Impact of MAX phase purity on performance of 2D layered MXenes in the energy sector

Rupesh S. Devan,

Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Indore, Khandwa Road, Sirmon, Indore 453552, India

Abstract

Ti_3C_2-X Menes have gained tremendous research momentum due to their 2D laminar morphology, which offers a range of functional applications. This motivates the synthesis of the pure MAX phase, which is essential for producing Menez at a large scale using simple and more cost-effective techniques. However, producing pure prerequisite MAX phase at atmospheric pressure and relatively lower temperatures remains a challenging task. Until now, researchers have mainly focused on optimizing the synthesis of the MAX phase. Various synthesis methods, including liquid or solid-state reaction processes and pulsed laser deposition, have been employed to obtain the MAX phase with enhanced purity. However, these techniques often result in remnant impurity phases, larger grain sizes, lower density of components, secondary phase formation, randomized morphologies, and low yield. Remnant impurity phases and low density of components, by and large, affect the interlayer spacing of the resultant MXenes. Therefore, removing the impurity phase and controlling the density of components is crucial for synthesizing pure MAX phases and, in turn, obtaining well-separated 2D laminar MXenes.

In this contest, I will discuss our recent efforts in synthesizing high-purity Ti_3AlC_2 MAX phase through molten salt shielding solid-state synthesis (MS^5) reaction process under atmospheric pressure conditions. This process has a significant impact on the interlayer spacing and electrochemical performance of the Ti_3C_2-F MXene electrode. The incorporation of F-terminal groups notably increases the interlayer spacing, resulting in a surface area of 8.9 m^2/g. This expanded structure provides more electroactive sites, enhancing the intercalation of sodium (Na) ions. As the purity of the MAX phase increases from 47% to 99%, the specific capacitance rises from 121.86 to 680.79 F/g. Furthermore, high-purity (i.e., >99 %) Ti_3C_2 MXene (Ti_3C_2-F) serves as an advanced anode material for Na-ion batteries, capable of operating at temperatures as low as -120°C. It also demonstrates significant potential for generating green hydrogen in a photocatalytic process and serves as an excellent catalyst for storing hydrogen to a great extent.