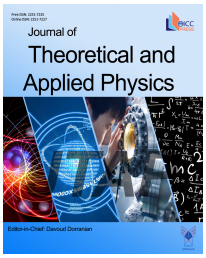

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Simulation-based analysis of the impact of lattice cavities on tungsten's mechanical properties

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Original Research

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Abstract:

Tungsten, as a plasma-facing material in nuclear fusion reactors like tokamaks, is exposed to extreme conditions, including high heat flux and neutron radiation. These conditions lead to the formation of vacancies and structural defects, significantly influencing its mechanical properties. This study investigates the impact of varying vacancy concentrations on the mechanical behavior of tungsten, focusing on Young's modulus and tensile strength. Using molecular dynamics simulations implemented in LAMMPS software, different levels of vacancy densities were introduced into tungsten's lattice structure. The results revealed that an increase in vacancy concentration correlates with a noticeable reduction in both stiffness and tensile strength of the material. These findings underscore the critical role of radiation-induced defects in altering the performance and durability of tungsten, providing valuable insights for its application in fusion reactor designs.

Keywords: Tungsten; Lattice vacancies; Mechanical properties; Young's modulus; Tensile strength molecular dynamics simulation

1. Introduction

Due to the significant intensity of high-energy particle radiation and neutron emissions resulting from nuclear fusion reactions, the radiation damage analysis in plasma-facing materials (PFMs) which are used in nuclear fusion reactors is of great importance. Generally speaking, Plasma-facing materials (PFMs) are exposed to the fusion plasma and are designed to handle the intense heat flux and energy deposition resulting from fusion reactions, while also managing particle exhaust effectively. These materials must withstand extreme thermal loads and efficiently dissipate the absorbed energy to ensure the safe operation of the reactor [1–8]. Therefore, PFMs should be able to withstand high-intensity rates of radiation as well as minimal damage to ensure the safe and efficient operation of the thermonuclear fusion reactor. However, one of the primary concerns of PFMs in nuclear fusion applications is radiation damage, predominantly caused by high-energy neutrons. Other high-energy particles, such as runaway electrons or low-flux high-energy neutral particles and ions, contribute minimally to the damage due to their relatively low energy levels, particularly in the divertor region [9–17].

Tungsten is a promising material for nuclear fusion applications due to its unique features:high melting point, high thermal conductivity, and strength at high temperature, which are necessary to maintain the structure of the fusion machines. In addition, tungsten has low sputtering efficiency, meaning that atoms are not easily knocked off the tungsten surface when exposed to high-energy particles in nuclear fusion facilities. This property of tungsten is very crucial to reduce the impurity concentration of the fusion plasma with high temperatures [18, 19].

The use of tungsten as one of the most widely used materials to be used in the divertor structure of magnetic confinement concepts such as tokamaks can lead to damage and localized

defects in the tungsten lattice due to the impact of neutrons and high-energy ions generated from the fusion process. Fusion radiation can lead to Frenkel pair generation, which creates vacancies in the tungsten structure, affecting its mechanical and physical properties [20, 21]. For this reason, extensive research has been conducted in recent years to investigate the effects of high-energy ions and neutron radiation on the surface and structural properties of tungsten [22, 23]. For instance, a research study conducted by Yu et al. examined the influence of hydrogen on the mechanical properties of tungsten, focusing on its effect on dislocation motion. While they observed some reduction in the binding energy at the dislocation core, their key finding was that hydrogen causes super pinning of defects, which enhances the hardness and strength of the material [24]. It was found that the presence of hydrogen in the tungsten structure decreases the energy of atomic bonding. In other relevant studies, the effect of helium plasma exposure on the surface morphology of tungsten for fusion-related applications was investigated [6, 25, 26].

Although tungsten is a promising material for nuclear fusion applications due to its unique characteristics, its behavior under irradiation of high-energy particles is still not well understood. For this reason, several theoretical studies have been conducted to simulate the interaction of high-energy particles with tungsten.

Molecular dynamics (MD) simulations have been widely used to study the behavior of PFMs such as tungsten under the extreme conditions of fusion [27–29]. As an example, the effects of fusion plasma exposure on the mechanical properties of tungsten were simulated. The simulation results indicated that the presence of vacancies in the tungsten lattice structure, formed due to the collision of neutrons and ions resulting from fusion reaction, leads to the propagation of tensile stress [30]. In a fusion-relevant theoretical research study based on molecular dynamic simulation, the effects of fusion byproducts such as helium ion and deuterium on the structural deformation of tungsten were investigated [31].

The main concern of the present study is to simulate the effects of void concentration on the essential mechanical properties of tungsten, namely Young's modulus and tensile strength, which are among the most critical mechanical properties of metallic materials. While it is well established that grain boundaries significantly influence these properties, the current study focuses specifically on the role of vacancies within the grains. This approach allows for a detailed investigation of the impact of void concentrations, providing a foundation for future studies that will include the effects of grain boundaries and their interactions with irradiation-induced defects.

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2. Simulation setup

Molecular dynamics simulations have become a powerful tool for studying the atomic-scale behavior of tungsten under various conditions, providing insights into its structural and mechanical properties. Recent advances in MD simulations have enabled the study of more complex systems and phenomena, such as the behavior of tungsten under simultaneous irradiation and high-temperature conditions. In this article, molecular dynamics simulations were performed by LAMMPS (Largescale Atomic/Molecular Massively Parallel Simulator) simulation code. In the simulation, the embedded-atom method (EAM) potential is considered which is an appropriate potential for atoms of hard metals. EAM potential is an approximation approach describing the energy between atoms and is a type of interatomic potential. Therefore, the energy is a function of a sum of functions of the separation between an atom and its neighbors [32, 33]. Generally speaking, the LAMMPS code uses neighbor lists known as Verlet lists to keep track of nearby particles. The lists are optimized for systems with particles that repel at short distances so that the local density of particles never grows too large [33].

In the present study, a $10 \times 10 \times 20$ simulation box is considered for 4000 tungsten atoms with a BCC lattice structure and a lattice constant of 3.165. The associated concentrations of vacancies of the lattice are 0, 1.25%, 2.5%, 5%, 7.5%, and 10% which are placed randomly in the tungsten structure. Fig. 1 shows the structure of tungsten, before and after the existence of different numbers of vacancies which are randomly distributed in the tungsten structure.

In this figure, blue circles represent tungsten atoms and red

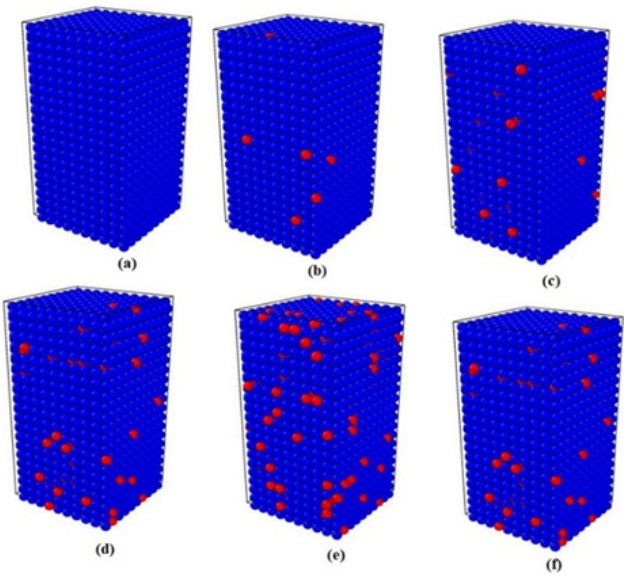

Figure 1. Simulated box of tungsten structure considering 0% (a), 1.25% (b), 2.5% (c), 5% (d), 7.5% (e), 10% (f) percentages of vacancies.

circles represent vacancies. The cause of these vacancies in the structure of tungsten is the radiation of high-energy neutrons resulting from nuclear fusion in fusion reactors. To better understand the presence of vacancies, the simulation box inside tungsten without the presence of tungsten atoms is shown in Fig. 2.

In molecular dynamics simulations, determining the time steps is critical. If the time steps are too large, the calculation of the motion of the atoms because of the integration error becomes impossible, and in such a case the results of the simulation may be incorrect. On the other hand, a very short time step also significantly reduces the simulation interval. In practice, a time step in the amount of a few percent of the atomic vibration period is usually considered. The time step in this simulation was set to 0.001 ps and then the simulation process was performed by applying periodic boundary conditions and the output files obtained from LAMMPS code were processed using OVITO software. To describe radiation damage to materials displacement per atom (DPA) parameter is introduced. In other words, DPA determines neutron radiation damage to the irradiated material. DPA parameter can be expressed in terms of atoms that are permanently displaced from their original position to a new stable position. To describe radiation damage to materials, the displacement per atom (DPA) parameter is introduced, which quantifies the number of atomic displacements caused by neutron or ion irradiation per lattice atom. DPA provides a measure of the extent of radiation damage but does not directly correspond to the concentration of vacancies in the material. The actual percentage of vacancies is influenced by additional factors, including defect recombination, migration, and clustering processes. In our simulations, the vacancy concentration (percentage) is modeled as a simplified representation of radiation-induced defects, which is informed by DPA estimates but not equivalent to it. This approach provides a practical means to study the mechanical effects of voids on tungsten without explicitly modeling all dynamic defect interactions.

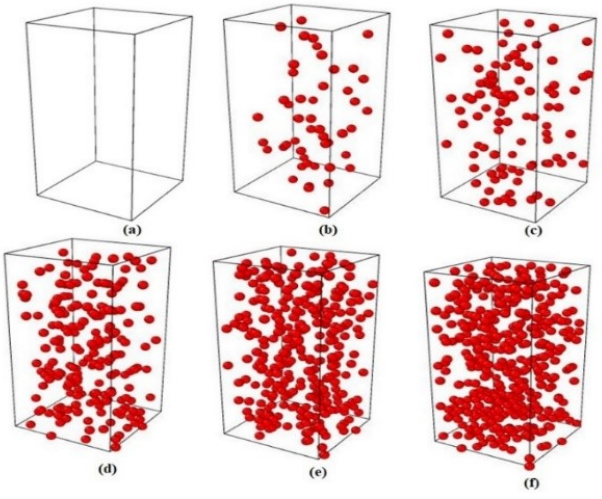

Figure 2. Distribution of holes in tungsten with no vacancy (a), 1.25% (b), 2.5% (c), 5% (d), 7.5% (e), and 10% (f) percentages of vacancies.

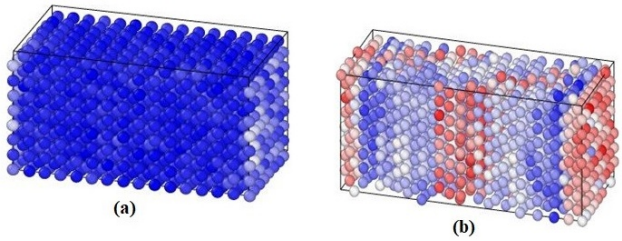

Figure 3. The structure of tungsten atoms in two states (a) no stretching force applied to them and (b) they are stretched under a force of 1.0×10^{10} eV/Å.

3. Results and discussions

For single-crystal BCC metal, the change of tungsten shape is mostly due to slip displacements of tungsten atoms that arise from vacancies. During MD simulations, slippages are observed and it is found that the sliding mechanism changes with the abundance of the vacancies. When the abundance of vacancies is low, most of the vacancies remain distributed within the lattice structure, and the integrity of the tungsten network is maintained. However, when vacancies cluster at specific locations, they can lead to localized disruptions and potential lattice instability.

Fig. 3 shows tungsten in two states. In a state where no force is applied to it and a state where tungsten atoms are pulled under a force of 1.0×10^{10} eV/Å.

If the atoms are in a relaxed state and no force is applied to them, their color tends to be blue. As more force is applied to the atoms and more tension they are subjected to, the intensity of the blue color is reduced and the atoms turn white and red colors respectively. As the number of vacancies increases, several tungsten atoms are removed from the lattice position and therefore, the shape of the tungsten lattice is changed. Consequently, the lattice change leads to more space for the accumulation of vacancies. Tensile stress in the direction can be obtained as [22].

$$\varepsilon_{xx} = \frac{L_x - L_{x0}}{L_{x0}}$$

where L_{x0} and L_x are respectively the primary and secondary lengths in the x direction. The general analysis of the stress-strain curve diagram is described in Fig. 4.

According to the figure, at lower strains, the stress-strain curve is linear, and the stress changes linearly (is proportional) with strain. The slope of the linear region of the stress-strain curve is defined as Young's modulus. The linear part of the stress-strain curve is also called the elastic region in which the material will return to its original state when the stress is removed. After the linear state, the stress strain curve tends to have non-linear behavior with a parabolic-like profile. The point at which the behavior of the curve changes from linear to non-linear is the point of yield strength of the material. As shown in the figure, the maximum of the stress-strain curve indicates the ultimate tensile strength or tensile resistance of the material. Tensile strength is a crucial mechanical property of a material that determines the ability of the material to resist deformation under tensile loads without being fractured, making it an essential consideration in material selection for various

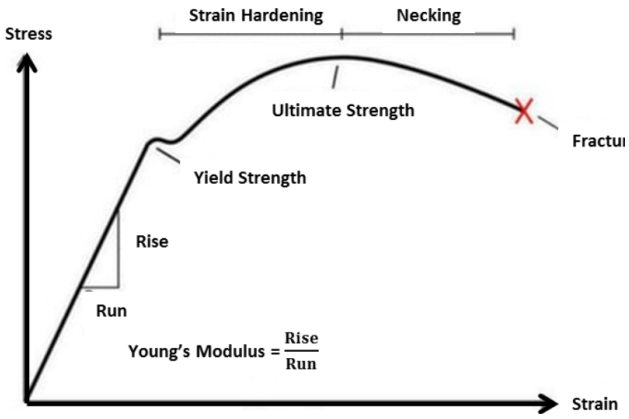

Figure 4. An overview of the stress-strain curve diagram and the physical meaning of the points on this diagram.

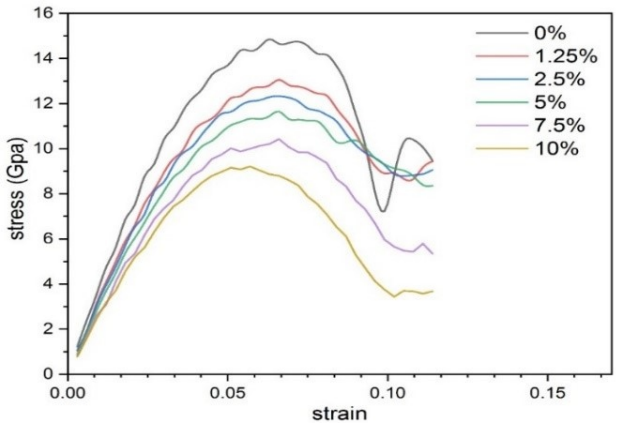

Figure 5. Stress-strain diagram of tungsten with different percentages of vacancies in its structure.

applications. The region between the yield point and the ultimate strength is known as the strain hardening zone. In this area, the material does not deform, but with increasing strain, the amount of stress in the material increases like a parabolic profile. After the point of tensile strength, as the strain parameter increases the material deforms, and the process of necking starts. As the strain in this area increases, the necking process intensifies to the critical point that leads to the fracture of the material. The end of the stress-strain curve describes the value of the strain at which the material is fractured.

Fig. 5 shows the stress-strain diagram of tungsten at a temperature of 300 K considering different concentrations of vacancies in the tungsten structure.

Regarding the figure, in the initial stage of the curve that is associated with the elastic regain, the stress parameter changes linearly with the strain which is in agreement with the linear profile of the reference diagram in Fig. 4. For small changes in the stress and strain parameters, the ratio of the stress to the strain (the slope of the linear part of the curve) gives the elastic or Young's modulus. Generally speaking, Young's modulus is a mechanical property parameter that measures the stiffness of the material under the applied lengthwise tension or compression force. It is understood from Fig. 5 that the tensile resistance decreases with increasing the number of vacancies in the tungsten structure. Increasing the number of vacancies in the tungsten structure reduces the energy of internal dependence of atoms and reduces the force of the W-W atomic bond. A range of non-linear behaviors can be observed in the stress-strain curves of Fig. 5 before the tension reaches a maximum value. The main reason for observing non-linear responses in simulations is the presence of surface defects in microscopic dimensions such as vacancies and displacements.

These defects are the main cause of the loss of material strength and progress in its deformation, and therefore, a wide range of nonlinear elastic changes can be observed.

The Young's modulus of tungsten was calculated with the presence of different percentages of vacancies. These values are in agreement with the expectations. Increasing the number of vacancies in the tungsten structure reduces the interaction of tungsten atoms with each other, which in turn reduces the Young's modulus. Results of Young's modulus and tensile resistance of tungsten with different percentages of the vacancies are given in Table 1.

The stress-strain curve obtained in the present article is validated with the results of Ref. 15 which is related to the presence of hydrogen atoms in the structure of tungsten. In the mentioned article, the Young's modulus of tungsten without the presence of hydrogen was reported 343.12 GPa which is in good agreement with the Young's modulus obtained in this article, without consideration of cavities in the structure of tungsten (330.39).

Regarding the stress-strain curve, it should be noted that it is not possible to observe the fracture phenomenon caused by the periodic boundary condition in all three directions. The end of these curves in Fig. 5 is not actually where the material is fractured, but is the point where the simulation stops. Since the same force is applied to the tungsten samples, according to the stress-strain curves of Fig. 5, it can be concluded that for the higher numbers of vacancies on the tungsten surface, the lower tensile strength of tungsten is expected due to the reduction of the energy dependency of the atoms and consequently, earlier fracture of the material occurs. For the higher percentages of the vacancies, more

Table 1. Young's modulus and tensile resistance with different percentages of vacancies in tungsten structure.

Percentage of vacancies	0	1.25	2.5	5	7.5	10
Young's modulus (G.Pa)	330.39	326.95	316.50	311.77	293.24	273.84
Tensil resistance (G.Pa)	14.58	13.05	12.32	11.65	10.42	9.21

-* no data available.

differences in the results are found. In the simulations of the present study, as the population of the vacancies increased from 5% to 7.5%, there was a significant difference in the tensile strength parameter. It should be also noted that the tensile resistance, as used in this study, refers to the yield strength of the material, which is the stress at which plastic deformation begins. The tensile strength, in contrast, indicates the maximum stress the material can endure before fracturing.

4. Conclusion

Through molecular dynamics simulations using the LAMMPS software, this study examined the impact of lattice vacancies on the mechanical properties of tungsten, including Young's modulus and tensile strength. The results demonstrated a clear correlation between increased vacancy concentrations and a decline in material performance. Specifically, as vacancy percentages rose from 0% to 10%, Young's modulus decreased significantly from 330.39 GPa to 273.84 GPa, while tensile strength dropped from 14.85 GPa to 9.21 GPa. These findings highlight the substantial influence of radiation-induced vacancies on the structural integrity of tungsten, underscoring the critical challenges posed by neutron interactions in nuclear fusion environments. Future research could expand on these findings by exploring the effects of substituting vacancies with fusion byproducts, such as hydrogen isotopes or helium, to evaluate their impact on tungsten's mechanical properties. Such investigations could provide deeper insights into the long-term viability of tungsten as a plasma-facing material in fusion reactor designs.

Authors Contribution
Mir Mohammad Reza Seyyed Habashi: Conceptualized the study, developed the methodology, conducted all molecular dynamics simulations, performed data analysis, and drafted the manuscript. Hadise Eslami: Contributed to data interpretation, provided insights on defect interactions in the tungsten structure, and assisted in manuscript editing. Mehdi Janbazi: Provided expertise in mechanical properties analysis, reviewed the stress-strain data, and contributed to the refinement of the methodology. Ehsan Noori: Supervised the project, provided critical feedback on the research direction, and reviewed the manuscript for scientific accuracy and consistency.

Availability of data and materials
The data that support the findings of this study are available from the corresponding author, upon reasonable request.

Conflict of interests
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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