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Understanding chemical vapor deposition (CVD) growth of MoS_2 layers by ReaxFF-molecular dynamics simulations[1] SUNGWOOK HONG, ARAVIND KRISHNAMOORTHY, CHUNYANG SHENG, PANKAJ RAJAK, SUBODH TIWARI, ANKIT MISHRA, RAJIV K. KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California, COLLABORATORY FOR ADVANCED COMPUTING AND SIMULATIONS TEAM — Recently, mono-layered MoS_2 has been widely studied for the next generation of electronic devices. A fundamental understanding of the CVD growth of MoS_2 layer is the key to manufacturing a high quality of MoS_2-based devices. However, reaction kinetics of the CVD growth of the MoS_2 layer has not been fully understood; and synthesis of uniform mono-layered MoS_2 up to the wafer-scale is still challenging. This is primarily due to the complexity of the CVD processes (*i.e.*, intermediate structures from MoO_3 to MoS_2 phases). Reactive molecular dynamic (MD) simulations can provide atomistic-scale insights into complex surface reactions during the CVD growth. For this reason, our work focuses on developing a ReaxFF reactive force field for $MoO_3/MoS_2/S$ interactions and performing massively parallel MD simulations of the sulfidation of MoO_3 systems. Our goal is to clarify the reaction mechanism of the sulfidation of MoO_3 clusters, and provide a theory-supported rational design for not only MoS_2-based applications but also for synthesis of other two-dimensional materials.

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