

The Effect of Platinum on Al Diffusion Kinetics in NiAl

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Thermal barrier coatings (TBCs) are applied to jet engine components to provide protection from the high operating temperatures of the engine. TBCs have three layers: a NiAl bond coat (BC), a yttria-stabilized zirconia (YSZ) topcoat, and a thermally grown oxide (TGO), $\alpha\text{-Al}_2\text{O}_3$, which forms between the BC and YSZ. While experiments have determined that adding platinum to the BC increases the lifetime of the coating, the reasons behind this beneficial effect remain ambiguous. One proposal is that Pt affects diffusivities in the BC. TBCs are constantly evolving at the high operating temperatures in the engine; for example, Al is diffusing through the bond coat to the BC/TGO interface to form the TGO. Since the atomic level mechanisms of diffusion cannot be studied *in situ*, we use density functional theory calculations to examine proposed mechanisms of diffusion in NiAl. We have characterized the diffusion pathways of Al in NiAl and determined that the triple defect mechanism and next-nearest-neighbor Al jumps are likely the dominant mechanisms for Al diffusion. Pt increases the rate of Al diffusion in NiAl by promoting the formation of defect clusters involved in the diffusion mechanisms. By lowering the formation energy of defects, Pt decreases the overall activation energy of diffusion, which contains in it the defect formation energy. Increasing the rate of Al diffusion may increase the levels of Al at the BC/TGO interface thereby preventing the formation of brittle, fast-growing Ni-rich oxides.