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Multiscale Physics Challenges For Plasma-Facing Materials[1]

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Plasma-facing materials undoubtedly experience some of the most demanding environments ever encountered by functional materials in engineered systems. They will be subjected to extremes of heat flux, ion and electromagnetic radiation bombardment, and neutron irradiation. The microstructure and hence all properties of the first few microns will be in a dynamic state, and will continuously evolve and change as the material is used in the plasma chamber. Several physical effects must be considered in the design and utilization of plasma-facing components, such as sputtering, erosion, re-deposition, de-gasing, blistering, embrittlement, and loss of ductility. Because of the severity of the operational environment, the development of plasma-facing materials must be based on the fundamental principles of physics, mechanics and materials science. We discuss here the multiscale modeling approach to the development of plasma-facing materials and components. The framework starts at the atomistic length scale, and utilizes both ab initio, molecular dynamics and kinetic Monte Carlo techniques. At the intermediate scale between the atomistic and continuum, mesoscopic methods (e.g. dislocation dynamics) are developed to describe the evolution of the materials microstructure. Finally, continuum methods are used to connect to experimental investigations. It will be shown that the proposed multiscale modeling framework, verified by experiments at each length scale, will lead to robust and rational development of reliable materials.

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