journal

J. Am. Ceram. Soc., **82** [4] 1073–75 (1999)

Effects of Interface Roughness on Residual Stresses in Thermal Barrier Coatings

Chun-Hway Hsueh,[*,†] James A. Haynes,[†] Michael J. Lance,[*,†,‡] Paul F. Becher,[*,†] Mattison K. Ferber,[*,†] Edwin R. Fuller, Jr.,[*,§] Stephen A. Langer,[§] W. Craig Carter,[*,§,¶] and W. Roger Cannon[*,‡]

Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831–6068; Department of Ceramics and Materials Engineering, Rutgers University, Piscataway, New Jersey 08855; and National Institute of Standards and Technology, Gaithersburg, Maryland 20899

Using a newly developed object-oriented finite-element analysis method, both an actual microstructure and model microstructures of a plasma-sprayed thermal barrier coating system were numerically simulated to analyze the full-field residual stresses of this coating system. Residual stresses in the actual microstructure were influenced by both the irregular top-coat/bond-coat interface and cracks in the top coat. By treating the microcracked top coat as a more-compliant solid microstructure, the effects of the irregular interface on residual stresses were examined. These results then could be compared to results that have been obtained by analyzing a model microstructure with a sinusoidal interface, which has been considered by some earlier investigators.

I. Introduction

CERAMIC thermal barrier coatings (TBCs) are commonly used to protect air-cooled superalloy hardware in the hot sections of gas-turbine engines, by reducing the surface temperatures of these components.[1–3] A typical plasma-sprayed TBC system consists of an oxidation-resistant metallic bond coat overlaid with a porous, thermally insulating ceramic top coat. Thermal-cycling experiments on plasma-sprayed TBC systems have shown that failure results from cracking and delamination of the top coat parallel to and near the interface. It is generally agreed that a rough bond coat surface can increase the lifetime of a typical plasma-sprayed TBC system during thermal cycling in a turbine engine. It has been commonly assumed that the roughness of the bond coat provides mechanical interlocking at the interface between the top coat and the bond coat. However, a recent theoretical analysis[4] showed that periodic undulations of the surface of the bond coat can provide oscillatory energy-release rates that cause cracking in the top coat to be arrested locally, which, in turn, prevents or postpones TBC spallation.

The purpose of the present study was to examine the effects of interface asperities on the residual-stress distributions in plasma-sprayed TBC systems. To achieve this objective, a recently developed object-oriented finite-element analysis (OOF)[5] method was used. OOF is designed to be used on microstructural images; thus, it incorporates the actual microstructure and interface geometry. Using an actual cross-sectional microstructure of a plasma-sprayed TBC system, the full-field residual stresses were analyzed. To examine the effects of interface asperities on residual-stress distributions, OOF also was performed on the actual microstructure, with the cracks removed, and a model microstructure with a sinusoidal interface.

II. The TBC System

The TBC system in this study consisted of an air-plasma-sprayed (APS) 8-wt%-Y_2O_3 partially stabilized ZrO_2 (YSZ) top coat that was deposited onto a vacuum-plasma-sprayed Ni-22Cr-10A1-1Y bond coat. The NiCrAlY bond coat was fabricated in a manner that induced significant surface roughness (R_A) (on the order of 14.2 μm). Deposition conditions have been reported elsewhere.[2] The substrate was a disk (2.2 cm in diameter) of single-crystal nickel-based superalloy (René N5, provided by GE Aircraft Engines, Cincinnati, OH). The thicknesses of the top coat, bond coat, and substrate were ~200 μm, ~125 μm, and ~3.175 mm, respectively. The specimen was subjected to 270 thermal cycles (~75% of its lifetime).[2] Each cycle consisted of a 15 min ramp to 1150°C, a 60 min isothermal hold, and 15 min forced-air cooling to ~25°C.

During high-temperature exposure, a thin oxide scale (predominantly α-Al_2O_3) formed along the irregular top-coat/bond-coat interface. A typical cross section of this specimen after thermal cycling is shown in Fig. 1(a), in which the dark-contrast oxide scale (thickness of ~5 μm) is visible. Large asperities were present along the interface, and numerous cracks were present within both the top coat and the oxide scale. The majority of cracks in the top coat were parallel to and near the interface, as has been observed previously.[6] The cracks in the oxide scale were predominately located on the convex portions of the interface asperities. Also, the oxide scale was typically thicker on the convex bond-coat surfaces, with some localized regions being as thick as 20 μm.

III. Numerical Simulations

Residual stresses exist in TBC systems because of the thermal mismatch strain and the oxidation strain. OOF, which uses a two-dimensional uniform grid (each grid consists of two triangular elements), was used to model the residual stresses. The thermal/mechanical properties used in the analysis are listed in Table I.[1,7] The temperature change used in calculating the thermal strain was −1125°C. Plastic deformation and creep deformation of the constituents were not considered in this analysis. However, creep of the top coat and the bond coat has been included in a recent finite-element model.[8]

An exact determination of the Young's modulus for the porous, microcracked ceramic top coat is difficult. The Young's modulus of a dense YSZ is ~200 GPa; however, Young's moduli of 5–50 GPa have been reported for free-standing deposits of APS YSZ.[7] In the present numerical simulation, a

A. G. Evans—contributing editor

Manuscript No. 190274. Received April 6, 1998; approved January 28, 1999.
Sponsored primarily by the U.S. Department of Energy, Division of Materials Sciences, Office of Basic Energy Sciences, under Contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.

[*]Member, American Ceramic Society.
[†]Oak Ridge National Laboratory.
[‡]Department of Ceramics and Materials Engineering, Rutgers University.
[§]National Institute of Standards and Technology.
[¶]Presently at Massachusetts Institute of Technology, Cambridge, MA 02139–4307.

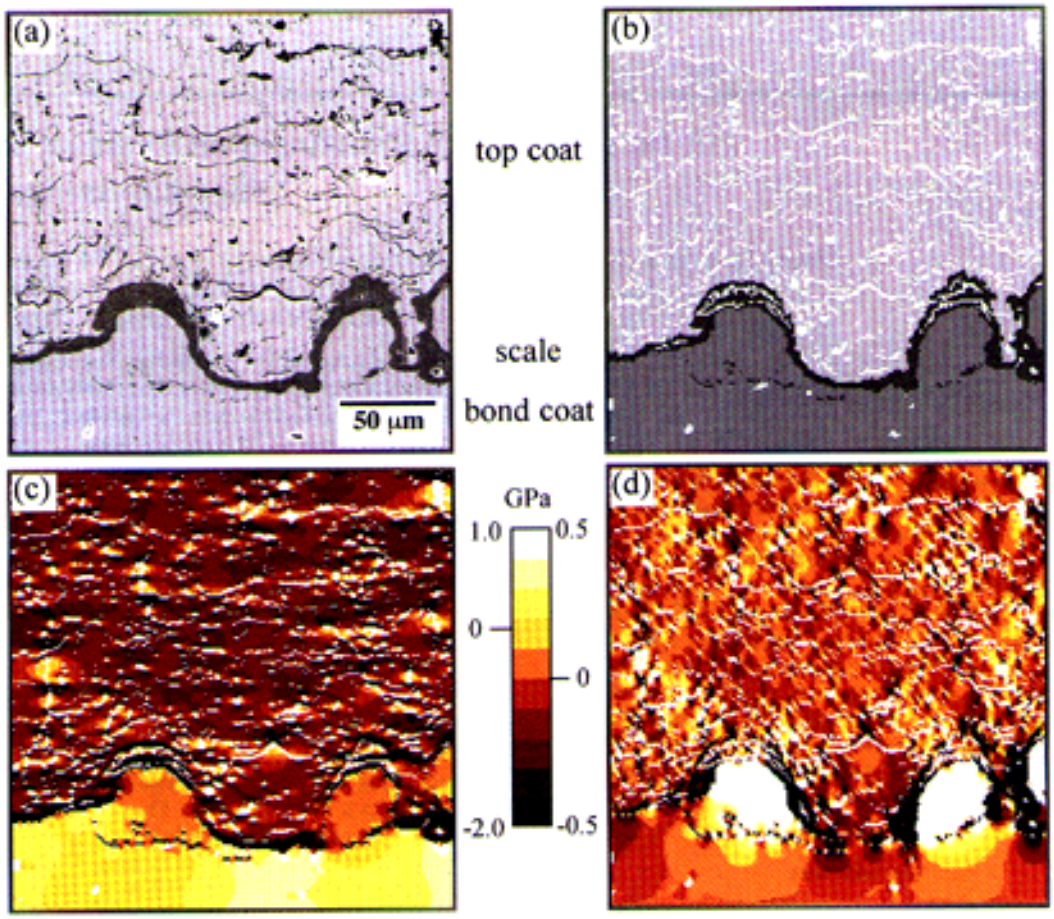

Fig. 1. (a) Actual microstructure, (b) processed image for numerical simulation, (c) calculated residual stress σ_x, and (d) calculated residual stress σ_y for the plasma-sprayed TBC system. The substrate is not shown.

Table I. Thermal/Mechanical Properties for the Plasma-Sprayed TBC System

Component	Young's modulus, E (GPa)	Poisson's ratio, ν	Coefficient of thermal expansion, CTE ($\times 10^{-6}$/°C)
Dense top coat	200	0.25	10
Porous top coat	50	0.1	10
Oxide scale	360	0.27	8
Bond coat	200	0.3	15.2
Substrate	213	0.25	14.5

Young's modulus of 200 GPa was adopted for the apparent dense region in the top coat prior to incorporation of the visible cracks (in the digitized image). For the analysis where all the cracks have been removed in the model microstructure, the reported upper bound of the Young's modulus (50 GPa) was adopted for the top coat.

Oxidation generally induces a volume expansion. This expansion can be readily incorporated in the OOF by replacing the coefficient of thermal expansion (CTE) of the oxide scale by an effective CTE, such that the thermal strain due to the effective CTE equals the sum of the thermal strain due to the actual CTE and the oxidation strain. However, the oxidation strain for converting the bond coat to the oxide scale is not well documented; therefore, replacement of the effective CTE for the oxide scale was not performed in this study. Hence, the important points in the present simulated results that will follow are trends in the residual-stress development with the interface morphology, rather than the absolute values of the stresses.

The TBC system is subjected to biaxial residual stresses in the plane parallel to the interface when interface asperities are not considered. While OOF is limited to a two-dimensional analysis, care should be taken in applying it to the cross section of the TBC system. For Fig. 1(a), the residual stress normal to the interface is expected to be much smaller than that parallel to the interface. For the plane-stress case, the elastic stress–strain (i.e., ϵ–σ) relationship parallel to the interface is described by $\epsilon = \sigma/E$, where E is the Young's modulus. For the biaxial stress case, the relationship becomes $\epsilon = \sigma(1 - \nu)/E$, where ν is the Poisson's ratio. Hence, to approximately capture the nature of the biaxial stress, E is replaced by $E/(1 - \nu)$ when the two-dimensional OOF is applied to the cross section of the TBC system in the present study.

(1) Analysis of the Actual Microstructure

First, the microstructure shown in Fig. 1(a) was digitized to a portable pixel map (ppm) format; each pixel then corresponded to two triangular elements. Hence, meshing in OOF was obtained simply by converting an image to a ppm format. The processed image (which consists of 78408 elements) is shown in Fig. 1(b). All visible cracks were included in the analysis (see the empty elements in Fig. 1(b)). The substrate (not shown in Fig. 1) was much thicker than the other constituents; thus, the thermal strain of the substrate (i.e., −0.0163) was used as the boundary condition at the right and left edges of the image in Fig. 1(b), to constrain its distortion in the x-direction.

Using OOF, the corresponding predicted-stress maps for the stress parallel and perpendicular to the interface (σ_x and σ_y, respectively) are shown in Figs. 1(c) and (d). The stresses in the system, minus the cracks (represented by empty elements), are indicated by the color bar in Fig. 1. In the absence of both interface asperities and cracks, σ_x values in the top coat, oxide scale, and bond coat should be −1.35 GPa, −3.6 GPa, and 225 MPa, respectively; $\sigma_y = 0$ in the system.[9,10] Perturbation of the residual-stress field due to the presence of interface asperities and cracks is obvious in Figs. 1(c) and (d). Specifically, σ_y is

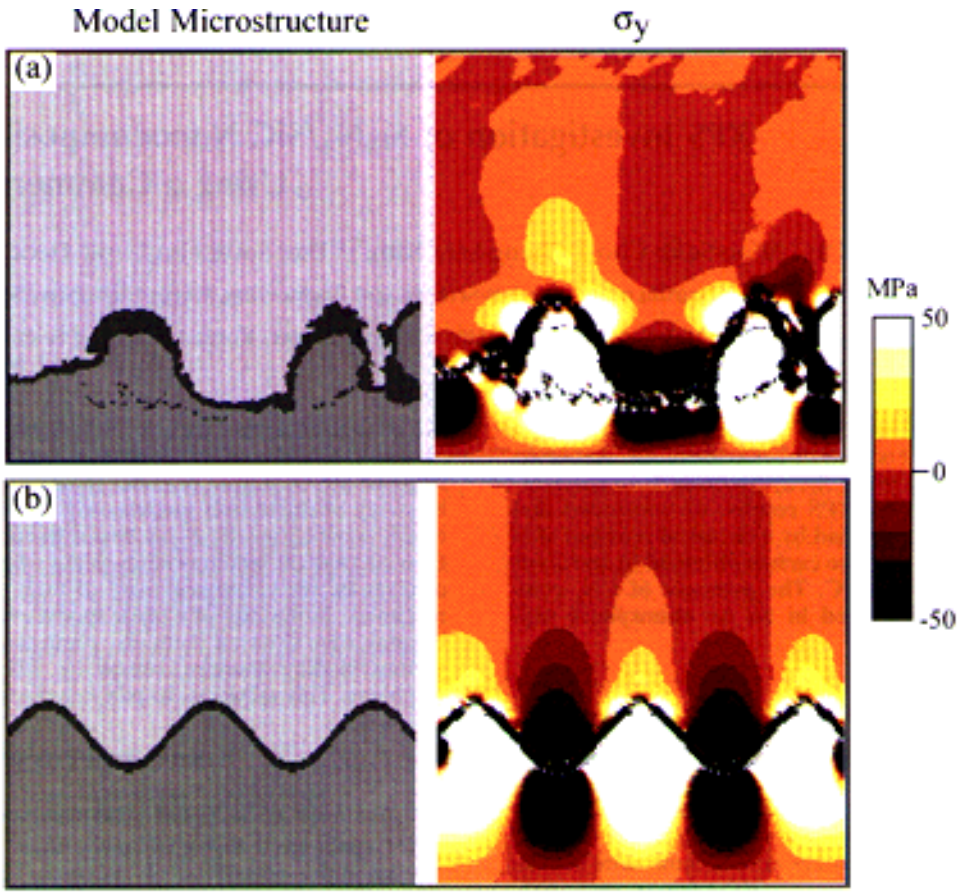

Fig. 2. Model microstructures and the calculated residual stress (σ_y) for the TBC systems ((a) cracks removed from the actual microstructure and (b) microstructures with an oxide scale and a sinusoidal interface topology).

tensile in the convex portions. To study how the geometry of the interface asperities influences the residual stresses, numerical simulations were performed on model microstructures as follows.

(2) Model Microstructures

The effects of interface asperities on residual stresses were somewhat obscured by the presence of cracks in Figs. 1(c) and (d). Removing the cracks from Fig. 1(b) and using 50 GPa as the Young's modulus for the top coat, the model microstructure and the predicted-stress map for σ_y are shown in Fig. 2(a). Also, assuming a periodic sinusoidal topology for the interface,[4,8,10,11] the model microstructure and the predicted σ_y are shown in Fig. 2(b).[††] The figure shows that tensile and compressive stresses normal to the interface (σ_y) occur in the regions of convex and concave asperities, respectively.

IV. Conclusions

Fracture and spallation of the plasma-sprayed Y_2O_3-stabilized ZrO_2 (YSZ) top coat are a major concern for thermal barrier coating (TBC) applications. A rough bond-coat surface can apparently increase the lifetime of plasma-sprayed TBCs. The present study attempts to analyze the effects of interface asperities on the residual-stress distributions in a plasma-sprayed TBC system. A newly developed object-oriented finite-element analysis (OOF) method was used to model the residual stresses. The uniqueness of OOF is that it can be used directly on microstructural images. OOF that is performed on the actual microstructure of the TBC system provides a full-field plot of the residual stresses. To systematically examine the effect of interface asperities on residual-stress distributions, OOF also can be performed on model microstructures with various interface geometries.[12]

[††]The stress should be strictly periodic if the boundary condition was imposed exactly. Because a uniform strain in the *x*-direction was imposed at the right and left edges of the image, the simulated results suffer the edge effect.

References

[1]W. Y. Lee, D. P. Stinton, C. C. Berndt, F. Erdogan, Y. D. Lee, and Z. Mutasim, "Concept of Functionally Graded Materials for Advanced Thermal Barrier Coating Applications," *J. Am. Ceram. Soc.*, **79** [12] 3003–12 (1996).

[2]J. A. Haynes, E. D. Rigney, M. K. Ferber, and W. D. Porter, "Oxidation and Degradation of a Plasma-Sprayed Thermal Barrier Coating System," *Surf. Coat. Technol.*, **86–87**, 102–108 (1996).

[3]M. J. Lance, J. A. Haynes, W. R. Cannon, and M. K. Ferber, "Piezospectroscopic Characterization of Thermal Barrier Coatings"; pp. 229–37 in Ceramic Transactions, Vol. 89, *Nondestructive Evaluation of Ceramics.* Edited by C. Schilling, J. N. Gray, R. Gerhardt, and T. Watkins. American Ceramic Society, Westerville, OH, 1998.

[4]M. Y. He, A. G. Evans, and J. W. Hutchinson, "Effects of Morphology on the Decohesion of Compressed Thin Films," *Mater. Sci. Eng. A*, **A245**, 168–81 (1998).

[5]S. A. Langer, W. C. Carter, and E. R. Fuller, "Object Oriented Finite Element Analysis for Materials Science," Center for Theoretical and Computational Materials Science and the Information Technology Laboratory at the National Institute of Standards and Technology, Gaithersburg, MD, 1997.

[6]A. H. Bartlett and R. Dal Maschio, "Failure Mechanisms of a Zirconia–8 wt% Yttria Thermal Barrier Coating," *J. Am. Ceram. Soc.*, **78** [4] 1018–24 (1995).

[7]R. V. Hillery, B. H. Pilsner, R. L. McKnight, T. S. Cook, and M. S. Hartle, "Thermal Barrier Coating Life Prediction Model Development," NASA Contractor Rept. No. 180807, 1988.

[8]A. M. Freborg, B. L. Ferguson, W. J. Brindley, and G. J. Petrus, "Modeling Oxidation Induced Stresses in Thermal Barrier Coatings," *Mater. Sci. Eng. A*, **A245**, 182–90 (1998).

[9]C.-H. Hsueh and A. G. Evans, "Oxidation Induced Stresses and Some Effects on the Behavior of Oxide Films," *J. Appl. Phys.*, **54** [11] 6672–86 (1983).

[10]A. G. Evans, G. B. Crumley, and R. E. Demaray, "On the Mechanical Behavior of Brittle Coatings and Layers," *Oxid. Met.*, **20** [5/6] 193–216 (1983).

[11]G. C. Chang, W. Phucharoen, and R. A. Miller, "Behavior of Thermal Barrier Coatings for Advanced Gas Turbine Blades," *Surf. Coat. Technol.*, **30**, 13–28 (1987).

[12]C.-H. Hsueh, P. F. Becher, E. R. Fuller Jr., S. A. Langer, and W. C. Carter, "Surface-Roughness Induced Residual Stresses in Thermal Barrier Coatings: Computer Simulations"; *Proceedings of 5th International Symposium on Functionally Graded Materials* (FGM '98) (Dresden, Germany, Oct. 26–29, 1998), in press. □