

Experimental and thermodynamic modelling of Al₂O₃ corundum and TiO₂ rutile structures forming on Ti-6Al-4V (TA6V) powder during oxidation

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Metallic additive manufacturing processes such as Laser Powder Bed Fusion (L-PBF) or Electron Beam Melting (EBM) are innovative developing technologies that are used for the fabrication of intricate metallic components in a relatively short timeframe. Ideally, these techniques are based on the local melting of metallic powder in a non-reactive atmosphere. Despite the intensive efforts that have been employed to control the chamber atmosphere, gaseous impurities such as dioxygen are still present. For example, the residual oxygen level is often as high as 1000 ppm using L-PBF [1]. This relatively high dioxygen partial pressure is sufficient to oxidize the metallic powder, especially if the alloy is highly reactive with oxygen.

TA6V is an extensively used alloy in additive manufacturing process for several aeronautical and biomedical applications. In this process, a minimal amount of TA6V powder is used for the final work piece, and the remaining powder loses its chemical and rheological properties. This aftermath may be the result of the interaction between the powder and the existing gaseous environment (dioxygen, humidity). Arafat et al. [2] found that the oxidation of TA6V powder under 15 ppm of dioxygen (oxygen concentration less than that present in a typical additive manufacturing chamber) at 750°C leads to the formation of a double oxide layer consisting of an inner layer of rutile TiO₂ and an outer layer consisting of a mixture of corundum α -Al₂O₃ and rutile TiO₂. It is important to note that the corrosion of TA6V alloy has been extensively studied in the literature for bulk material, especially regarding high temperature oxidation [3]. Generally, the main objective of all these studies is to investigate the corrosion products under several conditions, such as temperature, but until now there is no reactional mechanism that can explain the transport of the elements (point defects) in this duplex oxide presented previously. The unavailability of a complete explanation for this reactional mechanism can be attributed to the complex structure of α -Al₂O₃ and the diffusion of aluminum into TiO₂ rutile. Moreover, few kinetic studies have been carried out on powder and no rate law have been determined for such a geometry.

So, the main objective of this study is to go deeper in understanding the transport mechanism of Al³⁺ in TiO₂ and the defect structure of α -Al₂O₃ by taking into account the effect of the variations in temperature and in oxygen partial pressure on the dopant concentrations. The inert marker method revealed the anionic growth of the duplex oxide scale. The thermodynamic results highlighted that interstitial aluminum enters and diffuses fast within TiO₂ to form Al₂O₃ as the surface layer. Moreover, α -Al₂O₃ is shown to be a non-stoichiometric oxide with a very small excess of oxygen as dumbbells at high partial pressures of oxygen. A remarkable effect of the impurities on the concentration of native point defects is observed in this phase. Finally, a reactional mechanism with elementary steps for the oxidation of TA6V powder is proposed and solved to express the oxidation rate law.

References

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