Synthesis and Structural Characterization of Ultrathin Transition Metal Carbide/Dichalcogenide Heterostructures

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Abstract: Layered materials such as transition metal dichalcogenides (TMDs) can be stacked onto various materials to form heterostructures. While mechanical exfoliation of layered materials is a route to form heterostructures, developments in chemical synthesis have led to heterostructures with an atomically sharp interface and strong interfacial coupling. In this work, we have synthesized transition metal carbide (TMC) and TMD heterostructures through a post growth chalcogenization process and identified that the crystalline phase of the TMC is critical towards controllably synthesizing TMC/TMD heterostructures. Ultrathin, non-layered molybdenum and tungsten semi-carbide (Mo_2C, W_2C) and tungsten monocarbide (WC) TMC nanoplates were synthesized via a liquid metal chemical vapor deposition process. A heat treatment in chalcogen powder vapor or gaseous hydrogen chalcogenide (H_2S, H_2Se) converted the surface of TMC nanoplates into crystalline, layered molybdenum diselenide and tungsten disulfide. Following chalcogenization, Raman spectroscopy analysis identified a prevalence of multilayer TMD on the edge compared to the basal surface of the nanoplates. Through scanning/transmission electron microscopy (S/TEM) we observed the TMC nanoplates retain the initial morphology and high crystallinity. The chalcogenization proceeded along the TMC nanoplate edges with the top and bottom basal surfaces converted to epitaxial and polycrystalline TMD. Through planar and cross-sectional STEM energy dispersive X-ray spectroscopy we observed chalcogen concentrated along the surface of the nanoplates with a tendency to not dope or alloy with the TMC. Mo_2C and W_2C convert more readily for shorter times and lower temperatures than WC, with the facets being completely converted to multilayer TMD. The limited conversion of WC could provide a potential route to synthesizing few-layers of TMD on TMCs with distinct moiré patterns.