

Electronic properties of Ti-Al-C based MAX phases

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The MAX phases are the compounds comprising metals and nonmetals in a natural layered structure. They exhibit exciting physical properties which stem from a combination of covalent and metallic bonds. Their excellent mechanical properties including machineability and self-healing have already been relatively well described. However, the other basic physical properties such as the thermal and electrical conductivities, thermoelectric properties and their relation to the crystallographic order, local atomic structure, the nature and concentration of the electrical carriers, phonon properties as well as the spin and magnetic field effects are still poorly described.

Structurally, differences between the respective members of the family of MAX phases concern the number of M layers separating the A-layers: in the 211's there are two, whereas in the 321's three M-layers, Fig.1.

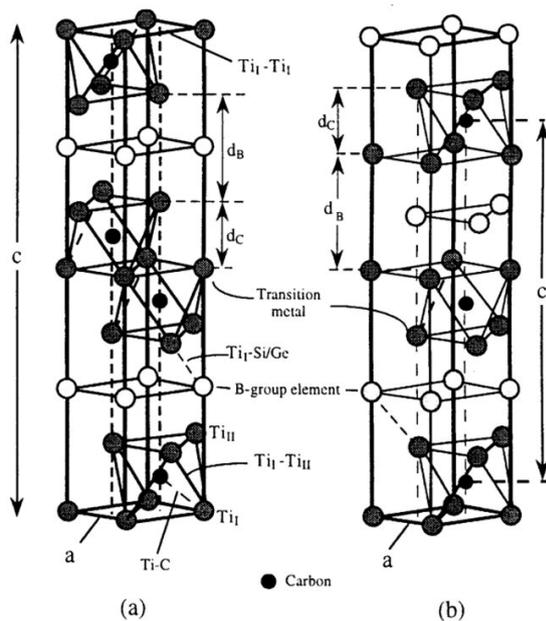


Figure 1. Structure of MAX phases compounds: a) 312 structure, b) 211 structure.

Examples of this type of structure materials are known among both naturally occurring minerals (layered silicates and aluminium silicates such as talc) and materials synthesised in technological processes, where a well-known example would be graphite or monolayered graphene form. This specific structure of MAX phases results with the features typical for structural ceramics (high bending strength and fracture toughness) combined with new set of properties, such as ductility, low hardness and, what is particularly interesting, wide spectrum of unusual properties in the field of electrical, magnetic, or heat characteristics which makes them attractive functional materials.

The aim of this work is to study the electronic properties of the Ti_2AlC and Ti_3AlC_2 , type MAX phases with XANES and band structure calculations, measurements of electrical transport and thermoelectric properties, as well as with the Raman spectroscopy.

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A Self-Propagating High-temperature Synthesis (SHS) was used to synthesize the precursor powders of polycrystalline nanolaminate materials of the Ti_2AlC and Ti_3AlC_2 groups. For the consolidation of powders an uniaxial hot pressing (HP) technique was used. The samples obtained were found to be of 95% purity MAX phases.

Measurements of the electrical resistivity of the sample of Ti_3AlC_2 show a small temperature coefficient and a considerable low temperature residual resistivity. This indicates a low mean free path of the electrical carriers due to scattering on structural defects. Measurements of Seebeck effect versus temperature and magnetic field show a change of its sign, which indicates that the character of dominant electrical carrier changes with temperature, Fig.2.

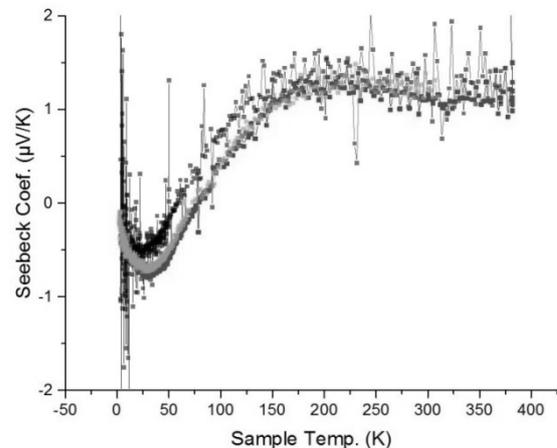


Figure 2. The temperature dependence of Seebeck coefficient of the Ti_3AlC_2 bulk sample at zero field (green symbols - cooling, red symbols - warming) and at the applied magnetic field of 8 Tesla (black symbols).

The XANES spectra have been preliminary computed using FEFF8.4 software package [6,7] – self-consistent real space multiple-scattering code for simultaneous calculations of x-ray absorption spectra and electronic structure. In Figures 3 and 4 calculated XANES spectra of carbon at the K-edge and titanium at the L_3 edge of Ti_3AlC_2 are presented. Also the spectra obtained for a vacancy in the nearest neighbor shell of the carbon and titanium are included.

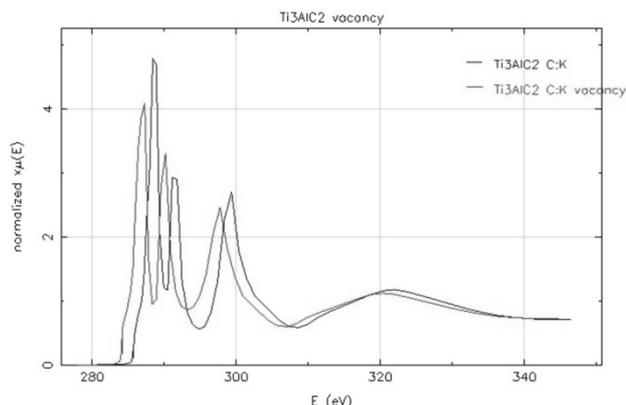


Figure 3. The calculated XANES spectra of carbon K-edge in Ti_3AlC_2 (Ti_3AlC_2 C:K) and for vacancy in the nearest neighbor shell of carbon (Ti_3AlC_2 C:K vacancy).

It is worth noting that the spectra at the carbon K-edge show a noticeable shift in the edge energy and shape with removal of one nearest neighbor to carbon from the structure. For titanium L_3 edge, L_2 edge (not shown) and also for the K edge (not shown) a minor effect is observed only.

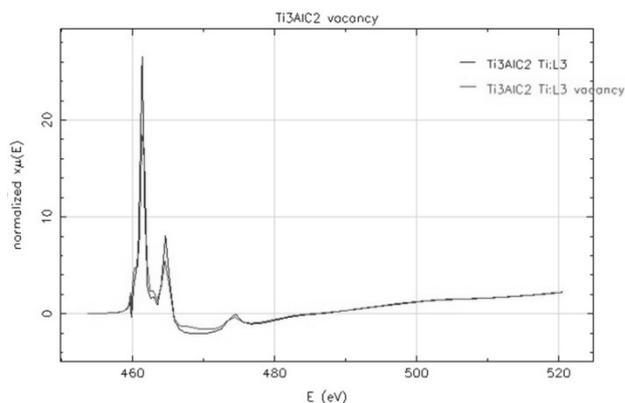


Figure 4. The calculated XANES spectra of titanium L_3 -edge in Ti_3AlC_2 (Ti_3AlC_2 Ti: L_3) and for vacancy in the nearest neighbor shell of titanium (Ti_3AlC_2 Ti: L_3 vacancy).

The results will be discussed and compared to the Raman spectroscopic study in order to elucidate vacancy, intermixing and possible carbon clustering effects as well as their impact on the electronic and thermal transport properties of the materials.

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