Modeling 2D Materials Growth Across Scales: Closing the MGI Loop

External User + In-house collaboration 2021

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A grand challenge towards widespread applications of 2D materials is their controllable and reproducible growth at large scale. Experimental efforts in the 2DDC-MIP on chemical vapor deposition (CVD) growth of wafer-scale crystalline monolayers are closely coupled with multi-scale simulation of the growth chambers to guide the way to the highest quality growth possible. Multiscale/multiphysics models couple continuum fluid mechanics and phase-field methods so that experimentally controllable macroscale (inlet velocity, temperature) and mesoscale (surface diffusion and deposition rates) growth parameters can be directly connected to the morphology of the as-grown 2D materials. Efforts on CVD growth of both WSe_2 and BN have established relationships between macroscale growth parameters and experimental growth coverage as a step on the path to synthesis-by-design.

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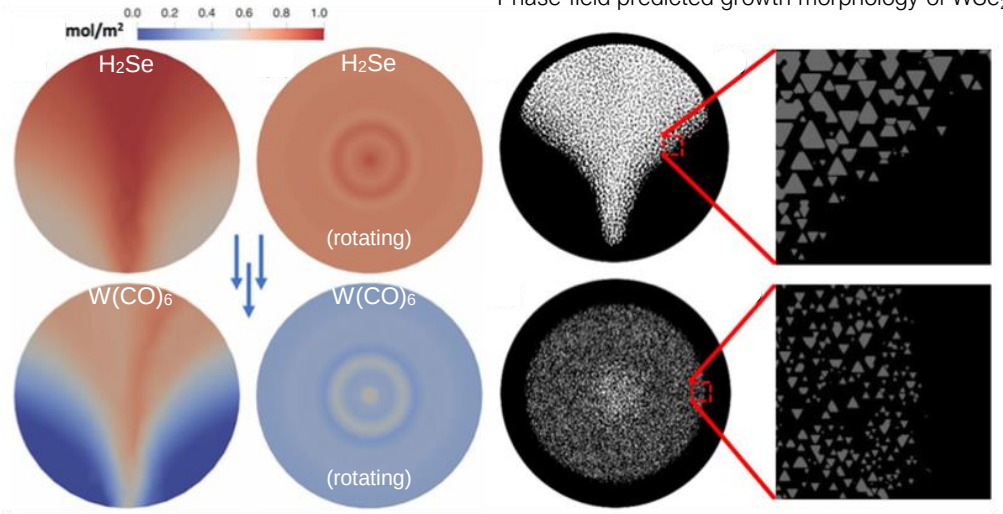
Phase-field predicted growth morphology of WSe_2



Simulated growth morphology of BN flakes