

Impact of aluminum concentration on the synthesis of highly pure Cr₂AlC MAX phase

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Abstract

In recent years, MAX phases achieved significant attention from scientists for their promising practical applications and theoretical values. This fascinating class of materials are layered ternary carbides and nitrides having hexagonal crystal structure. MAX phases exhibit a unique combination of properties of both metals and ceramics such as high thermal and electrical conductivity, excellent machinability, good damage tolerability and superb thermal shock resistance, as compared to binary carbides and nitrides. However, the wide applicability of MAX phases restricts due to cost effective synthesis and their phase stability. In this study, we have successfully synthesized Cr₂AlC MAX phase through pressure less sintering route. The impact of aluminum content (10 – 50 mol%) on the phase formation and structural properties of Cr₂AlC has been investigated. It is observed that the purity of Cr₂AlC MAX phase can be enhanced by varying the aluminum content, even at lower temperatures (1200–1300o C), as compared to previously reported Cr₂AlC MAX phase (> 1300o C). The highly pure Cr₂AlC is obtained at 1300o C, when the aluminum content in 40 mol%. Furthermore, the crystallite size is discovered greatest (28.14 nm) and cross section strain (4.03×10^{-3}) is least for profoundly unadulterated Cr₂AlC. Additionally, oxidation active investigation is performed to gauge initiation vitality (Eg) by following Kissinger-Akahira-Sunose (KAS) technique. The MAX phase demonstrated high oxidation resistance and no mass gain is observed in the TGA curve below 700o C. In addition, two exothermic peaks are observed at ~ 700o C and ~ 1050o C. The previous pinnacle is related the oxidation of abundance aluminum present on the outside of MAX stage. While later pinnacle speaks to the arrangement of Al₂O₃ layer over the surface MAX stage. MAX phases have attracted a lot of interest in the last years due to their unique combination of properties, bridging the gap between ceramics and metals. Among this large family of materials, with more than 70 different compositions and a huge number of solid solutions, Al-based MAX phases show the best performance to operate under high temperature (>1000°C) and aggressive environments. They combine the good properties of conventional MAX phases such as high elastic modulus, low density, high thermal and electrical conductivities, excellent thermal shock resistance and damage tolerance, with an outstanding oxidation resistance through the in situ formation of protective alumina scales up to 1300°C-1400°C. Furthermore, they show self-healing mechanisms at high temperatures under oxidizing environments. Among Al-based MAX phases, Cr₂AlC, Ti₂AlC, Ti₃AlC₂, Ti₂AlN, and Ti₃AlN₂ are the most well-studied and oxidation-resistant compositions. Based on these features, Al-based MAX phases are considered as potential candidates to increase the operating temperature, and consequently the efficiency, of turbine engines. The use of MAX phases might increase the performance of blades, vanes, shrouds, combustor

liners or other components in the hottest section of a gas turbine, either as bulk structural materials or as coatings. Even though most of the investigation has been focused on MAX phases as bulk component, coatings as protective material against oxidation and corrosion have gained considerable interest in the last years. For example, advanced turbine disks can be protected against Type I and II of low-temperature hot salt corrosion (LTHC). Cr₂AlC thin films have been deposited by high power impulse magnetron sputtering on a low γ 'solvus and a high refractory content alloy, named "LSHR" and developed at NASA Glenn Research Center. Cr₂AlC coatings with thicknesses of 25-30 μm prevented hot corrosion pitting, improving up to 90% the low cycle fatigue. Another interesting approach based on MAX phase coatings is to use them as bond coats for thermal barrier coating systems (TBCs) in gas turbines. The concept is feasible, although unfortunately it has not been reported up to know to the best of the authors' knowledge. Briefly, these systems are composed by different layers: an external TBC, an intermediate bond coat, a thermally grown oxide (TGO), and a substrate. TBC materials are oxides, such as YSZ, with low thermal conductivity, high porosity to be strain tolerant, and thickness about 500 μm . Its main functionality is to reduce the temperature that the substrate has to withstand. Bond coats are dense layers, typically based on MCrAlY (M = Co and/or Ni) or Pt-aluminide (Pt-Al) compositions with thickness around 100 μm . Bond coats are needed to protect the substrate against oxidation and corrosion, and to act as a bond between the substrate and the TBC. During the exposure of a TBC system at high temperature, a TGO layer grows between the bond coat and the TBC. This oxide layer should be dense, uniform, and chemically stable. The most preferred material is α -Al₂O₃ because it is thermodynamically stable and has low oxygen diffusivity. Finally, substrates are typically a Ni-base superalloy such as Rene'N5 or Inconel. As mentioned above, Al-based MAX phases present large potential as bond coat for different reasons. They can operate under aggressive environments at temperature up to 1300°C-1400°C³, which is around 100°C-200°C higher than the current bond coat materials. Bulk Al-MAX phases form also a dense, stable, and well-adhered α -Al₂O₃ layer. Probably the most attractive aim to use MAX phases as bond coat is the coefficient of thermal expansion (CTE) match with the surrounding materials. One of the main failures of TBC systems is caused by the thermal-expansion mismatch of stresses between the different layers. For example, CTEs of YSZ (TBC), Al₂O₃ (TGO), and Inconel738 superalloy are approximately $11 \times 10^{-6} \text{ K}^{-1}$, $9.3 \times 10^{-6} \text{ K}^{-1}$, and $16 \times 10^{-6} \text{ K}^{-1}$, respectively. NiCoCrAlY (bond coat) presents a CTE of around $17.5 \times 10^{-6} \text{ K}^{-1}$ depending on the exact composition, which generates a high stress. Replacing NiCoCrAlY by Cr₂AlC, which has a CTE of $13 \times 10^{-6} \text{ K}^{-1}$,¹⁸ might reduce the stress.

Finally, the self-healing capability at high temperature of Al-based MAX phases may play an important role in case of a crack penetrating into the bond of coat layer. Nevertheless, one of

the potential drawbacks for using MAX phases as bond coat is the inner diffusion of the metallic elements from the superalloy substrate.