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Unveiling Surface Chemistry and Hardening Mechanisms in Fusion and Nuclear Materials

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This work presents a combined theoretical and experimental approach to understand the complex surface phenomena occurring in fusion and nuclear materials.
Fusion Materials: We investigate the interaction of low-Z (lithium and boron) coatings with carbon under extreme fusion plasma conditions. A multi-scale approach using computational modeling, real-time plasma diagnostics, and ex-vessel in-situ experiments unravels the evolving characteristics of these surfaces. We explore the effects of these coatings on deuterium retention and chemical sputtering, with a focus on the critical role of oxygen in driving the surface chemistry during hydrogen irradiation. These findings can hold significant implications for fusion plasma confinement behavior. Additionally, computational studies expand beyond limitations of empirical methods, paving the way for a strategic approach integrating advanced modeling tools with in-vessel and ex-vessel diagnostics.

Nuclear Materials: We analyze the hardening behavior of irradiated and pristine BCC and FCC alloys for nuclear applications. Nanoindentation testing reveals significant hardening effects by both experiments and computational modelling. The observed qualitative agreement between experimental load-displacement data and MD simulations suggests sluggish dislocation diffusion, reduced defect sizes, and tetrahedral stacking fault nucleation as key strengthening factors. Notably, experimental observations point towards the nucleation of interstitial-type prismatic dislocation loops during loading, shedding light on the material's hardening mechanisms. In FCC materials specifically, these loops interact to form pyramidal stacking faults, primarily driven by $\frac{1}{3}\langle 100\rangle$ Hirth dislocation lines. The co-existence of both defect types observed in the plastic deformation zone further supports the combined experimental and computational approach. Reported mechanical data, experimental and numerical, are validated by microstructural SEM and TEM investigations. Finally, we discuss the advantages and limitations of conventional interatomic potentials and machine-learned models in simulating nanoindentation tests.

This work provides valuable insights into surface chemistry and hardening mechanisms in both fusion and nuclear materials, paving the way for advancements in material design and optimization for extreme environments.

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