Type of presentation: Poster

MS-2-P-5944 Structural investigation of single layer Ti_3C_2 MXene sheets

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2D materials are of great interest due to their unique properties, and granted the Nobel Prize recently [1,2]. Among 2D materials like Graphene, MoS_2, BN, WS_2, MXene is one of the most recent additions, exfoliated from the various MAX-phases. The MAX-phases consist of an M-element (transition metal), A-phase (usually an A-group element, commonly groups 13 and 14) and X-phase (C or N), in the form $M_{n+1}AX_n$ where n = 1, 2 or 3 [2]. These materials show unique properties, such as toughness, high temperature and corrosion resistance [3,4]. Exfoliating the MAX phase Ti_3AlC_2 in hydroflouric acid or ammonium bifluoride, NH_4HF_2, causes the A element to leave the chemical stable Ti_3C_2, which then form a layered structure of 2D crystals [5]. The 2D material, MXene, show unique properties as well, such as high conductivity and ductility [2]. The surface chemistry of the material depends on whether the surface is terminated by fluorine or hydroxyl groups [2].
In this contribution, low-kV (60 kV) high-resolution scanning transmission electron microscopy has been applied to investigate the atomic arrangement of single and double layer Ti_3C_2 MXene sheets in plan-view. Previous TEM investigations have shown that MXene nanosheets are a few nm thick and consist of Ti, C, O and H in a layered structure [2]. However, the exact position of the various elements has not been confirmed. In this study, the positions of the elements have been identified, while also the surface/edge termination and point defects has been investigated. In addition, the elemental properties have been investigating, addressing surface related groups which remain after the etching process.

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Acknowledgement: The Swedish Research Council (VR) is gratefully acknowledged for funding. The Knut and Alice Wallenberg (KAW) Foundation is gratefully acknowledged for the Ultra Electron Microscope Laboratory in Linköping. Jun Lu and Michel W. Barsoum are acknowledged for providing the MXene samples.