

Desorption Characteristics of Selenium Thin Films: A ReaxFF Molecular Dynamics Study

*M. Wang, N. Nayir, D.S.H. Liu, M. Hilse, R. Engel-Herbert, A.C.T. van Duin

Abstract: Two-dimensional layered chalcogenides possess unique properties that distinguish them from their bulk counterparts. Molecular beam epitaxy (MBE) has been adapted in several studies to achieve controlled growth of chalcogenide-based thin films with large area uniformity. However, MBE growth of chalcogenide-based thin films faces several challenges, as the high vapor pressure of chalcogens leads to their high volatility, which limits the growth rate and introduces vacancies into the film. The presence of less reactive polyatomic species in the chalcogen vapor also requires an increased oversupply of chalcogens to compensate for their lack of reactivity. In this study, the desorption kinetics of Se thin films in an MBE system have been investigated using a newly developed ReaxFF reactive force field. ReaxFF molecular dynamics (MD) simulations are used to investigate the temperature-dependent volatility of various chemical states of Se, providing insight into the molecular size and mass distribution of Se polymorphs in the effusion source. This study also examines the temperature-induced transitions in chalcogen vapor composition that significantly affect the rate of thin film deposition. These results provide theoretical guidance on the optimal growth temperature and chemical state of the evaporation sources, thereby advancing our understanding of the growth process of chalcogenide thin films.