ML-Driven Analysis of Self-Healing Properties in Tungsten Grain Boundaries

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Abstract

Nuclear fusion offers promising prospects for future energy supply due to its high energy yield and compatibility with the sustainability goals of the 2030 Agenda. A key challenge is the development of plasma-facing materials (PFMs) capable of withstanding the extreme irradiation and thermal loads present in commercial fusion reactors. Nanostructured tungsten (NW) is emerging as a strong candidate, with its dense grain boundaries (GB) facilitating the diffusion of H atoms and preventing their accumulation, potentially offering self-healing properties. However, the role of GBs in the behavior of He atoms remains unclear and requires further investigation to assess the viability of NW as a PFM.

Recently, this topic has received considerable attention, primarily through molecular dynamics (MD) simulations using empirical interatomic potentials (IP). While these empirical models offer advantages, they often struggle to accurately describe important phenomena such as electronic effects at interfaces or free surfaces. Density functional theory (DFT) simulations offer greater accuracy, but are limited by their high computational cost, which has traditionally limited their use in large-scale molecular dynamics simulations. Fortunately, the emergence of machine learning (ML) algorithms offers a promising solution to this challenge, enabling more realistic studies at longer time and length scales. In this work, we develop a specialized ML IP for W GBs. We apply this ML IP to study the recombination of intrinsic defects, such as vacancies and self-interstitial atoms (SIAs), as a function of defect density and temperature in the presence of light impurity atoms (LIAs), specifically H and He. Since the analysis of defects at GB using traditional methods can lead to inaccurate results, we employ a robust approach for automated defect analysis of crystalline materials. This approach transforms the local environment of each atom into a rotation-invariant descriptive vector ("fingerprint"). Finally, we discuss the advantages and limitations of our methodologies by comparing them to results obtained from published research on established methods.