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Improving the adherence of Thermal Barrier Coatings, thereby increasing the serviceable lifetime of coated components, is of paramount importance within the field of superalloys today. The main focus of this research is to characterise the behavior of titanium, an alloying element used in nickel based superalloys for its low density and $L1_2$ precipitate strengthening characteristics. Titanium forms rutile (TiO_2) at elevated temperatures, which is highly thermodynamically stable. It is not currently known how detrimental rutile formation is regarding alumina and TBC spallation and whether its formation is consistent between different TBC systems. These are the questions that we have endeavored to answer and in doing so, provide manufacturers with some insight into whether titanium removal from blades is warranted or not.

This research focuses on analysing the interaction between three commercially used diffusion coatings and a nickel based superalloy CMSX-4. The coatings applied are alumide, Pt-alumide and Pt-modifed γ/γ′. The research has two main themes, firstly diffusion and secondly oxidation. Results of quantitative EPMA show that titanium diffusion towards the surface varies between coatings, and has a strong correlation with the use of platinum within coatings. The concentrations of Ti within Pt-aluminide coatings after 100 hours oxidation in air at 1100°C were found to be twice as high as those within the plain aluminised CMSX-4 samples. Furthermore uphill diffusion of Ti was observed to occur within Pt-modifed γ/γ′ after the same exposure. In order to examine the effect of platinum additions on the diffusive behavior of titanium, first principle calculations using the density functional theory implementation CASTEP have been performed. In an ordered lattice structure, diffusion of a solute species must occur via the presence of defects, either anti-site (Ni_{Al}) or vacancy (V_{Ni}). Moreover clustering of these defects leads to increased opportunities for solute diffusion and hence increased diffusion rates within that structure. We have shown that the use of Pt strengthens defect formation and defect clustering within the Ni_3Al $L1_2$ phase. By increasing the amount of defect clusters Ti can diffuse more freely from the substrate through the coating to the surface.

By using XRD and EPMA mapping techniques we have shown that during both cyclic and isothermal oxidation in air at 1100°C, rutile particles form throughout the alumina scale. Rutile formation occurs for all three coating types although predominantly within plain aluminide coatings for reasons currently unknown. We have hypothesised that the use of Pt also decreases the porosity of the alumina scale, making it more difficult for the outwardly diffusing Ti to oxidise. Further analysis of these particles by precession TEM diffraction has helped to establish whether there is an orientation relationship between the rutile particles and the alumina matrix. By using Raman spectroscopic mapping, it has also been possible to obtain luminescence and Raman spectra over the same region of an oxidised specimen of Pt coated CMSX-4. By measuring the Cr^{3+} R-line peak shift in α-Al_2O_3 and rutile Raman signal, both TGO residual stress and rutile have been mapped for the same region. The formation of rutile increases the residual compressive stress for the surrounding region.

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