Simulating HF etching process of amorphous Si_3N_4 using machine learning potential

This research aims to advance the atomistic understanding of dry-etching processes crucial for semiconductor manufacturing. Current molecular dynamics (MD) simulations are limited by the lack of reliable force fields, hindering their application in etching studies. To address this, a neural network potential (NNP) was developed to simulate the etching of amorphous Si_3N_4 with HF molecules. The NNP was trained using surface reactions in diverse local environments: baseline structures, reaction-specific data, and general-purpose training sets; and refined through iterative comparisons with density functional theory (DFT) results to ensure high accuracy. The trained NNP allowed for detailed simulations of key aspects such as preferential sputtering, surface modification, etching yield, threshold energy, and product distribution. A continuum model, derived from MD results, was also developed to replicate surface composition changes effectively. This study establishes a robust computational framework for atomistic etching simulations, offering a pathway to more accurate and efficient etching process designs for the semiconductor industry. This work was published in ACS applied Materials & Interfaces 2024, **16**, 48457.