PiAI Seminar Series: Physics informed AI in Plasma Science
10:00-11:00, 10 June 2024 (CEST)
16:00-17:00, 10 June 2024 (CST)
17:00-18:00, 10 June 2024 (JST)
Web Seminar

Accurate atomistic morphology of plasma-oxidized copper using physics-informed neural network potentials

Yantao Xia

Hangzhou Institute of Medicine Chinese Academy of Sciences, Hangzhou, Zhejiang, China

The semiconductor industry is looking for an atomic-level engineering approach that is simultaneously capable of achieving high selectivity and high directionality. Plasma-thermal atomic layer etching (ALE) is one of the most promising techniques for this purpose, but currently a precise understanding at the atomistic scale is lacking, hindering process development. In this work, a physics-informed machine learning potential is developed to cover the entire range of potential energy surfaces from metallic copper, epitaxial oxide, full oxide, as well the interaction of their surfaces with energetic atomic and molecular oxygen ions. The neural network is coupled in a range-separated fashion to the ZBL potential. This approach ensure that the short-distance exponential repulsion behavior is preserved quantitatively, while the high-dimensional PES near equilibrium bond lengths is captured accurately by the neural network. The model is carefully validated to ensure accuracy close to that of first-principle calculations at the DFT level. Molecular dynamics (MD) simulation of the plasma oxidation of copper, covering a range of kinetic energy of ions up to 400 eV is performed, yielding simulation trajectories that are analyzed to reveal lateral and vertical

morphological features quantitatively matching experiments performed at similar conditions. Based on observed trends when plasma kinetic energy, temperature, and neutral-to-ion ratio are changed in our 'virtual reactor', it is predicted that self-limiting growth of the oxide is possible when the substrate temperature is lowered, and growth is only activated via kinetic energy imparted to the surface by the ions.