Xi Ling

Department of Chemistry, Division of Materials Science and Engineering. Boston University 590 Commonwealth Ave. Boston, MA 02215, USA

xiling@bu.edu

2D Metallic MXenes: Chemical Vapor Deposition and Structural Characterization

MXenes, a group of emerging two-dimensional (2D) transition metal carbides (TMCs) and nitrides (TMNs), are receiving growing interest given their excellent stability and intriguing properties, notably high conductivity.^[1,2] Progress has been made in the synthesis of MXenes via selective etching of the "A" layer from their bulk MAX phases, yet the 2D sheets produced in this manner suffer from small lateral size domains below 10 µm.^[3] This type of MXenes shows great potential in energy storage and electrochemical catalysis,^[4,5] but has limited applications in the field of electronic and optoelectronic devices. Developing method for large-area, continuous and crystalline MXenes, like what has been achieved on chemical vapor deposition (CVD) grown graphene and several 2D transition metal dichalcogenides (TMDs), is crucial to extend their applications, and enhance the functionality of the 2D materials family. In this work, I will present our recent work on CVD of ultrathin molybdenum carbide (Mo₂C), one of the widely studied MXenes. High-quality α -Mo₂C sheets with nanometer thickness are obtained.^[6] Moreover, through a systematic Raman spectroscopy study on the synthesized a-Mo₂C sheets with diverse shapes including hexagonal, triangular, pentagonal and truncated trapzoid morphologies, We realized that most of the a-Mo₂C sheets contain multiple domains and the c-axes of neighboring domains tend to form a 60° or 120° angle (Figure 1), due to the weak Mo-C bonds in this interstitial carbide and the low formation energy of the carbon chains along three equivalent directions. In addition, to overcome the challenges of conventional CVD method in obtaining diverse MXenes and their heterostructures with other 2D materials, we propose a chemical conversion strategy. A variety of MXenes are obtained successfully using this novel strategy (unpublished).

References

- [1] H. O. Pierson, Handbook of Refractory Carbides and Nitrides: Properties, Characteristics, Processing and Applications, William Andrew, **1996**.
- [2] Naguib Michael, Mochalin Vadym N., Barsoum Michel W., Gogotsi Yury, Adv. Mater. 2013, 26, 992.
- [3] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, *Adv. Mater.* **2011**, 23, 4248.
- [4] M. Naguib, J. Come, B. Dyatkin, V. Presser, P.-L. Taberna, P. Simon, M. W. Barsoum, Y. Gogotsi, *Electrochem. Commun.* **2012**, *16*, 61.
- [5] B. Anasori, M. R. Lukatskaya, Y. Gogotsi, Nat. Rev. Mater. 2017, 2, 16098.
- [6] T. Li, W. Luo, H. Kitadai, X. Wang, X. Ling, *Adv. Mater.* **2019**, 1807160.

Figures

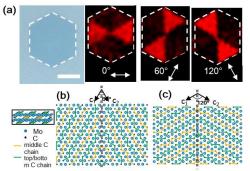


Figure 1. (a) Optical images and corresponding Raman maps of the intensity for a hexagonal α -Mo₂C flake under incident laser polarization at 0°, 60° and 120°. (b-c) Schematics of the atomic structure at the interface between two adjacent domains with a 60°-boundary (a) and 120° boundary (b) in one layer of α -Mo₂C.