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Hydrogen-Helium-coupled deformation of core-shell cavities in iron-based fusion structural materials

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Abstract

In fusion environments, transmutation-produced hydrogen (H) and helium (He) interact with irradiation-induced vacancies to form gas-filled cavities that degrade the mechanical performance of iron-based structural materials. However, how H and He jointly regulate cavity-mediated deformation remains unclear. Here, we establish an experimentally constrained multiscale framework integrating thermodynamic analysis, extended-timescale molecular dynamics (MD), and density functional theory (DFT) to bridge irradiation-induced cavity structures with their atomistic deformation

mechanisms. The framework determines representative core-shell configurations from experimental cavity statistics and thermodynamically preferred H occupancy. Atomistic simulations reveal that He remains preferentially confined within the cavity, whereas H is mainly stabilized at the cavity-matrix interface and redistributes under thermal and mechanical perturbations. Combined MD and DFT analyses reveal a complementary mechanism: He-induced internal pressurization sustains stress concentration, while interfacial H facilitates defect activation by lowering interstitial formation energies. This mechanistic picture establishes H-He coupling as an important consideration for designing irradiation-resistant iron-based structural materials in fusion environments.

Introduction

Fusion energy is widely regarded as a promising route toward sustainable and low-carbon energy production, yet its realization critically depends on the development of structural materials capable of maintaining mechanical integrity under extreme service conditions¹. In Deuterium-tritium (D-T) fusion reactors, these materials are simultaneously exposed to intense high-energy neutron irradiation, elevated temperatures, and complex stress states^{2,3}. Unlike fission environments, D-T fusion neutrons possess a high mono-energetic energy (~14.1 MeV), which not only causes severe displacement damage but also induces nuclear transmutation reactions^{4,5}. In particular, transmutation reactions such as (n, p) and (n, α) generate substantial quantities of low-solubility gaseous species, primarily hydrogen (H) and helium (He)¹⁻⁵. Irradiation-induced vacancies and vacancy (V) clusters act as effective trapping sites for these gas atoms, thereby promoting the nucleation and growth of gas-filled H-He-V complexes, bubbles and cavities^{6,7}. The synergistic interaction of these gas species can lead to the formation of characteristic microstructural defects that significantly degrade the macroscopic properties of the materials^{2,7,8}.

High-flux fusion-neutron sources are currently unavailable. Consequently, multi-ion beam irradiation^{6,7,9-15} and computational modeling have become essential¹⁶⁻²³. These approaches allow researchers to investigate the underlying mechanisms of displacement damage under fusion-relevant conditions. It is well established that the synergistic interaction between displacement damage and gas production at different temperatures promotes cavity swelling^{6,7,9-12}, leading to mechanical degradation such as irradiation hardening and He-induced grain-boundary embrittlement²⁴⁻²⁸. As a representative irradiation-induced microstructural feature in metals and alloys, the dynamic behavior of He bubbles plays a critical role in determining mechanical properties^{26,29-32}. Recent *in situ* transmission electron microscopy (TEM) studies have directly visualized the evolution of He bubbles under both irradiation³³⁻³⁵ and mechanical loading^{29,36-38}, thereby establishing important connections between nanoscale defect dynamics and macroscopic mechanical degradation. Reduced

activation ferritic/martensitic (RAFM) steels are among the leading candidate structural materials for ITER and DEMO because of their low activation characteristics and the inherent resistance of their body-centered cubic (BCC) structure to irradiation-induced swelling³⁹⁻⁴¹. It is worth noting that BCC-Fe is adopted as a representative model of the ferritic matrix of Fe-based fusion structural materials, allowing the atomic-scale effects of H and He on cavity-mediated deformation to be isolated. Although substantial progress has been made in understanding swelling behavior in RAFM steels under coupled displacement damage and H/He production^{6,7,9,11,42,43}, the deformation behavior and damage mechanisms associated with cavities containing both H and He remain insufficiently resolved.

A central unresolved issue concerns the formation and quantitative characterization of H-He-containing cavity structures under fusion-relevant conditions. Recent experimental studies using electron energy-loss spectroscopy (EELS) have provided important evidence for the interaction of H and He with cavities and the formation of H-He-V configurations in RAFM steels^{6,11}. Furthermore, our previous study²⁰ revealed the dynamic evolution processes and underlying physical mechanisms governing the formation of core-shell cavity structures, in which He is confined within the cavity core while H preferentially accumulates at the surface, under different environmental conditions. However, direct quantitative determination of the H and He contents in such cavities remains highly challenging. This is especially true for H, whose EELS signal is intrinsically much weaker than that of He because of its low elastic scattering cross section and the strong sensitivity of its spectral response to local bonding environments near surfaces^{11,44}. Consequently, the absence of quantitative compositional data restricts the development of physically realistic atomic models and impedes a rigorous evaluation of the respective roles of H and He in cavity-controlled mechanical degradation.

A second unresolved issue is the lack of systematic understanding of the deformation behavior and dynamic evolution of core-shell cavities composed of H and He atoms under applied loading. Owing to the shallow damage depth and limited

affected volume produced by ion irradiation, conventional tensile testing is generally not suitable for directly measuring the tensile response of ion-irradiated materials. Recent advances in small-scale mechanical characterization, particularly *in situ* micro-tensile testing^{29,31,32,36–38}, have provided more direct access to the tensile deformation behavior of irradiated layers than conventional nanoindentation. For example, Xu et al.³¹ demonstrated that *in situ* micro-tensile testing can effectively capture the irradiation-induced changes in strain-rate sensitivity, hardening behavior, and deformation heterogeneity in He-ion irradiated Ni single crystals. However, corresponding mechanical investigations of triple-ion irradiated materials involving simultaneous H and He implantation together with displacement damage remain very limited. This challenge primarily originates from the difficulty of obtaining reliable mechanical responses from highly heterogeneous near-surface irradiation layers, where steep damage gradients and dynamically evolving gas-defect complexes substantially complicate both micromechanical testing and interpretation. Existing computational studies have provided valuable complementary insight into H-He-V clusters and core-shell cavities^{16,17,20,45–48}. Density functional theory (DFT) calculations^{17,45,46} have provided key energetic parameters for H-He-V clusters, while molecular dynamics (MD) simulations^{18,19,47,48} have examined H trapping by He bubbles and the associated structural configurations. Nevertheless, these atomistic studies have focused on stable configurations, trapping behavior, or static properties. The influence of core-shell cavities on the mechanical response of the surrounding matrix, especially their role in stress concentration, dislocation emission, cavity growth, and secondary cavity nucleation during deformation, remains largely unresolved.

Another critical gap is that the specific role of H in cavity-mediated deformation and damage evolution has not been clarified across relevant loading conditions. Previous studies have introduced He bubbles with various structures (different sizes and He/V ratios) into various metallic systems to investigate their deformation behavior and mechanisms^{49–52}. These studies demonstrated that He bubbles subjected to external stress can grow through dislocation-mediated yielding processes. However, the

influence of H on the dynamic evolution of cavity nucleation and growth, particularly when H and He coexist within the same cavity (bubble), has received far less attention. Hatton et al.⁵³ demonstrated that H significantly influences He bubble growth and loop punching behavior, revealing a pronounced effect on dislocation generation and dynamics in mixed He-H gas bubbles compared to pure He bubbles in tungsten. Sanwar et al.⁵⁴ investigated the interaction of edge dislocations with H-He bubbles in tungsten and elucidated the synergistic effects of He and H on dislocation behavior in irradiated W during deformation. Moreover, our recent study²¹ examined the size dependence of the dynamic evolution of cavities containing both H and He under applied stress/strain fields, and further elucidated the role of H and its associated mechanisms within the cavities under specific conditions (723 K and 10^6 s^{-1}). Despite these advances, the mechanical response and defect evolution of H-He-containing cavities under varying conditions, including temperature, strain rate, and H/He implantation rate, remain insufficiently understood. Further investigation is therefore required to establish the role of H under these different conditions and to clarify its influence on cavity-mediated deformation and damage evolution.

To address these challenges, the present study establishes a multiscale computational framework integrating thermodynamic analysis constrained by experimentally derived cavity statistics, extended-timescale molecular dynamics (MD) simulations, and density functional theory (DFT) calculations to elucidate the mechanisms governing deformation and damage associated with irradiation-induced H-He core-shell cavities in BCC-Fe. Thermodynamic analysis first identifies physically representative cavity configurations expected under fusion-relevant irradiation conditions, providing experimentally informed initial states for atomistic simulations. Large-scale MD simulations then quantify the deformation behavior and defect evolution over a wide range of temperatures and strain rates, whereas DFT calculations reveal the atomistic origin of H-assisted interfacial defect activation. By integrating these complementary approaches across multiple length scales, this work establishes a multiscale mechanistic framework linking irradiation-induced cavity structures,

interfacial energetics, defect evolution, and mechanical response.

Results

Data-constrained framework for thermodynamic analysis

Recent triple-beam ion irradiation experiments using EELS elemental mapping have revealed a characteristic core-shell distribution in irradiation-induced cavities, with He preferentially localized in the cavity core and H enriched near the cavity surface^{6,11}. However, quantitative determination of the H and He contents within individual cavities remains challenging, particularly for H. A data-constrained thermodynamic framework was therefore developed to estimate the H occupancy of pre-existing cavities. This was achieved by combining experimentally constrained cavity sizes and He/V ratios with atomistic binding-energy data^{17,20,21,66}. To establish representative cavity configurations for the subsequent thermodynamic and MD analyses, experimentally measured and computationally derived He/V ratios for irradiation-induced bubbles in Fe-based alloys were compiled from previous irradiation experiments and MD simulations^{67–71}, as shown in Fig. 1 (a). Early measurements by Fréchal et al.⁶⁷ suggested an approximately linear dependence of He density on the inverse bubble radius. Subsequent positron annihilation spectroscopy (PAS) measurements⁷⁰ and MD simulations⁶⁹ covering a broader range of cavity sizes, however, indicated a logarithmic dependence of the He/V ratio on cavity size. The broader experimental and computational evidence was therefore used to constrain the size-dependent He/V range considered here, rather than directly extrapolating the experimentally measured EELS data to the sub-nanometer regime.

The upper bound of the He/V ratio was further constrained by reported cavity-stability limits from atomistic simulations⁷¹. Above the stability limit for a given cavity size, excessive He loading has been associated with loop punching and pronounced structural evolution of the cavity. Because the He content depends on irradiation temperature, He production, and implantation conditions, the He/V ratio is not expected to be unique for a given cavity size. Cavities formed under different irradiation conditions can therefore span a range of He/V ratios, including cavities with very low

He contents under relatively low He flux conditions. The lower bounds considered here were constrained primarily by available experimental measurements^{67,68,70}. Combining these experimental observations with the computationally established stability limits provides a size-dependent range of He/V ratios for the cavity configurations considered in this work.

The compiled cavity data were grouped into four representative size classes according to their measured size distributions, as shown in Fig. 1 (a). The mean cavity radius within each class was used to define the corresponding representative configuration. The resulting cavity radii and He/V ranges were 0.86 nm (He/V = 0.64 ~ 1.57), 1.43 nm (He/V = 0.28 ~ 1.26), 2.86 nm (He/V = 0.2 ~ 0.82), and 5.14 nm (He/V = 0.03 ~ 0.59). The decrease in the He/V ratio with increasing cavity size is consistent with the size dependence expected from the Young-Laplace relation^{72,73}. In addition, these representative radii are comparable to the characteristic cavity-size ranges and distribution peaks reported in multi-beam ion irradiation experiments on Fe-based steels^{6,7}. These four configurations were therefore used as representative cavity structures for the subsequent thermodynamic analysis.

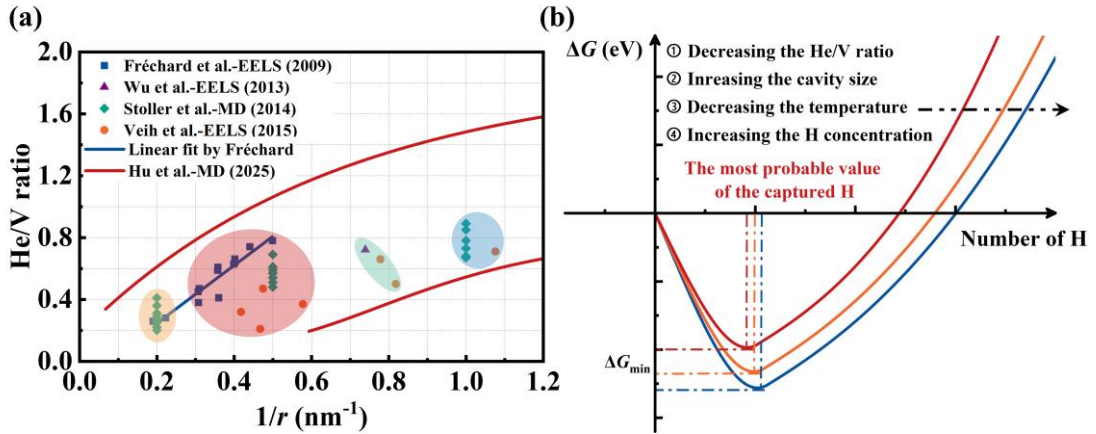


Fig. 1. (a) Compilation of experimental and computational data for the He/V ratios of irradiation-induced cavities in Fe-based steels^{67–71}. The data are grouped into four representative cavity-size classes, as indicated by the schematic geometries. (b) Schematic illustration of the data-constrained thermodynamic framework used to determine the thermodynamically preferred H occupancy of pre-existing cavities under specified cavity structures, temperatures, and matrix H concentrations through

minimization of the Gibbs free-energy change ($\Delta G_{\min}$).

Once the cavity size and He/V ratio were prescribed, the thermodynamic framework described in Supplementary Section S2 was used to determine the thermodynamically preferred H occupancy of each cavity under specified temperature and matrix H concentration, as schematically illustrated in Fig. 1 (b). The resulting Gibbs free-energy profiles indicate that the enthalpic contribution is primarily associated with the cavity structure, particularly its size and He/V ratio, whereas the entropy contribution depends strongly on the H concentration in the surrounding matrix. Within the parameter space considered here, larger cavities, lower He/V ratios, and higher matrix H concentrations increase the thermodynamic preference for H incorporation, whereas increasing temperature reduces this preference. Although the absolute H content increases with cavity size, the corresponding H/V ratio does not necessarily increase, reflecting the different scaling of cavity volume and H occupancy with cavity size. The calculated H occupancies for the different cavity configurations are summarized in Table 1.

A temperature of 723 K was selected for the main parametric analysis because it is close to the reported temperature range associated with maximum swelling in triple-beam irradiation experiments on Fe-based steels ^{6,7}. The matrix H concentrations considered here, 100 ~ 1000 appm, span the range adopted in previous irradiation studies and provide representative conditions for evaluating H retention in the cavity configurations considered ^{2,11}.

Table 1

Thermodynamically preferred H/V ratios for cavities with different sizes and He/V ratios in BCC Fe at 723 K under different matrix H concentrations.

Cavity structures	He/V ratios	H concentrations	H/V ratios
<i>R</i> = 0.86 nm	0.80	100 appm	0.59
	1.20		0.54
	1.50		0.49
	0.80		0.70
	1.20		0.66

(259 vacancies)	1.50		0.63
		500 appm	
	0.80		0.75
	1.20	1000 appm	0.70
	1.50		0.67
$R = 1.43$ nm	0.50		0.39
	0.80	100 appm	0.37
	1.20		0.33
	0.50		0.45
(1067 vacancies)	0.80	500 appm	0.42
	1.20		0.40
	0.50		0.48
	0.80	1000 appm	0.46
	1.20		0.43
$R = 2.86$ nm	0.20		0.21
	0.50	100 appm	0.20
	0.80		0.18
	0.20		0.24
(8393 vacancies)	0.50	500 appm	0.23
	0.80		0.22
	0.20		0.26
	0.50	1000 appm	0.25
	0.80		0.23
$R = 5.14$ nm	0.10		0.13
	0.30	100 appm	0.12
	0.50		0.11
	0.10		0.15
(48821 vacancies)	0.30	500 appm	0.14
	0.50		0.13
	0.10		0.16
	0.30	1000 appm	0.15
	0.50		0.14

Temperature and strain-rate effects on cavity-mediated deformation

The preceding thermodynamic analysis establishes the feasibility of H trapping in cavities with different sizes and He/V ratios under varying irradiation conditions. The resulting cavity configurations are consistent with the core-shell structures observed in multi-beam ion irradiation experiments on steels^{6,11} and provides a basis for constructing physically representative cavity configurations in Fe-based materials. The predicted H occupancies were therefore used to determine the initial H contents of core-

shell cavities for subsequent MD simulations. To examine cavity-mediated deformation while avoiding pronounced size effects identified in our previous study ²¹, a representative cavity radius of 2.86 nm was selected. For the temperature and strain-rate analyses, all initial core-shell cavities were constructed using the H contents predicted for a matrix H concentration of 1000 appm at 723 K, while the He/V ratio was varied within the experimentally constrained range. The corresponding H/V ratios are summarized in Table 1.

The effects of temperature and strain rate on the mechanical response of BCC-Fe containing H-He core-shell cavities were investigated using a cavity radius of 2.86 nm. For the temperature-dependent simulations, triaxial tensile loading was applied at a constant strain rate of $1 \times 10^6 \text{ s}^{-1}$, whereas the strain-rate dependence was examined at 723 K over strain rates from $1 \times 10^6 \text{ s}^{-1}$ to $1 \times 10^9 \text{ s}^{-1}$. A pure void was included as a reference to evaluate the effect of H and He confined within the cavity. The term temperature effect refers to the ambient temperature during mechanical loading.

The stress-strain responses in Fig. 2 exhibit a similar overall evolution across the investigated temperatures and strain rates. The initial elastic response is largely insensitive to the cavity structure, with the stress increasing nearly linearly before reaching the peak stress. In contrast, the peak stress and subsequent plastic response are strongly affected by the presence of H and He. At a given temperature or strain rate, the tensile strength decreases systematically with increasing He/V ratio. For a He/V ratio = 0.8 with the corresponding H content, the tensile strength is reduced by 17.5%, 19.4%, and 34.4% at 300, 723, and 973 K, respectively, relative to the pure-void reference. At 723 K, the corresponding reductions are 19.4%, 18.9%, 15.8%, and 13.6% at strain rates of $1 \times 10^6 \text{ s}^{-1}$, $1 \times 10^7 \text{ s}^{-1}$, $1 \times 10^8 \text{ s}^{-1}$, and $1 \times 10^9 \text{ s}^{-1}$, respectively. These results show that the strength reduction associated with cavities becomes more pronounced with increasing temperature, whereas the difference from the pure-void reference decreases progressively with increasing strain rate. The overall temperature dependence retains the characteristic thermal softening, while the increase in tensile strength with strain rate indicates positive strain-rate sensitivity under triaxial tensile loading ^{52,74–77}.

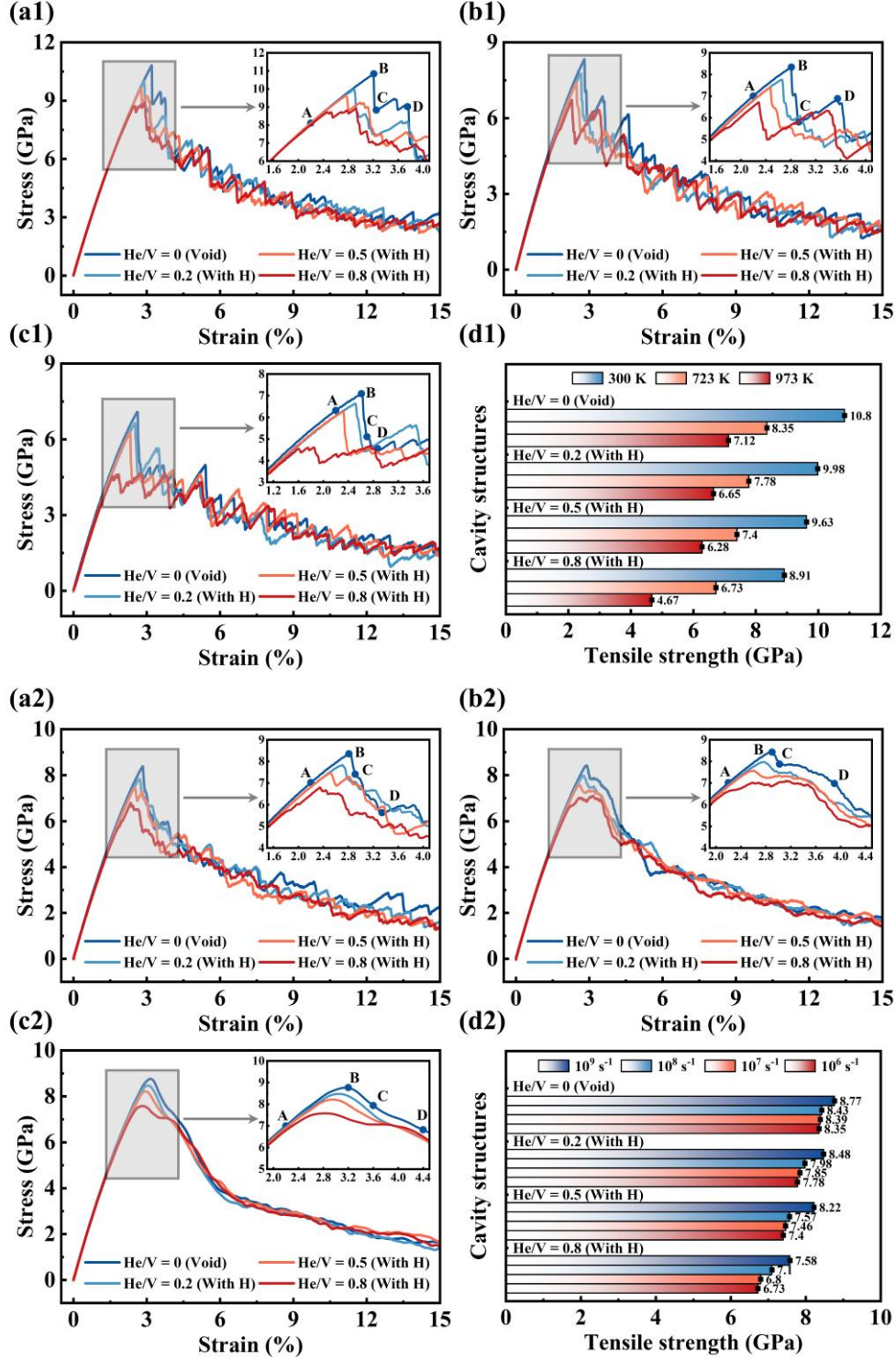


Fig. 2. Stress-strain responses of BCC-Fe containing a H-He co-occupied cavity under hydrostatic tensile loading at a strain rate of $1 \times 10^6 \text{ s}^{-1}$ and temperatures of (a1) 300 K, (b1) 723 K, and (c1) 973 K and at 723 K and strain rates of (a) $1 \times 10^7 \text{ s}^{-1}$, (b) $1 \times 10^8 \text{ s}^{-1}$, and (c) $1 \times 10^9 \text{ s}^{-1}$. The magnified insets correspond to the gray shaded regions and illustrate the evolution of curves for different cavity structures at various

temperatures. (d) Tensile strengths of BCC-Fe with cavities of different structures at each temperature, determined from the peak stresses in panels (a)-(c).

The evolution of defects further indicates that plastic deformation remains localized around the pre-existing cavity across the investigated conditions. As shown in Supplementary Figs. S2 and S3, dislocation activity emerges near the peak stress and coincides with the initial growth of the pre-existing cavity, indicating that plastic deformation is initiated in the cavity vicinity. Increasing the He/V ratio generally reduces the critical strain for dislocation nucleation at a given temperature and strain rate. With continued deformation, the dislocation density increases and reaches a maximum as dislocations interact and accumulate in the surrounding matrix. Secondary cavities subsequently nucleate at strains close to those associated with the peak dislocation density. This evolution suggests a sequential process involving cavity-associated dislocation emission, dislocation multiplication, and secondary cavity formation^{78,79}. The overall sequence is maintained across the investigated temperature and strain-rate ranges, although the critical strains and extent of defect evolution vary with the loading conditions.

Temperature and strain rate, however, regulate this process through different responses. Increasing temperature promotes earlier dislocation activation and reduces the critical strain associated with peak dislocation density and secondary cavity nucleation. The cavity morphology also changes from a more spherical to a faceted configuration at higher temperatures, while the presence of He contributes to cavity stabilization through internal pressurization. At the same time, H retention at the cavity surface decreases with increasing temperature, accompanied by H redistribution into the surrounding matrix. The simultaneous changes in cavity morphology and H distribution modify the local cavity environment during deformation and are consistent with the stronger strength reduction observed at higher temperatures. In contrast, increasing strain rate shifts dislocation emission, peak dislocation density, and secondary cavity nucleation to higher strains. The progressively smaller differences among cavity structures at higher strain rates suggest that the mechanical contribution

of the core-shell composition becomes less pronounced as the loading rate increases.

Overall, the same cavity-mediated deformation sequence is observed over the investigated temperature and strain-rate ranges, while temperature and strain rate modify its characteristic evolution in different ways. Temperature affects both the cavity structure and the redistribution of H during deformation, whereas strain rate primarily changes the time available for dislocation evolution and cavity-associated defect accumulation. Across the investigated conditions, cavities consistently exhibit earlier plastic activation than the pure-void reference, indicating that the presence of H and He alters the onset and subsequent evolution of cavity-mediated plasticity.

The corresponding microstructural evolution is shown in Figs. 3 and 4 for pure voids and cavities with a He/V ratio of 0.5 containing H. The selected configurations correspond to the elastic stage, peak stress, plastic deformation, and secondary cavity nucleation, marked as A, B, C, and D in Figs. 2 (a-c). Across all temperatures and strain rates, the elastic-stage configurations show little change in cavity morphology and no appreciable dislocation activity, consistent with the weak dependence of the elastic response on cavity composition and loading rate. Beyond the peak stress, plastic deformation initiates through dislocation emission from the cavity surface, followed by dislocation accumulation and secondary cavity nucleation in the surrounding matrix. Thus, despite variations in the kinetics of deformation, the overall sequence remains characterized by stress concentration, dislocation emission, dislocation multiplication, and secondary cavity nucleation.

Temperature primarily modifies the cavity structure and the subsequent evolution of H and defects. As shown in Fig. 3 (A11-A13) and (A21-A23), increasing temperature drives the cavity morphology from nearly spherical toward more faceted configurations⁸⁰, whereas He-induced internal pressure helps maintain the cavity structure. Meanwhile, H retention at the cavity surface decreases with increasing temperature because of thermally activated desorption²⁰. Dislocation emission after the peak stress originates from the cavity surface, as shown in Fig. 3 (C11-C13) and (C21-C23), and occurs at lower strains with increasing temperature and He/V ratio. At 300 K, H and He

remain largely confined within the cavity, and subsequent cavity growth and nucleation are dominated by dislocation-mediated deformation. At 723 and 973 K, partial H desorption and diffusion into the matrix become more pronounced. The mobile H can interact with lattice defects and dislocations under applied stress, which may contribute to the subsequent accumulation of defects and secondary cavity formation⁸¹. The newly formed cavities also exhibit H enrichment at their surfaces, as shown in Fig. 3 (D11-D13) and (D21-D23). These observations indicate that temperature affects cavity-mediated damage through the coupled evolution of cavity morphology, H redistribution, and He-induced pressure.

In contrast, strain rate mainly affects the kinetics of defect evolution. As shown in Fig. 4, the cavity morphologies at the elastic stage remain nearly identical over the investigated strain rates, with no detectable dislocation activity. Once plasticity begins, increasing the strain rate systematically shifts dislocation emission, the attainment of peak dislocation density, and secondary cavity nucleation to higher strains. The reduced time available for dislocation nucleation and defect rearrangement under rapid loading delays plastic activation and limits subsequent defect evolution. Accordingly, higher strain rates suppress dislocation accumulation and reduce the cavity volume generated during deformation, as further shown in Supplementary Fig. S4. The progressive convergence of the responses among different cavity structures at higher strain rates also indicates that the influence of H and He becomes less pronounced when defect evolution is kinetically constrained. Similar rate-dependent suppression of dislocation-mediated cavity growth has been reported for voids/He bubbles in BCC metals^{52,82}.

Taken together, Figs. 3 and 4 show that temperature and strain rate modify the same cavity-mediated deformation sequence through distinct pathways. Temperature affects cavity morphology and H redistribution while also modifying defect activation, whereas strain rate primarily constrains the time available for dislocation evolution and defect accumulation. Despite these differences, dislocation emission from the cavity surface remains the primary transition from elastic to plastic deformation, followed by dislocation accumulation and secondary cavity nucleation.

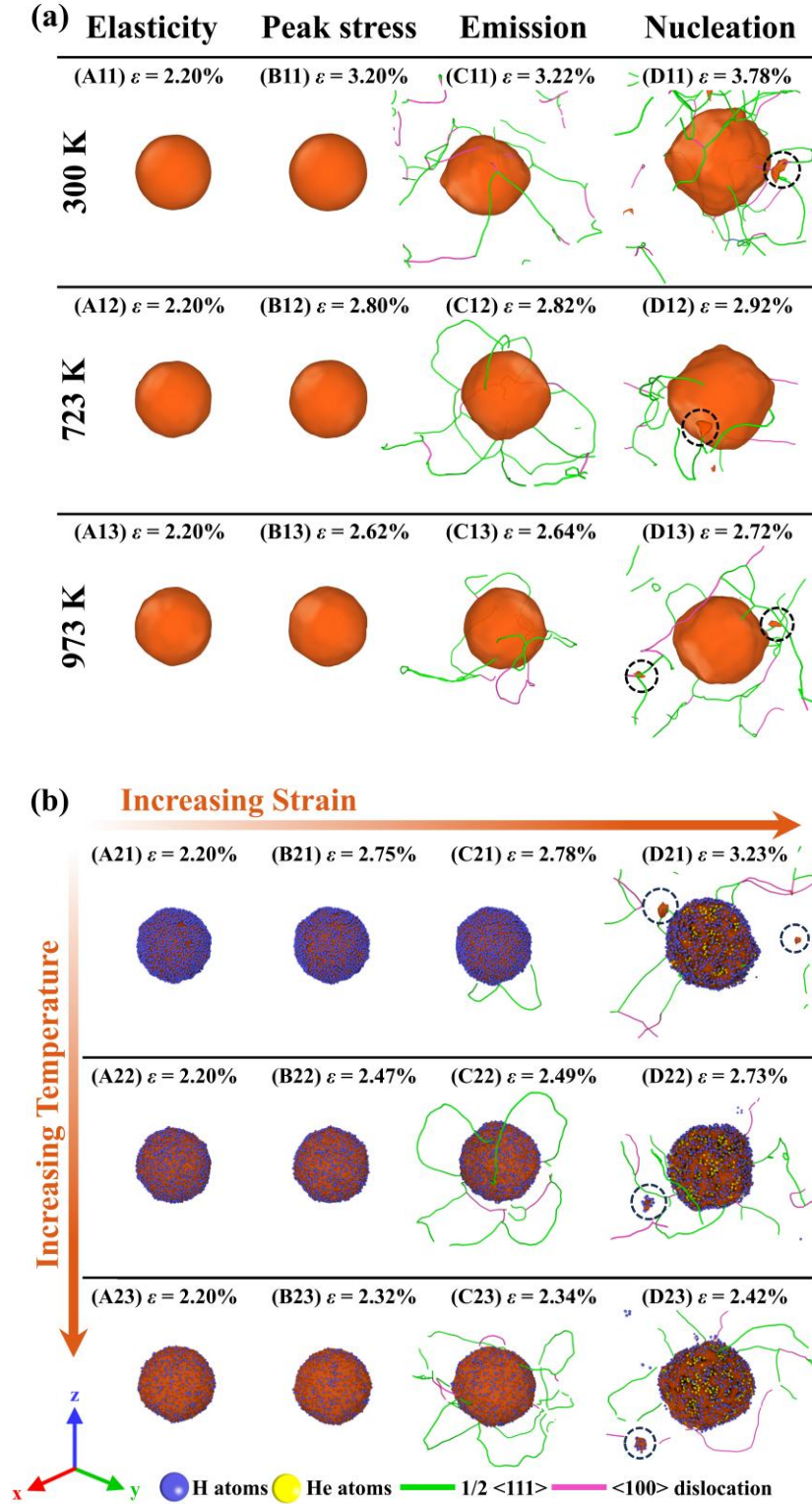


Fig. 3. Defect configurations in BCC-Fe at key deformation stages for (a) pure voids ($\text{He}/V = 0$) and (b) core-shell structured cavities ($\text{He}/V = 0.5$) under a hydrostatic strain (ε) field at different temperatures. The three-dimensional views corresponding to different temperatures and cavity structures are associated with the deformation

stages labeled as points (A), (B), (C), and (D) on the stress-strain curves shown in Figs. 2 (a1-c1). Dislocations within the matrix are identified using the DXA method, while cavity surfaces are rendered in orange using the CSM algorithm. Cavities nucleated during plastic deformation are highlighted by black circles.

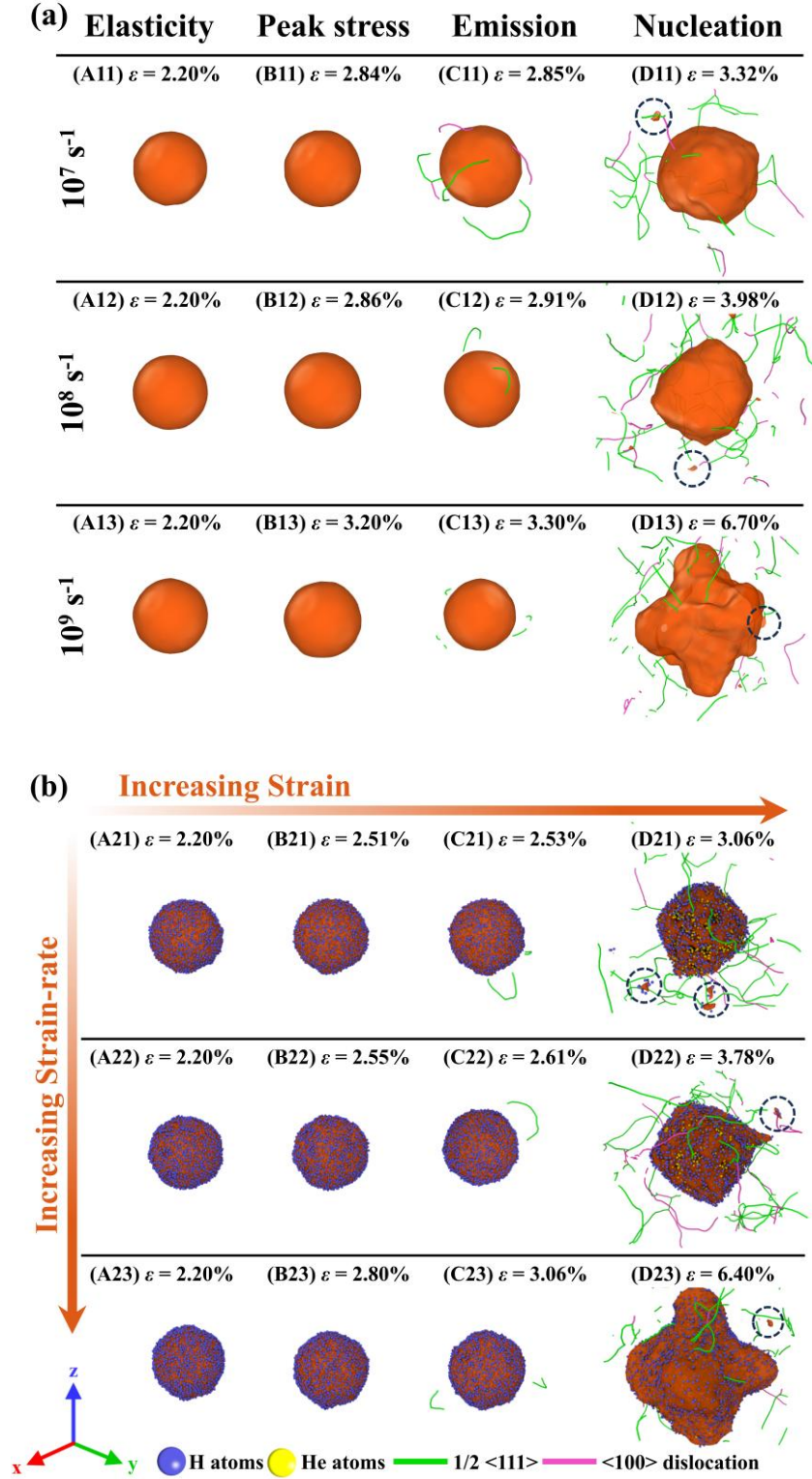


Fig. 4. Defect configurations in BCC-Fe at key deformation stages for (a) pure voids ($\text{He}/V = 0$) and (b) core-shell structured cavities ($\text{He}/V = 0.5$) under a hydrostatic strain (ε) field at different strain rates. The three-dimensional views corresponding to different strain rates and cavity structures are associated with the deformation stages labeled as points (A), (B), (C), and (D) on the stress-strain curves shown in Figs. 2 (a2-c2). Dislocations within the matrix are identified using the DXA method, while cavity surfaces are rendered in orange using the CSM algorithm. Cavities nucleated during plastic deformation are highlighted by black circles.

The role of H in cavity-mediated deformation

To isolate the role of H and its underlying mechanism within core-shell structured cavities, a systematic comparison was conducted between cavities containing both H and He and those containing only He under otherwise identical conditions. The cavity radius, He/V ratio, and loading mode were kept the same in each comparison, such that the differences in mechanical response were associated with H incorporation. Both temperature-dependent and strain-rate-dependent conditions were considered to determine whether the H contribution persists under different deformation conditions.

Effects of H on deformation under different conditions

At a given temperature or strain rate, the presence of H consistently reduces both the tensile strength and the strain required to reach the peak stress, as shown in Figs. 5 (a-c) and 6 (a-c). To quantitatively evaluate the effect of H in core-shell structured cavities on mechanically relevant deformation thresholds, three normalized dimensionless descriptors are introduced based on characteristic mechanical parameters. These include the normalized peak-stress factor (G_{peak}), the normalized dislocation-emission critical-strain factor (G_{emit}), and the normalized cavity-nucleation critical-strain factor (G_{nuc}), defined generally as:

$$G_i = \frac{M_i^{\text{sys}}}{M_i^{\text{ref}}}, i \in \{\text{peak}, \text{emit}, \text{nuc}\} \quad (1)$$

Where M_i^{sys} denotes the critical strain of the target system and M_i^{ref} denotes that of the reference system. The corresponding degradation parameter is defined as:

$$D_i = 1 - G_i = 1 - \frac{M_i^{sys}}{M_i^{ref}}, i \in \{peak, emit, nuc\} \quad (2)$$

Accordingly, D_{peak} , D_{emit} , and D_{nuc} represent the degradation in peak stress, dislocation-emission critical strain, and nucleation critical strain, respectively. By construction, all of these quantities are dimensionless. Together, these descriptors enable direct comparison of the influence of core-shell cavities and the H accommodated within them over different stages of deformation, while also providing a convenient basis for linking the atomistic results to larger-scale descriptions.

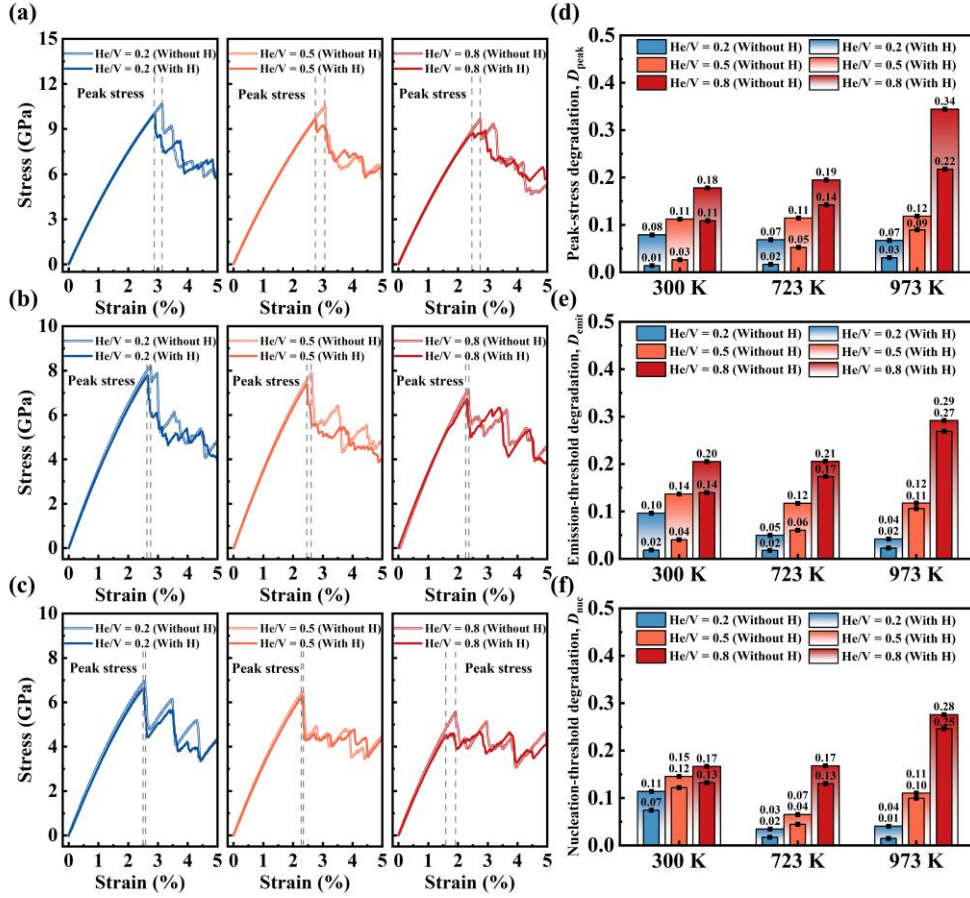


Fig. 5. (a-c) Stress-strain responses of BCC-Fe containing either H-He co-occupied cavities or He-only cavities under hydrostatic tensile loading at a strain rate of $1 \times 10^6 \text{ s}^{-1}$ and temperatures of (a) 300 K, (b) 723 K, and (c) 973 K. (d-f) Degradation of peak stress (d), critical strain for dislocation emission (e), and critical strain for secondary cavity nucleation (f) in BCC-Fe samples containing pre-existing cavities with different structures at various temperatures, relative to pure voids of the same size.

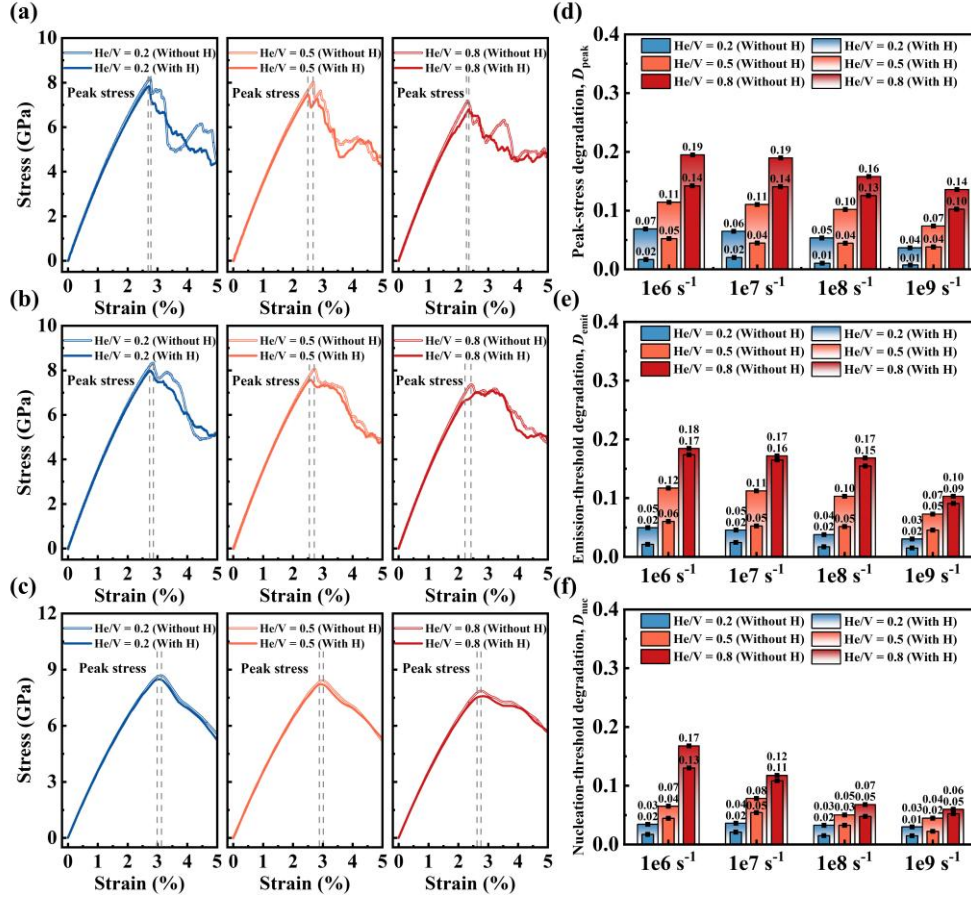


Fig. 6. (a-c) Stress-strain responses of BCC-Fe containing either H-He co-occupied cavities or He-only cavities under hydrostatic tensile loading at 723 K and strain rates of (a) $1 \times 10^7 \text{ s}^{-1}$, (b) $1 \times 10^8 \text{ s}^{-1}$, and (c) $1 \times 10^9 \text{ s}^{-1}$. (d-f) Degradation of peak stress (d), critical strain for dislocation emission (e), and critical strain for secondary cavity nucleation (f) in BCC-Fe samples containing pre-existing cavities with different structures at various strain rates, relative to pure voids of the same size.

The temperature-dependent results in Fig. 5 (d-f) show that H does not change the overall dependence of deformation degradation on He/V ratio, but modifies its magnitude. Increasing He/V generally increases the reductions in peak stress and the critical strain for dislocation emission, reflecting the increasing influence of He-induced internal pressure on the cavity surface. In contrast, the contribution of H depends strongly on its retention at the cavity surface. Higher temperature and larger He/V ratios reduce H retention through thermally activated desorption²⁰, thereby changing the extent to which H directly affects interfacial deformation. At lower temperatures and lower He/V ratios, retained H has a more pronounced effect on peak

stress and dislocation emission. At 973 K and $\text{He}/\text{V} = 0.8$, however, the presence of H produces a particularly large reduction in peak stress, which is associated with early dislocation activity at the cavity surface and accelerated local damage accumulation. For secondary cavity nucleation, H further reduces the critical strain as the He/V ratio increases, although the magnitude of this degradation does not vary monotonically with temperature.

The strain-rate-dependent results in Fig. 6 (d-f) show a similar overall effect of H, but with a clear kinetic dependence. At each strain rate, H reduces the peak stress and the critical strains for dislocation emission and secondary cavity nucleation. However, the magnitude of H-induced degradation decreases as the strain rate increases. This trend is consistent with the strain-rate dependence observed in Fig. 5. At high strain rates, the limited time available for dislocation nucleation, H redistribution, and defect rearrangement restricts the development of H-assisted deformation processes. The delay in reaching peak dislocation density, particularly at $1 \times 10^9 \text{ s}^{-1}$, further indicates that defect evolution is strongly constrained under rapid loading. Consequently, the influence of H on peak stress and dislocation emission is progressively reduced with increasing strain rate, whereas at lower strain rates sufficient time is available for H-assisted defect evolution to develop.

Taken together, Figs. 5 and 6 demonstrate that H facilitates earlier cavity-mediated plastic activation, but the magnitude of its contribution depends strongly on the loading conditions. Temperature modifies the H effect primarily through changes in H retention and redistribution, whereas strain rate limits the time available for H-assisted defect evolution. The distinct responses to temperature and strain rate therefore indicate that the mechanical role of H cannot be described by a single controlling parameter. The atomistic origin of this effect is examined further through the interfacial H distribution and DFT calculations.

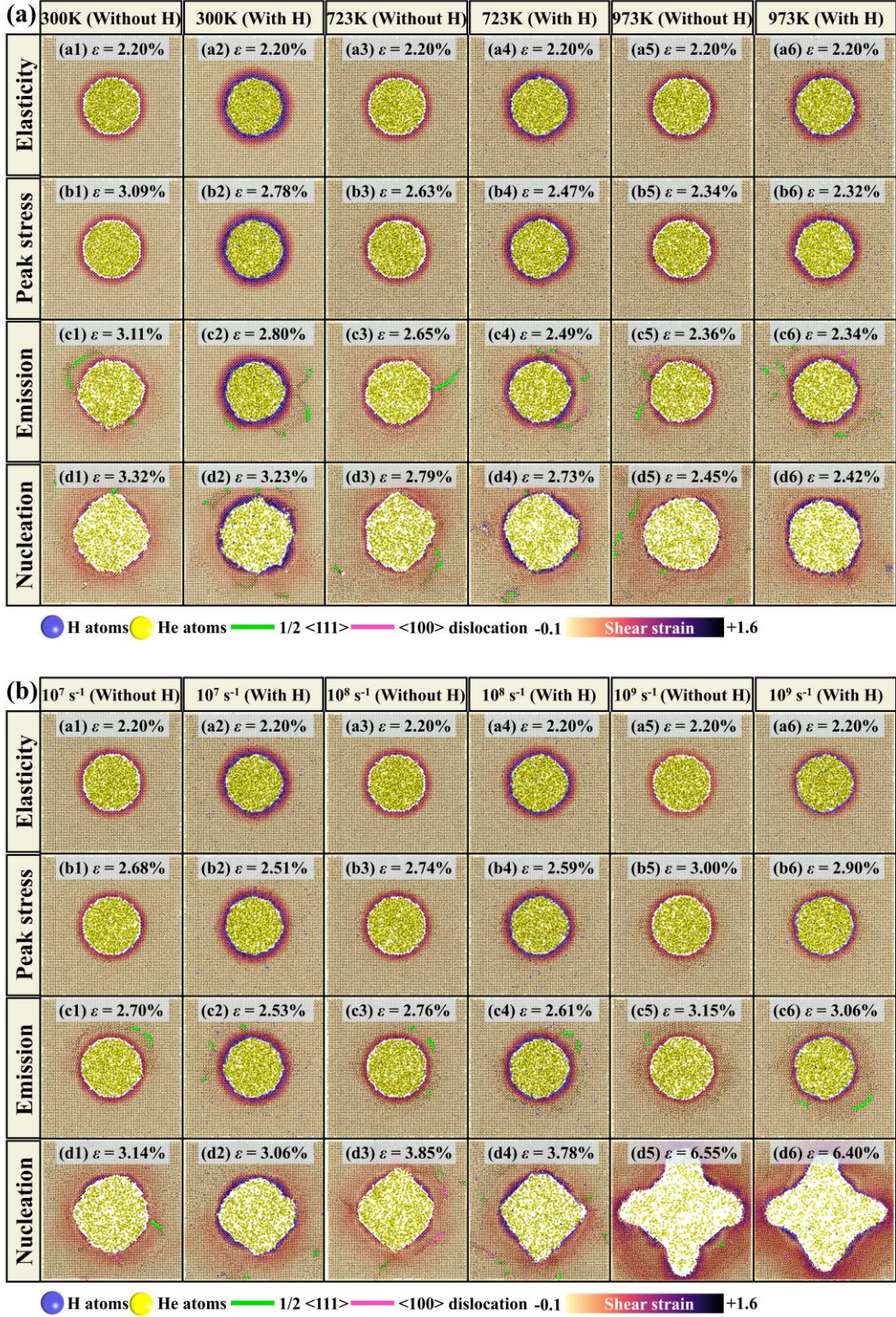


Fig. 7. Atomic distribution (colored by shear strain) and defect configurations (with dislocations identified using the DXA algorithm) in BCC-Fe containing cavities with a He/V ratio of 0.5 (with or without H) under a hydrostatic strain (ε) field at different (a) temperatures and (b) strain-rates. In the cross-sectional views, panels (a-d)

correspond to different stages of the deformation response along the stress-strain curves.

The atomic configurations corresponding to the characteristic deformation stages are shown in Fig. 7. These results provide direct atomistic evidence for the dependence of H-assisted deformation on temperature and strain rate. At all temperatures and strain rates, H enhances the local strain field around the cavity relative to the corresponding He-only cavity, whereas He remains confined within the cavity core because of its strong binding to the cavity (~ 2.0 eV)^{16,45}. In contrast, the lower binding energy of H (~ 0.8 eV)^{16,83,84} allows partial de-trapping during deformation. The extent of H de-trapping increases with temperature, leading to reduced H retention at the cavity surface and a weaker direct contribution of H to the local strain field.

The temperature-dependent configurations in Fig. 7 (a) suggest two distinct H-assisted pathways for secondary cavity nucleation. At 300 K, H remains largely trapped at the cavity surface and promotes dislocation emission from the cavity. The subsequent accumulation and interaction of dislocations provide favorable sites for micro-void nucleation^{78,79}, corresponding to a dislocation-mediated pathway. At 973 K, increased H migration into the matrix provides a second pathway. The mobile H can interact with lattice defects under the local stress field and promote vacancy formation, thereby facilitating vacancy-mediated cavity nucleation⁸¹. At 723 K, partial H retention at the cavity and limited H migration into the matrix allow both pathways to operate. The relative contributions of these two pathways therefore depend on the balance between H retention at the cavity and H transport into the matrix. At high He/V ratios, the increased internal pressure generated by He further enhances the local stress concentration, which can compensate for the reduced H retention at elevated temperature. This combined effect contributes to the non-monotonic temperature dependence of the cavity-nucleation degradation shown in Fig. 5 (f).

The strain-rate-dependent configurations in Fig. 7 (b) show a different response. The local strain enhancement associated with H becomes progressively weaker as the strain rate increases. Under rapid loading, the limited time available for atomic

rearrangement restricts H redistribution and defect evolution, thereby reducing the contribution of H to cavity-mediated deformation. At $1 \times 10^9 \text{ s}^{-1}$, the critical strain for secondary cavity nucleation is substantially increased, while dislocation emission and subsequent dislocation growth are strongly delayed. Newly generated vacancies also have insufficient time to diffuse and aggregate. Consistent with the evolution in Supplementary Fig. S3, the increase in pre-existing cavity volume precedes substantial dislocation accumulation, indicating a greater contribution from cavity growth to plastic accommodation under rapid loading. Similar competition between cavity growth and dislocation-mediated plasticity has been reported for He-containing cavities in metals at high strain rates ⁵². Overall, the atomic configurations demonstrate that H participates in multiple stages of cavity-mediated deformation, but its dominant pathway depends on the loading conditions. Temperature controls the balance between H retention at the cavity and H migration into the matrix, whereas strain rate limits the time available for H redistribution and defect evolution. These distinct responses account for the temperature- and strain-rate-dependent H effects observed in Figs. 5 and 6.

Atomistic origin of H-assisted dynamic deformation

To clarify the atomistic origin of the H effect, the radial pair distribution functions (PDFs) of H during deformation are presented in Supplementary Figs. S4 and S5. The peak at approximately 0.74 Å corresponds to H₂ molecules within the cavity core, whereas peaks in the range of approximately 1.7-1.77 Å indicate H atoms localized at the cavity surface ^{20,85}. Across all temperatures, H remains predominantly localized at the cavity surface throughout deformation (Fig. S4). At lower temperatures and lower He/V ratios, reduced H de-trapping and the larger available free volume favor the formation of H₂ molecules within the cavity interior. At 973 K, thermal activation enhances H de-trapping and redistribution, although some H still migrates into the cavity interior and recombines into H₂. Despite these changes, the dominant H population remains associated with the cavity surface. Thus, although molecular H₂ can form within the cavity, interfacial H remains the dominant H population relevant to the mechanical response.

A similar trend is observed under different strain rates (Fig. S5). At low He/V, increasing strain rate suppresses H redistribution and de-trapping, favoring H₂ molecules formation within the cavity interior, particularly at $1 \times 10^9 \text{ s}^{-1}$. Nevertheless, most H remains localized at the cavity surface over the investigated strain-rate range. The persistence of interfacial H, together with the degradation trends in Figs. 6 (d-f), indicates that surface-trapped H remains involved in cavity-mediated deformation even under rapid loading. The preferential localization of H at the cavity surface is consistent with its interfacial energetics. Previous DFT calculations showed that the standoff region at Fe-He interfaces provides a favorable site for H trapping because of the reduced host electron density^{46,86}. H₂ molecules formation in the cavity interior becomes favorable only under sufficiently high H coverage or thermally activated conditions. The present PDF results therefore support an interfacial mechanism in which surface-trapped H, rather than molecular H₂, makes the dominant contribution to the mechanical response.

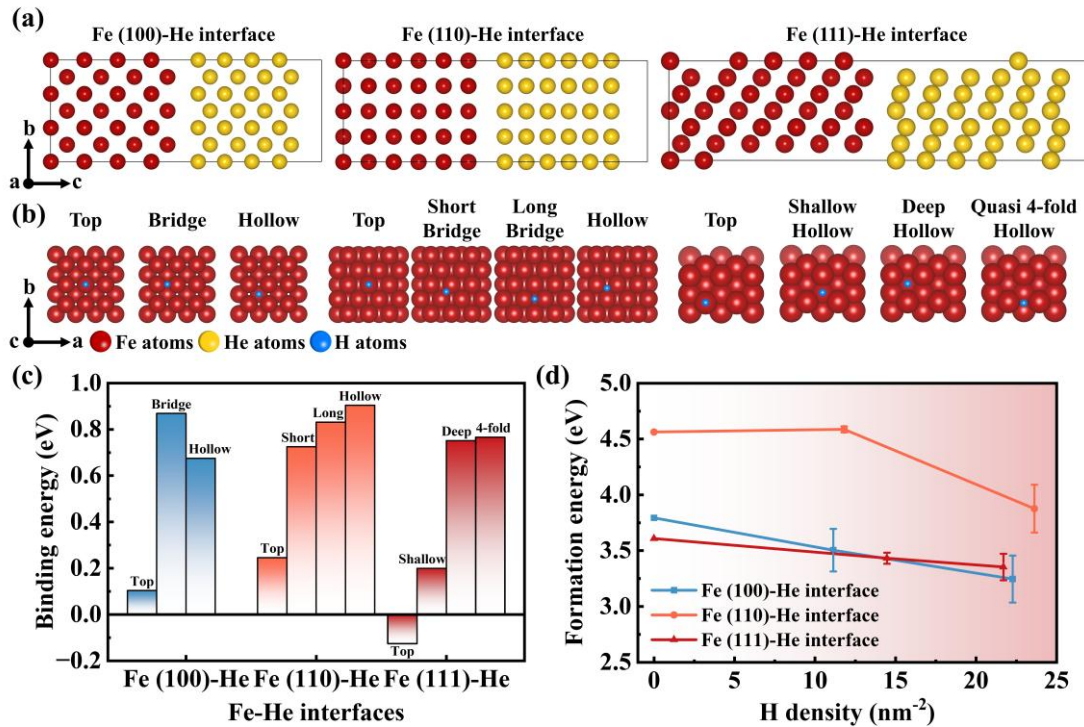


Fig. 8. Energetic interpretation of the effect of H on interstitial emission from Fe-He interfaces based on DFT calculations. (a) Relaxed atomic configurations of representative Fe (100)-He, Fe (110)-He, and Fe (111)-He interfaces. (b) Adsorption

sites of H at the Fe-He interfaces, where the red, yellow, and blue spheres represent Fe, He, and H atoms, respectively. (c) Binding energies of an individual H adatom at the adsorption sites shown in (b). (d) Effect of H on the formation energies of an interstitial at Fe-He interfaces as a function of H density.

To further examine the energetic origin of the H-associated defect response, DFT calculations were performed for Fe-He interfaces with (100), (110), and (111) orientations, as summarized in Fig. 8. The preferred H adsorption sites and corresponding binding energies vary with interface orientation, as shown in Figs. 8 (b) and (c). More importantly, the formation energy of an interstitial decreases systematically with increasing H coverage for all three interface orientations, as shown in Fig. 8 (d). The calculated H coverages encompass the range corresponding to the core-shell cavity configurations considered in the MD simulations. These results show that interfacial H thermodynamically facilitates interstitial formation at Fe-He interfaces by lowering its formation energy. This provides an atomistic energetic basis that is consistent with the enhanced dislocation emission observed in the MD simulations and suggests that H trapped at the Fe-He interface can facilitate the transition from localized interfacial deformation to defect emission and subsequent cavity-mediated plasticity.

Discussion

The results establish a common cavity-mediated deformation mechanism in BCC-Fe containing H-He core-shell cavities under hydrostatic/triaxial tensile loading. Regardless of temperature and strain rate, deformation proceeds through stress concentration around the cavity, dislocation emission from the cavity surface, dislocation accumulation, and secondary cavity nucleation. Temperature and strain rate primarily modify the critical conditions and kinetics rather than the sequence of events, as shown in Figs. 2-4. Temperature and strain rate primarily modify the critical conditions and kinetics of these processes rather than their overall sequence. Increasing temperature promotes thermal activation and defect evolution, whereas increasing strain rate restricts the time available for atomic rearrangement and defect development.

The resulting positive strain-rate sensitivity (PSRS) ⁷⁷ therefore reflects kinetic constraints on cavity-mediated plasticity rather than a change in the underlying deformation mechanism.

The distinct roles of H and He provide a physical basis for this coupled response. The MD and DFT results show that He remains preferentially confined within the cavity, whereas H is stabilized mainly at the cavity-matrix interface and can partially redistribute into the surrounding matrix. Confined He maintains internal pressure and contributes to the tensile stress concentration at the cavity surface, thereby providing a major mechanical contribution to defect activation. Interfacial H, in contrast, modifies the local interfacial energetics and facilitates localized defect formation and emission. The coupled H-He response can therefore be understood as a complementary interaction between cavity pressurization by He and interfacial defect activation mediated by H, rather than as an independent contribution from either species alone.

As shown in Figs. 5-8, the H-assisted defect response is consistent with the general concept of Hydrogen-Enhanced Localized Plasticity (HELP), in which H facilitates localized deformation near stress-concentrating defects ⁸⁷⁻⁹¹. The present results further indicate a more specific interfacial mechanism associated with H adsorption at Fe-He cavity interfaces. H retained near the cavity surface enhances local deformation and facilitates dislocation emission, whereas partial redistribution at elevated temperature provides an additional pathway for defect evolution in the surrounding matrix. This behavior is more closely related to the adsorption-induced dislocation emission (AIDE) framework ^{92,93}, in which adsorbed H modifies the local energetic conditions for defect emission. The DFT calculations support this interpretation by showing that increasing H coverage systematically lowers the formation energy of interstitials at Fe-He interfaces with different crystallographic orientations. Although this energetic result does not directly describe the barrier for dislocation nucleation, it provides an atomistic basis consistent with the enhanced defect emission observed in the MD simulations.

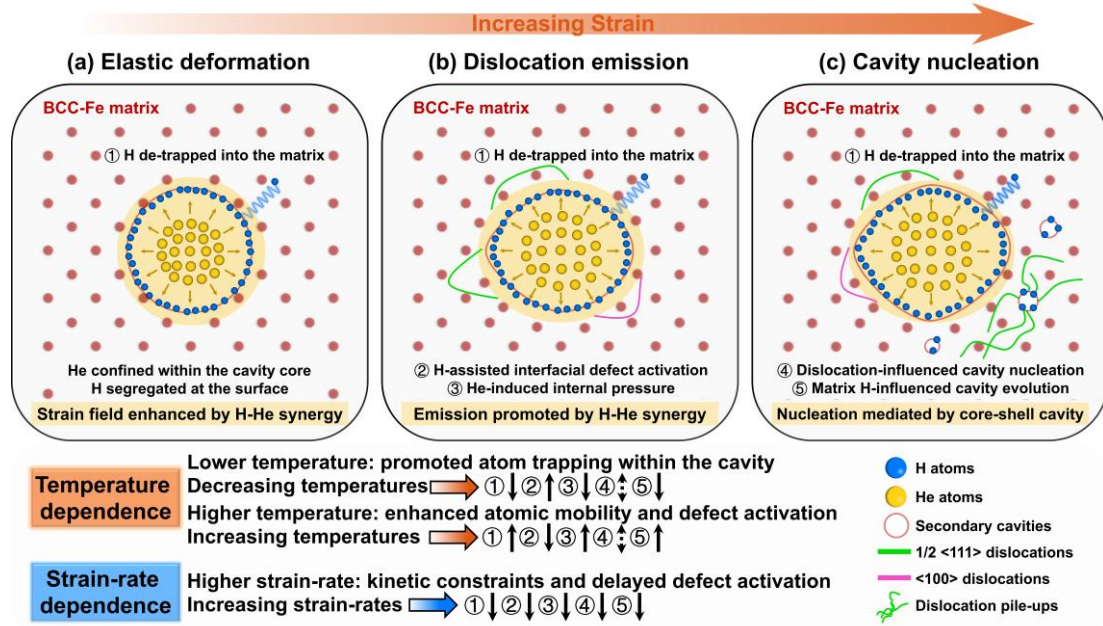


Fig. 9. Schematic illustration of the cavity-mediated deformation mechanism of BCC-Fe containing core-shell cavities under hydrostatic/triaxial tensile loading, highlighting the synergistic roles of H and He and the regulation of each deformation stage by temperature and strain rate.

To integrate these findings, Fig. 9 summarizes the deformation mechanism in three stages: elastic deformation, dislocation emission from the cavity surface, and secondary cavity nucleation in the surrounding matrix. During the elastic stage, He-induced internal pressure contributes to the primary stress concentration around the cavity, while interfacial H modifies the local strain and energetic state. Temperature can alter these interfacial conditions through changes in H mobility, retention, and cavity structure, whereas strain rate has a comparatively limited influence before significant defect evolution begins. During dislocation emission, He maintains the stress concentration required for defect activation, while interfacial H facilitates defect formation and emission through its modification of the local interfacial energetics. Increasing strain rate delays this process by restricting atomic rearrangement, H redistribution, and defect evolution. Temperature produces competing effects: H retention at the interface decreases with increasing temperature, whereas thermal activation and He-induced internal pressure promote defect activity. The balance between these contributions leads to the observed temperature dependence of the H-associated deformation response.

During subsequent secondary cavity nucleation, dislocation accumulation and interaction generate local stress concentrations that can provide favorable sites for micro-void formation ⁷⁹. H may affect this stage indirectly through its earlier influence on interfacial defect activation and, at elevated temperatures, through redistribution into the surrounding matrix. Redistributed H may interact with lattice defects under the applied stress and contribute to vacancy-related defect evolution ⁸¹. In contrast, increasing strain rate suppresses H redistribution and defect evolution by reducing the available time, weakening this H-associated pathway. The resulting deformation response thus reflects the coupled effects of He retention and pressurization, H interfacial trapping and redistribution, thermal activation, and loading-rate-dependent kinetic accessibility.

The atomistic simulations presented here should not be regarded as definitive predictions of irradiation-induced deformation under service conditions. Rather, they provide a physically grounded framework for connecting experimentally relevant cavity structures with their underlying atomistic mechanisms and for evaluating mechanistic hypotheses proposed to interpret irradiation-induced damage. By combining experimentally constrained cavity sizes and He/V ratios with thermodynamically preferred H occupancy, extended-timescale MD simulations, and DFT calculations, this work establishes a direct link between irradiation-induced cavity structure, interfacial H behavior, defect activation, and mechanical response. The results further indicate that the mechanical consequences of H and He cannot be described by He/V ratio, temperature, or strain rate alone, but depend on the coupled evolution of He pressurization, H interfacial retention and redistribution, and defect kinetics. This mechanistic understanding provides a basis for incorporating H-He coupling into the design and assessment of irradiation-resistant iron-based structural materials for fusion applications, where controlling H retention and its coupling to He-containing cavity evolution may help mitigate irradiation-induced plasticity and damage.

Methods

Thermodynamic analysis

To evaluate the thermodynamic tendency of H trapping by cavities under varying irradiation conditions, the He/V ratio, temperature, and matrix H concentration were taken into consideration. The Gibbs free-energy change, referred to as (ΔG), associated with the incorporation of H atoms into a pre-existing cavity was evaluated. The free-energy change for the formation of a stable $H_iHe_nV_m$ complex is expressed as:

$$\Delta G(i, n, m) = -\left\{\sum_{z=2}^m E_b^v(0, 0, z) + \sum_{y=1}^n E_b^{He}(0, y, m) + \sum_{x=1}^i E_b^H(x, n, m)\right\} - \left\{(m-1)k_B T \ln \frac{C_V}{1-C_V} + nk_B T \ln \frac{C_{He}}{1-C_{He}} + ik_B T \ln \frac{C_H}{1-C_H}\right\} \quad (1)$$

Where k_B represents the Boltzmann constant, and C_V , C_{He} , and C_H denote the corresponding concentrations in the surrounding matrix. The parameters E_b^v , E_b^{He} , and E_b^H represent the binding energies of vacancies, He atoms, and H atoms, respectively, to the cavity. Here, (m), (n), and (i) denote the numbers of vacancies, He atoms, and H atoms in the resulting stable $H_iHe_nV_m$ complex. The binding-energy parameters were obtained from our previous atomistic studies^{11–14}.

For a cavity with a prescribed size and He/V ratio, the thermodynamic favorability of capturing an additional H atom can be assessed from the incremental free-energy change. Specifically, if $\Delta G(i+1, n, m) - \Delta G(i, n, m) < 0$, the capture of the ($i+1$)-th H atom is thermodynamically favorable under the specified matrix H concentration and temperature. Accordingly, the H occupancy of a cavity is determined by the minimum of the Gibbs free-energy profile, (ΔG_{min}), with the corresponding H content taken as the thermodynamically preferred H occupancy under the prescribed conditions. This treatment therefore provides a thermodynamic estimate of H retention in pre-existing cavities without explicitly resolving the time-dependent H exchange process. Further details of the thermodynamic formulation are provided in Supplementary Section S2.

Molecular dynamics simulations

All molecular dynamics (MD) simulations were carried out using the LAMMPS

(Large-scale Atomic/Molecular Parallel Simulator) ⁵⁵ software package. Interatomic interactions in the Fe-H-He ternary system were described by the embedded-atom-method (EAM) potential of Huang et al. ¹⁸, which has been shown to reproduce the energetics of H and He interacting with vacancies and self-interstitial atom clusters in BCC-Fe with satisfactory accuracy ^{18,20,21}. The simulation model consisted of a pre-existing spherical cavity containing He and H within a BCC Fe single-crystal matrix, as illustrated in Supplementary Fig. S1. The defect-free BCC-Fe matrix was built as a $50 \times 50 \times 50 a_0$ box ($a_0 = 2.8553 \text{ \AA}$ at 0 K) containing 2.5×10^5 Fe atoms, with the x -, y -, and z -axes aligned with the $[100]$, $[010]$, and $[001]$ directions, respectively. Periodic boundary conditions were applied in all three directions. Spherical cavities with prescribed radii were generated by removing Fe atoms from the center of the simulation cell. The simulation-cell dimensions were maintained at no less than five times the cavity radius to reduce interactions between the cavity and its periodic images ^{52,56,57}. The resulting structures were first energy-minimized using the conjugate-gradient (CG) method and then relaxed for 50 ps under isothermal-isobaric (NPT) ensemble.

Helium atoms were subsequently introduced into the cavity to achieve the prescribed He/V ratios, followed by CG minimization. The number of H atoms was determined from the thermodynamically preferred H occupancy predicted by the Gibbs free-energy analysis described in the above thermodynamic analysis. The resulting H-He-containing cavities were then thermally relaxed and equilibrated at the target temperature and zero pressure for at least 100 ps to obtain mechanically stable core-shell configurations. The equilibrated systems were subsequently subjected to extended-timescale molecular dynamics (ET-MD) tensile simulations, in which triaxial tensile deformation was applied over a temperature range of 300-973 K and a strain-rate range of 10^6 s^{-1} to 10^9 s^{-1} . All loading simulations were performed in the canonical (NVT) ensemble at the prescribed temperature. At each loading increment, the simulation cell was deformed by affine scaling, and the atomic configuration was subsequently relaxed under NVT conditions with the updated cell dimensions fixed. Thus, the volume was held fixed during each relaxation step while evolving

continuously over the entire loading process as the applied tensile strain accumulated.

The lowest strain rate considered here, 10^6 s^{-1} , approaches the lower end of the strain-rate range that can be practically accessed using conventional MD while retaining computational tractability. At this strain rate, each loading simulation required several hundred million MD timesteps, motivating the use of the extended-timescale loading protocol. Post-processing and visualization were carried out with the Open Visualization Tool (OVITO) program⁵⁸. The local atomic environments, defect configurations, and damage evolution under dynamic tensile loading were resolved by combining the dislocation extraction algorithm (DXA), the construct surface mesh (CSM) procedure, Coordination analysis, Atomic Strain analysis, and Bond analysis.

Density functional theory calculations

Density functional theory (DFT) calculations^{59,60} were performed using the VASP code⁶¹ to investigate H trapping and defect activation at Fe-He interfaces. Following Refs.^{46,62}, Fe-He interfaces were used to represent the local environment of H at He-containing nanocavities. The projector augmented-wave (PAW) method⁶³ and the PW91 generalized gradient approximation (GGA) functional⁶⁴ were employed. A plane-wave cutoff energy of 500 eV and a Γ -centered $1 \times 4 \times 4$ Monkhorst-Pack k -mesh⁶⁵ were used. The Methfessel-Paxton smearing width was 0.2 eV. Total energies were converged to $-0.02 \text{ eV}/\text{\AA}^{-1}$. Spin polarization is considered in all DFT calculations. Fe-He interfaces with (100), (110), and (111) orientations were considered. For each orientation, H binding at the standoff region was evaluated from the difference between the H solution energies in bulk Fe and at the Fe-He interface, following Refs.^{46,62}. The formation energies of Fe interstitials were then calculated for different H coverages to quantify the effect of interfacial H on defect activation. The interstitial formation energy was defined as the energy difference between the total energy of the H-containing interface system with the interstitial defect and the corresponding defect-free constituent states.

Data availability

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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Declaration of competing interest

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

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