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Sintering and microstructure evolution in columnar thermal barrier coatings

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Abstract

Sintering of thermal barrier coatings changes their key properties, such as thermal conductivity and thermal shock resistance, thus adversely impacting their reliability. We present a novel modeling approach to study the evolution of coating structure during sintering. We model the sintering of individual columns using a thermodynamic principle, and incorporate the center-to-center approach rates for the columns calculated using this principle in a larger scale discrete dynamics model for the evolution of a large number of columns. Surface energies, grain boundary energies and strain energies associated with the deformation of the columns are all included in this framework, while sintering is assumed to occur by the concerted action of surface and grain boundary diffusion. Two sets of initial conditions corresponding to different extents of pre-sintering among neighboring columns are considered. When the extent of pre-sintering is small, we observe that small clusters containing 5–20 columns are formed. In contrast, where a larger amount of pre-sintering exists, we observe, especially at large column densities, that clusters containing 50–100 columns separated by large inter-cluster pores/channels that appear to organize themselves into a network are formed. These observations are in good agreement with recently published experimental observations. We also explain how these results can explain the development of a "mud-crack"-like pattern.

Keywords: Kinetics self-organization and patterning; Thermal barrier coatings; Sintering; Non-equilibrium processes; Micromechanical modeling

1. Introduction

Thermal barrier coatings enable the operation of aircraft engines and industrial gas-turbine engines at gas temperatures close to the melting point of the engine material [1]. Higher gas temperatures imply higher efficiency engines. A typical thermal barrier coating system (TBC) consists of four integral parts: an yttria-stabilized zirconia (YSZ) topcoat, a thin layer of thermally grown oxide (TGO), an alloy bondcoat and a superalloy substrate (see Fig. 1). The YSZ topcoat has a low thermal conductivity, thus enabling it to sustain large thermal gradients. Consequently, the superalloy can be maintained at a considerably lower temperature than the gas. The bondcoat provides adhesion between the ceramic topcoat and the superalloy substrate, and oxidizes to produce alumina, which protects the superalloy from oxidation. High temperature oxidation of the bondcoat produces the TGO.

The YSZ topcoat is 100–500 μm thick and is routinely deposited by air-plasma spray deposition (APS) or electron beam physical vapor deposition (EBPVD). The APS coatings have a nearly equiaxial, "splat" grain microstructure; the "inter-splat" cracks and porosity make the coating strain-tolerant. EBPVD coatings, on the other hand, have a columnar microstructure, with columns that are 5–20 μm thick and 100–200 μm tall. In the as-produced form, the EBPVD columns are predominantly separated from one another/have pore channels normal to the bondcoat–topcoat interface. This is responsible for the topcoat's high

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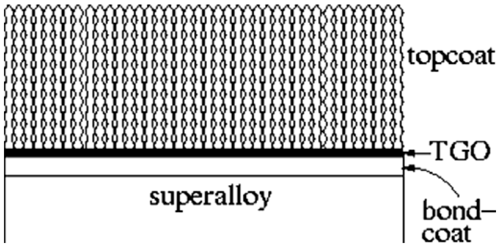

Fig. 1. A schematic of a typical thermal barrier coating system with an EBPVD topcoat.

thermal shock resistance. Fine, nanometer-scale, porosity is also found within the columns. The porosity and cracks in these coatings render the effective thermal conductivity significantly lower than the intrinsic conductivity of the coating. The EBPVD coatings have a comparatively smooth as-deposited coating–substrate interface and higher resistance to interface failure than do the APS coatings, and are preferred for demanding applications, such as aircraft engine turbines [1]. This study will focus on EBPVD topcoat microstructures.

Several mechanisms may contribute to the delamination and spallation of thermal barrier coatings. Among these, probably the most important is interface delamination (at the bondcoat/topcoat or superalloy/bondcoat interfaces) driven by the concerted action of stresses generated in the TGO due to thermal expansion, oxide growth and thermal cycling, and the interaction of these stresses with interface imperfections [2]. Other possible mechanisms include the formation of brittle spinel phases associated with Al depletion from the bondcoat, foreign body impact, erosion of the topcoat and, in the case of very high temperature operation, attack by molten siliceous dust ingested from the turbine environment [1,3]. Which coating failure mechanism dominates depends upon the specific materials chosen for the different layers of the TBC. For example, interface delamination and failure driven by the elongation of the TGO as it thickens are commonly observed in TBC systems containing an EBPVD topcoat and a Pt-aluminide bondcoat. In contrast, crack formation in the coating in TBC systems containing a two-phase (β, γ') NiCrAlY bondcoat is believed to be initiated at foreign oxide “pegs” formed at the bondcoat/TGO interface. The compressive stress generated in the TGO during oxide growth can also vary widely depending upon the bondcoat material; for example, this stress is 1000 ± 100 MPa for FeCrAlY bondcoats and 50 ± 50 MPa for NiCoCrAlY bondcoats (growth stresses are insignificant in the latter case).

Phase and microstructure changes that occur in the topcoat in-service alter its key properties, such as thermal conductivity and strain tolerance, and can accelerate the failure of the coating system via any of the mechanisms discussed above. For example, the transformation of tetragonal YSZ to a monoclinic allotrope (with its accompanying volume change) can lead to topcoat cracking [4]. Sintering of the topcoat columns also occurs at turbine operating temperatures, leading to an increase in the in-plane stiffness of the coating and an accompanying loss in compliance [5]. Sintering also increases the effective thermal conductivity of the topcoat. This results in a higher temperature at the bondcoat surface with accompanying enhancements in bondcoat oxidation and creep [1]. This has adverse implications for coating life, since stresses generated as a result of bondcoat oxidation are the principal drivers of interface delamination. Sintering can also result in an increased propensity for the topcoat to develop through-thickness cracks [4]. Sintering can also lead to an increase in the width of some of the pore channels, thus enhancing the possibility that hot, molten siliceous material comes into contact with the superalloy. Differential sintering along the thickness of the coating can lead to gradients in the elastic modulus of the coating, which could initiate cracks parallel to the surface.

The above discussion illustrates the effect of topcoat sintering on thermal barrier coating reliability and failure. While earlier studies have examined the effect of sintering on the properties of the topcoat, only recently has there been a concerted effort to understand the mechanisms underlying topcoat sintering and the associated changes in coating microstructure [4–6]. Such understanding is essential to correlate sintering-related changes in the topcoat to coating failure. Recently, Lughi et al. [6] performed a series of experiments that investigate the microstructural changes accompanying topcoat sintering. They found that isothermal exposure to turbine operating temperatures leads to topcoat densification; primarily by sintering between undulations along the column length on neighboring columns (see Fig. 1). These undulations form at relatively short times via diffusional smoothing of the characteristic “feathery” structure of the as-deposited coating. They also found that sintering resulted in the formation of clusters containing multiple columns with intercluster pore channels separating the clusters. In the case where the topcoat was deposited on a superalloy substrate, the clusters organized themselves in patterns reminiscent of “mud-cracking”. Closer examination of these “mud-cracks” revealed that they were similar to other inter-cluster channels, with the exception that the channels associated with the mud-cracks were wider.

In this study, we examine how multiple-column clusters form during the sintering of the undulations on neighboring column surfaces. We also examine how these clusters organize into the pattern discussed above. We develop a two-level modeling approach to address this problem. At the microscopic level, we examine the sintering of individual column pairs by neck formation and coalescence between undulations along the surfaces of neighboring column pairs. At the macroscopic level, we examine the coating densification and cluster formation that results from the interaction of a large number of discrete columns. At this level of description, we neglect the sintering of individual undulations and replace it with a pairwise column interaction from the microscopic level. The displacement of