



# Void bias in irradiated model metals

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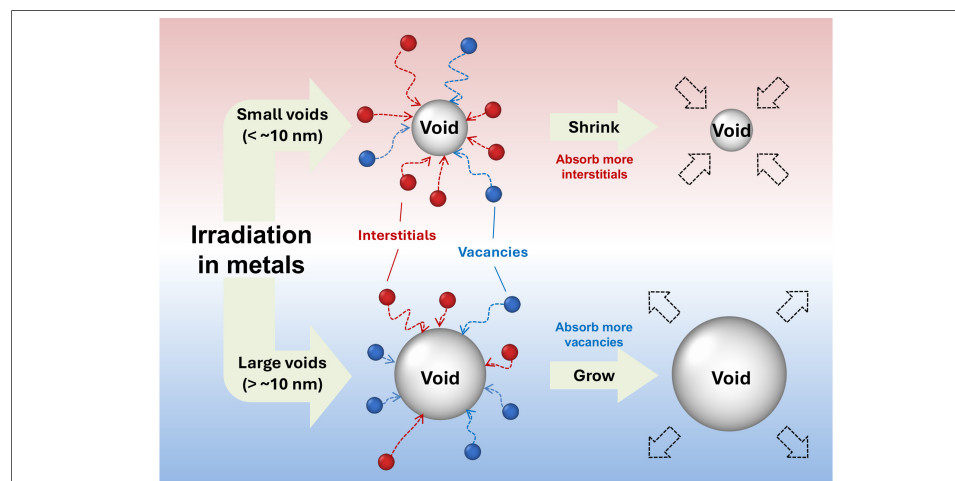
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## Abstract

Void swelling plays a critical role in the microstructural evolution and mechanical property degradation observed in irradiated materials. The preferential absorption of mobile point defects by microstructural sinks (e.g., dislocations) is postulated to be the driving force behind this phenomenon. While most studies treat voids as neutral sinks, this assumption has been challenged both theoretically and experimentally, emphasizing the necessity of quantitatively determining the void bias under various irradiation conditions. This study employs a state-of-the-art atomistic Kinetic Monte Carlo approach to determine the void bias in irradiated pure Fe, Cu, and Ni, examining the effects of size, temperature, density, and void morphology. Our findings reveal that voids in all examined metals act as non-neutral sinks for mobile point defects, particularly at small sizes (e.g., ~2 nm). Furthermore, this study demonstrates that voids have lower efficiency in absorbing mobile point defects compared to dislocation loops and stacking fault tetrahedra. These findings provide quantitative estimates of the competition of different sinks, which is responsible for the growth and shrinkage of voids under different irradiation conditions. The implications of void bias on swelling rate calculations in both fcc and bcc metals are also discussed, offering crucial insights for predicting void swelling behaviors, microstructure evolutions, and related properties in irradiated metals.



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## INTRODUCTION

Void swelling is a key degradation phenomenon that may cause intolerable volumetric expansion in irradiated metals and alloys<sup>[1,2]</sup>. The underlying mechanism of this phenomenon is known as the bias of microstructural sinks<sup>[3]</sup>. For instance, dislocations have long been considered to absorb more self-interstitials (SIAs) than vacancies, resulting in an excess concentration of vacancies and the growth of voids<sup>[4]</sup>. Thus, the bias of each type of sink is crucial for microstructural evolutions and swelling behaviors in irradiated materials. Since voids serve as reference sinks for the point defect flux<sup>[5]</sup>, their bias is critical for understanding and predicting void swelling<sup>[6]</sup>. Furthermore, the void bias has crucial implications for dislocation loop nucleation and growth<sup>[7]</sup>, radiation-induced segregation<sup>[8]</sup>, and irradiation hardening<sup>[9]</sup> in irradiated materials. These phenomena are highly correlated and determined by the competitive absorption of mobile point defects among various sinks. In many studies<sup>[5,10–13]</sup>, voids are assumed to be neutral sinks, with their bias neglected in void swelling calculations (e.g., flux models). However, this cannot explain the experimental observations that voids may shrink or grow under different irradiation conditions<sup>[14–24]</sup>. The underlying challenge is that void swelling is inherently multiscale in both length and time and depends on the capture efficiencies and sink strengths of all relevant sinks, despite the long history of studying void swelling in structural materials.

Following the initial observation of voids in irradiated steels<sup>[14]</sup>, subsequent studies using a high-voltage electron microscope (HVEM) in annealed nickel<sup>[16]</sup> and neutron-irradiated stainless steel<sup>[17]</sup> revealed void growth. Both works reported a rapid increase in void size alongside a decrease in void number density with rising irradiation temperature, highlighting the importance of incorporating voids as point defect sinks in theoretical models. The bias model was then developed to elucidate the underlying mechanism of void growth<sup>[6]</sup>, suggesting a lower void bias compared to dislocations or dislocation loops. However, Loomis and Gerber<sup>[18]</sup> observed both growth and shrinkage of voids in ion-irradiated Nb at varying temperatures, indicating evolving interactions between voids and mobile point defects. In a recent *in situ* Transmission Electron Microscopy (TEM) investigation, Chen *et al.* reported the shrinkage of voids in Kr-irradiated Ni below  $\sim 0.5 T_m$  (the melting temperature) and the growth above this temperature, with faster shrinkage noted for smaller voids<sup>[20]</sup>. This aligns with other heavy ion irradiation studies that observed the void shrinkage<sup>[21–24]</sup>. Small voids are suggested to capture point defects more rapidly and exhibit higher shrinkage rates than large voids in irradiated copper samples with abundant nanovoids and twin boundaries<sup>[22]</sup>. More recently, Niu *et al.* reported continuous shrinkage of pre-existing nanovoids in irradiated fcc copper<sup>[23,24]</sup>. Additionally, the shrinkage phenomenon was also observed for nanopores in Au<sup>[21]</sup>, which was attributed to the higher tensile stress generated by smaller voids, leading to preferential absorption of mobile SIAs over vacancies. These experimental observations underscore the significant variability of void bias based on critical parameters such as void size and irradiation temperature.

Theoretically, most void bias calculations rely heavily on elasticity theory<sup>[6,13,25–27]</sup>. For instance, Wolfer and Ashkin<sup>[27]</sup> formulated equations grounded in elastic interactions between spherical voids and point defects in an idealized isotropic elastic medium, using a flux model. Their findings indicated a tendency for voids to preferentially absorb interstitials over vacancies, with void growth occurring only when interstitials interact more strongly with dislocations than with voids. This was subsequently supported by Dubinko *et al.*, highlighting the importance of void size in absorbing SIAs and the consequent evolution of voids under irradiation<sup>[13]</sup>. To improve the accuracy, Borodin *et al.* delved into the anisotropic effects of point defect diffusion by introducing averaged point defect dipole tensors<sup>[28]</sup>. The significance of the anisotropic diffusion of point defects was then systematically determined by Carpentier *et al.*<sup>[29]</sup>. Additionally, several studies challenged the notion of voids as neutral sinks. For instance, a molecular dynamics (MD) study by Wang *et al.* stated that small vacancy clusters are highly biased sinks for point defects<sup>[30]</sup>. Additionally, Samaras *et al.* also reported bias void based on very short-scale displacement cascade simulations at room temperature,

which only serves as the starting point for realistic long timescale diffusion and defect evolution<sup>[26]</sup>. These calculations face two main limitations. First, elasticity theory approaches neglect a significant amount of core effect. The core effect here refers to their substantial anisotropic stress/strain field and impact on point defect diffusion near the void, varying with void size. Due to the atomistic configuration, we find that the smaller the voids, the more pronounced the core effect. This effect is further complicated by variations in configurations of SIAs during the diffusion processes, which have been found to dramatically influence the bias estimations<sup>[29,31,32]</sup>. Second, bias calculations rooted in elasticity theory lack comparability due to varied assumptions and inconsistent underlying approximations made for different sinks. For instance, Wolfer *et al.* employed a flux model to estimate the bias of dislocations<sup>[3]</sup> and voids<sup>[33]</sup>, assuming dislocations as a perfect cylinder and voids as spheres. These result in the bias values of dislocations and voids primarily depending on a few parameters, e.g., capture radius of dislocations and surface energy of voids. The choice of these parameters could potentially introduce significant variations in bias values and influence the analysis of void growth and shrinkage. Furthermore, the lack of consistency in theoretical models also leads to challenges in comparing different works<sup>[13,25,27,28,33,34]</sup>. In these works, various approaches have been employed to calculate the interactions between point defects and sinks, e.g., estimations based on strain field, in either isotropic<sup>[3]</sup> or anisotropic elastic mediums<sup>[35]</sup>, or atomistic binding energies<sup>[12]</sup>, complicating the assessment of the overall bias trend among different sinks.

In this study, we have employed a recently developed atomistic kinetic Monte Carlo (AKMC) approach<sup>[31]</sup> to calculate the void bias in typical irradiated structural metals. This AKMC approach is found to yield quantitative agreement with experimental results for dislocation loops and SFTs. We focus on pure Cu, Ni, and Fe, considering the complexity of the problem, yet these metals also underpin many important alloys<sup>[1,2]</sup>. The factors that influence the void bias, as identified in previous theoretical studies<sup>[13,25,27,28,33,34]</sup>, including void size, temperature, void density, and metal structures (bcc vs. fcc), are systematically examined. Experimental values of these parameters across different metals and irradiation conditions are employed in our model<sup>[36–39]</sup>. The effect of void morphology is also analyzed in this study, as various void shapes have been observed in experimental investigations<sup>[40–43]</sup>. Furthermore, a comparative assessment of point defect absorption efficiencies of major sinks in both bcc and fcc metals, including dislocations, dislocation loops, and stacking fault tetrahedra (SFTs, exclusively in fcc systems), is conducted. This simulation system has also been employed to calculate dislocation bias and loop bias in bcc Fe, exhibiting close alignment with experimental observations<sup>[31]</sup>. Using this model, a quantitative prediction of void swelling is feasible, regardless of the type of defect included.

## METHODS

### Simulation setup

The atomistic configurations of voids are constructed by removing the atoms in a spherical region of 2, 4, and 10 nm diameters using LAMMPS<sup>[44]</sup>, followed by a relaxation process. The interatomic potentials for bcc Fe, fcc Cu, and fcc Ni are those developed by Ackland *et al.*<sup>[45]</sup>, Mishin *et al.*<sup>[46]</sup>, and Mendelev *et al.*<sup>[47]</sup>, respectively. These potentials have been tested and used extensively for understanding irradiation effects in these systems.

The scheme of the atomistic KMC simulation system is provided in Figure 1. This AKMC simulation is employed to determine the lifetime of mobile point defects (both SIAs and vacancies), which is defined as the duration it takes for a point defect to diffuse from its initial position to the void. Point defects start their diffusion from the surface of this spherical simulation system. When a point defect diffuses out of the simulation system, another defect of the same type is randomly placed on the system surface. This ensures that the distance between the point defect and the void remains constant. Such a boundary condition is defined as Random Boundary Condition (RBC), which has been previously employed in dislocation bias

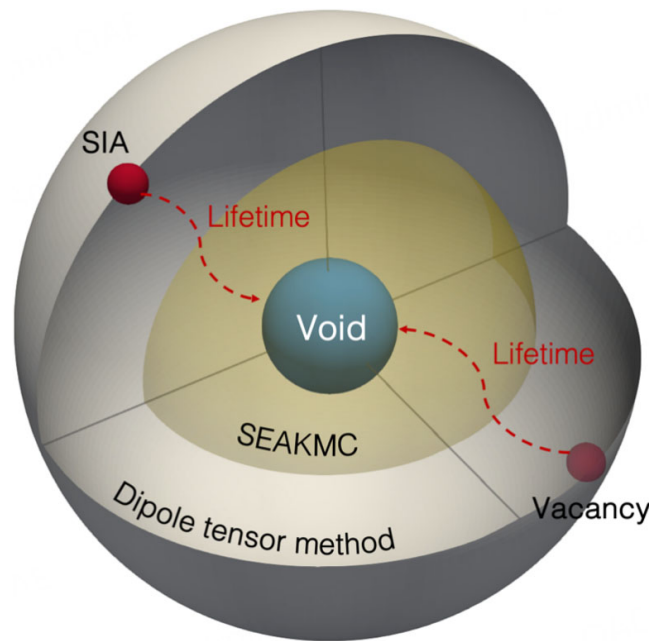


**Figure 1.** The scheme of the AKMC simulation system. The trajectories of mobile point defects are illustrated by dotted lines, starting from the boundary of the simulation system, and continuing until point defects are absorbed by the void. The duration along this trajectory is termed the lifetime.

calculations<sup>[48]</sup>. Periodic Boundary Conditions (PBCs) are avoided because the centrosymmetric strain field of the void imposes identical driving forces on the point defect before and after boundary crossing. This effect artificially influences the point defect diffusion but diminishes with increasing simulation system size. The time for each diffusive step is determined by the migration energy barrier (MEB) at its current atomic position and point defect configuration. The details of MEBs are shown in Section "Migration energy barriers". A point defect is considered absorbed upon entering the spontaneous absorption region (SAR). When a point defect diffuses into the SAR, it is considered spontaneously absorbed by the void. The SAR for the void is determined through binding energy calculations, with the criteria set as  $-0.1$  eV for SIAs and  $-0.05$  eV for vacancies, respectively. Four simulation system sizes between 57 and 80 nm have been applied, corresponding to void densities between  $3 \times 10^{21} \text{ m}^{-3}$  and  $10^{22} \text{ m}^{-3}$ . Since a linear relationship is observed between the point defect lifetime and the volume of the simulation system (shown in [Supplementary Section I](#)), the point defect lifetime for void densities outside this range can be extrapolated from the fitted values. The density of voids is defined as the inverse volume of the simulation system, corresponding to a scenario where the voids are evenly distributed. Three void sizes (2, 4, and 10 nm) are considered in this work to investigate the void size effect. Larger voids were not considered due to computational limitations and the general expectation that their bias values approach zero. For a given void size, density, and temperature, a KMC simulation is performed with 500 randomly selected starting positions and 4,000 trajectories for each point defect, balancing calculation efficiency and accuracy. A detailed standard error test of the obtained lifetime is provided in the [Supplementary Section II](#).

### Migration energy barriers

Migration energy barriers (MEBs) of mobile point defects are the saddle point energy when a point defect migrates to its first nearest neighbor lattice points, which is crucial for AKMC simulations and analyses of their interactions with sinks. The MEBs of two types of point defects, interstitials (dumbbells) and single vacancies, are considered in bcc Fe, fcc Cu, and fcc Ni. Specifically, for bcc iron, there are six dumbbell configurations ( $\langle 110 \rangle$ ,  $\langle 101 \rangle$ ,  $\langle 011 \rangle$ ,  $\langle \bar{1}\bar{1}0 \rangle$ ,  $\langle 10\bar{1} \rangle$ , and  $\langle 01\bar{1} \rangle$ ). For each dumbbell configuration, eight

saddle points are found associated with the lowest energy barrier (bulk value 0.308 eV) to diffuse to four of their eight first nearest neighbors along the  $[111]$  direction. For vacancies, comparatively, there are eight saddle points to diffuse to the eight first nearest neighbors in bcc iron, the bulk value of which is 0.640 eV. In fcc metals, there are three typical dumbbell configurations ( $\langle 100 \rangle$ ,  $\langle 010 \rangle$ , and  $\langle 001 \rangle$ ). For each dumbbell configuration, eight saddle points are found toward four of their first nearest neighbors, with bulk values of 0.099 eV for Cu and 0.123 eV for Ni. As for a vacancy, there are twelve saddle points, the bulk value of which is 0.692 eV for Cu and 1.036 eV for Ni.

To calculate the MEBs in the region close to the void, we use the self-evolving atomistic kinetic Monte Carlo (SEAKMC)<sup>[49]</sup>, which accounts for the non-elastic interactions between a void and a point defect with atomistic fidelity. The point defect is inserted into the atomic system as the initial configuration, and the saddle point energies for migrations are obtained within an active volume, the radius of which is around 15 Å in this work. This approach enables the calculation of millions of saddle points with an accuracy within  $\pm 0.002$  eV. The core region where the SEAKMC approach is applied is in yellow in Figure 1 and is adjacent to the absorption region, approximately 2–3 nm away from the void surface.

Beyond this core region, shown in grey in Figure 1, the dipole tensor method<sup>[29]</sup> based on elasticity theory is utilized for estimations of MEBs. The equations based on the elastic interactions between the point defect and the dislocation loop are listed below,

$$E^m[\varepsilon] = E_0^m + P_{ij}^{ini} \varepsilon_{ij}(\vec{r}_{ini}) - P_{ij}^{sad} \varepsilon_{ij}(\vec{r}_{sad}) \quad (1)$$

$$P_{ij} = -V \langle \sigma_{ij} \rangle \quad (2)$$

where  $\varepsilon_{ij}$  is the strain tensor,  $E^m$  is the point defect MEB considering elastic interaction, and  $E_0^m$  is the bulk value. The elastic dipole tensors at the initial stable position  $\vec{r}_{ini}$  and the saddle point  $\vec{r}_{sad}$ ,  $P_{ij}^{ini}$ , and  $P_{ij}^{sad}$ , are calculated using a supercell.  $P_{ij}$  in Equation (2) works with fixed periodicity vectors between the defective and original supercells, where  $V$  is the supercell volume and  $\sigma_{ij}$  is the residual stress. Since the region where the dipole tensor method is applied is far from the core area, deviations in MEB values can be neglected. The boundary between the core region (SEAKMC) and the dipole tensor method region is determined by a discrepancy threshold in MEBs of  $\pm 0.002$  eV, ensuring both precision and computational efficiency.

### Void bias and sink strength using the KMC approach

In AKMC simulations, a random number is drawn to select one saddle point  $i$  from the saddle point list based on the relative probability  $P_i$  in each KMC step, which is given by,

$$P_i = \frac{\Gamma_i}{\sum_{j=1}^n \Gamma_j}, \quad (3)$$

where  $n$  represents the total number of saddle points for migrating to the first nearest neighbor.  $\Gamma_i$  is the probability of the diffusive step passing through the saddle point  $i$ ,

$$\Gamma_i = v_0 \exp\left(-\frac{E_{m,i}}{kT}\right), \quad (4)$$

where  $v_0$  is the attempt frequency, which is set as  $10^{12} \text{ s}^{-1}$ .  $E_{m,i}$  stands for the MEB of saddle point  $i$  corresponding to a specific atomic position with a specific dumbbell configuration.  $k$  is Boltzmann's constant, and  $T$  is the temperature in Kelvin. The lifetime of mobile point defect  $\alpha$  ( $\tau_\alpha$ ) is determined by summing the duration of each diffusive step ( $\Delta\tau$ ) using the residence-time algorithm,

$$\tau_\alpha = \sum \Delta\tau, \quad (5)$$

$$\Delta\tau = \frac{-\ln(x)}{\sum_{j=1}^n \Gamma_j}, \quad (6)$$

where  $\alpha$  is  $i$  or  $v$  for interstitials or vacancies, respectively, and the random number  $x \in (0, 1]$ . For instance, a point defect takes  $10^6$  steps before being absorbed by the void, with each step having a unique value of  $\Delta\tau$ . The value of  $\tau_\alpha$  is the sum of these  $10^6$   $\Delta\tau$  values. In Equation (6),  $n$  saddle points are considered for the given point defect, with 12 and 8 corresponding to vacancy first-nearest-neighbor diffusions in fcc and bcc metals, respectively. Additionally, 8 first-nearest-neighbor diffusion saddle points and 4 rotational saddle points are considered for dumbbells in both fcc<sup>[50]</sup> and bcc<sup>[31]</sup> metals. The flux of point defect  $\alpha$ ,  $J_\alpha$ , represents the number of defects absorbed per unit time by a closed surface  $S$ . This point defect flux is proportional to the total number of introduced point defects  $N$ , divided by the total diffusion time  $t_N$ . The inverse of this value is the average lifetime of the point defect  $\alpha$ ,

$$J_\alpha = \frac{dn}{Sdt} \propto \frac{N}{t_N} = \frac{1}{\tau_\alpha}. \quad (7)$$

Subsequently, the capture efficiency is determined using a flux model<sup>[3]</sup>, where, far from the sink, a reservoir of point defects exists, which is maintained at a constant concentration:

$$Z_\alpha = \frac{J_\alpha}{J_\alpha^r}. \quad (8)$$

Note that Wolfer defined  $Z_\alpha$  as “bias” and  $B$  as “net bias”, which in this work correspond to the capture efficiency and bias, respectively. Thus, the capture efficiency of the void to point defect  $\alpha$  is obtained as

$$Z_\alpha = \frac{\frac{1}{\tau_\alpha}}{\frac{1}{\tau_\alpha^r}} = \frac{\tau_\alpha^r}{\tau_\alpha}, \quad (9)$$

where  $\tau_\alpha$  symbolizes the lifetime of the point defect when influenced by a void, while the superscript  $r$  denotes random walk, representing the absence of any interaction between the point defect and the void (MEBs are set to bulk values for random walk). The point defect random walk ends upon reaching the SAR. The bias of voids is derived based on the capture efficiency,

$$B = \frac{Z_i - Z_v}{Z_v} . \quad (10)$$

Moreover, the sink strength of a given void for point defect  $\alpha$  ( $k_\alpha^2$ ) can be determined based on the derivation of Mansur *et al.* [51] using the obtained capture efficiency,

$$k_\alpha^2 = Z_\alpha k^2 , \quad (11)$$

where the capture efficiency  $Z_\alpha$  is introduced to represent the interactions between the void and point defect, and  $k^2$  represents the sink strength for random walks, where the elastic interactions are absent. This parameter is typically used to represent the interaction between mobile defects and the sink in rate theories, with higher values indicating stronger interactions. Here, the value of  $k^2$  can be obtained in the KMC simulation, where only one mobile point defect is present in the simulation system at a time. In KMC simulations, the sink strength is defined as the inverse of the square of the mean free path in 1D/3D diffusion [52–54],

$$k^2 = \frac{2n}{d_j^2 \langle n_j \rangle} , \quad (12)$$

where  $n$  is the dimensionality ( $n = 3$  in this study),  $\langle n_j \rangle$  is the average number of jumps made by point defects (the number of jumps needed for a mobile point defect to be absorbed), and  $d_j$  is the jump distance. This framework has been utilized to calculate the sink strength of dislocation loops, SFTs, and straight dislocations in irradiated Fe and Cu [31,32], providing a close agreement with experimental observations. Finally, the relation between the bias value and sink strength can be obtained based on capture efficiencies,

$$B = \frac{Z_i}{Z_v} - 1 = \frac{k_i^2}{k_v^2} - 1 . \quad (13)$$

## RESULTS

### Migration energy barriers in the core region of voids

Migration energy barriers (MEBs) for SIAs ( $\langle 110 \rangle$  dumbbell in bcc Fe and  $\langle 100 \rangle$  dumbbell in fcc Cu/Ni) and vacancies near voids of different sizes have been determined in the investigated metals. As an example, the core effect of voids is illustrated using a 10 nm void and a 4 nm void in Fe, as shown in Figures 2 and 3, respectively. The  $[110]$  dumbbell MEBs are provided as representative examples. Since there are eight saddle points for first-nearest-neighbor diffusion in bcc iron [31,32], and the two saddle points along the diagonal of the unit cell lead to the same final configuration, four MEB maps for the  $[110]$  dumbbell are presented with their final dumbbell configurations. The comparison among SEAKMC results, dipole tensor method results, and their differences (calculated by subtracting dipole tensor method results from SEAKMC results) is shown in 3-D views. MEBs that are too close to the bulk value (within 0.002 eV) and differences smaller than 0.002 eV are hidden. Since voids at the atomic scale are not perfectly spherical due to atomic-scale irregularities, their shapes deviate from ideal spheres. These deviations arise from factors such as surface reconstruction and local atomic distortions, leading to anisotropic interactions between voids and mobile point defects, defined as the core effect.

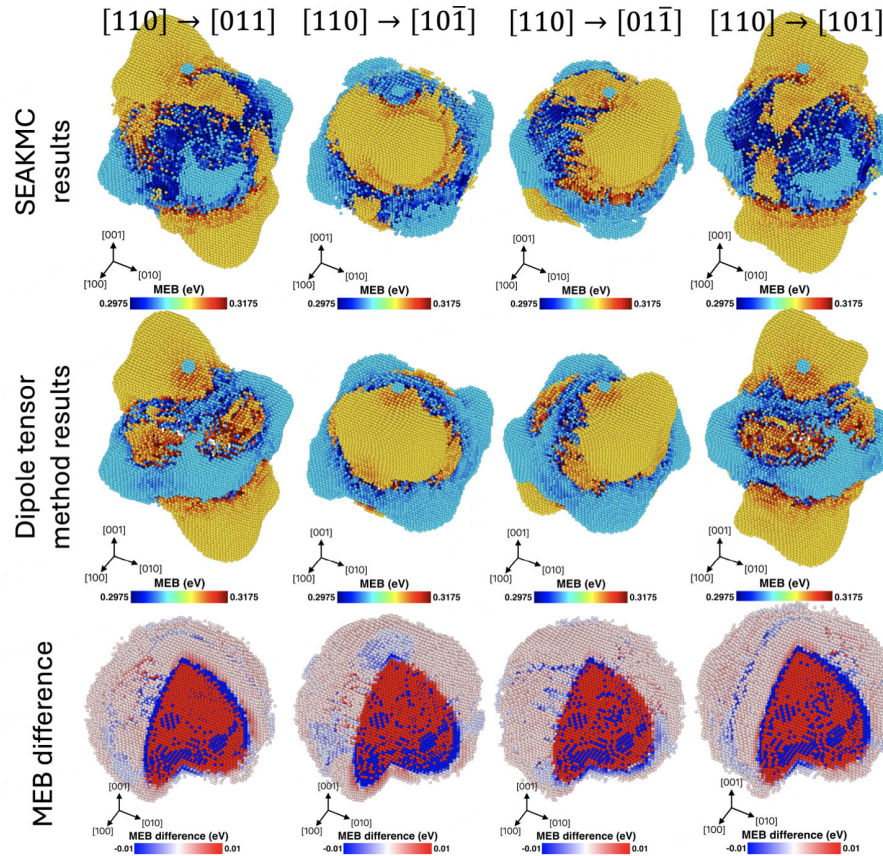


**Figure 2.** The 3-D MEB maps of a [110] dumbbell near a 10 nm void calculated using SEAKMC and dipole tensor method are compared, and the difference is displayed in red and blue. 1/4 of the MEB difference map is hidden for a clearer view in the core region.

MEBs exhibit strong anisotropy due to the atomistic interaction between mobile point defects and voids within the core regions, approximately 2 nm from the void surface in bcc Fe. Such an impact range remains relatively the same in Cu and Ni regardless of void sizes, details of which are presented in [Supplementary Section III](#). Because of this, the interactions between voids and point defects are expected to decrease as the void size increases. The void size increase is usually accompanied by a density decrease in experiments<sup>[37,38,55,56]</sup>. Therefore, the core effect in irradiated samples with high-density smaller voids is comparatively more pronounced than in samples with large voids, resulting in stronger interactions with point defects.

This core effect is quantitatively presented in [Figures 4 and 5](#), showing its long-range impact on defect lifetimes and void bias. [Figure 4A and B](#) presents the interstitial lifetime as a function of position near a 10 nm void at 573 K, calculated using MEBs from SEAKMC and the dipole tensor method, respectively. In general, the lifetime of interstitials is longer when the atomic-scale core effect is neglected, as shown in [Figure 4B](#). A direct comparison is made in [Figure 4C](#), where the ratio  $\tau^{\text{dipole}}/\tau^{\text{SEAKMC}}$  is plotted. Because of the fluctuations of the ratio at each atomic position, an averaged value is provided every 3 nm from the void center, and the regions are labeled as A, B, and C based on increasing distance from the void. In region A, close to the void core, the lifetime is overestimated by more than 30% on average when the core effect is ignored. This overestimation reduces to 13.6% in region B and further converges to approximately 10% in region C and beyond. This deviation, especially near the void surface, originates from differences in MEBs between SEAKMC and the dipole tensor method within about 2 nm of the void surface. However, the effective core effect shows long-range impact on lifetime calculations, as demonstrated by the  $\sim 1.1$  ratio instead of 1.0 persisting outside region C.

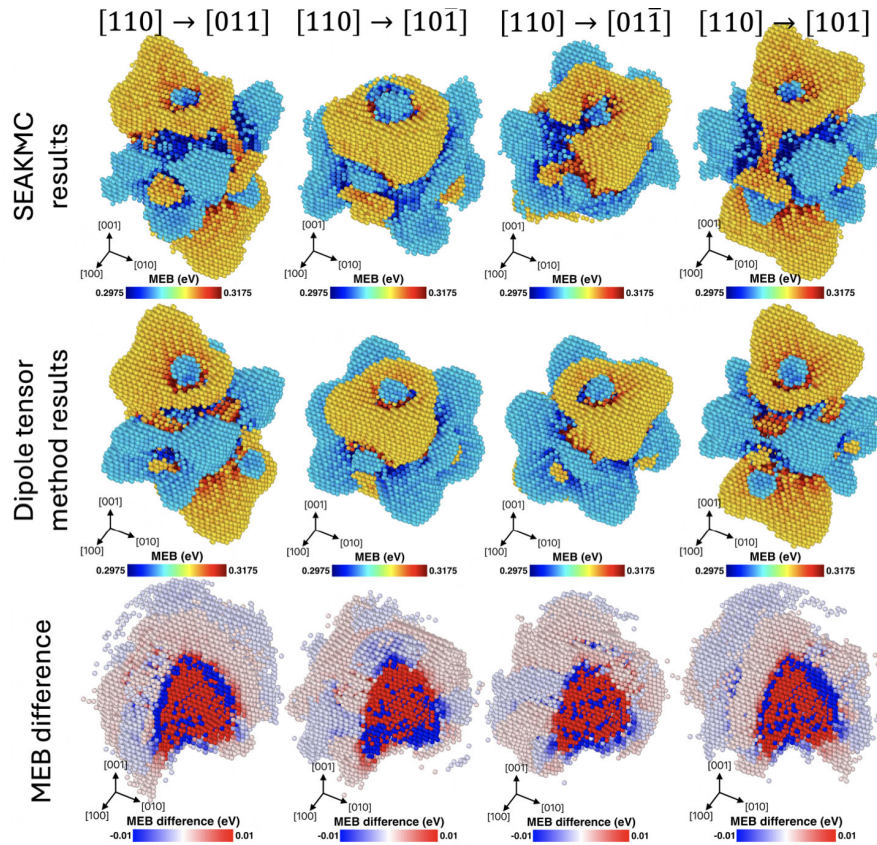


**Figure 3.** The 3-D MEB maps of a  $[110]$  dumbbell near a 4 nm void calculated using SEAKMC and dipole tensor method are compared, and the difference is displayed in red and blue. 1/4 of the MEB difference map is hidden for a clearer view in the core region.

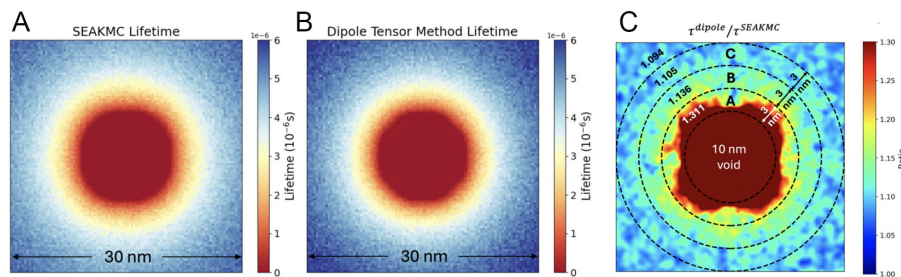


**Figure 4.** Interstitial lifetimes as a function of position near a 10 nm void, calculated using MEBs from (A) SEAKMC and (B) the dipole tensor method. The lifetime comparison is shown in (C), illustrating the significant deviations in the void core region. All figures are based on data from a  $[100]$  section plane passing through the center of the void.

The bias value as a function of positions near a 10 nm void, calculated using MEBs from SEAKMC and the dipole tensor method, is shown in Figure 5A and B, respectively. In general, the bias values calculated using SEAKMC are lower than those obtained from the dipole tensor method. This discrepancy occurs due to regions repelling interstitials, where negative bias values are observed, as labeled in blue in Figure 5A. The local atomic structure of the void along the  $\langle 100 \rangle$  direction exhibits compressive regions, as illustrated in Figure 5C, while other directions lead to tensile regions [Figure 5D], where interstitials are preferred. This phenomenon leads to an overall positive bias with specific regions exhibiting a negative bias, which is a counter-intuitive and concrete representation of the core effect. However, this effect is underestimated by elasticity theory, leading to the uniformly positive bias distribution seen in Figure 5B. Notably, the distribution and shape of repulsion regions vary depending on the crystal structure (e.g., bcc or fcc) and void

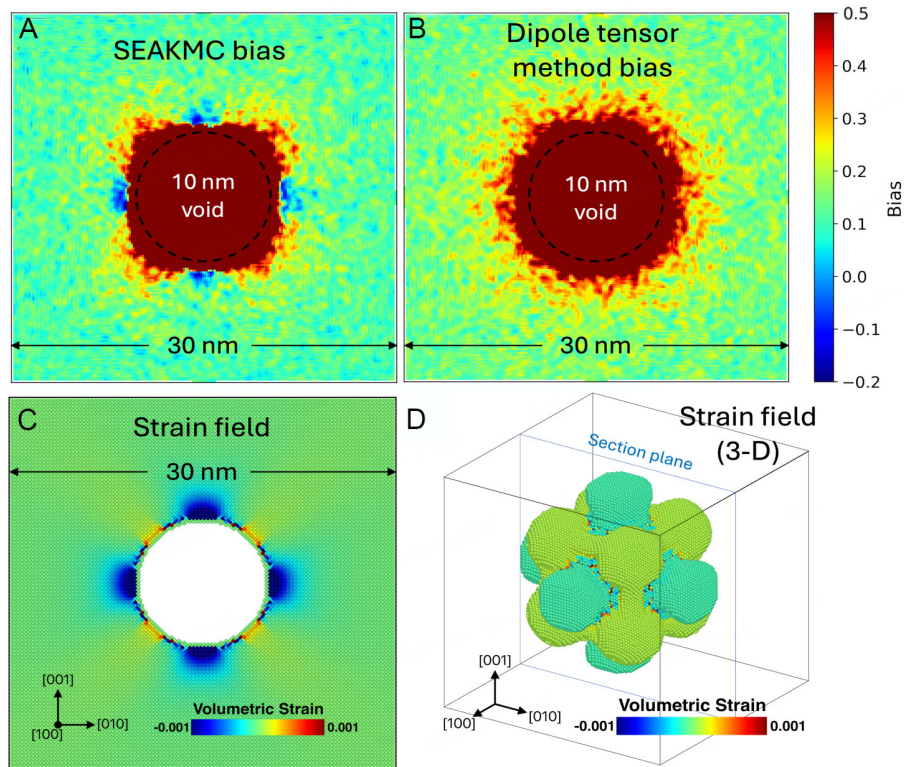


**Figure 5.** Bias values at each atomic position near a 10 nm void obtained using (A) SEAKMC and (B) the dipole tensor method. The volumetric strain field corresponding to the same section as (A and B) is shown in (C), where compressive regions correspond to the negative bias regions identified by SEAKMC. A 3D representation of the strain field is provided in (D) for reference, with the section plane corresponding to Figure 4 and (A-C) labeled.

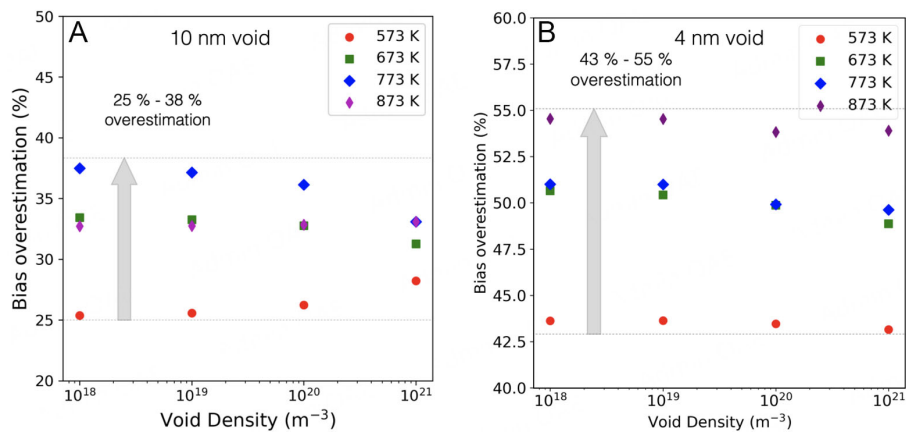


**Figure 6.** The bias overestimation using the dipole tensor method compared to SEAKMC is shown for (A) a 10 nm void system and (B) a 4 nm void system.

size, with the impact diminishing for larger voids. A detailed analysis of the shape effect is provided in the [Supplementary Section IV](#).

The core effect also leads to distinct void bias predictions with a given void density. For a 10 nm void, the dipole tensor method overestimates the bias by 25% to 40% from 573 to 873 K, considering commonly observed void densities ( $10^{18}$  to  $10^{21}$   $\text{m}^{-3}$ ), as shown in [Figure 6A](#). In contrast, the overestimation for a 4 nm void is notably higher, ranging from 42% to 55% compared to the bias derived from SEAKMC MEBs [[Figure 6B](#)], attributed to stronger core effect from small voids as discussed above. Although the absolute bias difference appears minimal, this relative change significantly impacts void swelling predictions. Accurate atomistic data are crucial for upper-length-scale modeling, e.g., rate theory calculations.

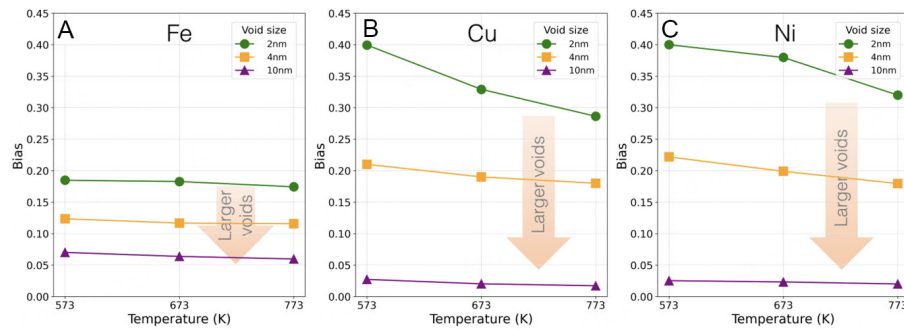


**Figure 7.** Void bias as a function of void sizes and temperatures in (A) Fe, (B) Cu, and (C) Ni. A commonly observed void density at  $10^{20} \text{ m}^{-3}$  is selected for this comparison.

**Table 1.** Bias of 2 and 10 nm voids with various number densities at 673 K

| Densities        | $10^{22} \text{ m}^{-3}$ | $10^{20} \text{ m}^{-3}$ | $10^{18} \text{ m}^{-3}$ |
|------------------|--------------------------|--------------------------|--------------------------|
| 2 nm void in Fe  | 0.190                    | 0.183                    | 0.182                    |
| 2 nm void in Cu  | 0.336                    | 0.329                    | 0.328                    |
| 2 nm void in Ni  | 0.345                    | 0.320                    | 0.318                    |
| 4 nm void in Fe  | 0.130                    | 0.117                    | 0.116                    |
| 4 nm void in Cu  | 0.182                    | 0.170                    | 0.165                    |
| 4 nm void in Ni  | 0.191                    | 0.180                    | 0.175                    |
| 10 nm void in Fe | 0.084                    | 0.064                    | 0.062                    |
| 10 nm void in Cu | 0.024                    | 0.020                    | 0.019                    |
| 10 nm void in Ni | 0.026                    | 0.020                    | 0.019                    |

### Void bias in Fe, Cu, and Ni

Void bias values have been determined in pure Fe, Cu, and Ni, varying void size and temperature, as shown in Figure 7. Three different void sizes (2, 4, and 10 nm in diameter) and temperatures (573, 673, and 773 K) have been investigated. The impact of void density is analyzed in Section "Temperature and void density effects" with data shown in Table 1.

### Void size effects

The void bias in Fe, Cu, and Ni decreases as void size increases, as demonstrated in Figure 7A–C. Specifically, in Fe, the void bias of a 2 nm void ranges from 0.17 to 0.19 between 573 and 773 K. This value decreases to 0.11–0.13 for a 4 nm void and further reduces to 0.06–0.07 for a 10 nm void. In comparison, voids in Cu and Ni show greater bias reduction with size increase than those in Fe. In Cu and Ni, the bias of 2 nm voids is mostly higher than 0.3, which decreases to around 0.2 with 4 nm voids. The bias of 10 nm voids is approximately 0.02, substantially lower than that of a 10 nm void in Fe.

This observed pattern is attributed to the core effect of voids, which are primarily caused by deviations from perfect sphericity due to atomic-scale irregularities. For smaller voids, the core effect strongly enhances the preferential absorption of interstitials over vacancies. As voids increase in size, their geometries approach ideal spherical symmetry while simultaneously exhibiting diminished absorption preferences, thereby reducing discrepancies between atomistic simulations and elasticity theory approaches. Therefore, it is reasonable to expect that the deviation of conventional calculations based on elasticity theory<sup>[13,28,33]</sup> will decrease and become negligible with large voids on the order of hundreds of nanometers in size.

### *Temperature and void density effects*

A reduction in bias is observed with increasing temperatures across the three studied metals, as shown in [Figure 7](#). This is because the impact of migration energy barrier  $E_{m,i}$  [from Equation (4)], which reflects the interaction between the void and mobile point defect, decreases at higher temperatures. The effect of temperature is notably more pronounced with small void sizes in fcc metals. For example, the bias of a 2 nm void in Cu shows a decrease from 0.40 to 0.29 as the temperature increases from 573 to 773 K. Comparatively, within the same temperature range, the bias of a 10 nm void in Cu reduces from 0.027 to 0.017. In contrast, the temperature effect is relatively weaker in Fe, with a bias difference of  $\sim 0.01$  observed between 573 and 773 K across various void sizes.

Compared to the temperature effect, the impact of void density on bias values is less significant. The bias values at three different void number densities ranging from  $10^{18}$  to  $10^{22} \text{ m}^{-3}$  at 673 K are presented in [Table 1](#). Generally, the void bias tends to decrease with lower number densities due to the extended diffusion distance of a point defect before it reaches the void. However, such a decrease in bias value converges at low densities ( $10^{18}$  to  $10^{20} \text{ m}^{-3}$ ) in all the investigated metals. This tendency is reflected by a tiny variation of approximately 0.001, despite significant changes in number density or the void size (2 to 10 nm).

Additionally, the key factor behind the difference between fcc and bcc metals remains unclear but may stem from the nature of their crystal structures or the anisotropic diffusion of point defects. BCC Fe exhibits higher capture efficiency for both interstitials and vacancies than fcc metals ([Supplementary Section V](#)), suggesting voids in bcc Fe absorb defects more effectively. In contrast, the difference between Cu and Ni is negligible.

## **DISCUSSION**

### **Efficiency of point defect absorption by voids**

Although voids are found biased sinks with a preference for absorbing SIAs over vacancies, this finding does not conflict with the conventional dislocation bias model, attributing the growth of voids to a net vacancy flux entering the voids<sup>[4]</sup>. This is because different sinks, e.g., dislocation, dislocation loops, precipitates, and SFTs, compete in point defect absorption. The corresponding defect partition can be analyzed from the following two aspects: the specific bias and the sink strength.

### *The specific bias of point defects*

We propose a conceptual framework to explain the competition among different defect clusters for point defect absorption. Here, specific bias is defined as the ratio of the bias to the number of vacancies or SIAs within a sink. This parameter characterizes the normalized ability of a sink to absorb SIAs relative to vacancies. A sink with a low specific bias indicates either a low bias value or a large size (which correspondingly implies low densities in irradiated metals and a reduced impact on diffusion of point defects). Note that this definition is claimed for a more direct comparison, while the bias values will be used in rate theory calculations, rather than the specific bias. [Figure 8A](#) compares the specific bias of various sinks in Cu, Ni, and Fe at 573 K. In fcc metals (Cu and Ni), a SFT with a size of 2 nm encapsulates 36 vacancies and exhibits bias efficiencies of the order of  $10^{-2}$ . In comparison, a 10 nm interstitial loop containing  $10^3$  interstitials has a specific bias of  $10^{-4}$ , while a 10 nm void with roughly  $10^4$  vacancies has a specific bias of around  $10^{-6}$ . The voids exhibit a specific bias that is roughly two orders of magnitude lower than loops and is much lower overall. Thus, the absorption of SIAs by 10 nm voids is considerably weaker compared with dislocation loops and SFTs in Cu and Ni. In bcc Fe, the specific bias of voids is also significantly lower than that of dislocation loops.

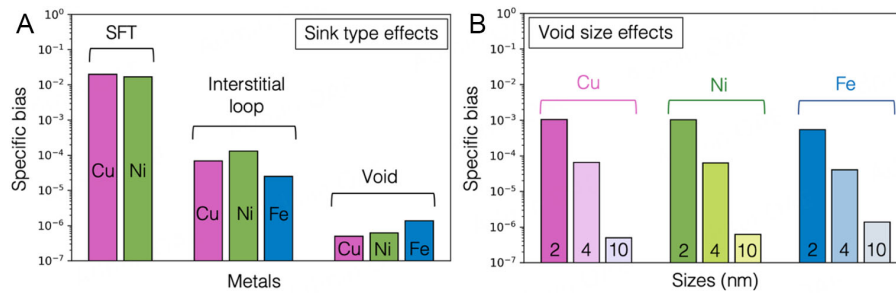


**Figure 8.** Specific bias of (A) voids with different sizes and (B) different sinks in Cu, Ni, and Fe. In (B), the SFT has a size of 2 nm, while both the loop and void have diameters of 10 nm. Dislocation loop types are selected based on experimental observations:  $1/3\langle 111 \rangle$  Frank loops observations for fcc Cu<sup>[57]</sup> and fcc Ni<sup>[39]</sup>, and  $\langle 100 \rangle$  Frank loops for bcc Fe<sup>[37]</sup>.

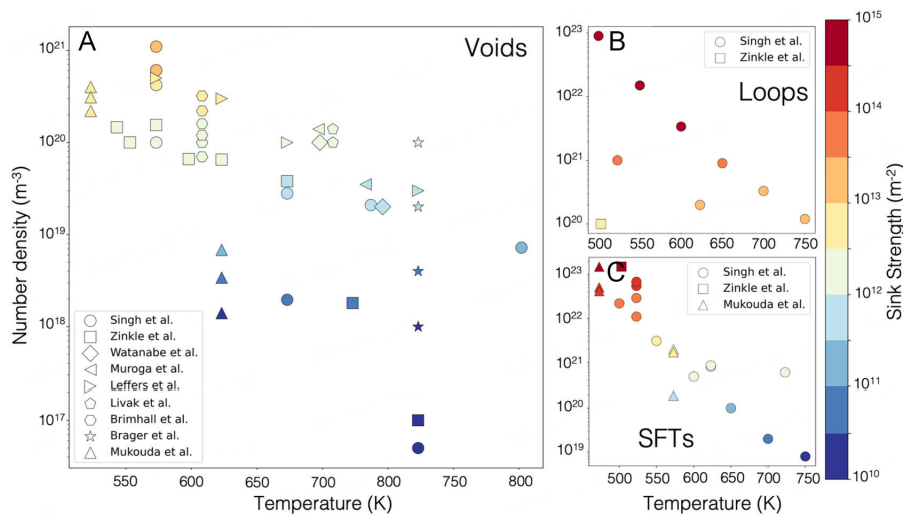


**Figure 9.** Comparative analysis of sink strengths among voids, loops, and SFTs in Cu. The range of temperatures and number densities for each sink varies based on experimental observations. (A) Voids; (B) Loops; (C) SFTs.

Voids with a size of 4 nm exhibit a specific bias similar to 10 nm interstitial loops [Figure 8A], both around  $10^{-4}$ . The specific bias of smaller voids significantly exceeds that of 10 nm voids, as depicted in Figure 8B. Moreover, 2 nm voids show an ability to absorb SIAs that is roughly an order of magnitude greater than 4 nm voids. This demonstrates that smaller voids ( $\leq 4$  nm) are strongly biased sinks for mobile SIAs and must be included in predictions of void swelling. Such a tendency is also observed in experiments in irradiated Cu and Au<sup>[21,22]</sup>. Experiments reveal that smaller voids (typically  $\leq 10$  nm) demonstrate higher efficiency in absorbing irradiation-induced interstitials for void shrinkage compared to larger voids.

### Sink strength of point defect sinks

Sink strength not only characterizes the capture efficiency for point defect absorption but also reflects the effect of sink number density. Therefore, sink strength can be used to understand the overall effects of different types of sinks. Figure 9 illustrates the sink strength of a 10 nm void, 10 nm interstitial loop, and a 2 nm SFT in Cu for SIA absorption, considering commonly observed densities and temperatures in experiments<sup>[38,39,43,55,57–66]</sup>. The sink sizes are selected based on a balance between typical sizes observed in experiments and the limitations of computational capabilities. Following Equation (11), the  $Z_\alpha$  value for voids is assumed to be the same as that of a 10 nm void. This assumption is based on the expectation that the core effect of larger voids would be even lower, and their capture efficiency is presumed equivalent to the  $Z_\alpha$  value of a 10 nm void. The sink strength  $k^2$  is estimated using the derivation by Golubov et al.<sup>[5]</sup>,  $k^2 = 4\pi N_{void} \langle R \rangle$ , where  $\langle R \rangle$  is the average value of void radii and  $N_{void}$  is the void number density.

Void sink strength typically ranges between  $10^{10}$  and  $10^{13} \text{ m}^{-2}$  and increases with decreasing temperatures and rising densities as shown in Figure 9A. Small voids (4.5–7.7 nm) have the highest sink strengths ( $> 10^{13} \text{ m}^{-2}$ )<sup>[66]</sup>, the bias of which is not negligible as mentioned in Section "Void bias in Fe, Cu, and Ni". However, when compared to SFTs and dislocation loops, voids generally exhibit the lowest sink strength. This observation is attributed to the prevalence of large voids ( $> 10 \text{ nm}$ ) with low density and bias, primarily observed in experiments with doses exceeding  $0.01 \text{ dpa}$ <sup>[55]</sup>. In contrast, the sink strength of loops is mostly between  $10^{13}$  and  $10^{15} \text{ m}^{-2}$ , as illustrated in Figure 9B. On the other hand, SFTs are found with number densities higher than  $10^{22} \text{ m}^{-3}$  under 550 K with bias values as high as around 0.6 for the most commonly observed sizes (1.5–3.5 nm). In this case, SFT sink strength is found between  $10^{13}$  and  $10^{15} \text{ m}^{-2}$ , showing its strong capability to absorb SIAs. Thus, voids capture point defects with relatively low efficiency, leading to the diffusion of point defects toward other biased sinks. A similar observation is also found in Ni and Fe, illustrating the universality of the weak attraction of voids to mobile point defects in the three investigated metals.

### The impact of void bias on void swelling

Voids have been treated as neutral sinks ( $Bias = 0$ ) in many previous swelling rate calculations<sup>[5,10–13]</sup>. However, it is essential to take into account the actual void bias and sink strength in the swelling rate estimations because the void serves as the reference for all sinks. According to the rate theory<sup>[5]</sup>, the swelling rate can be derived from the relation between the generation rate ( $G$ ) and concentrations ( $C_i$  and  $C_v$ ) of point defects (also called balance equations),

$$G + G_v^{\text{th}} - k_{\text{void},v}^2 D_v C_v - \Sigma k_{\text{sink},v}^2 D_v C_v - \mu_R D_i C_i C_v = 0 \quad (14)$$

$$G - k_{\text{void},i}^2 D_i C_i - \Sigma k_{\text{sink},i}^2 D_i C_i - \mu_R D_i C_i C_v = 0 \quad (15)$$

Here,  $k_{\text{void},v}^2$  and  $k_{\text{void},i}^2$  represent the void sink strength for vacancies and SIAs, respectively.  $k_{\text{sink}}^2$  stands for the sink strength of other sinks that will absorb mobile point defects, including edge or screw dislocations, dislocation loops, and SFTs. The term  $\Sigma k_{\text{sink},v}^2 D_v C_v$  represents the summation of the effects of various types of sinks, excluding the void. The recombination of point defects is included in the  $\mu_R D_i C_i C_v$  term and vacancy emission is represented using  $G_v^{\text{th}}$ . The values of  $D_v C_v$  and  $D_i C_i$  can be derived as follows,

$$D_v C_v = \frac{G}{k_{\text{void},v}^2 + \Sigma k_{\text{sink},v}^2} \quad (16)$$

$$D_i C_i = \frac{G}{k_{\text{void},i}^2 + \Sigma k_{\text{sink},i}^2} \quad (17)$$

The swelling rate is thus obtained from the net flux of vacancies to voids,

$$\frac{dS}{d\phi} = k_{void,v}^2 D_v C_v - k_{void,i}^2 D_i C_i = \frac{k_{void,v}^2 (k_{void,i}^2 + \Sigma k_{sink,i}^2) - k_{void,i}^2 (k_{void,v}^2 + \Sigma k_{sink,v}^2)}{(k_{void,v}^2 + \Sigma k_{sink,v}^2) (k_{void,i}^2 + \Sigma k_{sink,i}^2)} \quad (18)$$

Here,  $S$  stands for the total volume of voids and  $\phi = Gt$  is the irradiation dose in dpa<sup>[5]</sup>. The sink strengths are obtained from capture efficiencies and bias of each type of sink following Equations (11–13). Considering the correlated defect recombination, a survival fraction at 0.1<sup>[67]</sup> is multiplied by the obtained swelling rate  $\frac{dS}{d\phi}$ . Additionally, vacancy evaporation has been considered for 10 nm voids, with evaporation rates exceeding 60% at 773 K. Since the evaporation rate is proportional to the void size, this phenomenon is negligible in very small voids and shrinking voids.

$$Swelling\ rate = \varepsilon^* \frac{dS}{d\phi} * \left(1 - \frac{J_v^{em}}{N}\right). \quad (19)$$

$J_v^{em}$  is the vacancy emission rate<sup>[5,68]</sup>, and  $N$  is the number of vacancies contained in a void. Detailed calculations are provided in the [Supplementary Section VI-IX](#), including the swelling rate derivation and the representative densities of various sinks.

As shown in Equation (18), the bias of the void (the ratio between  $k_{void,i}^2$  and  $k_{void,v}^2$ ) is a critical parameter that significantly influences the void swelling prediction, which can be quantitatively shown based on experimental data. Singh *et al.*<sup>[66]</sup> observed voids with densities around  $1.1 \times 10^{21} \text{ m}^{-3}$  and mean sizes around 16 nm in a 0.3 dpa neutron-irradiated Cu sample and measured the swelling rate around 0.43% dpa<sup>-1</sup>. Based on the framework in this study, the estimated swelling rate is 0.41% dpa<sup>-1</sup>, considering the void bias, showing a close agreement with the experimental observation. For comparison, if the void bias is neglected (assume  $k_{void,v}^2 = k_{void,i}^2$ ), the predicted swelling rate is 0.5% dpa<sup>-1</sup>. Notably, this overestimation from neglecting the void bias is predictably more significant with smaller void sizes or higher void densities, as small voids exhibit higher bias values. The bias is around 0.02 with the void size in the above example, which can be up to 10 times greater with smaller voids. For instance, as reported by Wakai *et al.*<sup>[69]</sup>, pure Ni irradiated by He<sup>+</sup> ions at 773 K with a dose of  $4 \times 10^{20} \text{ ions}\cdot\text{m}^{-2}$  shows void sizes between 3 and 7 nm and densities over  $10^{23} \text{ m}^{-3}$ . In this case, the void bias is estimated to be  $\sim 0.2$ . The number density of dislocation loops is reported as  $1.5 \times 10^{22} \text{ m}^{-3}$  and the bias is 0.17 at 773 K based on the same framework for void bias calculation in this study. Assuming a dislocation density of  $10^{13} \text{ m}^{-2}$  and the SFT density of  $10^{19} \text{ m}^{-3}$  at 773 K, we predict the swelling rate is 0.82% dpa<sup>-1</sup>, the value of which increases to 4.37% dpa<sup>-1</sup> if the void bias is neglected. As a reference, the experimentally observed swelling rate is around 0.67% dpa<sup>-1</sup>. Since this deviation is over an order of magnitude, neglecting void bias will heavily affect the interpretation of the swelling behavior in irradiated metals. Additionally, numerous experimental works have reported either small void sizes ( $\leq 10 \text{ nm}$ ) or high void densities ( $\geq 10^{20} \text{ m}^{-3}$ ), e.g., in irradiated Ni<sup>[36,70]</sup>, Cu<sup>[59,61,62]</sup>, or Fe<sup>[37]</sup>, which demonstrate that small voids with high densities are commonly found in irradiated metals, further emphasizing the need to incorporate void bias in the calculation of swelling rates.

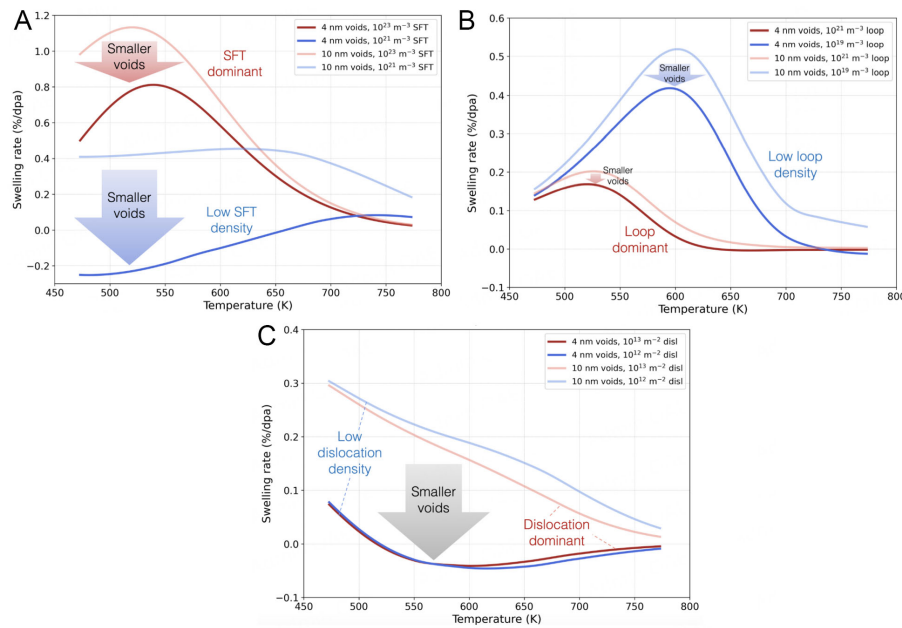


**Figure 10.** Predicted swelling rates based on representative sink densities. The effects of (A) SFT density, (B) dislocation loop density, and (C) dislocation density on predicted swelling rates are presented. Predictions with void sizes of 4 and 10 nm are presented in each figure to illustrate the void size effect.

### The competitive absorption of point defects and their effects on void swelling/shrinkage

The evolution of voids is critically affected by the competitive absorption of mobile point defects across various sinks. The material exhibits positive swelling when the sink strengths of voids are smaller than those of other sinks. Comparatively, the system may have potential negative swelling rates (corresponding to void shrinkage) when voids exhibit higher sink strengths than other sinks. We analyze the impacts of various major sinks on void swelling/shrinkage based on Equation (18) and provide the situations in which void shrinkage is likely to happen. Here, we take irradiated Cu as an example. Representative densities of voids, dislocation loops, and SFTs as a function of temperature are obtained by linear regressions of the experimental data [38,39,43,55,57–66]. Specifically, SFT density decreases from approximately  $10^{23}$  to  $6 \times 10^{18} \text{ m}^{-3}$  as the temperature increases from 473 to 773 K. Concurrently, dislocation loop density decreases from  $10^{22}$  to  $10^{19} \text{ m}^{-2}$ , and void density decreases from  $10^{20}$  to  $10^{18} \text{ m}^{-3}$  within the same temperature range. Based on experimental observations, the representative density for dislocations is typically on the order of  $10^{12}$  to  $10^{13} \text{ m}^{-2}$ . The representative sizes of SFTs and dislocation loops are 2 and 10 nm, respectively. To investigate the roles of various sinks in void swelling and shrinkage, the densities of SFTs [Figure 10A], dislocation loops [Figure 10B], and dislocations [Figure 10C] are used as variables for swelling rate prediction. For each scenario, the densities of other sinks are maintained as representative values as a function of temperature. Voids with sizes of 4 nm (bias values around 0.2) and 10 nm (bias values around 0.02) are employed to illustrate the size effect of voids in each scenario. The bias values for all the sinks have been calculated in a previous study [32].

Void shrinkage is generally observed only when the void size is small. In Figure 10A, both the SFT-dominant scenario (red curves, with a number density of  $10^{23} \text{ m}^{-3}$ ) and low-SFT-density (blue curves, with a number density of  $10^{21} \text{ m}^{-3}$ ) scenario demonstrate that 4 nm voids significantly reduce swelling rates and even lead to shrinkage under low SFT densities at temperatures below approximately 650 K. For the same void size, SFTs result in high swelling rates (peak bias exceeding  $1\% \text{ dpa}^{-1}$ ) under 600 K. This behavior corresponds to experimental observations [39,55,57,61,62,66,71], illustrating that SFTs are highly competitive in point defect absorption under these conditions. In comparison, dislocation loops [Figure 10B] tend to reduce the swelling

rate due to their low bias values (approximately 0.1) and high sink strength (over  $10^{14} \text{ m}^{-2}$ ). The peak swelling rate with a loop number density of  $10^{19} \text{ m}^{-3}$  is around  $0.52\% \text{ dpa}^{-1}$  for 10 nm voids and  $0.42\% \text{ dpa}^{-1}$  for 4 nm voids. These values decrease to approximately  $0.2\% \text{ dpa}^{-1}$  when the loop density increases by two orders of magnitude. In contrast to SFTs and dislocation loops, the density of straight dislocations does not significantly influence the swelling rate, as shown in Figure 10C. Since the experimentally observed dislocation densities are relatively stable (mostly between  $10^{12}$  to  $10^{14} \text{ m}^{-2}$ ), and the dislocation bias is found to be relatively insensitive to density variations within this range<sup>[32]</sup>, the contribution of dislocations to void swelling remains consistent.

In conclusion, small voids tend to shrink, while large voids consistently swell, with the critical size falling between 4 and 10 nm. Biased sinks, especially SFTs and dislocation loops, are more effective in absorbing mobile point defects than small voids at high densities, thereby limiting the void shrinkage processes. Notably, the quantitative data obtained in this study are based on specific empirical interatomic potentials. Although these potentials are widely accepted and employed in numerous published studies, they still present certain limitations. Additionally, since all the density parameters are derived from irradiation experiments and the size parameters are based on estimations, the calculated swelling rates serve primarily as a guideline. Other parameters, such as void morphologies and sink distributions, may also influence swelling rate predictions. However, performing a systematic analysis of nanoscale void shapes or distributions observed in experiments remains challenging, as they can evolve during void growth.

## CONCLUSIONS

This study systematically calculates the MEBs in the core region of voids and subsequently determines the void bias in irradiated Fe, Cu, and Ni using a recently developed atomistic KMC approach. The effects of void size, irradiation temperature, void density, and void morphology on bias values are presented. Small voids exhibit high bias values that decrease with increasing size, with a more drastic reduction observed in fcc metals compared to bcc Fe. Additionally, void bias consistently decreases with higher temperatures and lower void densities across all investigated metals.

The evolution of voids is found to be decisively influenced by the competitive absorption of mobile point defects among various sinks. Two crucial factors, the specific bias and sink strength, are employed to demonstrate such competition. Small voids (< 4 nm) are identified as highly biased sinks and display higher specific bias and sink strengths with high void densities, leading to the shrinkage of nanovoids. Moreover, the high bias values of small voids could potentially impede the growth of interstitial dislocation loops. In contrast, voids with diameters exceeding 4 nm exhibit a weaker capacity to absorb mobile point defects than dislocation loops and SFTs, leading to the growth of voids. These results reconcile the seemingly contradictory phenomena of void growth and void shrinkage, providing a consistent framework for predicting void evolution under irradiation.

Overall, the inclusion of precise void bias values addresses previous discrepancies arising from neglecting void bias or treating voids as neutral sinks. Furthermore, the bias values and sink strength derived from this study have broader applications, such as informing the modeling of other irradiation-induced processes and microstructural evolution or incorporating them into higher-scale simulations. Nevertheless, the current approach faces limitations in precipitation-based alloys due to the drastically increased computational load from solute-defect interactions and the added complexity of precipitate diffusion dynamics. Expanding this approach would be helpful for broader and more mechanistic insights into void swelling phenomena across different alloy systems.

## DECLARATIONS

### Authors' contributions

Investigation, methodology, validation, formal analysis, writing - original draft, visualization: Yu, Z.  
Conceptualization, methodology, formal analysis, writing - review & editing, supervision, project administration, funding acquisition: Xu, H.

### Availability of data and materials

The raw data supporting the findings of this study are available within this Article and its [Supplementary Materials](#). Further data are available from the corresponding author upon reasonable request.

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### Conflicts of interest

All authors declared that there are no conflicts of interest.

### Ethical approval and consent to participate

Not applicable.

### Consent for publication

Not applicable.

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### Supplementary Materials

[Supplementary Materials](#)

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