Helium Effect on Self-Healing at Tungsten Grain Boundaries Using a DFT-Based Machine Learning Interatomic Potential

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Nanostructured tungsten is a leading candidate for plasma-facing materials in future fusion reactors because its high grain boundary (GB) density can promote radiation-damage mitigation through intrinsic defect recombination ("self-healing") under specific conditions [1]. However, helium is simultaneously generated and implanted in fusion environments, where it binds strongly to vacancies, GBs, and other crystal defects, and subsequently nucleates into clusters due to its positive He–He binding energy [2]. This competes with self-interstitial atoms for available sinks and suppresses recombination.

Although this effect has been widely observed experimentally [3], a deeper understanding of the underlying competition requires an accurate atomistic description of defect migration and trapping, which is highly sensitive to the specific GB character. While such a description remains prohibitive for *ab initio* methods due to their inherent time- and length-scale limitations, empirical interatomic potentials (IPs) are often unreliable because their simple functional forms fail to capture the complexity of highly distorted GB environments. Consequently, the characterization of transition pathways between energy minima remains limited despite their critical role in governing defect migration and relaxation dynamics.

Here, we address the central question of the extent to which helium hinders intrinsic defect recombination near a tungsten GB and how this behavior depends on irradiation conditions. To answer these questions, we use large-scale molecular dynamics simulations driven by an MLIP based on a neural network [4] that was specifically developed in this work [5]. This model accurately reproduces the potential energy surface by repeating electronic structure calculations over a grid in the configuration space of interest. In particular, the model is explicitly trained on bulk tungsten and on a representative semicoherent GB frequently observed in sputter-deposited nanocrystalline tungsten (see Figure 1), and includes configurations containing intrinsic point defects and helium atoms over a wide temperature range. We employed an active-learning strategy to robustly train the model in complex atomic environments where multiple defect species coexist, a task that, to the best of our knowledge, has not been explicitly addressed in previous MLIPs for W–He systems [6,7].

Our results demonstrate that helium consistently suppresses intrinsic defect recombination, and this effect intensifies with higher helium concentrations, defect densities, and temperatures. Under irradiation-relevant conditions, helium is therefore expected to largely inhibit self healing. Nevertheless, GBs play a crucial mitigating role by redistributing helium away from the grain interior toward interfaces, where the larger free volume reduces local pressurization. Consequently, nanostructured tungsten exhibits broader He/V ratio distributions and a reduced tendency to form highly pressurized He–V clusters compared to bulk tungsten, providing an improved resistance. However, these results highlight the need to continue developing and investigating new materials that can withstand extreme irradiation conditions over an extended operational lifetime, enabling fusion to become a viable energy source.

References

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Figures

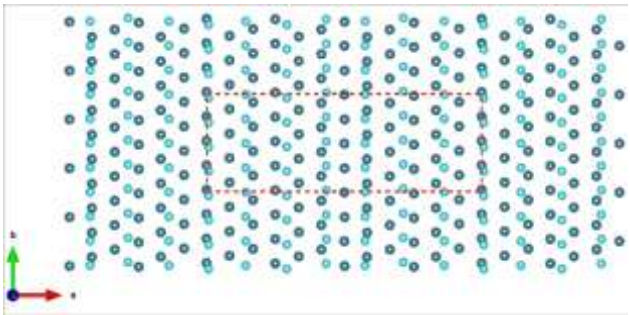

Figure 1. Frontal view of the W <110> (light blue)/W <112> (dark blue) GB. The red dashed rectangle indicates the in-plane dimensions of the simulation cell used for training the MLIP.