Chemical bonding and electronic-structure in MAX phases as viewed by X-ray spectroscopy and density functional theory

Martin Magnuson, Maurizio Mattesini

PII: S0040-6090(16)30690-3
DOI: doi:10.1016/j.tsf.2016.11.005
Reference: TSF 35606

To appear in: *Thin Solid Films*

Please cite this article as: Martin Magnuson, Maurizio Mattesini, Chemical bonding and electronic-structure in MAX phases as viewed by X-ray spectroscopy and density functional theory, *Thin Solid Films* (2016), doi:10.1016/j.tsf.2016.11.005

Chemical bonding and electronic-structure in MAX phases as viewed by X-ray spectroscopy and density functional theory

Martin Magnuson[1] and Maurizio Mattesini[2,3]

[1]*Thin Film Physics Division, Department of Physics, Chemistry and Biology, IFM, Linköping University, SE-58183 Linköping, Sweden.*
[2]*Departamento de Física de la Tierra, Astronomía y Astrofísica I, Universidad Complutense de Madrid, Madrid, E-28040, Spain.*
[3]*Instituto de Geociencias (CSIC-UCM), Facultad de CC. Físicas, E-28040 Madrid, Spain.*

Abstract

This is a critical review of MAX-phase carbides and nitrides from an electronic-structure and chemical bonding perspective. This large group of nanolaminated materials is of great scientific and technological interest and exhibit a combination of metallic and ceramic features. These properties are related to the special crystal structure and bonding characteristics with alternating strong M-C bonds in high-density MC slabs, and relatively weak M-A bonds between the slabs. Here, we review the trend and relationship between the chemical bonding, conductivity, elastic and magnetic properties of the MAX phases in comparison to the parent binary MX compounds with the underlying electronic structure probed by polarized X-ray spectroscopy. Spectroscopic studies constitute important tests of the results of *state-of-the-art* electronic structure density functional theory that is extensively discussed and are generally consistent. By replacing the elements on the M, A, or X-sites in the crystal structure, the corresponding changes in the conductivity, elasticity, magnetism and other materials properties makes it possible to tailor the characteristics of this class of materials by controlling the strengths of their chemical bonds.

Keywords: Nanolaminates, chemical bonding, X-ray emission spectroscopy, electronic structure calculations, elastic and magnetic properties, Seebeck measurements

Contents