DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering

PhD Defense

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Mechanism and Kinetics of 2D Transition Metal Carbides (MXenes) Synthesis

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Abstract

Two-dimensional (2D) nanomaterials including graphene, hexagonal boron nitride (*h*-BN), transition metal dichalcogenides (TMDs), and MXenes have attracted much attention because they present a wide range of physicochemical, optoelectronic, and mechanical properties along with various atomic structures and compositions. MXenes represent the larges and rapidly growing family of 2D transition metal carbides and/or nitrides, which exhibit unique combinations of properties, including metallic conductivity, hydrophilic surface chemistry, redox-active surface, and plasmonic behavior that make them attractive as electrodes for pseudocapacitive energy storage to coatings for electromagnetic interference shielding, transparent conducting displays for optoelectronics, conductive yarns for functional textiles, implantable electrodes for medicine, and many other applications. MXenes are typically derived via topochemical etching of atomically thick layers from precursor layered MAX phases using corrosive aqueous etchants. However, the chemical etching process is only somewhat optimized for one composition, and is nonetheless often slow, with low-yield, and results in defects in the materials.

This thesis focuses on understanding the fundamental mechanism and kinetics of the selective etching of layered MAX phases using aqueous HF-based etchant solutions for topochemical synthesis of MXenes. Despite their importance, such studies have been challenging because of the atomic thickness of the A-element layers being etched and the aggressive etchants that hinder in situ studies. To achieve this, analytical setups for measuring etching kinetics, in situ microscopic cells for observing the etching mechanism, and spectrometric characterization techniques for chemical depth-profiling of MAX and MXene particles are developed and used to study the influence of critical process parameters on synthesis. Spatial mapping of the etching front and models of the etching kinetics are thus developed to enable tailored synthesis for specific applications, rational high-throughput optimization of synthesis for all MXene compositions, and scaling up synthesis towards industrial levels.