A series of MAX phases with MA-triangular-prism bilayers and elastic properties

With the support by the National Natural Science Foundation of China and the Chinese Academy of Sciences, the research team led by Prof. Chen XiaoLong (陈小龙) at the Laboratory of Advanced Materials and Electron Microscopy, Institute of Physics, Chinese Academy of Sciences, discovered a series of MAX phases with novel crystal structures and outstanding elastic properties, which was published in *Angew Chem Int Ed* (2019, 58: 4576—4580).

MAX phases belong to a family of non-van-der-Waals layered compounds with a general formula of $M_{n+1}AX_n$ (n=1, 2, 3) in which M=transition metals, A=main group elements, and X=C/N. Some of them host high thermal and electrical conductivity, good elastic performance, excellent resistance to corrosion, oxidation, and thermal shock, easy machinability and unusual damage-tolerance. These combined elastic, electrical and thermal properties enable them to be promising materials for various applications, especially in the structural or conductive components under high temperatures. Besides, MAX phases also have drawn much attention as the precursor of MXenes.

The study of MAX phases started from the 1960s when the H-phases were found by Nowotny's group. Now, over 60 MAX phases are found. Depending on the value of n, the M_2AX, M_3AX_2, and M_4AX_3 phases are usually named 211, 312, and 413 phases, respectively. The multi-layering of MA layers, however, has never been found among the known MAX phases.

Based on structural design, the research team discovered new MAX phases in As-, P- containing systems, namely, Nb_3As_2C, V_3As_2C, Nb_3P_2C, and Ta_3P_2C. Their crystal structures are determined by X-ray diffraction and high resolution transmission electron microscopy. These isostructural phases can be regarded as the formation from alternate stacking of one MX layer and two MA layers in their unit cells. In contrast to the known MAX phases, the multi-layered MA sheets are first observed in 321 phases. It is noteworthy that the new 321 phase, Nb_3As_2C, exhibits a bulk modulus up to 225(3) GPa as determined by high-pressure synchrotron X-ray diffractions (through a cooperation with the researcher at the BSRF), one of the highest values among MAX phases. First-principles calculations confirm the elastic stiffness. These 321 phases, represented by a chemical formula $M_{n+1}A_nX$, broaden the scope of the MAX family and novel properties are expected in these new phases.

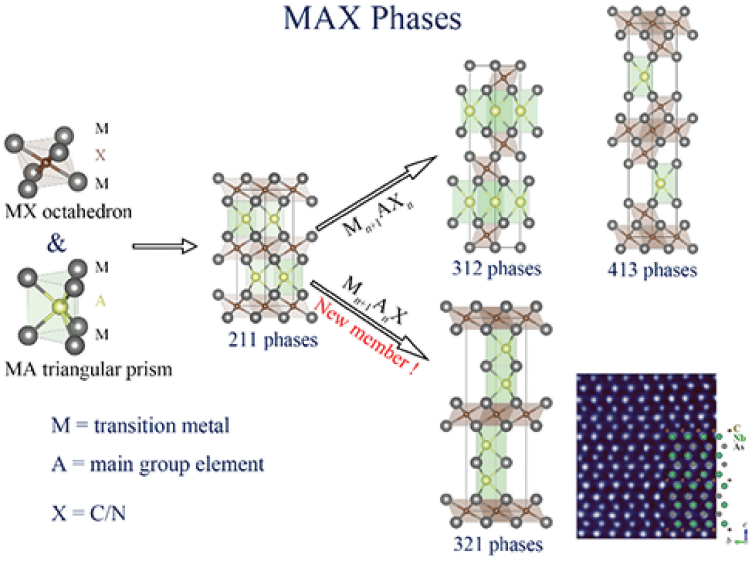

Figure The crystal structures of traditional and new $M_{n+1}AX_n$ phases.