The Role of Grain Boundaries and Surfaces on Irradiation Defect Evolution in Tungsten

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Background & Motivation

Fusion energy can be a potential source of safe, non-carbon emitting, and sustainable energy. Harnessing the power of fusion will be a key step in balancing our energy portfolio [1-6]. The heat flux on ITER’s divertor is estimated at 10 – 20 MW/m² and the Scrape-off Layer (SOL) hitting the blanket will introduce a particle flux of 10¹³ m⁻²s⁻¹. Thus, good resistance against the drastic radiation damage, practical heat conductivity, and high stability against thermal shock will be the governing properties of plasma facing components (PFCs).

Tungsten as Plasma Facing Material

Tungsten, the PFC material of choice in ITER’s divertor, exhibits the most advantageous properties for the forward-looking reactor platforms [2,7-13]. Tungsten has the highest melting temperature (3695K) of any metal, stable behavior at high temperature, and a small density with T. For the concern of the ion contamination: with W only in the divertor, W was hardly detectable inside the main plasma (with a sensitivity about 100 times above the measured signals) and no restrictions in plasma operation were reported [3, 9, 12, 14, 15].

Objectives of the Simulation Objectives and Procedures

Molecular Dynamics simulations were performed in the LAMMPS software package to explore the role of grain boundaries and surfaces in defect formation and damage evolution during collision cascade simulations. Primary knock-on atoms were sequentially impacted into the system to produce 400 cumulative impacts each with an energy of 1 keV.

Two grain sizes was explored – 6 and 12 nm – containing two grain boundary GB structures – Σ3, Σ5 CSL GBs. Damage accumulation on the surface, in the matrix, and in grain boundaries was quantified focusing on accumulation and depletion on the surface and point defect formation in the matrix and GBs.

Damage Accumulation at the Surface

Cascade overlap transpires during cumulative PKA impacts and controls the overall defect evolution trends. The effect of cumulative impacts was first quantified with vacancies shown in blue and interstitials in red.

• For 12 nm grain size model, the collision cascade does not interact with the GB. Consequently, all the defects form within the grain matrix for both GB configurations.
• Defect trends show that the vacancy production rate followed the cascade overlap probability.
• Net surface accumulation and depletion also scaled with the overlap probability.

Summary

We find that defect formation during low energy collision cascades is impacted by the presence of a surface, thereby influencing the response of tungsten at the plasma-material interface. Grain boundaries also strongly influence the evolution of point defects, and intrinsic material characteristics such as grain size and grain boundary character will ultimately govern the role of grain boundaries in accommodating radiation damage.

References


Identification of the Cascade Size from the Peak Damage Region

• Damage is most severe in the core of the collision cascade were the majority of Frenkel Pairs are created. This occurred within 5ps following PKA impact.
• However, as is shown in (c) on the right, displacement sequences also occurred outside of the peak damage region that ultimately led to the formation of interstitials outside of the collision cascade core.

Those sequences are usually referred to as Replacement Collision Sequences (RCS).

Replacement Collision Sequences

• An RCS with smaller energy will not create an interstitial defect, which is demonstrated for a 60 eV RCS in (a) on the right.
• When the RCS energy exceeds the threshold displacement energy along the preferential <111> direction, a split Frenkel Pair is created as shown in (b) – (d) on the right.

Grain Boundary Interstitials

• The GB-RCS interactions in the 6 nm grain size structure resulted in interstitials forming preferentially in the GBs.
• GB type influenced the effective trapping strength for the interstitials.

GB Interstitial Contributions from Different Mechanisms

As shown above in (a), the interstitial formation based on RCS-GB interactions is a stochastic process depending on the probability of a RSC to reach a GB. For crowdion migration in (b), the gradient in the interstitial segregation energy influences the sink efficiency.

• Interstitials can also be annihilated through two main processes, thus affecting total interstitial loading in the GB: (1) migration to the surface as shown in (c), and (2) recombination outside of the GB plane in (d).

The balance of formation, migration, and recombination events dictate the role of the GBs in accommodating point defects in tungsten, which scales with the GB character and grain size as well as other extrinsic driving forces such as PKA energy and temperature.