TWO-DIMENSIONAL NANOCRYSTALS OF TRANSITION METAL CARBIDES PRODUCED BY EXFOLIATION OF MAX PHASES

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Two-dimensional (*2-D*) free-standing crystals are attractive as they exhibit properties that differ from those of their three-dimensional, *3-D,* counterparts. Currently, there are relatively few such atomically layered solids. Herein, we report on the fabrication of a new family of *2-D* $M_{n+1}X_n$ sheets from *MAX* phases. [1, 2] *MAX* phases are a large family of machinable layered ternary carbides and nitrides, where *M* is an early transition metal, *A* is a group 13 to 16 element and *X* is C and/or N. [3]

The exfoliation process was carried out by immersing selected *MAX* phase powders in hydrofluoric acid, HF, at room temperature, which results in the selective etching of the *A* layers from the *MAX* phases. We are labeling those *2-D* layers *MXene*s to denote the loss of the *A* element from MAX and emphasize their structural similarities with graphene. Several examples are discussed, such as Ti_2C, Ti_3C_2, $(Ti_{0.5}Nb_{0.5})_2C$, $(V_{0.5}Cr_{0.5})_3C_2$, Ta_4C_3, and $Ti_3(C_{0.5}N_{0.5})_2$.[2] The most characterized material to date is Ti_3C_2 produced by the room temperature exfoliation of Ti_3AlC_2 in HF for 2h.[1] Not only are individual layers formed, but also multi-layer particles and conical scrolls with radii less than 20 nm. [1]

The large elastic moduli predicted by *ab initio* simulation and the possibility of varying their surface chemistries render these nanosheets attractive as polymer composite fillers. Cold pressed discs of *MXenes* showed hydrophilic behavior and electrical conductivity compared to multilayer graphene.[2] We also predict that their band gaps can be tuned by varying the surface terminations. Preliminary results have shown that the *MXene* are promising materials for anoded in lithium ion batteries.[4] At C/25, the steady state capacity was 225 $mAh \cdot g^{-1}$; at 1C, it was 110 $mAh \cdot g^{-1}$ after 80 cycles; at 3C, it was 80 $mAh \cdot g^{-1}$ after 120 cycles; and at 10C, it was 70 $mAh \cdot g^{-1}$ after 200 cycles. [4]

Since there are over 60 *MAX* phases known to date, this discovery opens the door to the synthesis of a large number of other 2-D transition metal carbides and nitrides.

References

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