A Genomic Approach to Study Properties of MAX Phase Compounds

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The anisotropic laminated transition metal compounds with hexagonal crystal structure called MAX phases or $M_{n+1}AX_n$ is a special class of ternary alloys having some outstanding mechanical and electronic properties [1]. They behave both like metals and ceramics which roots from its highly anisotropic crystal structure and diverse chemical composition. Depending on their unique combination of M, A, X atomic species, structural arrangement and bonding pattern, these ternary alloys possess some of the most diverse and desirable properties such as damage-tolerance, oxidation resistance, excellent thermal and electric conductivity, machinability etc. suitable for applications as advanced materials in many different technologies and under extreme conditions. So far, only about 60 such MAX phases have been confirmed.

We report a comprehensive assessment using *ab initio* methods on the elastic, mechanical and electronic properties of 792 possible MAX phases with M = Sc, Ti, Zr, H, V, Nb, Ta, Cr, Mo; A = Al, Ga, In, Tl, Si, Ge, Sn, Pb, X = C or N and n = 1-4. These crystals are then screened for mechanical and thermodynamic stability using Cauchy-Born criteria and heat of formation calculations, resulting in a large database of 665 viable crystals. All the experimentally verified MAX phases passed the screening (see **Figure 1**). Various correlations among and between them are fully explored. In particular, the key elements in the interdependence between the mechanical properties and the electronic structure are identified. We designate the Pugh modulus ratio (Shear modulus G over bulk modulus K) and the total bond order density (TBOD) as the two most relevant parameters to represent the mechanical properties and electronic structure respectively. It is shown that the distribution of K and G and the Pugh ratio covers a wide range signifying the diversity of the mechanical properties of the MAX phases (see **Figure 2**). Detailed analysis of various correlation plots shows that there is a clear correspondence between bulk modulus K and TBOD, especially with the M-A part of the TBOD even though the M-X part of the TBOD makes largest contribution and this correlation varies with n. The correlation becomes less clear for the Shear modulus G and other mechanical parameters. Sc appears to be an exception and there are marked differences between carbides and nitrides.

This large data base is also used to test the efficacy of data mining algorithm and statistical machine learning approach [2] for materials genome. It is shown that by using 50% of the data as the training set, we can predict the properties of the other 50% of the data with very

good accuracy. The TBOD is the key descriptor that controls the predictability of the materials properties in MAX phases. We further identified several thermodynamically stable new MAX phases that have never been synthesized in laboratory or theoretically investigated.

References

[1] Barsoum, M.W., *MAX Phases: Properties of Machinable Ternary Carbides and Nitrideds*. 2013: Wiley-VCH.

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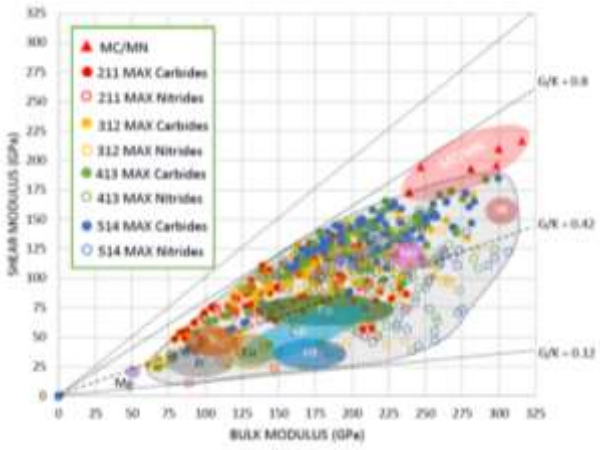

Fig.1 Bulk modulus vs shear modulus for all screened MAX phases. Solid circles for carbides and open circles for nitrides. Different color is used for different n. The locations of other metals and binary MC/MN compounds are also shown.

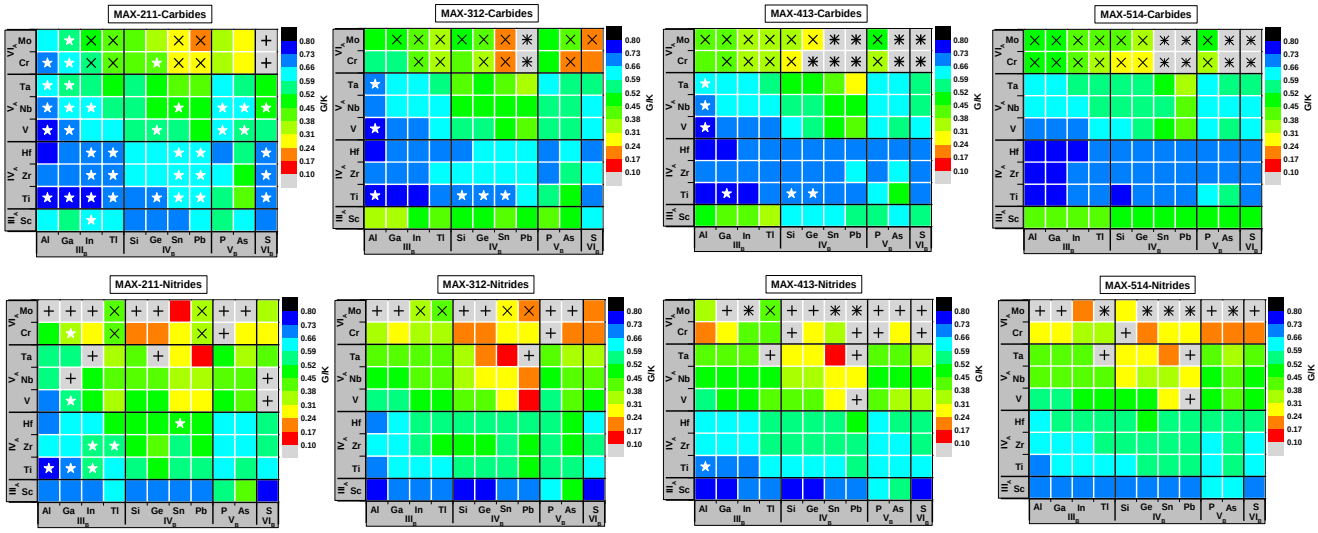

Fig.2. G/K maps for all the MAX carbides (upper) and nitrides (lower) according to M (Y-axis) and A (X-axis) elements. Color in the box represents calculated G/K values. Stars in the box indicate these phases have been synthesized. '+' stands for elastic instability and '×' indicates thermodynamic instability due to positive heat of formation.