Evokinetics: A software tool for the analysis of CVD growth of novel 2D materials?

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Planar synthesis technologies, such as Chemical Vapor Deposition (CVD), are currently attracting increasing attention as an alternative to mechanical exfoliation in order to supply a complete, new generation of atom-thick materials, including semi-metals (graphene, NiTe2, VSe2,...), semiconductors (WS2, WSe2, MoS2, MoSe2, MoTe2, TaS2, RhTe2, PdTe2,...), insulators (hexagonal-BN, HfS2,...), superconductors (NbS2, NbSe2, NbTe2, TaSe2,...) and topological insulators (Bi2Se3, Bi2Te3, Sb2Te3). During CVD growth, however, many flakes of the 2D material are nucleated at different locations, leading to the formation of a polycrystalline 2D sample, characterized by the presence of numerous grain boundaries, which deteriorate the electronic, thermal and mechanical properties of the material. Therefore, control over the actual shape and size of the flakes before coalescing is essential in order to enable tailor production and quality management of the grown 2D materials by both researchers and CVD synthesis industries.

By showing that the shape and size of the flakes are dominated by the relative kinetics of different atomistic processes, such as adsorption, desorption, dissociation, nucleation, terrace/perimeter diffusion, etc..., the talk presents the idea that a software tool can possibly be used in the near future in order to analyze the atomistic kinetics by directly extracting information from microscopy images of the surface morphology during growth. Refered to as Evokinetics, we show that the approach, is able to describe the activation energies of the various atomistic processes, simultaneously providing clear information about which atomistic processes are relevant (i.e. active) and which are accessory, implicitly describing the effect of temperature, partial pressures, inlet fluxes and other experimental parameters.

This autonomous determination of the kinetic competition between atomistic processes can possibly be performed in a wide range of fields, including heterogeneous catalysis, chemical synthesis, wet etching and epitaxial growth. In the same way as researchers currently may try to optimize manually surface-mediated processes by varying the experimental conditions, measuring total yields and analyzing morphology images, Evokinetics offers the possibility to automatize and speed up such a search while making it completely objective. In this manner, Evokinetics may perhaps be used in the future in order to accelerate/optimize the setup/development of CVD equipment for the synthesis of novel 2D materials.