Dissertation Proposal

Computational modeling of refractory metals and alloys

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Table of Contents

[1. Statement of Research Objectives 4](#_Toc124230466)

[2. Introduction 4](#_Toc124230467)

[2.1. Motivation 4](#_Toc124230468)

[2.2. Objectives and Tasks 5](#_Toc124230469)

[3. Background 6](#_Toc124230470)

[3.1. Irradiation damage in body-centered cubic (BCC) tungsten (W) 6](#_Toc124230471)

[3.2. Properties of HEAs 8](#_Toc124230472)

[3.3. Simulation methodologies 10](#_Toc124230473)

[3.3.1. Molecular dynamics & LAMMPS 10](#_Toc124230474)

[3.3.2. Density functional theory & VASP 11](#_Toc124230475)

[3.3.3. Transition state theory 11](#_Toc124230476)

[3.3.4. Cluster expansion 13](#_Toc124230477)

[4. Preliminary Results 15](#_Toc124230478)

[4.1. Strain Effects on the Diffusion Properties of Near-Surface Self-Interstitial Atoms and Adatoms in Tungsten [61] 15](#_Toc124230479)

[4.1.1. Methodology 15](#_Toc124230480)

[4.1.2. Result 16](#_Toc124230481)

[4.2. Rate of edge dislocation escape from a void in bcc tungsten 23](#_Toc124230482)

[4.2.1. Methodology 24](#_Toc124230483)

[4.2.2. Result 25](#_Toc124230484)

[5. Research Plan 28](#_Toc124230485)

[5.1. Study the vacancy diffusion mechanism in the dislocation core 28](#_Toc124230486)

[5.2. Screw dislocation mobility in helical configuration 29](#_Toc124230487)

[5.3. Design and develop a novel refractory high entropy alloy (ARPA-E) 30](#_Toc124230488)

[6. Potential Original Contribution and Broader Impacts for Science 31](#_Toc124230489)

[7. Statement on Personal Contribution to the Formulation of Ideas and Plans of Research 32](#_Toc124230490)

[8. Reference 33](#_Toc124230491)

# Statement of Research Objectives

The overall research objective is to study the mechanical and thermal properties of refractory metals and alloys relying on theory and modeling, and to develop a novel material for enhanced performance in plasma-facing components (PFCs). PFCs are used in the Tokamak fusion device which is intended to provide clean energy through nuclear fusion reactions between deuterium and tritium. The material will be exposed to extreme irradiation environments of neutron, helium, and heat fluxes that induce defects and change the microstructure and mechanical properties of the material.

# Introduction

## Motivation

In the foreseeable future, fusion energy will provide human beings with stable and environmentally friendly energy. Tokamak devices can be used as controllable fusion reactors, which generate plasma contained by a magnetic field. Deuterium (D) and Tritium (T) collide, react, produce helium (He) atoms and neutrons, and release a huge amount of energy [1]. Most helium atoms eventually deposit in the divertor which is at the bottom of the reaction vessel [2]. Neutrons are neutral particles and will escape the plasma to collide with the materials forming the vessel, generating the heat that will be used to generate electricity. After the reaction, helium atoms and neutrons have a very high energy and can cause irradiation damage to the plasma-facing materials (PFM). Tungsten (W) is used as one of the common PFMs since it has a high sputtering threshold, high thermal conductivity, high melting point, and low sputtering yield [3, 4]. As a consequence of irradiation in W, scientists observe helium interstitials, helium bubbles, dislocation loops, and transmutation products in W bulk, and, under certain conditions, the formation of a surface nanostructure denoted as “fuzz” [5, 6, 7, 8]. Defects significantly modify the material properties, for example, increasing the strength of the material but reducing the ductility [9, 10, 11, 12], making W brittle and reducing the operational lifetime of the facilities, and therefore, their efficiency. Understanding the mechanisms of irradiation hardening in W can help optimize the manufacturing process, and predict property changes in operation. Designing materials with better response will improve efficiency making fusion more attractive to investors, which will speed up its deployment. High-entropy alloys (HEAs) are a new class of materials with potentially enhanced properties compared to traditional alloys. HEAs are made of at least 4 different elements and can form a stable solid solution single phase [13, 14]. Previous reports mentioned that HEAs show a sluggish diffusion effect [15, 16, 17, 18] and can combine the advantages of each component (cocktail effect) [19, 20]. The sluggish diffusion of particles might enhance recombination and increase irradiation resistance and the cocktail effect enables a wide variety of HEAs.

## Objectives and Tasks

The overall objective of this project is to investigate the mechanism of irradiation damage of tungsten and try to design and develop novel tungsten-based HEAs. We target to learn the mobility of self-interstitial atoms (SIAs) in tungsten in the presence of strain fields and its relation to the formation of fuzz. In addition, we will analyze the interaction of a void with an edge dislocation to understand how the absorption time depends on the size of the void, which relates to the hardening effect of the voids. Screw dislocations can also absorb defects, generating helical turns along the line, which modify the dislocation mobility, which also relates to hardening. For HEAs, we plan to design and develop a novel refractory HEA (rHEA) teaming up with external collaborators. In this project, we will explore the order-disorder transition process depending on temperature and composition, and calculate the enthalpy of mixing and free energy at different temperatures to predict the stability of rHEA. Also, we will investigate the behavior of vacancies, He interstitial atoms, and H interstitial atoms in the rHEA.

# Background

## Irradiation damage in body-centered cubic (BCC) tungsten (W)

BCC tungsten is one of the most common PFMs because of its excellent properties. It has a high melting temperature, a low vapor pressure at the melting point, a low sputtering yield, and a high sputtering threshold. The thermal conductivity of W is 145 W/mK at room temperature and only slightly reduces with increasing temperature [21, 22, 23]. Other properties are listed in table 1 below.

|  |  |  |  |
| --- | --- | --- | --- |
| Density at RT, g/cm3 | 19.3 | Melting point, °C | 3410 |
| Thermal expans. Coeff. at RT, 10−6/K | 4.5 | Vapor pressure at 2000°C, Pa | 1.3 × 10−7 |
| Thermal cond. at RT/1000°C, W/mK | 145/113 | Atomic number/Atomic weight | 74/183.8 |
| Elastic modulus at RT, GPa | 410 | Ductile to Brittle Transition Temp. (DBTT), °C | 100 - 400 °C |
| Poisson ratio | 0.28 | Recrystallization temperature, °C | 1150 - 1350 |

*Table 1. Properties of tungsten. [21]*

After being exposed to plasma, the effect of neutron and helium irradiation is considerable. After absorbing neutrons, W can transmute to a variety of radioactive elements, like rhenium, osmium, tantalum, hafnium, iridium, etc [9, 24, 25, 26]. Furthermore, during helium (He) irradiation, He atoms can implant in W bulk and encounter other He atoms to form He clusters. Clusters will grow bigger after absorbing more He atoms. When the cluster is big enough, it can eject W self-interstitial atoms (SIAs) to bulk and generate vacancies at the bubble to release pressure [27]. After enough W SIAs are formed, they can agglomerate into prismatic <111>-dislocation loops, glide to the surface and annihilate there. This process is called ‘loop punching’ [27, 28, 29], which will decrease the thickness of the ligaments between bubbles and the surface. Once a ligament is thin enough, He bubbles can break and release He atoms, leaving a crater behind [27]. The increasing number of craters leads to the formation of nanotendrils, which eventually result in the ‘fuzz’ structure. Figure 1 shows a scanning electron microscopy (SEM) micrograph of the fuzz structure [30].

A picture containing graphical user interface

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*Figure 1. Cross-sectional SEM micrograph of a single crystal W target. Symbols to the right indicate target cross-section orientation in SEM field of view and plasma material interaction (PMI) surface [30].*

## Properties of HEAs

The first publication in multicomponent alloys dealing with the development of a HEA crystal dates from 2004 [19, 31, 32]. In the early studies, HEAs were defined as alloys with 5 or more metal elements, with the composition of each element between 5% to 35%. Currently, the definition is less restrictive including alloys with 4 elements, and the range of composition is wider [17, 33, 34, 35]. HEAs are fascinating because of four main effects:

1) high entropy effect

High entropy alloys have a high configurational entropy as their name implies, and according to the Gibbs free energy G = H-TS (G is Gibbs free energy, H is enthalpy, T is temperature, S is entropy), the high entropy of the disordered system will stabilize a single solid solution phase at high temperature. The solid solution phases usually have higher entropy than intermetallic, although enthalpy can stabilize ordered phases. Thus, in some cases, intermetallics may become the most stable phases, usually at low temperature. A phase transition between solid solution and intermetallic can occur, which is called ‘order-disorder transition’ [36].

2) Sluggish diffusion effect

The slow diffusion of particles in HEAs has been reported in both experiments and simulations [14, 16, 17, 18, 37], which is likely to be a reason for the strong resistance to high-temperature softening [17]. This effect might be due to the complexity of the local environment. When atoms and/or defects diffuse in the HEA bulk, the neighbors before and after jumping into a new site are different which modifies the activation energies for migration. The low-energy sites can trap defects, with large activation energies that prevent fast diffusion.

3) Severe-Lattice-Distortion Effect

The components of a HEA have different atomic volumes. Big atoms push away neighbors, and small atoms have extra free volume around them. As a result, the crystal lattice is severely distorted. The distortion can affect the deformation mechanisms, modifying the dislocation properties and plastic deformation pathways [38, 39]. It also affects diffusion properties.

4) Cocktail Effect

The properties of HEAs relate to the properties of its composing element [40]. For example, metals that have a high melting point (such as W, tantalum, and chromium) are widely used in refractory HEAs [17, 41, 42].

## Simulation methodologies

## Molecular dynamics & LAMMPS

Molecular dynamics (MD) is a standard tool for investigating the properties of metals and alloys, developed by B. J. Alder and T. E. Wainwright in 1959 [43]. The idea of MD is to solve Newton’s equations of motion to get the trajectory of atoms provided forces are known. In our studies, we use the LAMMPS [44] code to perform MD simulations. Initial configurations are read from the data files, simulation commands are in input files, and the interatomic potentials that describe the atom-atom interactions (result from the Born-Oppenheimer approximation, which considers electrons are always at the ground state) are in the potential files.

The data file includes information such as: The number of atoms in the system, the size of the sample, the number of atom types, and the position of each atom. There are many data file generators, the most used one in our project is Atomsk [45], which can generate pure element bulks, different kinds of defects, polycrystals, etc.

The Langevin thermostat [46] can be used in Lammps to constrain the temperature of the system through the modification of Newton's equations of motion. The force in the Langevin equation of motion is given by:

is the interaction force between atoms, is a frictional drag or viscous damping term, which can be calculated as , D is the damping factor, is velocity, is the stochastic force to simulate random kicks by a heat bath, which is proportional to where is the Boltzmann constant, T is the temperature, m is the mass, dt is the timestep size, and D is the damping factor [46].

## Density functional theory & VASP

Density functional theory (DFT) is a reformulation of the many-body Schrödinger equation based on two seminal theorems by Hohenberg, Kohn, and Sham, which provided theoretical support for the development of the theory [49, 50]:

1. The ground-state electron density uniquely determines the electronic wavefunction.
2. The energy of an electron distribution can be described as a functional of the electron density, and this functional is a minimum ground-state density.

One of the most widely used computer codes to solve the DFT equations is the Vienna Ab initio Simulation Package (VASP). DFT codes, including VASP, apply approximations to compute the so-called exchange-correlation functional (to calculate electron-electron interactions). A broadly used approach, and the one that we use here, is called generalized gradient approximation (GGA) [51]. GGA considers both electron density and its gradient to describe the inhomogeneous nature of electronic densities. Projector augmented wave (PAW) pseudopotentials [52] are widely used to calculate and save computational time as they coarse grains the inner core electrons that usually do not participate in bonding. The solution of the Schrödinger equation, the wavefunction, is usually written as an expansion in basis functions. In the PAW method, those basis functions are plane waves. Increasing the number of plane waves increases the accuracy of the method but decreases efficiency, making this method computationally costly.

## Transition state theory

The description of the energy change in a reaction process is that an activated complex with higher free energy is formed between the reactant state and the product state. Such state is denoted as transition state [53]. We apply harmonic transition state theory to analyze the diffusion rate of atoms or defects:

In equation (2), is the rate (number of events per unit time), is a pre-exponential factor, is the activation energy determined by the difference of the potential energies of initial configuration and activated complex, is the activation stress tensor related to the difference of the stress tensor at the saddle point and at the initial configuration, is the applied strain tensor, is the atomic volume, is the Boltzmann constant, and T is the temperature.

We use the nudged elastic band (NEB) method to find out the minimum energy path (MEP) two configurations [47, 48]. N-1 replicas are interpolated between the initial and final state. The force acting on a replica consists of a spring force along the local tangent and a true force normal to the local tangent. The spring force restrains replicas not to move too far apart or close to each other, and the true force which is proportional to the gradient of the energy of the system takes replicas to the MEP. An example is shown in Figure 2.

Diagram

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*Figure 2. An example of NEB calculation, black solid lines are potential energy surfaces, black dots are stand for replicas.*

## Cluster expansion

When analyzing the properties of HEA, considering the complexity of the local environment is a challenge. The cluster expansion method predicts the energy of an atomic configuration. The enthalpy of mixing of a K-component alloy is defined as:

is the total energy of the alloy, is the average concentration of the p component, and is the cohesive energy of the pure element. The cluster expansion predicts as [54, 55, 56, 57, 58]:

is the configurational occupation vector, is the cluster number, m is the multiplicity factor that indicates the number of clusters that are equivalent by symmetry (divided by the number of lattice sites), J is the concentration-independent effective cluster interactions, that we fit to DFT results applying the structure inversion method, and is the average correlation function that can be calculated as [59]:

where are point functions denoting the occupancy of each cluster, (s) = {j1, j2…jk} is the decoration of the cluster by point functions. The point functions need to be orthogonal, and for a K-component system [60] we can use:

Hence, the enthalpy of mixing now can be written as:

# Preliminary Results

## Strain Effects on the Diffusion Properties of Near-Surface Self-Interstitial Atoms and Adatoms in Tungsten [61]

In section 3.1, we have introduced how ‘fuzz’ forms in bcc W. Here, our target is to explore the strain effects on the diffusion properties of SIAs and adatoms.

## Methodology

We used MD simulations as implemented in the LAMMPS [44] code to model the behavior of SIAs and adatoms in bcc W with an embedded atom method (EAM) interatomic potential developed by Marinica et al. [62]. Three different sets of simulations are used to investigate different properties, with samples all oriented in the , , directions, with free surfaces in z and a time step of 2 × 10−3 ps.

The first set employs a sample of dimensions 61.5 × 76.1 × 86.6 Å3, with 26,880 atoms. This orientation has been chosen since the surface is the lowest energy in W [62]. A SIA is added at the middle of the sample and the time it takes to reach the surface is computed as a function of temperature and equibiaxial strain. We have used three different temperatures, 700, 850, and 1,000 K, enforced using a Langevin thermostat [46] with relaxation time equal to 1 ps, and strains ranging from −0.007 to 0.007. The biaxial strain in the x and y directions was applied after the steady-state thermal expansion was reached at each temperature running at 0 pressure for 200 ps. Twenty independent simulations were run for each case.

The second set of simulations intended to compute the effect of strain on the diffusivity of adatoms on a W surface. In this case, we ran simulations at five different temperatures, from 1,000 K to 1,400 K, five different equibiaxial strains, in the range from −0.008 and 0.008, and carry out five independent runs for each set of conditions. Again, the strain was applied after the steady-state thermal expansion was reached at each temperature. These dynamical simulations were complemented by performing NEB [47, 48] computations to obtain the MEP between two neighboring equilibrium adatom sites at the various levels of applied equibiaxial strain. These NEB simulations were performed in the samples with the volume obtained at 1,000 K for the different strains.

The last simulation set aimed at analyzing the effect of biaxial strain on the morphological evolution of a W surface. Five strains, from −0.008 to 0.008 were applied following the same methodology as above at a temperature of 1,000 K and one SIA was inserted randomly into the system every 200 ps, mimicking the ejection of SIAs from He bubbles. The initial sample size was 123.0 × 152.2 × 86.6 Å3 with 107,520 atoms. These conditions result in a flux of SIAs of 2.67 × 1025 m−2 s−1, overestimating experimental He implantation fluxes that range from 1021 to 1023 m−2 s−1. Such overestimation highlights one of the main limitations of MD models in terms of the total time that can be simulated. Nevertheless, these simulations provide valuable information about the basic mechanisms occurring in the W slab as SIAs are added and diffuse towards and on the surface, and the strain effect on such processes.

The configuration changes and the positions of SIAs changes are tracked using a common neighbor analysis (CNA) [63] algorithm as implemented in the OVITO visualization tool. For the first passage time simulations, a SIA is specified to reach the surface when all the atoms in the bulk crystal are arranged in bcc lattice sites.

## Results

The most probable time for a diffusing particle to reach a point in space from a given origin in 1D is given by [64]:

is the travel distance of SIAs, and the diffusivity can be calculated through transition state theory, , with the jumping distance, the rate (see equation (2)) and a prefactor. For W, the atomic volume is 15.8 Å, and by fitting simultaneously the values gathered from MD we obtain activation energy is 0.19 eV, activation stress = 110.6 GPa, and a prefactor 12.9 Å ps-1. Figure 3 shows the MD results (square symbols with error bars) and theoretical model (solid lines) for a SIA migrating from the center of the sample to the surface. We observe a significant effect of strain on the first passage time, which may result in differences between the estimated times by almost two orders of magnitude. As we biaxially compress the material the time decreases as the diffusivity increases. The temperature effect seems to follow the usual Arrhenius relation for the cases studied in this work.

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*Figure 3. First passage time for a SIA to reach the free surface traveling a distance = 4.4 nm as obtained with MD and the theoretical model as a function of (A) applied equibiaxial strain, and (B) inverse temperature.*

For an adatom on the W surface, the diffusivity D is calculated following Einstein’s relation on 2D:

is the mean-squared displacement of adatoms, and t is the time. Then we fitted the diffusivity following transition state theory and have prefactor = 44.35 Å ps-1, = 0.8 eV, The results are shown in Figure 4. We observe again that the compressive biaxial strain increases the diffusivity, although the effect is weaker than in the bulk, being within one order of magnitude. The adatom hops follow mostly one of the two ⟨111⟩ directions on the plane, leading to an isotropic diffusion, which has been reported in the literature [65].

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*Figure 4. Diffusion coefficient of an adatom in a W surface as a function of (A) equibiaxial strain, and (B) inverse temperature.*

To rationalize the results, we performed NEB simulations to compute MEPs and the respective activation barriers of an adatom hopping along a ⟨111⟩ direction on a W surface at various applied strain levels. As shown in Figure 5, we observe the compressive equibiaxial strain leads to a decrease in the activation energy , and the value at zero strain is 0.68 eV, which is smaller than 0.8 eV obtained from the dynamics runs. We attribute this difference to statistical errors in the fitting procedure, small anharmonic effects, but also the fact that other hopping mechanisms with higher activation barriers, such as the exchange and crowdion mechanisms might co-exist. The maximum difference in the energy barrier is 0.08 eV between 0.008 and −0.008 strain.

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*Figure 5. MEPs for an adatom hopping along a ⟨111⟩ direction on a W surface at various applied equibiaxial strain levels.*

To explain the evolution of surface morphology as added SIAs diffuse to the surface and migrate on it to form clusters and aggregate, leading to an increase in surface roughness depending on the applied equibiaxial strain, we compute the surface roughness as [66]:

We divided the surface into small cells, is the average height for each cell and is the average height for the whole surface. We have run the MD simulations for 2 µs, adding a total of 10,000 SIAs to the W slab. To compute the SR values, we have discretized the domain in N cells in x and y, with indices i and j, and found the atoms belonging to each of the surfaces. The size of the cells was chosen such that the minimum number of atoms per cell is one, with cell sizes ranging between 9 and 25 Å2.

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*Figure 6. Surface roughness evolution at various levels of applied equibiaxial strain.*

Initially, we see that equibiaxial compression leads to a slightly larger SR since the SIAs migrates fast to the surface. However, as we add more atoms, the SR at compressive strains plateaus. At this point, extra atoms create new bcc layers under compression and do not increase the SR, while under tension, the SR continues to grow, leading to a crossover at around 1 µs.

The evolution of the W slab in the simulation supercell when an equibiaxial tensile strain ε = 0.008 is applied is shown in Figure 7. Only atomic arrangements with structures different from that of a bcc crystalline lattice following a CNA [63] are presented and colored according to their potential energy. Dislocation lines are shown in light green as obtained by the dislocation-extraction algorithm (DXA) [67], which identifies the generated dislocations as edge in character with Burgers vector Figure 7A displays the structure after 1 µs, where we observe a large density of dislocations and SIA clusters. Dislocations are close to the surface of the slab, and at 1.032 µs (Figure 7B) one dislocation segment reaches the surface, generating a depletion or groove on the surface, that increases the surface roughness. Surface diffusion leads to the flattening of the depletion and, hence, grooves are unstable at this stage. As the structural evolution proceeds, dislocations annihilate at the surface leading to the configuration shown in Figure 7C after 1.6 µs, where two dislocation segments impinge on the surface. As the top dislocation is absorbed (Figure 7D) at a time of 1.8 µs, some extra depletions in the surface are formed.

Diagram

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*Figure 7. Evolution at different simulated times denoted in each subfigure, of a W slab with   surfaces under equibiaxial tensile strain ε11 = ε22 = 0.008 showing the presence of edge dislocations (green lines) generated as aggregates of SIAs and annihilating at the surface, forming grooves that dissolve due to diffusive processes.*

## Rate of edge dislocation escape from a void in bcc tungsten

Previous studies regard irradiation-created voids as immobile obstacles for edge dislocations, with the edge dislocation bowing under stress until the void is overcome [68, 69, 70]. These studies are performed with MD, which requires an extremely high strain rate due to the time limitation. However, to the best of our knowledge, there is no work analyzing the time for void absorption by dislocation in the irradiation hardening of tungsten. If the dislocation absorbs the void (partially or fully) in a short time and escapes, the contribution to hardening would be weaker than previously predicted. To enhance our understanding on the irradiation hardening mechanism of tungsten, in this project, we study the escape rate of an edge dislocation from a void in bcc W.

## Methodology

We use MD simulations as implemented in LAMMPS [44] to study the interaction between an edge dislocation and a single void of different sizes. Samples are oriented in [-111], [1-10], [112], an edge dislocation with Burgers vector 1/2[-1 1 1] is placed in the center of the system with the dislocation tangent to the z-direction. In the initial structure, we also delete a spherical cluster of atoms to form a void at the center of the dislocation line. The radii of the voids were 0.22 nm, 0.3 nm, 0.335 nm, 0.35 nm, 0.38 nm, 0.4 nm, 0.5 nm, and 0.6 nm, which corresponds to 3, 5, 10, 13, 15, 20, 34, and 58 vacancies. Different temperatures are applied depending on the void size, ranging from 1000 K to 2400 K, enforced using a Langevin thermostat [46] with relaxation time equal to 1 ps. The escaping rate is slower as the size of the void increases. To overcome this challenge, we increase the temperature in those cases to be able to compute the escaping rate within MD times. The void size and temperature information is listed in table 2.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Radius of void(nm) /number of vacancies in void | Temperature (K) | | | | | | |
| 0.22/ 3 vacancies | 1000 | 1100 | 1200 | 1300 | 1400 |  |  |
| 0.3/ 5vacancies | 1000 | 1100 | 1200 | 1300 | 1400 |  |  |
| 0.335/ 10 vacancies | 1200 | 1300 | 1400 | 1500 | 1600 |  |  |
| 0.35/ 13 vacancies | 1400 | 1500 | 1600 | 1700 | 1800 | 1900 | 2000 |
| 0.38/ 15 vacancies | 1600 | 1700 | 1800 | 1900 | 2000 |  |  |
| 0.4/ 20vacancies | 1800 | 1900 | 2000 | 2100 | 2200 |  |  |
| 0.5/ 34 vacancies | 2000 | 2100 | 2200 | 2300 | 2400 |  |  |
| 0.6/ 58 vacancies | 2000 | 2100 | 2200 | 2300 | 2400 |  |  |

*Table 2. Void size and temperature information.*

## Results

Figure 8 shows the initial and final configuration of a void absorption process. All the atoms in this figure are with structures different from bcc following a CNA [63] in OVITO. In the final configuration, the edge dislocation absorbs all vacancies in the void, climbs and forms a jog. Absorption of vacancies at the dislocation core has been reported before [68]. We measured the rate of absorption/escape as the inverse of the time taken by the dislocation to absorb/escape the void, by visually inspecting from the first simulation step to when we consider the void is fully absorbed or detached from the edge dislocation. The MD data is fitted with the exponential function following transition state theory, shown in equation (11). Γ is the escaping rate, and compared with equation (2), the strain term equals 0. a, b, c, and d are 4 parameters indicate the prefactor and activation energy is considered as a linear function of the radius of void, the fitting is tested by calculating the coefficient of determination R2:

Chart

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*Figure 8: a) Atomic structure of the dislocation core and the void; b) atomic structure of the dislocation after the absorption of the void. Atoms are colored according to their potential energy.*

Figures 9 and 10 show the MD results (as solid circle symbols) and the theoretical model (solid lines), all the lines are fitting together, and have a = 0.59, b = , c = 0.28, and d = -0.03. R2 equals to 0.732, which proves the fitting model.

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*Figure 9. Absorption rate as a function of inverse temperature for different void sizes, ranging from 0.22 nm to 0.6 nm.*

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*Figure 10. Absorption rate as a function of void radius.*

# Research Plan

## Study the vacancy diffusion mechanism in the dislocation core

We plan to apply the NEB method to calculate the activation energy for a vacancy hopping in the dislocation core. Different possible hopping paths will be considered in an area including the jog. The goal is to find the hopping mechanism and estimate the diffusivity. Our hypothesis is that the jogs are traps for vacancies, slowing down the overall diffusion constant. The challenge is twofold: (1) the number of paths for the vacancy to hop is large and (2) the vacancy might delocalize complicating the analysis.

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*Figure 11. A sketch of different vacancy pathways in the dislocation center. White atoms arrangements with structures are different from that of a bcc crystalline lattice.*

## Screw dislocation mobility in helical configuration

Under irradiation, screw dislocations act as sinks for irradiation-created defects, absorbing vacancies and SIAs generated during displacement cascades. This absorption process leads to changes in the dislocation morphology that starts developing helical-like configurations [71]. It is not well understood how such configurations modify the characteristics of the dislocation glide. Our hypothesis is that the helical morphology considerably modifies the dislocation mobility affecting the ductile-to-brittle transition temperature. The movement of screw dislocations in bcc alloys is thermally activated due to the large Peierls barrier they need to overcome. The presence of the helix will modify the potential energy landscape, but it is not clear in what sense if it makes the dislocation to move more easily or it might hinder the dislocation motion. Using a well-validated interatomic potential for W in molecular dynamics (MD) simulations performed with the LAMMPS code, we will study this effect from an atomistic viewpoint in terms of a dislocation mobility function. How does the presence of the helix modify the dislocation mobility? The MD results will be fitted to a functional form for the dislocation velocity depending on the resolved shear stress and the temperature. This non-linear mobility function might be employed in mesoscale discrete dislocation dynamics models to solve the equations of motion, , to study the time evolution of a dislocation ensemble, with the driving force and T the temperature. We will study correlations between the radius of the helical turn, the density of helical turns, and the number of absorbed vacancies/SIAs.

## Design and develop a novel refractory high entropy alloy (ARPA-E)

In this research, we will focus on designing and developing a novel rHEA with unique composition based on W, Ta, Cr, V and Hf, and an optimized microstructure using advanced and additive manufacturing processing techniques for enhanced performance in plasma-facing components (PFC). Our collaborators at Los Alamos National Laboratory and University of Wisconsin-Madison will perform experiments to manufacture different rHEAs, and to characterize samples using Transmission electron microscopes (TEM), energy dispersive spectroscopy (EDS), and electron backscattered electron diffraction (EBSD). Samples will be tested under different exposures and study the irradiation damage under different conditions.

Our role will be to test different compositions using atomistic simulations based on DFT and CE methodologies (which are introduced in section 3). Monte Carlo simulations will be performed to predict the thermodynamics of the alloys with different compositions. In particular, we will focus on the free energy to understand the stability of each composition and the order-disorder transition temperature, below which intermetallic phases precipitate. The presence of intermetallics is often deleterious in structural components as their presence embrittles the material. The W38-Ta36-Cr16-V11 system has been shown to perform extremely well under irradiation, showing little change in properties compared to pure W [72]. We will start with a similar composition to the W-Ta-Cr-V alloy and will vary the composition in 5% intervals. We plan to calculate the mixing entropy, enthalpy of mixing, and short-range order, to figure out which compositions can have a stable structure and to investigate the order-disorder transition temperatures of these compositions. In addition, the formation and migration energies of vacancies, hydrogen interstitial atoms, helium interstitial atoms, and the binding energy between different point defects will be calculated to correlate the results with experimental observations and to guide experiments on the optimal composition to enhance the material response to irradiation.

# Potential Original Contribution and Broader Impacts for Science

We propose to use MD simulations to study the absorption/escape rate of an edge dislocation from a void, which can potentially modify our understanding of the role of irradiation-created defects in the observed irradiation hardening effect. Current hardening models depend on the number density of defects. Our development will potentially dictate what is the critical size for voids to affect the dislocation motion. Hence, the current models may need to be modified to account for the fact that the average glide velocity of the dislocation depends on the rates that we compute with this study. The proposed methodology can be applied to different types of crystalline structures and alloys, opening up the possibility of improving our understanding in a wide variety of systems.

Concerning the HEA study, the development of a material capable of withstanding the extreme conditions posed by fusion plasmas will revolutionize the field and will take us a step further on the development of fusion reactors as clean energy generation devices. Mitigating climate change is a priority and this work tries to help on this direction, potentially opening research lines on novel materials with optimal properties.

Shape

Description automatically generated

*Figure 12. An example of Cr30Ta30V10W30 high entropy alloy*

# Statement on Personal Contribution to the Formulation of Ideas and Plans of Research

I declare that the formulation of all ideas and research plans in this proposal are developed in consultation with my advisor. The proposal is based on my personal knowledge of the subject matter through literature review, preliminary results and analysis of data.

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