions and magnitudes influence the diffusion behavior of point defects. This approach is primarily used to study the dynamic behavior and properties of the system when it is far from equilibrium. Fig. 2 [Figure 2: see original paper] illustrates a schematic of the stress gradient along the X-axis. A 60$×8×10*supercellboxcontaining*19200*atomswascreated*, *andaunidirectionalexternalforcealongtheX*−
axiswasappliedtoeachatomthroughoutthesimulation.*Thecollectiveeffectofthesedirectionalforcesgenerates*
and−*errormethodtopreventstructuralinstabilityfromexcessiveloading*.*Afterapplyinganappropriateforceal*
directiontoeachatomandmakingseveraladjustmentstotheX−*axisstrainofthebox*, *astablestressgradientinthe*
*directionwasachievedthrough*20*psofequilibrationinthecanonical*(*NVT*)*ensemble*.*Thesamestrategywasused*
supercells, respectively. The resulting stress distribution is shown in Fig. 3 [Figure 3: see original paper], with three different magnitudes of gradients considered for each direction. Note that all positive stress values in this paper represent tensile stresses, while negative values indicate compressive stresses. After the stress gradient is established, a point defect is introduced into the center of the box, and the simulation is continued for 50 ns under the NVT ensemble. The temperature was set to 700 K to ensure that sufficient diffusion occurred, and the MSD of the point defect was calculated to determine the diffusion coefficient. Repeat the simulation 20 times for each stress condition to obtain statistically robust results.

The temperature gradient model was constructed using the NEMD method [**?**], as shown in Fig. 4 [Figure 4: see original paper] (with the temperature gradient in the X direction as an example). A 50 × 6 × 8 supercell simulation box is constructed, and a vacuum layer of 10 Å thickness is introduced at both ends of the box by removing U atoms. This prevents interaction between the cold end (heat sink) and hot end (heat source) through periodic boundary conditions. The heat sink and heat source each consist of a 10 Å thick atomic layer, with the temperature of the heat sink set to 300 K, and the temperatures of the heat sources set to 500 K, 700 K, and 900 K, respectively. Before the temperature gradient is established, the entire system is relaxed in the NPT system for 100 ps at the specified temperature and zero pressure. This specified temperature is determined by the intermediate value of the temperature gradient interval to be established, e.g. 600 K for a temperature gradient interval of 300-900 K. This is done to expand the system volume to an equilibrium volume corresponding to the average temperature of the entire system in order to eliminate as much as possible the unevenness of thermal stresses due to differences in local thermal expansion after the temperature gradient is established. The maximum thermal stress gradient introduced, even at a heat source temperature of 900 K, is only 1.3 MPa/Å. Therefore, the effect of the thermal stress gradient caused by the temperature gradient during the simulation is considered negligible. The simulation is then performed in the microcanonical (NVE) ensemble, with only the heat source and heat sink thermally equilibrated by the velocity rescaling method to maintain their respective temperatures. After 20 ps of dynamic equilibrium, a stable temperature gradient is established, as shown in Fig. 5 [Figure 5: see original paper]. The temperature gradient is approximately 14.3 K/nm when the heat source temperature is 500 K, and increases to 28.6 K/nm and 42.9 K/nm as the heat source temperature rises to 700 K and 900 K, respectively. This gradient is nearly five orders of magnitude higher than that observed in nuclear fuel. However, such large gradients are essential for visualizing the effect of temperature gradients on the motion of point defects on the MD timescale.

After a stable temperature gradient was established, a point defect was introduced at the center of the box and allowed to evolve for 50 ns. Its MSD was recorded and used to calculate the diffusion coefficient. A simulation box with $10 \times 24 \times 8$ and $10 \times 6 \times 28$ supercells is used to establish temperature gradients in the Y and Z directions, respectively. This setup ensures that the heat flow in all three directions travels similar distances from the heat source to the heat sink, avoiding inconsistencies in the gradient magnitudes due to differences in lattice constants. Simulations were conducted 20 times for each temperature gradient condition to ensure the reliability of the results.

III. RESULTS AND DISCUSSION

A. Diffusion of point defects in equilibrium fields

The structure of orthorhombic α-uranium can be thought of as corrugated, with closely packed atomic layers centered around the (010) planes, loosely stacked in the [010] direction [**?**]. As a result, the physical properties of α-uranium show significant anisotropy both in the corrugation plane and in the direction perpendicular to the plane. The aim of this section is to explore the mechanisms of point defect diffusion and investigate the anisotropy in migration caused by different mechanisms. The diffusion coefficients of vacancy and SIA in α-U were investigated at different temperatures, as shown in Fig. 6 [Figure 6: see original paper]. Overall, the diffusion coefficients of the SIA are higher than those of the vacancy at all temperatures. The higher diffusivity of SIAs suggests they will migrate to sinks within the microstructure more rapidly than vacancies, resulting in an excess of vacancies within the material under irradiation, which favors the formation of vacancy loops or voids. Furthermore, both species display marked diffusion anisotropy in their migration behaviors.

Interestingly, we find that the diffusion coefficients of the SIA in the X- and Y-directions vary with temperature in a fixed ratio (DX /DY is approximately 0.22). By analyzing the motion trajectories of the defect, it is found that the SIA primarily diffuses in a dumbbell structure. The schematic is shown in Fig. 7 [Figure 7: see original paper] (a), and the cutaway view is presented in Fig. 7 (b). The SIA shares a lattice site with a lattice atom to form a $< 110 >$ dumbbell, which migrates as one of the split atoms kicks out the neighboring U atoms to form a new dumbbell structure one lattice site away, while the other atom moves to the regular site. This migration process occurs along the $< 110 >$ direction, and therefore involves diffusion in both the X and Y directions, which is the primary reason for the variation of DX and DY in a fixed ratio. It follows that DX /DY = $(0.5a0/0.5b0)^2$ from equation 1, considering the lattice constants a0 and b0 at 0 K, which are approximately equal to 0.23.

The diffusion of SIA along the Z-direction involves a special structure as shown in Fig. 7 (c). It involves three lattice sites, denoted as a three-site interstitial. Atoms b and c are aligned almost along the [001] direction, and atoms a and d are pushed off-site noticeably. This configuration has also been observed in DFT study [?] and shows highly favorable energies at 0 K. For long-range diffusion along the Z-direction, atoms a and b undergo rotation and reorientation around vacancy e, forming a $< 110 >$ dumbbell configuration as depicted in Fig. 7 (a). Concurrently, atoms c and d return to their respective lattice sites f and g. This process exhibits a migration barrier of 0.2 eV. The $< 110 >$ dumbbell formed by atoms a and b can diffuse within the X-Y plane. Alternatively, it may undergo further rotation, where atom b pushing atom h upwards to create a new three-site interstitial configuration. This sequence completes the migration of the SIA along the Z direction.

As illustrated in Fig. 6, the vacancy exhibits an exceptionally low diffusion coefficient along the Y-axis. This phenomenon can be attributed to the significant energy barrier encountered during migration along this direction, with our potential calculations yielding a migration barrier of 1.48 eV (compared to 1.24 eV from DFT calculations [?]). Such high activation energies make long-range vacancy diffusion along the Y-direction thermodynamically difficult on standard MD time scales. Consequently, the diffusion of vacancies in α-U is confined to the corrugated plane, as shown in Fig. 8 [Figure 8: see original paper]. Vacancies can only diffuse along the a-atom or b-atom, but not to neighboring corrugated planes.

The obtained diffusion coefficients are fitted to the Arrhenius relation $D(T) = D0\exp(-Em/kT)$, where k is the Boltzmann constant, and T is the temperature. The results are shown in Fig. 9 [Figure 9: see original paper], the pre-exponential factor D0 and the migration energy barrier Em, for the total diffusivity, as well as for the diffusivity in each crystallographic direction, are provided in Table 1 for each defect species. For vacancy diffusion, we are unable to obtain the diffusion coefficients along the Y-direction accurately due to its slow diffusion. As a result, the fit to the Arrhenius relation for vacancy diffusion in this direction was omitted. A comparison with the previously reported DFT study [?] of individual vacancy and interstitial at 0 K is also presented. As expected, the SIA demonstrates identical diffusion barriers of 0.16 eV along both the X and Y axes, marginally lower than the 0.20 eV barrier observed in the Z direction. However, the DFT study reveals that the SIA displays a lower migration barrier along the Z-axis direction. This discrepancy can be attributed to the high-temperature-induced lattice expansion within the α-uranium crystalline structure. The lattice expansion along the Z-axis results in less favorable migration due to increased diffusion path lengths. Although the same thermal expansion occurs along the X-axis at elevated temperatures, this effect is counterbalanced by concurrent lattice contraction along the Y-axis. The Y-axis compression reduces interatomic distances in this crystallographic direction, which lowers the activation energy potential barriers for planar migration. Based on our fitting results, the total diffusion barrier is approximately equal to the average of the barriers in the three directions. For the diffusion barrier of vacancy, the simulation results at high temperatures show a significantly lower barrier in the Z direction compared to DFT calculations. This difference is attributed to the negative thermal expansion in the Y direction, which reduces the curvature of the corrugated surface in Fig. 8. Specifically, the decrease in the y-value shortens the diffusion path of the vacancies to the b-atoms, thereby promoting the occurrence of diffusion. Meanwhile, the large D0 and higher migration barrier suggest that the diffusion coefficients are more sensitive to temperature changes. The diffusion coefficient of vacancy in the X direction increases rapidly with temperature compared to the other directions, and the diffusion rate of vacancy in this direction is faster than that of the SIA. This disparity between vacancy and interstitial mobility significantly diminishes their recombination probability, particularly pronounced at elevated temperatures. This suggests that vacancies may primarily migrate in the X direction at high temperatures. In contrast, the SIA exhibits the highest diffusion rate in the Y direction, making SIA diffusion in the Y direction particularly significant. These results provide supporting evidence for the hypothesis of Seigle et al. [?], which suggests that irradiated growth is primarily driven by anisotropic net fluxes of point-defect diffusion. The vacancy diffusion rate in the X direction is higher than that of the SIA, and the resulting net vacancy flux ultimately causes contraction in the X direction. Meanwhile, the high diffusivity of the SIA and the very low diffusivity of vacancies in the Y direction lead to lattice dimensional growth in this direction. The diffusivities of vacancies and SIA in the Z direction are of comparable magnitude, with the diffusion coefficient of SIA being slightly higher than that of vacancies at high temperatures. As a result, the material experiences only a slight elongation in this direction. Another related phenomenon is the formation of void superlattices observed in α-U at 773 K and 873 K [?]. We hypothesize that this may result from the diffusional anisotropy of interstitial atoms and vacancies, as previous studies have suggested that diffusional anisotropy, particularly one-dimensional diffusion, is the mechanism behind the formation of void superlattices in cubic metals [**?**]. Our simulation results reveal the complex anisotropic behavior of point defects in α-U at the atomic scale, providing a theoretical basis for understanding irradiation growth and the evolution of material structures under irradiation. Given that the diffusive behavior of individual defects may not be directly applicable to defect clusters or loops, rate theory or cluster kinetic theory is needed to further investigate the collective behavior of point defects at diffusional length and time scales at low burnups.

B. Diffusion of point defects in temperature gradient fields

Diffusing particles experience a drift motion in addition to random diffusion when an external driving force is applied. Temperature gradients in a material can also act as a driving force on diffusing atoms. This section investigates the effect of temperature gradients on the diffusion behavior of point defects in α-U by simulating temperature gradients along three different directions and considering three distinct gradient magnitudes for each direction. The diffusion coefficients obtained are shown in Fig. 10 [Figure 10: see original paper], which clearly indicates that the diffusion coefficient of the point defects increases differently with the increasing temperature gradient, both in terms of the total diffusion coefficient and the directional component, regardless of the direction in which the temperature gradient is applied. However, this trend does not extend to vacancy diffusion along the Y-axis direction, which remains unaffected by temperature gradient variations. The analysis of atomic motion trajectories reveals that the diffusion mechanism of point defects under temperature gradients aligns with that in the equilibrium field. The SIA continues to diffuse in the form of a dumbbell, as shown in Fig. 7. Vacancies also fail to diffuse along the Y-direction in the inter-planar region of the corrugation, even when a temperature gradient of 300-900 K (42.9 K/nm) is applied in this direction. Interestingly, although the temperature gradient was applied in only one direction, the diffusion coefficient components of the SIA in the other two directions were correspondingly enhanced as the temperature gradient increased. This was later found to be due to the directional migration of the SIA towards the high-temperature region, which raised the localized temperature at its location, thereby promoting the diffusion rate in the other two directions. The diffusion rate of vacancy similarly increases with the temperature gradient, except in the Y direction. Our subsequent study found this effect to be caused by the increase in localized temperature due to the diffusion of vacancies towards the high-temperature region. When the temperature gradient is applied in the Y direction, no long-range diffusion of vacancy along the Y direction into the high-temperature region is observed. However, the location where the vacancy was initially introduced experiences different localized temperatures depending on the magnitude of the temperature gradient, leading to effects similar to those in the direction of the other two applied temperature gradients.

To investigate the effect of the temperature gradient on the direction of defect motion, the number of forward and reverse diffusions of vacancy and SIA along the temperature gradient, as a percentage of the total number of diffusions, was counted based on the results of 20 independent simulations. As shown in Fig. 11 [Figure 11: see original paper], we define the direction of the gradient as the positive direction, that is, the direction in which the temperature increases. As seen on the right side of Fig. 11 (a), the number of vacancy diffusions along the positive direction of the gradient in the X-direction temperature gradient field is significantly higher than that in the negative direction, when compared to the diffusion in the equilibrium field (left side of Fig. 11 (a)). This trend becomes more pronounced as the temperature gradient increases, suggesting that the temperature gradient along the X-direction promotes the directional diffusion of vacancies towards the high-temperature region. The same conclusion can be drawn from the results for the temperature gradient along the Z-axis, as shown in Fig. 11 (b). Additionally, for the results of SIA (Fig. S2 in the supplementary material), the temperature gradient in all three directions shows that SIA tends to diffuse towards the high-temperature region. This suggests that in the presence of a temperature gradient, vacancies and SIAs diffuse simultaneously toward the high-temperature region, increasing the likelihood of their combined annihilation. As a result, the excessive defect concentration caused by the difference in diffusion coefficients is reduced. Shockley [**?**] proposed that if a temperature gradient exists in a crystal and the defect density at any point is assumed to correspond to a characteristic equilibrium value for the local temperature at that point, a continuous flow of defects will occur within the crystal. The nature of and analytic expressions for the driving forces can be deduced from the thermodynamics of irreversible processes or kinetic theory, the net flux (one-dimensional) of vacancies under a temperature gradient is given by the following equation [**?**, **?**]:

$$J_v = -\frac{D_v}{kT^2}\frac{dT}{dx}Q_v$$

where Dv is the diffusion coefficient of vacancy, λ is the lattice spacing, k is Boltzmann's constant, T is the absolute temperature, and Qv, known as the 'heat of transport' [**?**], represents certain energies characteristic of the system. Brammer [**?**] and LeClaire [**?**] assumed Qv to be the algebraic difference between the vacancy formation energy Ef and the migration activation energy Em, such that Qv = Ef - Em. Therefore, the direction of the vacancy flow is primarily determined by the relative magnitudes of Ef and Em. The vacancy formation energy calculated by our potential is 1.72 eV, which is much larger than the migration energy of vacancies along the X and Z directions. As a result, Qv is a positive value, and the direction of the vacancy flow aligns with the temperature gradient, moving towards the high-temperature region. The defect flow for SIAs can be described using a similar kinetic model, with the detailed reasoning provided in the supporting material. The net flux of interstitial atoms can be expressed as:

$$J_i = -\frac{D_i}{kT^2}\frac{dT}{dx}Q_i$$

where Di is the diffusion coefficient of interstitial, B is a positive constant, and here Qi is equal to the migration energy Em of the SIA. Since this value is positive, the direction of the defect flow for the SIA is also towards the high-temperature region. Ultimately, we conclude that the temperature gradient present in α-U promotes the diffusion of point defects and produces directed migration. We predict that the concentration of point defects in the high-temperature region of the temperature gradient field will exceed the equilibrium defect concentration, which increases the chances that the vacancies and interstitials will recombine with each other to annihilate, but may also lead to the formation of more stable defect clusters and ultimately affect the microstructure and material properties.

C. Diffusion of point defects in stress gradient fields

Temperature changes and irradiation-induced growth can generate internal stresses of up to hundreds of MPa within the material [**?**, **?**]. To gain insights into stress-driven cracking and plastic flow, the kinetic behavior of point defects in a stress gradient and the static energy within the stress field are investigated. The diffusion coefficients of SIA and vacancy in the stress gradient field are shown in Fig. 12 [Figure 12: see original paper], with the simulations conducted at a temperature of 700 K to ensure sufficient diffusion. Atomic trajectory analysis reveals that the diffusion mechanism of SIA and vacancy in the stress gradient field is consistent with that in the equilibrium field. From Fig. 12 (a)-(f), it is evident that the stress gradient as an additional driving force has a facilitating effect on the diffusion of point defects. This effect is observed not only in the direction parallel to the stress gradient but also in the perpendicular direction. However, vacancy is still unable to diffuse along the Y direction, even in the presence of a stress gradient. The applied stress gradient in different directions exerts varying levels of influence on the diffusion of SIA and vacancy. Specifically, the stress gradient in the X direction promotes SIA diffusion the most, while the Y and Z directions show comparable levels of enhancement. In contrast, the stress gradient in the X direction has the least favorable effect on vacancy diffusion, compared to the Y and Z directions. Note that the gradient magnitude in the Z-direction reaches a maximum of only 0.021 GPa/Å, as applying excessive loads may lead to structural changes in the system. In addition, the direction of the diffusion driving force induced by the stress gradient was investigated. The number of forward and reverse diffusions of SIA and vacancy along the stress gradient, as a percentage of the total number of diffusions, was counted based on the results of 20 independent simulations, as shown in Fig. S3 and S4 in the supplementary material, respectively. We define the tensile stress state as positive, with the positive direction of the gradient pointing from compressive to tensile stress. Fig S3 (a)-(c) show that the frequency of SIA diffusion into the positive direction of the gradient is significantly higher than that in the negative direction. This indicates that SIA tends to diffuse into the tensile stress region in the stress gradient field, with this tendency becoming more pronounced as the gradient magnitude increases. The diffusion behavior of vacancy in the stress gradient field is opposite to that of SIA. As shown in Fig. S4 (a)-(b), vacancies tend to diffuse toward the region of compressive stress concentration.

To reveal the chemomechanical origin of anisotropic stress on the diffusion behavior of point defects, we calculated the formation energy of defects under varying uniaxial stress conditions. The formation energy of SIA in the stress field is given by [**?**]:

$$E_{SIA}(\sigma_{ij}) = E(N+1;\sigma_{ij}) - \frac{N+1}{N}E(N;\sigma_{ij})$$

where E(N + 1; σij) and E(N ; σij) are the total energies of the supercell containing N atoms with and without a SIA under the stress tensor σij, respectively. The structure of the examined SIA is a three-site interstitial, as shown in Fig. 7 (c), which is the most stable SIA structure observed after relaxation and reorientation at high temperatures during our simulations. The formation energy of vacancy in the stress field is defined as:

$$E_{Vac}(\sigma_{ij}) = E(N-1;\sigma_{ij}) - \frac{N-1}{N}E(N;\sigma_{ij})$$

where E(N - 1; σij) and E(N ; σij) are the total energies of the supercell containing N atoms with and without a vacancy under the stress tensor σij, respectively. The calculation results are shown in Fig. 13 [Figure 13: see original paper]. The stress-strain state of the system at the point of defect formation energy calculation is also provided in Fig. S5 of the supplementary material, and the linear stress-strain relationship indicates that the studied stress interval remains within the elastic deformation stage.

Fig. 13 (a) shows the variation in the formation energy of SIA with applied stress under uniaxial stress conditions along the X, Y, and Z axes. The formation energy of SIA is higher in the compressive stress region (negative stress values) and decreases monotonically as the stress state transitions from compressive to tensile stress, indicating that SIA tends to form in the region of tensile stress concentration. In addition, among the three axial stresses, the change in the stress state along the X-axis has the most significant effect on the formation energy of the SIA. Meanwhile, Fig. 13 (b) shows that the formation energy of vacancy is lowest in the region of compressive stress concentration, and the stress changes in the Y-axis have the greatest impact on the formation energy of vacancy. The above conclusions suggest that the concentration of interstitial atoms will exceed the equilibrium concentration in regions of tensile stress concentration, while the concentration of vacancies will be significantly higher in regions of compressive stress concentration. Next, we analyze the energy changes associated with the diffusion of point defects in the stress field. As seen in Figs. 7 and 8, both SIA and vacancy in α-U primarily diffuse along two paths. We designate the diffusion of SIA in the X-Y plane as SIA diffusion path 1, and the diffusion along the Z-direction as SIA diffusion path 2. Similarly, the diffusion of vacancy towards the a-atom is referred to as vacancy diffusion path 1, and the diffusion towards the b-atom is vacancy diffusion path 2. The potential barriers for these four diffusion paths under different stress conditions have been calculated using the Nudged Elastic Band (NEB) method [?]. The results for SIA and vacancy are shown in Fig. 14 [Figure 14: see original paper]. The stress-strain relationship of the system during the calculation is provided in Fig. S6 and S7 of the supplementary material, respectively. The linear variation of stress-strain indicates that the system is in the elastic deformation stage. Within the studied stress intervals, we observe that the trend of the diffusion barrier with stress exhibits clear anisotropy. For example, when stress is applied along the X or Y direction, the potential barrier of the SIA diffusion path 1 changes non-monotonically with the magnitude of the stress. However, when the applied stress is along the Z-axis, the potential barrier decreases monotonically. We investigate the dominant mechanism behind this phenomenon using elasticity theory, which can predict the change in energy when a simulated box is subjected to a uniform strain . The effect of strain on point defects in solids is typically analyzed through the concept of the force dipole tensor P [?]. Another more intuitive quantity for assessing anisotropic behavior is the formation volume tensor Vf [?, ?], which effectively quantifies the volume change induced by point defects in each direction. In the elastic region, P and Vf are correlated by [?]:

$$P_{ij} = -\Omega_{bulk}\sigma_{defect} = \Omega_{bulk}C_{ijkl}\varepsilon_{defect} = C_{ijkl}V^{f}$$

where Ωbulk is the volume of the simulation box, σdefect the stress induced by the point defect, Cijkl is the elasticity constant of the material, and defect is the strain induced by the point defect. In the presence of external stresses, the evaluation of the defect formation energy Edefect (σ) must account for the strain work required to deform the system under the applied stress field. This expression can be written as [?]:

$$E_{defect}(\sigma) = E_{defect}(0) - \sigma : V^{f}$$

where Edefect(0) is the defect formation energy under stress-free conditions, Vf is the formation volume tensor, and σ is the external stress tensor. From equation (8), it is evident that the defect formation energy is inversely proportional to the tensor product of the formation volume tensor and the stress tensor, which allows us to characterize how the formation energy of point defects responds to stress in different directions. The formation volume tensor is expected to be anisotropic and dependent on the external deformation. This is due to the fact that the formation energy calculated in Fig. 13 is anisotropic and exhibits a nonlinear dependence on the applied stress. When the elastic constants of the material and the volume of the simulated system are known, it can be seen from Eq. (7) that there are two methods for calculating the formation volume tensor of point defects [**?**]. The first approach involves obtaining the residual stress introduced by the point defect. In the particular case where the volume and shape remain fixed between the defective and perfect supercells, the formation volume tensor is proportional to the residual stress. This residual stress corresponds to the increase in stress following atomic relaxation due to the introduction of point defects into the simulation box. Another approach considers the opposite scenario, where a uniform strain is applied to the defect-containing supercell to eliminate the residual stresses introduced by the point defects. The formation volume tensor is proportional to this uniform strain. In this paper, the first approach is used to calculate the formation volume tensor during the diffusion of SIA and vacancy. Another tensor involved in the diffusion process is the migration volume tensor, denoted as Vm. It corresponds to the difference in the formation volume tensor between the saddle point of the diffusion path and the initial relaxed structure, Vmsaddle - Vfinitial, characterizing the additional volume change introduced by the point defect at the saddle point [**?**, **?**]. The migration barrier is determined by the enthalpy difference between the saddle-point configuration and the initial configuration, while the first-order effect of stress on the migration barrier is reflected in the difference between the two formation volume tensors of the respective configurations [**?**, **?**]. Therefore, the degree of response of the migration barrier to stress can be quantified by the migration volume tensor. The formation volume tensor for the saddle point can be obtained by calculating the residual stress introduced by the point defect at the saddle point. The formation volume tensors for the initial configuration and saddle point of the SIA and vacancy are shown in Fig. 15 [Figure 15: see original paper] and Fig. 16 [Figure 16: see original paper], respectively. The migration volume tensor is also presented as their difference. It can be observed that the volume tensor for the formation of SIA and vacancy changes with stress, arising from the atomic relaxation on and around the defects, which strongly depends on the deformation of the system. In most stress regions, SIA causes volume expansion (positive formation volume tensor), while vacancies cause volume contraction (negative formation volume tensor), both aimed at minimizing the elastic energy in the region surrounding the defect. The SIA has the largest formation volume tensor in the X direction, indicating that stress variations in this direction have the most significant impact on the formation energy. In contrast, vacancies exhibit the largest negative formation volume tensor in the Y direction, indicating that the maximum contraction occurs in this direction, making the formation energy of vacancies most sensitive to stress variations in the Y direction. Furthermore, we find that when the sign of the migration volume tensor changes, the monotonicity of the migration potential barriers under different stress conditions also changes accordingly. The stress values corresponding to the inflection points of the migration barriers in Fig. 14 exactly coincide with the stress values at which the sign of the migration volume tensor changes in Figs. 15 and 16. Therefore, we conclude that the trend of the migration barriers with stress variation is primarily governed by the sign of the migration volume tensor. To clarify the mechanism behind directional diffusion, the driving force of the stress gradient on the diffusion of point defects was investigated. The thermodynamic properties of point defect transport under external stresses, as influenced by the chemical potential, can be expressed as [**?**]:

$$\mu(\sigma_{ex}) = \mu(0) - \sigma_{ex} : (V^f + V^m)$$

where (0) is the potential without stress effects. From the equation (9), the change in chemical potential during point defect transport under different stress conditions can be calculated, as shown in Fig. 17 [Figure 17: see original paper]. It can be observed that the chemical potential of SIA increases in the compressive stress region and decreases in the tensile stress region, with the magnitude of this decrease varying depending on the direction of the applied stress. The change in stress along the X-direction has the most pronounced effect on the chemical potential of SIA, and it can be expected that the impact of stress in this direction on the diffusion behavior of SIA will also be the most significant. This is consistent with the results of our kinetic simulations (Fig. 12). The chemical potential of vacancy decreases in the compressive stress region and increases in the tensile stress region. The stress change along the Z-axis has the most pronounced effect on the chemical potential, while the X-direction exhibits the least sensitivity. This discrepancy may provide a potential means of regulating matter flow transport in α-U single crystals. In summary, we conclude that when a stress gradient is present, the resulting chemical potential gradient generates a driving force for the SIA to diffuse toward the tensile stress concentration zone, while the vacancies diffuse toward the compressive stress zone. This supports our previous proposal that, due to the anisotropic thermal expansion of the lattice and irradiation-induced growth, compressive stress concentrations may form between grains, acting as vacancy sinks and leading to the formation or growth of voids.

IV. SUMMARY

Due to the asymmetric crystal structure, the transport, aggregation, and recombination of vacancies and interstitials within the crystal, as well as their loss to sinks, are anisotropic and vary with temperature. These behaviors become even more complex when an external gradient field is applied. In this work, the diffusion behavior of irradiation defects in α-U under both equilibrium and gradient fields is investigated using a classical molecular dynamics approach. We find that SIA exhibits a unique diffusion mechanism in the X-Y plane and along the Z direction. In the X-Y plane, diffusion primarily occurs in the form of a $< 110 >$ dumbbell via a kick-out mechanism, with the diffusion coefficients of SIA in the X and Y directions being coupled and varying with temperature in a fixed ratio (approximately 0.22). Diffusion along the Z direction involves a configuration denoted as the three-site interstitial, also diffusing via a kick-out mechanism and involving an intermediate process. Vacancy diffusion occurs only within the corrugation planes and hardly spreads between the corrugation planes along the Y direction. At high temperatures, vacancies predominantly migrate along the X-direction, while SIAs preferentially migrate in the Y-direction. This result may provide supportive evidence for the irradiation growth mechanism hypothesis, which proposes that changes in each dimension of α-U are caused by differences in the net flux of diffusion along that direction.

In a temperature gradient field, the migration rate of SIA and vacancy increases with the magnitude of the gradient. This is primarily due to the additional driving force generated by the temperature gradient, which causes the SIAs or vacancies to migrate toward the high-temperature region, thereby increasing the local temperature in their vicinity and promoting their diffusion rate. We use a kinetic theory model to characterize this driving force. For vacancies, the direction of the transport driving force is determined by the sign of the difference between the vacancy formation energy and the vacancy migration energy, as well as the direction of the gradient. In contrast, the direction of the driving force for SIA is determined solely by the direction of the temperature gradient.

The stress gradient accelerates the diffusion rate of SIA and vacancies and causes a separation motion effect. Regarding the intergranular cavities observed in the experiments, we propose a stress-driven vacancy growth mechanism. Through elasticity theory, we find that the effect of the stress gradient on diffusion behavior is induced by the generation of different strains, which in turn affect the energetics of the defects. The stability of point defects is closely related to the stress state. Within the studied stress range, the diffusion barriers of SIA and vacancies show either monotonic or non-monotonic variations with the stress magnitude, depending on the direction of the applied stress. This phenomenon is primarily determined by the sign of the migration volume tensor of the point defects during diffusion. A change in the sign of the migration volume alters the monotonicity of the migration barrier with respect to the stress magnitude accordingly. The chemical potential of SIA decreases in the tensile stress region, while it increases in the compressive stress region, with the opposite trend observed for vacancies. Combining this with the simulation results from our kinetics analysis, we conclude that the effect of the stress gradient on the diffusion behavior of point defects essentially arises from the chemical potential gradient.

In this work, the effects of temperature and stress on the diffusion behavior of point defects in α-U are systematically investigated. These results contribute to a better understanding of the microstructural evolution of the fuel under in-reactor conditions. This study provides a foundation for mesoscale simulations that consider the behavior of defect aggregation and diffusion in interaction with external gradient fields. Furthermore, in addition to experimental irradiation and characterization, further computational work on extended defects using classical molecular dynamics should be conducted to more thoroughly elucidate the potential mechanisms of defect clustering and their interaction with the α-U crystal structure.

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