

Presence of Oxygen in Ti-Al-C MAX Phases-Based Materials and their Stability in Oxidizing Environment at Elevated Temperatures

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MAX-phases or nanolaminated ternary complex carbides and nitrides were firstly classified by M. W. Barsoum and can be characterized by general formula $M_{n+1}AX_n$, where $n = 1, 2$ or 3 ; M – early transition metals (in our case Ti and Nb); A – elements of A-group (in our case Al) and X is C or N. They have perovskite-like crystal structures and the most abundant stoichiometries are M_2AX (211), M_3AX_2 (312) and M_4AX_3 (413), which in fact differ by the amount of carbide or nitride layers in the unit cells separated by layers of A-group metal elements. These compounds have attracted extensive attention due to their extremely high thermal shock and mechanical damage tolerance, as well as a combination of metallic and ceramic properties. They have self-healing abilities because of oxidation. MAX-phase based materials are promising for application in different industries: power electrical, hydrogen, nuclear industries; aviation; cosmonautics; mechanical and chemical engineering, etc.

Incorporation of O was first observed in the Ti_2AlC . An initial study showed experimental indications of O substituting C while still retaining the MAX phase structure [1], suggesting O as a potential X element besides C and N. Subsequent calculations indicated that O prefers the C site under oxygen-lean conditions and high temperature [2] and that up to at least 50% of C may be replaced by O.

The testing at 600 °C for 1000 h in air of (I) Ti_3AlC_2 –based material (89 wt.% of Ti_3AlC_2 ; 6 wt.% of TiC and 5 wt.% of Al_2O_3), (II) $(Ti,Nb)_3AlC_2$ –based (60 wt.% $(Ti,Nb)_3AlC_2$, 37 wt. % TiC, 3 wt.% Al_2O_3), and (III) Ti_2AlC –based (73 wt.% Ti_2AlC , 10 wt. % $AlTi_3$, 7 wt.% TiO, 10 wt.% $Al(N,C,O)$) showed that all tested materials turned out to be more resistant in such conditions than Crofer JDA steel, but the amounts of oxygen absorbed by the materials for 1000 h were different. Material III demonstrated the lowest oxygen uptaken, material II absorbed a somewhat higher amount and the highest amount is absorbed by material I. SEM and Auger study showed that amounts of oxygen in the MAX phases before the exposure in air was as well different: main matrix phases in material I was $Ti_{3.1-3.2}AlC_{2-2.2}$, II - $Ti_{1.9-4}Nb_{0.06-0.1}AlC_{1.6-2.2}O_{0.1-1.2}$ and material III contained two main phases with near $Ti_{3.6}AlC_{1.9}O_{0.6}$ and $Ti_{2.3}AlCO_{0.2}$ stoichiometries (before the study the surfaces of the materials were etched by argon ions in the chamber of microscope JAMP-9500F to remove the oxidized layer). So, oxygen present in the MAX phases did not liberate during long-tem heating and provides higher resistance against oxidation. Material III was prepared using Al with high amount of oxides at the surface.

- [1] J. Rosen, P.O.Å. Persson, M. Ionescu, A. Kondyurin, D.R. McKenzie, and M.M.M. Bilek, Oxygen incorporation in Ti_2AlC thin films, *Appl. Phys. Lett.* **92** (2008) 064102.
[2] T. Liao, J. Wang, M. Li, and Y. Zhou, First-principles study of oxygen incorporation and migration mechanisms in Ti_2AlC , *J. Mater. Res.* **24**(10) (2009) 3190-3196.