Atomistic kMC simulation on TiN ALD

The atomic layer deposition (ALD) process of titanium nitride (TiN) thin films is widely used in microelectronics, but the detailed growth mechanism is still elusive at the atomistic level. In this work, we carry out kinetic Monte Carlo (kMC) simulations on the ALD process using $TiCl_4$ and NH_3 precursors. Based on the on-lattice model, we sort out key reactions relevant for the ALD process. Considering the local environments, the reaction energies are calculated at the level of density functional theory (DFT) while the activation barriers are linearly fitted to sampled cases. The resulting kMC model produces the temperature-dependent growth rates and the amounts of Cl residues, which is in reasonable agreement with experiments. Our growth pathway underscores the critical role of surface Cl atoms in the ALD process by generating HCl gas molecules. By revealing the atomistic mechanisms in the TiN-ALD process, this work would help optimize material properties of TiN thin films. This work was published at Computational Materials Science, 213, 111620.