(MPT-3) Molecular Dynamics and Density Functional Simulations of Tungsten Nanostructure Formation by Helium Plasma Irradiation

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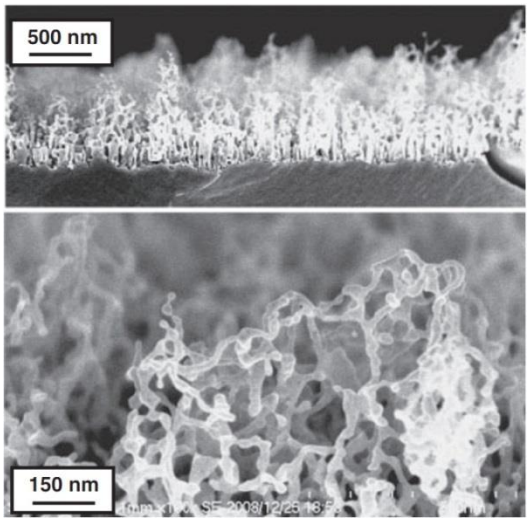

tungsten fuzzy nanostructure

- To clarify the tungsten fuzzy nanostructure formation by helium plasma irradiation, He penetration process, He diffusion and agglomeration process, and He bubble growth process were explained by using binary collision approximation (BCA), density functional theory (DFT), and molecular dynamics (MD), respectively.
- Molecular dynamics and Monte-Carlo (MD-MC) hybrid simulation achieved to represent the formation process of the fuzzy nanostructure.
- Thus, multi-scale simulations and hybrid simulation approaches accelerate reactor material researches.

MD-MC hybrid simulation