

## AN ANALYTICAL MODEL OF OXIDE RUMPLING AS THE MECHANISM LEADING TO FAILURE IN THERMAL BARRIER COATINGS

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*Summary* A model providing an analytical approximation of undulation growth in the oxide layer of a multi-layer thermal barrier coating incorporating most of the important details is presented for a realistic cyclic thermal history; thickening, yield and lateral growth within the oxide layer are included, and creep in the metallic bond-coat and ceramic top-coat is modeled using a power-law description. Common observations are explained and the connection between rumpling and fracture in the top-coat is elucidated.

### INTRODUCTION

Ceramic films with low thermal conductivity are used to protect internally cooled machine components from the extreme temperatures of their surroundings by establishing a thermal gradient across the coating that can lower the temperature of the underlying substrate by several hundred degrees. Perhaps the most important application of thermal barrier coatings at present is on the blades in turbine engines used for aircraft and power generation. Internal temperatures can be well in excess of 1000 °C. A thermal barrier system consists of four layers. The ceramic top-coat is typically zirconia and 100-200  $\mu\text{m}$  thick. Beneath the top-coat is a metallic bonding layer that is attached to a thick superalloy substrate. The bond-coat is roughly 50  $\mu\text{m}$  thick and is usually PtNiAl or FeCrAl. At elevated temperatures a film of aluminum oxide forms between the bond-coat and the zirconia top-coat that is several  $\mu\text{m}$  thick and acts as a barrier that prevents oxidation of the superalloy substrate. The bond-coat and porous ceramic top-coat creep easily at temperatures in excess of 600 °C. Both layers are modeled at elevated temperatures as power-law creeping materials. The oxide is modeled as elastic at temperatures below 1150 °C and elastic/perfectly-plastic at 1150 °C based on recent high-temperature indentation data. In addition, thickening and growth within the oxide layer are incorporated that drive changes in the oxide stress.

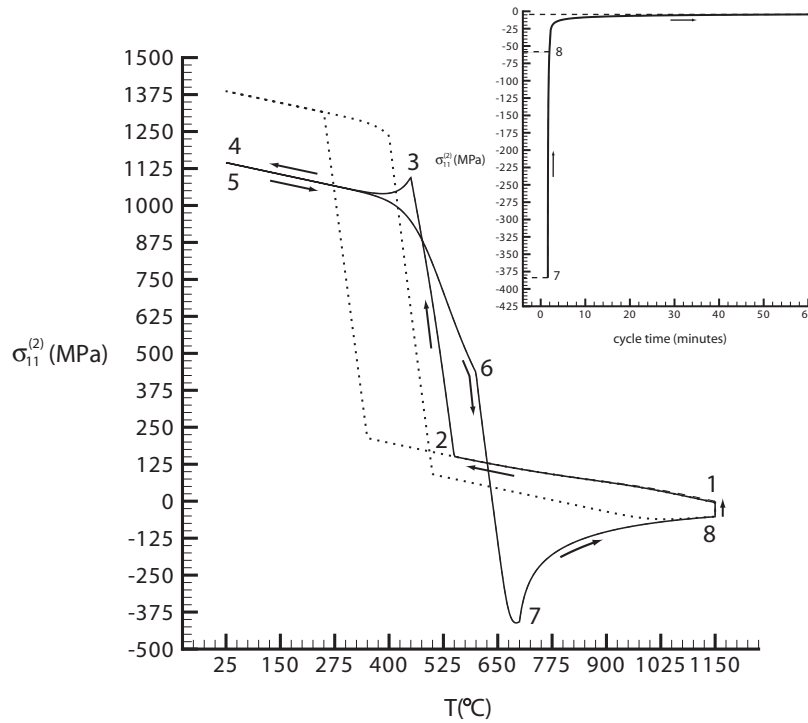
It is becoming increasingly clear that development of undulations in the oxide layer, otherwise known as oxide rumpling, and the stresses they induce in the ceramic top-coat and on the oxide/bond-coat interface are perhaps the main factors affecting the lifetime of thermal barrier coatings. At the present time, no comprehensive understanding exists of the mechanics of rumpling, and a model that captures the behavior of both PtNiAl and FeCrAl systems is lacking. A model providing an analytical approximation of undulation growth in the oxide layer of a complete four-layer thermal barrier system, incorporating most of the important details, is presented for a full cyclic thermal history.

### RESULTS AND CONCLUSIONS

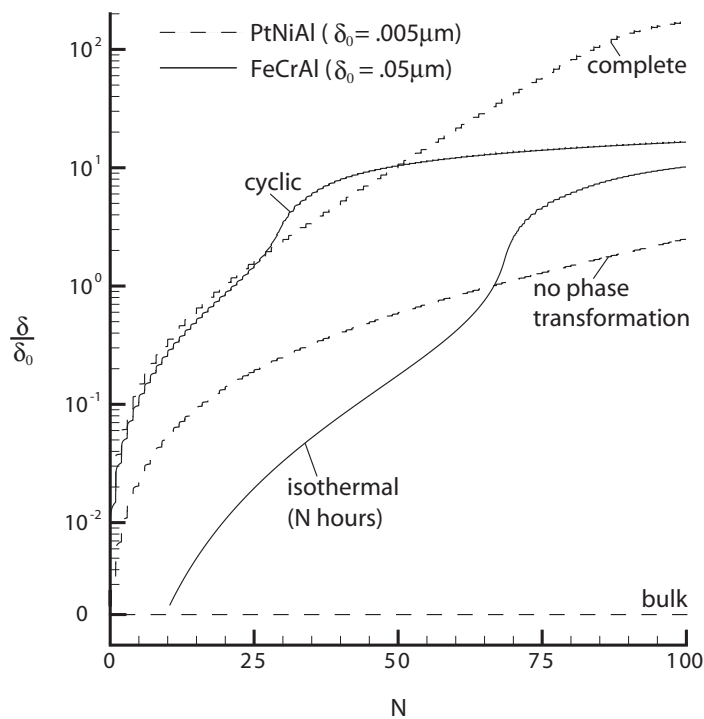
Details of rumpling as predicted by the model depend on the bond-coat material. In all cases, rumpling driven by a compressed, undulating oxide film relies upon the highly nonlinear power-law creep behavior of the bond-coat. Results suggest that the differences between PtNiAl and FeCrAl that are most relevant to rumpling are that PtNiAl experiences a large mismatch strain when the system is cycled, whereas FeCrAl does not (c.f. Fig. 1). For appreciable undulation growth to occur, the model requires amplitudes of undulations in FeCrAl systems prior to thermal cycling to be approximately an order of magnitude larger than they are in PtNiAl systems. In addition, the yield stress of oxide grown on FeCrAl is roughly 3 times larger than for PtNiAl, which leads to a higher driving force for undulation growth. Both systems are predicted to rumple appreciably upon thermal cycling with FeCrAl also rumpling under isothermal conditions, consistent with observations (c.f. Fig. 2).

The mechanics underlying rumpling differs between the two systems. PtNiAl has a relatively large mismatch with the substrate, i.e. the equi-biaxial stress in the bond-coat is essential (c.f. Fig. 1). The change in volume that accompanies the reversible phase transformation in PtNiAl is critical, as it is the primary cause of large bi-axial stress in the bond-coat. An undulation with an amplitude of 5 nm in a PtNiAl system can grow by nearly 1  $\mu\text{m}$  in 100 cycles. Any perturbation in the surface of a PtNiAl bond-coat is highly unstable. Thus, controlling the bond-coat stress appears to be the most feasible way to suppress rumpling in PtNiAl systems. Modifying the phase transformation by shifting the hysteresis to lower temperatures, which decreases the stress in the bond-coat at elevated temperatures (c.f. Fig. 1), can dramatically reduce rumpling; a shift of  $-200$  °C reduces total undulation growth by 90%. This is a potentially viable way to modify the design of PtNiAl thermal barrier coatings for longer lifetimes.

FeCrAl systems have little or no mismatch with the substrate. Thus, bond-coat equi-biaxial stress does not play a major role in FeCrAl rumpling. The normal traction at the interface between bond-coat and oxide controls rumpling in FeCrAl systems. Much less rumpling would occur if the initial undulations were comparable in size to those in PtNiAl systems. Decreasing the initial amplitudes, which seems feasible, would be sufficient to effectively suppress growth in FeCrAl systems; this is not true of PtNiAl. The model predicts that the difference between cyclic and isothermal rumpling for FeCrAl systems is not nearly as large as in PtNiAl systems, which is consistent with experimental observations (c.f. Fig. 2).



**Figure 1.** The equi-biaxial stress cycle in a PtNiAl bond-coat when subjected to a typical cyclic thermal history. Most of the total undulation growth per cycle occurs between points 7 and 1, when the creep strength is low and the stress is large (c.f. inset). Although the stress is relatively small at point 8, approximately -60 MPa, the creep strength of the bond-coat is sufficiently small to allow further undulation growth to occur during the 1-hour isothermal period that lasts from point 8 to point 1. The dotted line shows the stress cycle for a modified phase transformation; the hysteresis of the phase transformation is shifted by  $-200^{\circ}\text{C}$ .



**Figure 2.** Shown here: 1) no undulation growth occurs on oxidized bulk PtNiAl (i.e. not attached to a thick substrate) 2) the phase transformation leads to much more undulation growth in PtNiAl systems ( $\delta_{N=100} = .875 \mu\text{m}$  with the transformation included,  $\delta_{N=100} = .0125 \mu\text{m}$  without it) 3) significant undulation growth ( $\delta_{N=100} = .75 \mu\text{m}$ ) can occur on FeCrAl despite having little or no mismatch with the substrate because the initial undulations are larger than PtNiAl and the oxide yield stress is higher 4) there is little difference between cyclic and isothermal histories for FeCrAl, i.e. significant undulation growth can occur for FeCrAl under isothermal conditions ( $\delta_{N=100} = .5 \mu\text{m}$ ).