

Cluster dynamics modeling of hydrogen saturation retention in tungsten with a universal trapping-site sink strength

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Abstract

Hydrogen isotope (HI) retention poses a key issue for tungsten (W)-based plasma-facing materials (PFMs) in fusion devices, where microstructures such as dislocations (DLs) and grain boundaries (GBs) play a dominant role. Existing theoretical sink strength models for microstructures like DLs and GBs fail to account for the observed saturation of HI retention. In this study, we propose a novel universal trapping-site model that dynamically represents sink strengths as time-dependent site concentrations, which is incorporated into an improved cluster dynamics model for high-fluence HI irradiation. Our simulations quantitatively reproduce the saturated low-energy deuterium (D) retention and depth profiles in W, in good agreement with experiments. A critical saturation fluence of approximately 10^{23} m^{-2} is identified, below which unsaturated D retention is governed by both GBs and ion-induced defects, whereas above this threshold GBs dominate D retention by trapping free D and approaching their theoretical saturation limit. The trapping-site sink strength model enables quantification of H trapping by diverse microstructures via unified effective site concentrations, providing mechanistic insights into microstructural effects and facilitating direct evaluation of HI retention in PFMs under different irradiation conditions.

Full Text

Preamble

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1 Key

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Abstract

Hydrogen isotope retention poses issue tungsten (W)-based plasma-facing materials (PFMs) fusion devices, where microstructures dislocations (DLs) grain boundaries (GBs) dominant role.

Existing theoretical strength models microstructures account observed saturation retention. study, propose novel universal trapping-site model dynamically represents strengths time-dependent concentrations, which incorporated improved cluster dynamics model high-fluence irradiation. simulations quantitatively reproduce saturated low-energy deuterium retention depth profiles agreement experiments. critical saturation fluence approximately identified, below which unsaturated retention governed ion-induced defects, whereas above threshold dominate retention trapping approaching their theoretical saturation

limit. trapping-site strength model enables quantification trapping diverse microstructures unified effective concentrations, providing mechanistic insights microstructural effects facilitating direct evaluation retention under different irradiation conditions. words: clear fusion, Tungsten, Deuterium retention, Cluster dynamics, Trapping-site strengths, Microstructures

1. Introduction

plasma-facing materials (PFMs) fusion reactors subjected thermal loads, high-energy neutron irradiation, particle impacts generated reactions, resulting radiation damage formation basic defects vacancies, self-interstitial atoms (SIAs), hydrogen isotope (HI), helium [1,2] These defects evolve dislocation loops, cavities, bubbles, absorbed inherent sinks dislocations (DLs) grain boundaries (GBs). addition, hydrogen (H)/He atoms easily combine vacancies clusters bubbles, which sources crack growth, volume expansion, radiation hardening [3,4] Tungsten (W)-based materials considered promising candidate future fusion devices, thermal conductivity, melting point, mechanical strength, sputtering yield, retention erosion significant amount retention usually occurs during tokamak operation, mainly influence surface damage/microstructures basic diffusion, trapping accumulation behaviors species persistent enhancement underscores retentions W-based critical challenge directly governing safety operational stability fusion reactors.

Microstructures materials significantly affect retention behaviors W-based PFMs, including impurities (such second phase particles (oxide/carbide dispersion-strengthened particles), solution atoms (such proven trapping sites, pathways preferential diffusion through density, distribution further influence these effects modifying defect efficiencies strain gradient.

Similarly, served trapping centers drive segregate towards them, leading large amount accumulation [13,14] addition, accelerate diffusion, promoting rapid accumulation retention through enhanced interfacial mobility localized trapping Second-phase particles introduce interfaces strain

fields trapping sites while solute atoms could alter solubility diffusion lattice distortion chemical interactions. summary, influence diverse microstructures behavior exhibits significant complexity.

Inherent defects, particularly primary candidates responsible trapping atoms under sub-threshold plasma energy exposure conditions necessary investigate fundamental mechanisms retention inherent microstructures W-based PFMs. experimental researches retention commonly

methods

include

Analysis

(IBA), Secondary Spectrometry (SIMS), Residual

Analysis

(RGA), Nuclear Reaction

Analysis

(NRA), Thermal Desorption Spectroscopy (TDS) These techniques offer valuable insights behavior under various conditions, determining concentration, diffusion characteristics trapping behaviors.

However,

method

inherent limitations. example, quantify concentration struggles distinguish between different trapping sites, estimate trapping energies desorption spectra cannot directly resolve dynamic desorption pathways complex defect interactions Additionally, these techniques sensitive experimental conditions temperature irradiation dose, making challenging infer microscopic mechanisms static observations Crucially, complex, non-equilibrium processes involved radiation damage, defect evolution clustering, difficult time.

These limitations highlight theoretical simulations complement experimental studies.

Computational approaches, especially mesoscale, preferred alternative approach providing insights retention mechanisms modeling defect evolution diffusion, trapping desorption. theory, Object Kinetic Monte Carlo (OKMC) models describe interactions microstructures (such discrete objects defined energy states geometries typically idealized infinite sinks, exemplified Jansson cylindrical dislocation model Valles perfect-sink

approximation where defects reaching these microstructures permanently removed absorbed. spatial correlation random distribution defects system, commonly adopted describe dynamic evolution complex clusters microstructures, quantify trapping efficiency under non-equilibrium conditions However, computational complexity makes difficult apply large-scale long-time systems.

Cluster dynamics crucial studying long-term defect dynamic evolution retention behavior materials especially under high-dose irradiation based numerical solution equations absorption microstructures strength calculated using steady-state equations proposed Brailsford Bullough during 1970s 1980s However, these analytical expressions, derived under mean-field approximation, characterize dynamic trapping-detraping behavior under non-steady-state conditions.

Furthermore, existing models inherit critical limitation assumption infinite microstructural absorption capacity, mobile defects produced irradiation irreversibly trapped. neglects saturation desorption processes, contradicts experimental observed saturation behavior retention.

Therefore, necessary develop universal strength model incorporating finite trapping capacities dynamic defect-microstructure interactions, accurately describe saturation desorption behaviors complex microstructures. widely proved atomic-scale calculations density functional theory (DFT)/molecular dynamics (MD)) atoms ferentially occupy discrete lattice sites, particularly tetrahedral interstitial sites (TIS) Based fact, propose trapping capacity microstructures fundamentally determined density their interactions uniformly characterizing microstructural features through concentration establishing functional relationships between occupancy defect geometry, strength directly linked time-dependent concentration

microstructures. approach eliminates parametric dependence complex defect morphologies traditional analytical models, provides self-consistent description retention dynamics microscopic trapping.

Furthermore,

method

could extended study synergistic effects various types microstructures, providing universal formulation strength multiscale modeling interaction microstructures. paper, propose universal trapping-site strength model describe non-steady state variations strength microstructures improved model developed simulate retention considering saturation trapping emission processes based trapping-site strength model. model successfully reproduces experimental retention depth distribution, particularly saturation phenomenon retention. microscopic mechanisms saturation retention explored.

Finally, predict trapping capabilities various typical microstructures W-based under typical irradiation conditions.

methods

model based mean-field theory (MFRT) employed which extensively simulate radiation damage, microstructural evolution, effects during plasma-material interactions. model account defect generation, diffusion, reactions trapping processes.

IRatMat developed based scheme successfully investigated retention polycrystalline under different irradiation conditions, including H/He-neutron synergistic irradiation different incident energies, fluxes, fluence temperatures study, developed improved code, IRatMat-Site (CD-site), proposing universal trapping-site strength model describe reaction rates various types microstructures. differ-

steady-state diffusion equations, while CD-site incorporates trapping-site strength model, which further detailed Section following, briefly introduce basic framework IRatMat-Site focusing strength theory proposed trapping -site strength model.

- $\frac{3}{4}\frac{3}{4}\frac{3}{4}\textcircled{\text{R}} =$

I I V

- $\frac{3}{4}\frac{3}{4}\frac{3}{4}\textcircled{\text{R}} =$

I I V denotes absorption point defects inherent sinks including here. models based typically treat follows, which addition various sinks defect absorption considering existing multiple types microstructures system.

People study absorption behavior defects various materials fission/ fusion reactor

stainless steels, zirconium, ferritic alloys, molybdenum Furthermore, researchers introduced additional terms improve accuracy reality simulation results, considering temperature effects emission transforming linear concentrations volume concentrations Ahlgren expressed dissociation mobile defects sinks following that,

$$\epsilon \approx \bar{\epsilon} = - \hat{e} \cdot \hat{u} \zeta \div \bar{\epsilon} \approx \bar{\epsilon} \hat{u}$$

stochastic cluster dynamics model developed Jourdan further takes account forms densities, makes following modifications

$$\epsilon \approx \bar{\epsilon} = - \hat{e} \cdot \hat{u} \zeta \div \bar{\epsilon} \approx \bar{\epsilon} \hat{u}$$

where GBs), strength microstructure mobile defect represents atomic volume, where system.

Burgers vector. linear concentration defect binding energy between

2.2 Trapping-s

strength model absorption emission strength microstructure mobile defect which represents absorption defects.

Taking inherent microstructures example, model given Brailsford around 1980s mostly simulation methodologies models.

Those model based MFRT, incorporating prescribed boundary conditions treating defect fluxes within lossy continuum approximation solving steady-state diffusion equation under these conditions, model yields analytical solutions strength approximate asymptotic solutions

under limiting regimes. examples development trapping-site strength model.

Typically, dislocation regarded cylindrical lossy effective medium radius cylindrical coordinate system.

Considered defects system, strength given follows

- $d l - \theta \theta d k Z r = , (5)$

Several different expressions strength derived using either embedded cellular models cellular model assumes polycrystals single spherical isolated grains without defined medium around them, interaction between particle interfaces. particles originate diffusion defects within grains, conditions gains similar cells. expression cellular strength given

- limit approximations extreme cases Here, size, total strength single crystal microstructures within grain.

Those formulations, given steady-state equation solutions, inherently capture transient micro-dynamics sinks.

Furthermore, kinetic formulations would introduce computational inefficiencies impede systematic identification generalizable mechanisms governing trapping. break through these limitations, propose universal trapping-site strength model describe trapping emission behaviors within microstructures. relatively small radius ability energy tends occupy channeling experiments [26,43] observation further supported simulations employed calculations obtain formation energies substitutional, Octahedral interstitial sites vacancies. found lowest formation energy occurs specific Based these facts, propose fundamental hypothesis trapped sinks composed series sites, regardless their structural configurations. atoms generally exhibit repulsion between other, exist single distributed evenly possible equivalent sites microstructures [46,47] which supports validity hypothesis.

effects inherent defects essentially described trapping them. principle, interactions between these negligible compared interaction between indicated atomic simulations fourth reaction right represented instead follows, where represents geometric factor, absorption radius radius detailed derivation geometric factor provided Supplementary Information. dimensionless factor representing absorption efficiency

total number which usually density length/area/volume zero/one/two dimensional (0-D/1-D/2-D) sinks, which governs maximum trapping capacity saturation concentration) typical metals, denotes unoccupied density varies time.

$$(\quad) + H S - H S H S S S 2 (\quad) k r r Z n t p r = + (10)$$

description variations strength. Compared lytical model strength, trapping-site model offers several advantages.

Secondly, finite density effectively explains gradual saturation retention under high-fluence irradiation.

Finally, trapping-site model universal applicable various sinks voids, impurities, ODS/CDS, others. geometric structure, density, interaction energy, other characteristics these sinks incorporated which further simplifies calculation process implementation.

parameters verification reliability CD-site model verified comparing experimental

directly ensure reliability accuracy model, carefully choose fundamental kinetic energetic parameters considering published values DFT/MD calculations experiments, shown Table binding energies various types typically exhibit Gaussian distribution simplicity, their values adopted study, primary focus effects newly proposed trapping-site model. fact, multi-trapping effects treated previous Specifically, binding energies mobile defects large defect clusters estimated using Capillary while binding energies clusters estimated through simple formula reaction types chosen previous research which reasonably described be-

behavior retention desorption under deuterium irradiation. reaction coefficients comprehensively illustrated elsewhere [29,31,36,50]

shows initial depth distribution D-induced defects under low-energy implantation.

D-induced defects obtained following formula mentioned Section ion-induced defects localized within near-surface region ions.

D-induced defects under implantation energy Parameter symbol references

pre-exponential factor Migration energy Migration energy Migration energy Formation energy Formation energy Formation energy Binding energy Binding energy Binding energy Binding energy Binding energy Binding energy [12,58] [15,30] (m/n) shown retention depth distribution profiles simulated, implantation fluence ranging (Fig. 4 Figure 4: see original paper) implantation fluence (Fig. 4(b)) Overall, 4(a), CD-site simulation

results

exhibit gradual saturation increasing fluence, consistent experimental observations. contrasts CD-pre curve, following linear increase increasing fluence. 4(b), CD-site

results

consistent experimental compared CD-pre results, particularly following aspects: surface layer (0-0.2 order magnitude experimental value; plateau region (0.7-7 within order magnitude deviation experimental values contrast continuous decline depth

CD-pre profile. retention mainly being trapped inherent defects considered types inherent defects analyzing sites them, leading prediction saturation retention. fluence, retention exhibits near-linear fluence dependence, efficient trapping abundant unoccupied sites. intermediate fluence, growth becomes sub-linear sites gradually occupied, leading fewer available sites decline trapping efficiency.

Above critical saturation fluence about saturation sites shifts retention plateau, where further accumulation becomes negligible. fluence 4(a), simulated retention smaller experimental values. differences complex properties different

analysis

techniques (such could essentially affect experimental

results

retention [1,3,63,64] other hand, fundamental energetic parameters, other defects (such impurities) density DLs/GBs model differ experimental conditions. incident fluence influence these factors total retention greater compared fluence, simulation

results

noticeably lower experimental values. worth noting retention experimental inherently exhibit deviations about orders magnitude other, complex changeable microstructures differences experimental conditions.

Therefore, discrepancy between simulation

results

experimental values study remains within acceptable range variation discrepancy between CD-site experimental absence near-surface concentration CD-site results.

Cavities/blisters formed increase dislocation density induced supersaturation surface under low-energy, high-flux plasma irradiation which complex should studied future research.

Fluence dependence retention under implantation compared experimental

results

implantation [59,60,65] Depth profiles after implantation fluence

3.2 Effect

various defects/sinks retention Identifying which microstructure plays saturation retention essential understanding microscopic mechanisms evolution behavior quantifies retained clusters trapping under different fluences.

CD-site simulation

results

indicate retention gradually approaches saturation value fluence increasing, which similar 4(a). contrast, CD-pre simulation

results

linear increase retained increasing fluence. retained clusters simulated CD-site CD-pre overlap completely, which saturation trend increasing fluence clusters reach their maximum number trapped Thus, infer saturation retention mainly

originates saturation trapping Furthermore, since theoretical limit concentration retained grain about least orders magnitude higher (with dislocation density dominant saturation retention low-energy arises trapping

Cluster under implantation different fluences where solid lines represent CD-site CD-pre results, respectively. order understand microscopic mechanisms retention contributions different forms retained shown shows concentration profiles obtained using CD-pre CD-site, during implantation fluence distribution CD-pre CD-site nearly identical fluence while notable differences emerge between terms fluence particular, CD-site

results

distinct platform depth discrepancy arises because provide sufficient sites fluence, fluence increases, these sites become progressively saturated occupation.

CD-pre, assumption infinite trapping leads overestimation retention Overall, retained -surface region comes clusters concentration primarily dominated clusters, explained detailed trapping mechanism

analysis

clusters shown Vacancies, migration energy temperature, combine near-surface irradiated region clusters. contrast, lower migration energies, diffuse deeply. rapid migration promotes recombination irradiation region,

which decreases vacancies concentration, causing shift backward become narrower. retained primarily originates especially these types inherent sinks contain larger number sites capable capturing substantial amounts finite concentration sites imposes theoretical upper limit amount retained CD-site. increasing fluence, trapping capability gradually decreases limit concentration approached, allowing diffuse deeper bulk.

Consequently, CD-site simulation

results

exhibit better agreement experimental measurements compared those CD-pre, shown 4(a). trapped clusters (D-Cluster), (D-DL) (D-GB) during implantation fluence retained Cluster during implantation fluence

3.3 Distribution

evolution trapping above

results

indicate inherent microstructures including dominate saturation retention under implantation fluence higher. Within framework, typically assumed spatially uniform distributions.

Accordingly, ratio occupied density total density serve metric evaluating D-trapping capacity inherent microstructures along depth materials under different irradiation conditions. shows depth fluence dependence occupied black (with occupied sites density percent density percent) divides distribution regions, unoccupied region saturated region where sites fully occupied noted. Section theoretical limit concentration retained order order causing reach saturation lower fluence threshold (less exhibit broader saturation region (Fig. 8 Figure 8: see original paper). shown 8(b), density occupied sites fluence divided three distinct regions.

Region (unsaturated), total sites concentration exceeds implanted concentration, resulting sites remaining unoccupied minimal retention.

Region saturation occurs primarily near-surface region (within region, ion-induced defects incoming preventing saturation region extending deeper region fluence exceeds critical saturation fluence saturated rapidly expands. interval, sites irradiated region occupied, diffuse trapped

density ratios depth fluence implantation Black lines represent occupied density ratios. trapping-site strength model quantifies trapping behavior inherent defects/microstructures converting their structural characteristics equivalent densities. addition, concentration ion-induced vacancies converted concentrations, allowing retention behavior evaluated within unified framework. total trapping capacity these sinks characterized ratio total retained

0 D

black total concentration available sites

0 D

which corresponds threshold saturation retention. represents

0 D

trapping sites fully occupied indicating saturated

0 D

$S / 1 C C < ,$ some defects/sinks remain available for further D

retention. trapping, unsaturated retention. study, found contribute dominantly retention, accounting 40-60% surface beyond Vacancy-type clusters contribute

approximately 10-30% surface, their contribution decreases increasing fluence enhanced recombination. contrast, contribute retention across depths, their concentration sites, which always negligible.

These

results

highlight dominant governing low-energy saturation retention

0 D

percent depth fluence implantation black represents

0 D

$S / = 1 C C$.

Basic prediction retention microstructures trapping-site strength model offers practical unified framework quantify trapping capacity diverse microstructures. converting their structural characteristics effective concentrations, model enables direct evaluation their influence retention PFMs. realistic applications, irradiation material design introduce extra traps beyond including voids, pre-irradiation bubbles, impurities, second-phase particles (ODS/CDS) solute atoms. evaluate contribution various microstructures retention, common ranges their structural parameters selected W-based reported literatures, given Table ODS/CDS under typical irradiation conditions. trapping-site model approximately treats centers, whose strength related their respective concentrations radii. shown Table taking monovacancy example vacancy-type defects,

estimated larger-size voids/cavities, assumed occupy positions similar vacancy similar radius, whose density interface sinks ODS/CDS estimated about regarding second-phase particles ensemble impurity atoms. densities sinks described detail Section Table shows under typical conditions vacancies ODS/CDS provide highest concentrations dominate trapping followed impurities, while provide several orders magnitude lower concentrations, contributing least retention.

Based trapping-site strength model, evaluate influence different types sinks retention behavior under unified framework.

Under three typical irradiation conditions plasma irradiation alone, synergistic irradiation neutrons heavy ions), retention polycrystalline arises contributions different types sinks (especially vacancy clusters GBs). low-energy irradiation, H-induced vacancies mainly distributed near-surface region nanometer scale, contributing little total retention.

Therefore, retention primarily originates trapping synergistic irradiation low-energy neutrons, neutron irradiation generates large number uniformly

distributed vacancy-type clusters. These vacancy clusters large amounts thereby significantly increasing retention. In case, dominant contributions retention irradiation-induced vacancy clusters synergistic irradiation low-energy heavy ions, heavy introduce numerous vacancy-type clusters within micrometer-scale depth range leading retention irradiation damage region.

Meanwhile, rapidly diffusing atoms trapped deeper locations mainly forming spatially partitioned retention mechanism.

densities diverse sinks typical characteristics. strengths Typical Theoretical

0 S

Formula range strengths density Impurities Ultimately, behavior retention radiation damage W-based under realistic conditions basically predicted, providing guidance optimal regulation density. temperatures below migration vacancies activated, there exists significant effect between vacancies sinks which means higher density leads poorer radiation damage resistance.

Moreover, density increases retention. Therefore, low-temperature regions first-wall, materials density should selected simultaneously reduce radiation damage retention temperatures above effect between vacancies sinks neglected increasing density effectively enhances absorption intrinsic defects, thereby improving radiation damage resistance.

However, competes tendency higher densities increase retention.

Therefore, high-temperature regions divertor, optimal density should carefully selected maximize radiation damage

resistance while minimizing H retention.

4. Conclusion

universal trapping-site strength model developed quantitatively describe retention behavior replacing conventional various analytical strength equivalent concentration framework. model accurately reproduces saturation depth profiles retention under low-energy implantation.

Distinct spatial retention mechanisms revealed follows: irradiated regions, trapping governed combined effects ion-induced vacancies; bulk, dominate trapping diffuses inward. concentration framework provides unified metric evaluating strength across various microstructures. contributions total trapping vacancies competitive near-surface irradiated regions, account bulk, whereas negligible (<0.1%) across depths. model quantitatively reveals retention originates H-irradiation-induced vacancies sinks through concentration analysis, proposing tailored inhibition strategies different irradiation conditions. approach provides efficient optimizing irradiation performance fusion reactors, enabling basic predictions retention behavior through simplified assessment trapping capacities

various microstructures, rather relying large-scale simulations.

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