Synthesis of Large-area Ultra-thin Mo_2C Films Using Chemical Vapor Deposition

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Abstract

Two-dimensional (2D) materials are strong candidates for addressing critical technological challenges in modern society. Their high surface area-to-volume ratios, combined with tunable electronic properties ranging from insulators to superconductor, make them an exceptionally versatile platform for the development of next-generation sustainable devices. Although quantum confinement effects are typically associated with van der Waals layered structures, they are not exclusive to them. For example, transition metal carbides (TMCs) can also be synthesized as ultrathin nanoplatelets (less than 50 nm in thickness), expanding the scope of 2D materials. Among ultrathin TMCs, molybdenum carbide (Mo_2C) has garnered significant interest due to its potential applications in catalysis and energy storage. However, a key challenge in the application of Mo_2C is the synthesis of large-area films which necessitates the quantification of the lateral film coverage as a function of growth parameters. In this work, we employ a liquid copper (Cu) melt to facilitate molybdenum (Mo) diffusion to the surface, enabling the one-step chemical vapor deposition (CVD) of large-area, continuous Mo_2C films. We demonstrated that several parameters, such as thickness of the copper foil, time, and methane-hydrogen gas ratio, significantly influenced Mo_2C synthesis. Thinner Cu foils and longer growth times enhanced Mo diffusion to the surface, leading to improved lateral film uniformity and overall film coalescence. As a result highly crystalline Mo_2C films spanning centimetre-scale areas were synthesized as demonstrated by X-ray diffraction (XRD) and Raman spectroscopy measurements. Raman spectroscopy further revealed the presence of multilayer graphene on the film surface, as confirmed by distinct contrast variations in scanning electron microscopy (SEM) images. We hypothesized that graphene, grown simultaneously during the synthesis, serves as a diffusion barrier for Mo, enabling the growth of nanometre-thin Mo_2C films. The resulting large-area films, characterized by their large-area and high crystallinity, show great promise as electrodes for electrocatalytic applications. Future work involves benchmarking the electrocatalytic and electronic transport properties of these films and analysing the effects of defects such as pinholes, step-edges, and grain boundaries on the resulting properties.

Keywords: *Transition metal carbides, chemical vapor deposition*