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Positron Annihilation Spectroscopy for vacancy defects studies in irradiated tungsten: Combination of modelling and experiments for vacancy size distribution and impurities interaction determination

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Tungsten has been selected as the divertor material for ITER and is also considered for the first wall in fusion reactors due to its exceptional properties, including a high melting point, excellent thermal conductivity, low thermal expansion, high strength at elevated temperatures, and a high sputtering threshold energy. In these environments, tungsten will be exposed to neutron irradiation, intense Helium and Hydrogen fluxes, and extreme thermal loads, with temperatures reaching up to 1780 K. These harsh conditions could drastically affect its macroscopic properties, potentially causing embrittlement and swelling as a result of microstructural evolution.

Multi-scale modeling plays a crucial role in understanding and predicting tungsten microstructure evolution in future fusion reactors. To validate these models, experimental data are essential, particularly regarding the behavior of radiation-induced defects. Additionally, one of the key open questions is the interaction between these defects and impurities present in both the material and the plasma. Theoretical studies suggest strong interactions that could significantly influence microstructure evolution under irradiation.

This work combines modeling and experimental approaches to investigate the nature and properties of irradiation-induced defects in tungsten. On the experimental side, well-controlled irradiations are followed by advanced characterizations using Positron Annihilation Spectroscopy (PAS), including lifetime and Doppler Broadening (PAS-DB), along with Transmission Electron Microscopy (TEM) to analyze defects across different scales, from single vacancies to nanoscale cavities. On the modeling side, calculations using Two-Component Density Functional Theory (TC-DFT) provide positron annihilation characteristics—lifetimes and Doppler broadening spectra—essential for defect identification. Additionally, defect evolution is simulated as a function of irradiation conditions and impurity concentration using Molecular Dynamics, Cluster Dynamics, and Object Kinetic Monte Carlo methods.

A novel approach is introduced to estimate vacancy-type defect concentrations from experimental PAS data [1]. This method utilizes a quadratic solver calibrated with a positron trapping model [1], incorporating TC-DFT-calculated annihilation characteristics for various vacancy defects [2]. The analysis reveals small vacancy clusters that are undetectable by TEM, with concentrations significantly exceeding those of TEM-visible defects (10^{24} m^{-3}) in self-irradiated tungsten at 0.02 dpa and 500℃ [1]. Moreover, the effect of the tungsten purity on the vacancy type defects distribution is shown [2,3]. Accounting for positron trapping in oxygen-vacancy complexes enables an accurate reproduction of high-temperature irradiation experimental data [1].

References

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