Atomistic Investigation of Interstitial Dislocation Loop Formation in Tantalum and Tantalum-Tungsten Alloy under by Low Temperature Irradiation under Local Deformation

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1. Introduction

This article focuses on the properties of tantalum (Ta) and its alloys, which are considered refractory metals with unique properties for high-temperature and nuclear applications [1][2]. These materials exhibit high ductility, corrosion resistance, and the ability to form highly stable anodic films on their surface [1] [3] [4]. Additionally, they have a high neutron yield under spallation conditions, making them promising materials for use as target cladding or in a spallation neutron source target. The article examines the impact of radiation and local strains on Ta and tantalum alloys and aims to understand the effect on their structural integrity. Molecular dynamics (MD) simulations were used to investigate the behavior of cascades and the production of defects in Ta, W, and their alloys, providing insights into their dynamic characteristics. This research aims to further explore the collision cascade interactions and strain effects on pure Ta and tantalum alloys under irradiated conditions, as relatively little research has been conducted in this area.

2.Simulation methods

This study used Molecular Dynamics simulations with the LAMMPS code [5] integrated with the Materials-Square Platform [6]. The EAM potential chosen to model the behavior of pure Ta and Ta-W alloys under irradiation [7]. The simulations were performed at 30 K and 0 K, and multiple runs were carried out for each displacement direction to minimize the effects of thermal vibration and time correlations on the results as per described in previous work [8]. Various random distributions of Ta and W atoms were created to simulate the alloy structures, and each system was subjected to six incremental hydrostatic strain values ranging from -1.6% to 1.4%. The results were analyzed to determine the formation of defects, including self-interstitial atoms (SIAs) and vacancies. The dislocation loops were analyzed using the OVITO code[9]. The study provides specific modeling parameters and simulation duration used in the work.

3. Results and discussion

3.1 The Effect of Local Deformation on the Survived Frenkel Pairs in Ta-W Alloy

This study investigated how local deformation affects the creation and survival of Frenkel pairs (FPs) in Ta-W alloy under irradiation. The results show that both PKA energy and strain type have a significant impact on the number of FPs produced. Tensile strain generates more FPs than compressive strain, and the number of FPs increases with higher PKA energy in both strained and unstrained systems (Fig.1).

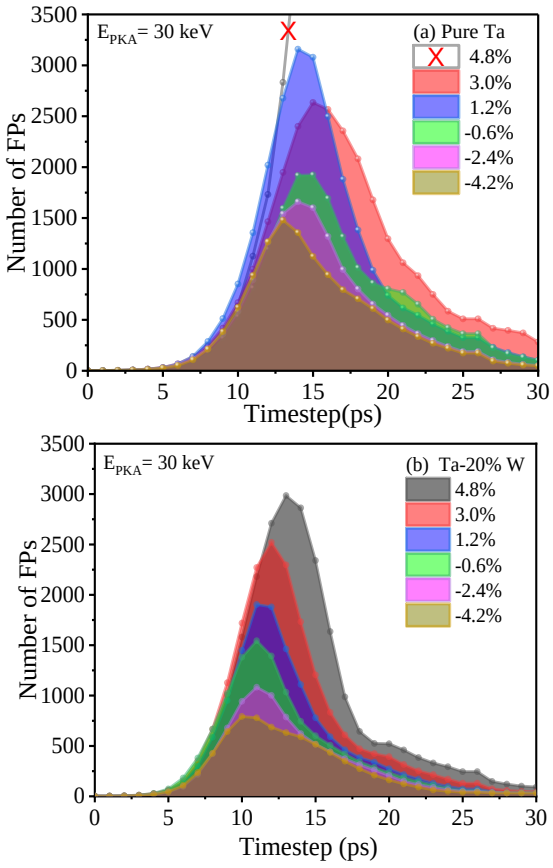


Fig. 1 illustrates the number of Frankel pairs (FPs) produced during collision cascades with a primary knock-on atom energy of 30 keV for both pure (a)Ta and (b)Ta-W alloy systems under varying levels of strain resulting in volume changes ranging from -4.2%

to 4.8%. Each data point represents the average of sixteen unique samples, including four different displacment directions and four distinct vibration timings. The **X** in red color denoted to the struacure failure occurred at this strain level.

The study also found that the alloyed structure exhibited better structural stability and fewer defects under larger strain compared to pure Ta. This is likely due to the addition of W, which creates lattice strain and restricts the movement and accumulation of defects like vacancies and interstitials. W's higher melting point also makes it an interstitials and vacancies sink, preventing the formation of defects. We also found that 20% W addition led to increase into the threshold displacement energy (TDE) by 15 eV as compared to the pure Ta as per our previous work [10] which is 60.5 eV for pure Ta and 76 eV for Ta-20W.

3.2. Strain effects on clusters and dislocation loops

3.2.1 Cluster analysis

In addition to studying the effect of PKA energy and strain on Frenkel pairs, this study also investigated the cluster size distribution and the fraction of point defects in clusters at the end of the cascade in Ta and Ta-W alloys. The results showed that the number of formed clusters increased with increasing PKA energy, and the existence of small interstitial clusters (SIA) in pure Ta was roughly twice that observed in the alloyed structures. It was also found that clusters consisting of small numbers of vacancies and SIA atoms were prevalent in both pure and alloyed systems (Fig.2).

Furthermore, the study found that the fraction of interstitial clusters among the total number of formed clusters in alloy systems was higher by ~0.3 than the fraction of vacancy clusters, which was consistent with findings reported in previous studies for other alloy systems for the W-Re [11] and Fe-Cr [12,13] alloys. While vacancy clusters can form in larger volumes compared to interstitial clusters, they occur less frequently in such larger sizes. The formation energy of vacancies is lower than that of SIAs, which facilitates the formation of vacancy clusters more easily than SIA clusters.

Moreover, the rate of increase in the number of interstitial clusters was faster in pure Ta than in alloyed structures when subjected to strain. Additionally, both pure and alloyed structures exhibited a higher number of clusters under tensile strain compared to non-strain or compressed strain conditions, with the alloyed structure showing fewer cluster counts in the latter case. These findings suggest that the addition of W to Ta can restrict the movement and accumulation of defects, leading to fewer and smaller clusters when the material is irradiated.

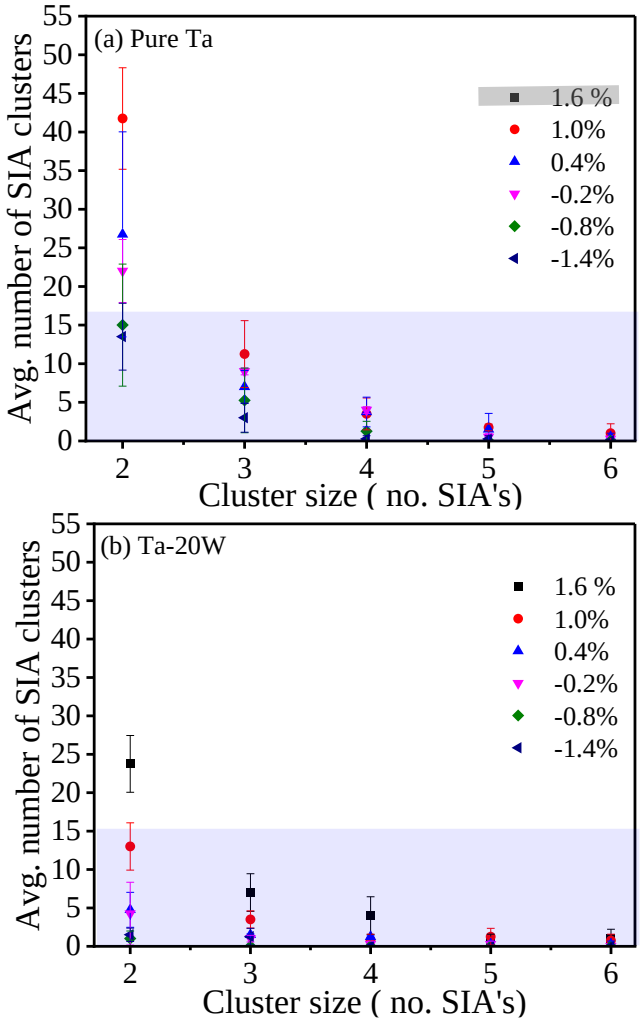


Fig. 2. (a) The average number of formed clusters (from 2~6 SIA's sizes) for various strain levels and 30 keV of PKA energies. The reported number of clusters were averaged over 4 different displacement directions as the standard deviation is shown. (a) and (b) for SIA clusters. At 1.6% the structure was deformed thus no applicable data to be shown of that strain range fir the Pure Ta.

3.2.2 Interstitial Dislocation loop formation

We found that under tensile strain, certain regions had significantly increased defect formation and clustering. Using the DXA algorithm, we were able to investigate the mechanisms of defect formation and found that only ½<111> interstitial dislocation loops (IDLs) were observed at a PKA level of 30 keV. Lower PKA values

did not result in IDL observation in either pure or alloyed structures. The frequency of IDLs was higher in the pure structure, and their length was longer than those observed in the alloyed structure (Fig.3). The alloyed structure only showed IDLs when subjected to tensile strains of 1.0% and 1.6%, while the pure structure exhibited IDLs even at a lower strain of 0.4%. At 1.6% tensile strain, the pure structure showed complete deformation, while the alloyed structure remained stable.

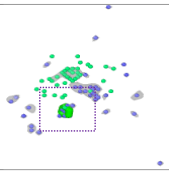
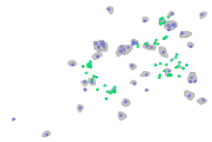
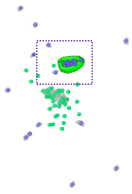
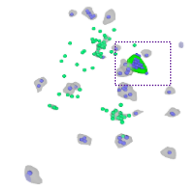
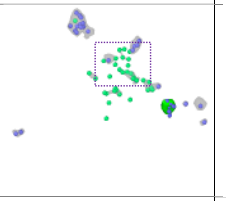
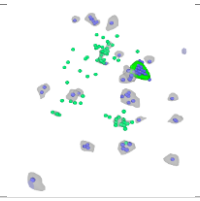
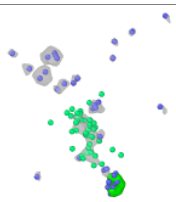
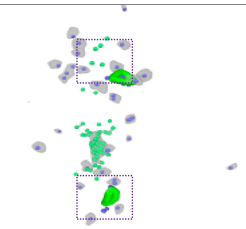
Displacement direction,	Alloyed Ta	Pure Ta
<111>		
	½ ⟨111⟩ (22.72 Å)	0 [1]
<110>		 [2]
	½ ⟨111⟩(41.96 Å)	½ ⟨111⟩ (43.35 Å)
<100>		 [3] [4]
	½ ⟨111⟩ (20.05 Å)	½ ⟨111⟩ (25.06 Å)
<321>		 [5]
	½ ⟨111⟩ (28.04 Å)	½ ⟨111⟩ (74.12 Å)

Fig. 3 displays different stages of FP evolution and the formation of IDLs at various displacement directions. These simulation events were conducted using a 30 keV PKA and a 1.6% level of strain, and the snapshots were taken within a time span of 30 picoseconds. The red-colored atoms indicate vacancies, blue atoms represent Self-Interstitial Atoms (SIA), while the green loops signify ½<111> IDLs.

Conclusion

In this study, we used molecular dynamic simulations to investigate the effects of strain on the primary defects and interstitial dislocation loops (IDLs) in pure Ta and Ta-20W alloy systems. Our results show that increasing tensile strain leads to more Frenkel pairs and self-interstitial atom clusters, while compression reduces them. Pure Ta has larger and longer IDLs than the alloyed Ta, which has smaller and shorter IDLs. Additionally, strain reduces the barrier for IDL formation, causing material degradation. These findings have implications for radiation-resistant materials and can help inform decisions about structural materials in critical infrastructure.

REFERENCES

[1] T.T.W. (Stanford U. JW, Behavior and Properties of Refractory Metals, Stanford Calif Press. (1965). http://books.google.com/books?id=CttRAAAAMAAJ.

[2] S.N. Mathaudhu, K. Ted Hartwig, Grain refinement and recrystallization of heavily worked tantalum, Mater. Sci. Eng. A. 426 (2006) 128–142. https://doi.org/10.1016/j.msea.2006.03.089.

[3] J.N. Brooks, L. El-Guebaly, A. Hassanein, T. Sizyuk, Plasma-facing material alternatives to tungsten, Nucl. Fusion. 55 (2015) 43002. https://doi.org/10.1088/0029-5515/55/4/043002.

[4] S. Nogami, I. Ozawa, D. Asami, N. Matsuta, S. Nakabayashi, S. Baumgärtner, P. Lied, K. Yabuuchi, T. Miyazawa, Y. Kikuchi, M. Wirtz, M. Rieth, A. Hasegawa, Tungsten–tantalum alloys for fusion reactor applications, J. Nucl. Mater. 566 (2022) 153740. https://doi.org/https://doi.org/10.1016/j.jnucmat.2022.153740.

[5] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J. Comput. Phys. 117 (1995) 1–19. https://doi.org/10.1006/jcph.1995.1039.

[6] Engel, Virtual Lab Inc, Pap. Knowl. . Towar. a Media Hist. Doc. (2016).

[7] M.S. Daw, M.I. Baskes, Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals, Phys. Rev. B. 29 (1984) 6443–6453. https://doi.org/10.1103/PhysRevB.29.6443.

[8] M.J. Banisalman, S. Park, T. Oda, Evaluation of the threshold displacement energy in tungsten by molecular dynamics calculations, J. Nucl. Mater. 495 (2017) 277–284. https://doi.org/10.1016/j.jnucmat.2017.08.019.

[9] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO–the

Open Visualization Tool, Model. Simul. Mater. Sci. Eng. 18 (2010) 15012. http://stacks.iop.org/0965-0393/18/i=1/a=015012.

[10] M.B. Salman, M. Park, M.J. Banisalman, Atomistic Study for the Tantalum and Tantalum – Tungsten Alloy Threshold Displacement Energy under Local Strain, (2023).

[11] J. Fu, Y. Chen, J. Fang, N. Gao, W. Hu, C. Jiang, H.-B. Zhou, G.-H. Lu, F. Gao, H. Deng, Molecular dynamics simulations of high-energy radiation damage in W and W–Re alloys, J. Nucl. Mater. 524 (2019) 9–20. https://doi.org/https://doi.org/10.1016/j.jnucmat.2019.06.027.

[12] L. Malerba, D. Terentyev, P. Olsson, R. Chakarova, J. Wallenius, Molecular dynamics simulation of displacement cascades in Fe–Cr alloys, J. Nucl. Mater. 329–333 (2004) 1156–1160. https://doi.org/https://doi.org/10.1016/j.jnucmat.2004.04.270.

[13] D.A. Terentyev, L. Malerba, R. Chakarova, K. Nordlund, P. Olsson, M. Rieth, J. Wallenius, Displacement cascades in Fe–Cr: A molecular dynamics study, J. Nucl. Mater. 349 (2006) 119–132. https://doi.org/https://doi.org/10.1016/j.jnucmat.2005.10.013.