Stress development during bond coat oxidation

The generation of stresses in polycrystalline oxide films formed via the oxidation of a substrate is analyzed using a new continuum model. The model includes a description of the polycrystalline microstructure in two dimensions. The diffusion of all independent components, the rate of the oxidation reaction and the effect of stresses on these are accounted for in a thermodynamically self-consistent manner. Grain boundaries serve both as high diffusivity paths and as sites for new oxide formation. Different diffusion controlled oxidation regimes (rapid cation / oxygen diffusion, comparable cation / oxygen diffusivities) and different grain boundary / bulk diffusivity ratios are examined within this framework. A homogenized 1-D treatment captures the correct signs of stresses and through-thickness stress gradients observed in experiments. Numerical solutions of the 2-D polycrystalline situation reveal large lateral stress gradients, with stresses concentrated around the grain boundaries. While the average in-plane stress is compressive and the stress at the film/substrate interface near the grain boundary highly so, large tensile stresses are observed near the grain boundary at the film surface. The grain boundary diffusivity has a significant effect on the stress gradients, with larger diffusivities leading to smaller stress gradients. We also present analytical approximations for the stress distribution in the film that capture the essential features of the numerical results. The predictions are compared with experimental measurements/observations of stresses and stress gradients in oxide scales. The implications of these results for understanding the fundamental nature of the self-stresses generated during bond coat oxidation and in other oxides are discussed.