

XAS study of Ti-Al-C and Ti-Al-N based MAX phases

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The compounds called MAX phases comprise metals and non-metals crystallising in layered structures. Their exciting physical properties originate from the interplay of covalent and metallic bonds. They exhibit excellent mechanical properties including machineability and self-healing, which have already been broadly investigated and relatively well described. However, the other physical features, such as the thermal and electrical conductivities, thermoelectric properties and their relation to the crystallographic order, local atomic structure and electronic properties are still far from a complete description.

Structural differences between the respective members of the family of MAX phases concern the number of M layers separating the A-layers, e.g. in the 211's there are two, whereas in the 312's - three M-layers. This specific structure of MAX phases results in features typical for structural ceramics (high bending strength and fracture toughness) combined with new set of properties, such as ductility and low hardness. It also brings about unusual properties concerning their electrical, magnetic or thermal characteristics, which makes them attractive functional materials.

The aim of this work is to study the local structure and electronic properties of the Ti₂AlN and Ti₃AlC₂ MAX phase compounds with X-ray Absorption Spectroscopy (XAS) in the XANES (X-ray Absorption Near Edge Structure) and EXAFS (Extended X-ray Absorption Fine Structure) ranges. To synthesize the precursor powders of polycrystalline nanolaminate materials the Self-Propagating High-temperature Synthesis (SHS) was used. Subsequently, uniaxial hot pressing (HP) technique was used for the consolidation of powders. The samples obtained were found to be of 95% purity MAX phases.

XAS measurements have been carried out at the SuperXAS beamline of the Swiss Light Source, PSI,

Switzerland (partial fluorescence yield mode, room temperature). The spectra in the XANES range of the Ti:K-edge are shown in Fig.1.

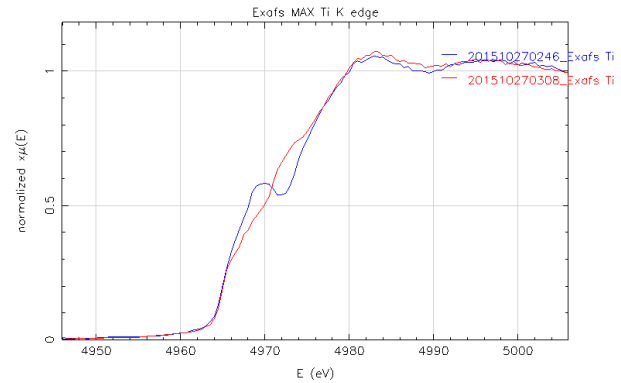


Figure 1. The XANES spectra of titanium K-edge in Ti₃AlC₂ (blue) and Ti₂AlN (red).

The EXAFS functions $\chi(R)$ obtained by Fourier transformation of the oscillations above the Ti:K-edge are shown in Fig.2.

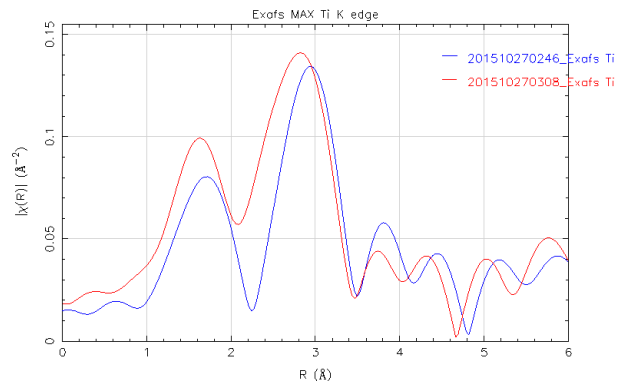


Figure 2. The EXAFS functions at titanium K-edge in Ti₃AlC₂ (blue) and Ti₂AlN (red).

The XANES spectra reveal a pronounced bump in the middle of the absorption edge of Ti₃AlC₂ (blue), whereas two smooth steps are observed there for Ti₂AlN. The EXAFS function $\chi(R)$ shows the intensity of the 1st neighbor peak (N or C) higher for Ti₂AlN than for Ti₃AlC₂ due to a higher scattering factor for nitrogen than for carbon. Also the 1st and 2nd neighbor peaks are at slightly smaller distance for Ti₂AlN. The results are compared with the simulated XAS data and discussed in terms of their relation to the electronic and thermal transport properties of the materials.

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