MXene Particle Synthesis and their Scalability

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Introduction

- **MXene** is a 2-Dimensional nano particle with electrical properties surpassing graphene opening possibilities of replacing graphene as carbon-based nanomaterial for electrical applications.
- MXene has a general formula $M_{n+1}X_nT_x$ where **M is an early transition metal, X is carbon and/or nitrogen, and T is a functional group** on the surface of a MXene (typically O, OH and F)
- The traditional method of MXene synthesis involves **etching of MAX phase with HF** to break the **M-A bond** which is metallic while **the M-X bond** is a mix of covalent/metallic/ionic bond.
- HF is hazardous and the yield from HCl etching is inadequate. The replacement **in-situ HCl from HCl + LiF** has been suggested which is less hazardous as it can be stored as HCl and LiF which are easier and safer to handle.

Experimental Method

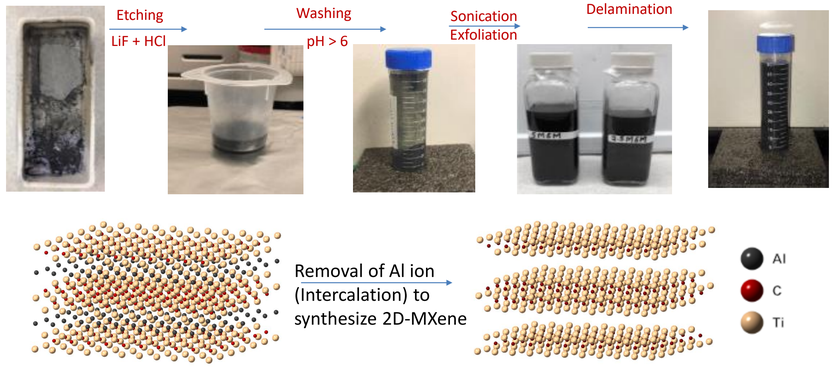

Fig. 1- (a)MAX Phase (b) in-situ HF + MAX phase (c) 2D MXene flakes after intercalation. (d) Sonicated solution with 2D flakes delaminated (e) pure 2D-MXene solution in DI water (f) Microstructure of MAX phase with ions (g) Microstructure of MXene after removal of ions

- The MAX phase is reduced to powder form using a ball mill up to a few micrometer size to improve yield by better etching.
- The **molar ratio Ti_3AlC_2 is 1:7.5:23.4** and etching is done using in-situ HF on a magnetic hot plate with **500RPM at 35°C for 24hrs**.
- After etching, solution is washed till **pH>6** is achieved followed by sonication to get high quality **2D-MXene** in the solution.
- This solution is passed through a vacuum filtration setup to get dry MXene sheets.

Results and SEM images

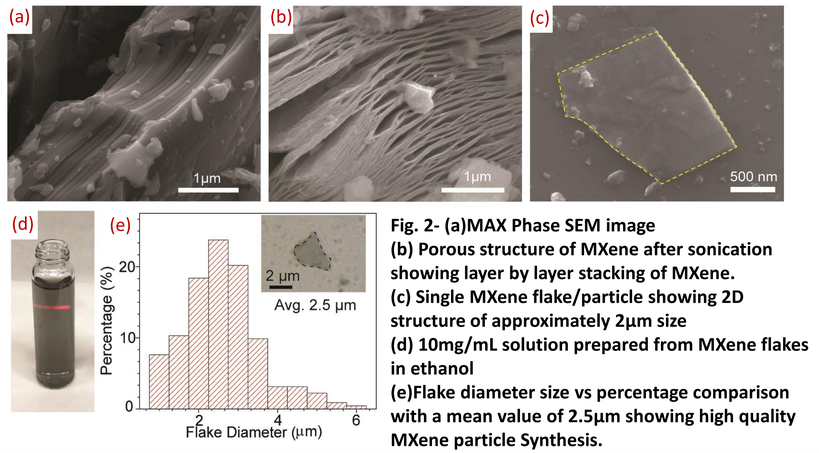

Fig. 2- (a)MAX Phase SEM image (b) Porous structure of MXene after sonication showing layer by layer stacking of MXene. (c) Single MXene flake/particle showing 2D structure of approximately 2µm size (d) 10mg/mL solution prepared from MXene flakes in ethanol (e)Flake diameter size vs percentage comparison with a mean value of 2.5µm showing high quality MXene particle Synthesis.

Experimental Method – II (Proposed Future Work)

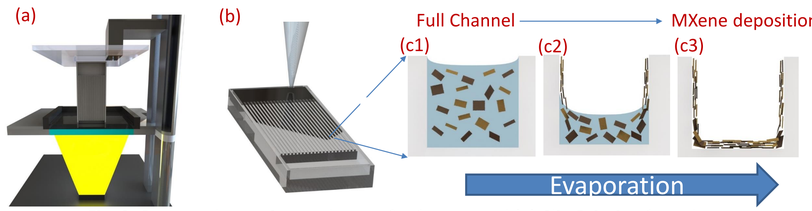

Fig. 3- Proposed experimental setup for future work(a) Clip Printing for substrate (b) deposition of MXene solution (c) Front view of microchannel during evaporation

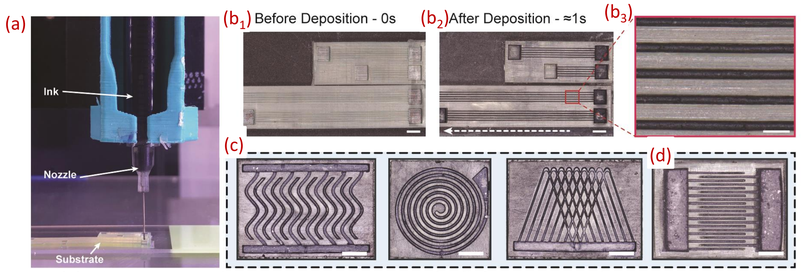

Fig. 4- (a) Inkjet printing of MXene-ethanol solution (b_1/b_2) deposition of MXene solution via inkjet (b_3)Enlarged image of microchannels (c) Proposed substrate design for capacitance and sensing (d) Proposed design for supercapacitor applications.

Simulation Results for deposition

- Optimal parameters for the post-synthesis experimental setup decided using **ANSYS FLUENT based solver** by comparing velocity profiles, viscosity, discrete phase concentration and residence time of particles with a **transient-discrete phase study.**

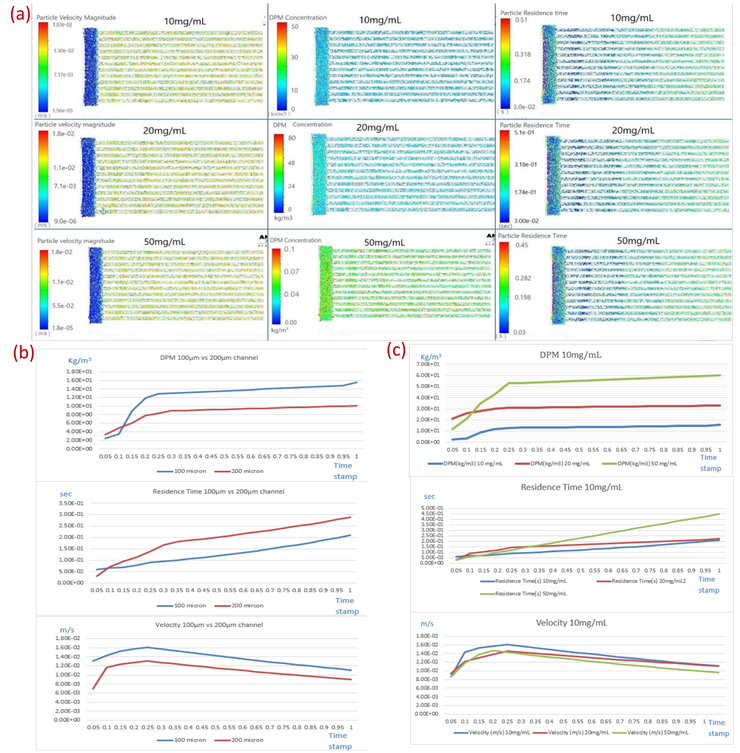

Fig. 4- (a) Particle residence time/velocity profile and particle distribution contour plots from ANSYS for 10-20-50mg/mL MXene solution respectively. (b) Comparison of particle properties between 100µm and 200µm channel for 10mg/mL MXene solution (c) Comparison of particle properties between 10-20-50mg/mL MXene solution

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