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Influence of pores on the surface microcompression mechanical response of thermal barrier coatings fabricated by atmospheric plasma spray—Finite element simulation

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ABSTRACT

Surface microcompression is a very important technique to characterize the mechanical properties of film and coating systems. In this paper, surface microcompression simulation for $La_2Zr_2O_7$ (LZ) thermal barrier coatings (TBCs) was implemented by finite element method, especially, the influence of pores on the surface microcompression mechanical response of the thermal barrier coatings fabricated by atmospheric plasma spray (APS) was focused on. The simulation results indicate that the pores not only affect the stress distribution beneath the contact area between the indenter and coating surface, but also affect the shape of the force–displacement curve and the plastic deformation behavior of TBCs. The micromechanism was discussed in detail in this study. At the same time, by using the surface microcompression technique, a new direction or method was proposed to characterize the pore content of the coating quantitatively.

1. Introduction

In the present, typical thermal barrier coatings (TBCs) usually with the content of 7 ± 1% wt Y_2O_3 partially stabilized ZrO_2 (YSZ) are deposited on the nickel based superalloy substrate with the MCrAlY (where M = Ni and/or Co) as the metallic coat in order to protect the substrate against being subjected to the high temperature, corrosion and wear. The technique of electric beam physical vapor deposition (EB-PVD) and atmospheric plasma spray (APS) are usually adopted to prepare the TBCs [1–3]. The ceramic layer of TBCs prepared by EB-PVD usually has the characteristic of columnar grain and inner sub-grain distributed between the columnar grains, while the conventional TBCs fabricated by APS exhibits lamellar layer structure, but the characteristic is not evident in the nanostructured TBCs. Nanoindentation is regarded as “fingerprint” of materials, it is usually adopted to characterize the mechanical properties of films and coatings such as elastic modulus and microhardness [4,5]. Microindentation is a novel technique which has also been adopted recently to evaluate the mechanical properties of films and coatings system and it was advanced by some researchers recently [6–8].

As the indentation technology has been widely used to characterize the mechanical properties of the materials (films or coating system, and some bulk materials), the development of the indentation testing instruments combined with finite element technology enables us to investigate the material properties more conveniently than before. Recently, the low-load and depth-sensing nanoindentation method has been successfully utilized to measure the mechanical properties of materials at the sub-micro and nanoscales, like ultra-thin films. Nanoindentation or microindentation experiments are fast to perform and do not require removing the films or coatings from their substrates. Thus, this method is routinely employed to investigate the elastic and plastic properties of various thin films and coating systems. However, the indentation itself generally only provides information on hardness *H* and Young’s modulus *E*. Moreover, thin films and thin/thick coatings are supported by their substrates, hence substrate-independent measurements of thin-film and coating system properties are complicated due to the small thickness of films and coating systems and the measuring instrument resolution. Another factor that convolutes the analytical deviation of a thin film’s mechanical properties is the complex deformation of the film/substrate or coating/substrate bimaterial or multilayed system [9–11].

Some research work about the characterization of the mechanical properties of materials by using the microindentation technique has been published. Zhang and Li [12,13] have investigated the interfacial failure mechanisms for Cu–ceramic and Al alloy–ceramic interfaces and the interfacial bond strengths of regularly grained and nanograined Al_2O_3/TiO_2 composite coatings using a newly developed lateral force-sensing microindentation method. Lugscheider et al. [14] have investigated the mechanical properties of EB-PVD zirconia TBCs by nanoindentation. Because of the

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microstructure of EB-PVD-coatings, as expected different behavior at the grain boundaries and the grain, the mechanical properties in the vertical and the horizontal direction are completely different. Bouzakis et al. [15] have investigated the mechanical properties of the EB-PVD ZrO_2 coating by means of advanced experimental analytical procedures. Stress–strain curves for the coatings examined were determined by a continuous, finite element method (FEM)-supported simulation of indenter penetration into the coating surface. Panich and Sun [16] have investigated the nanoindentation process of a soft coating on a harder substrate by the finite element method. The author discussed the relationship of the critical indentation depth with the yield strength ratio of the soft coating to the harder substrate and the indenter tip radius in detail. Chen et al. [17] have investigated the plastic deformation behavior and densification of TBC with a columnar microstructure as well as the column distortions caused by the impression by finite element method, the author thought that it was also capable of exploring the deformation heterogeneities observed experimentally, such as shear bands, by embodying salient constituent properties, such as the column width, contact friction and inter-columnar friction. Comparisons with measurements, finite element simulation result could provide some understanding of the plastic response of several thermal barrier systems.

Zirconate based TBCs is expected to be a new candidate of TBCs material in the future, because of its low thermal conductivity, good sintering resistance ability at high temperature, higher melting point and chemical stability than the conventional YSZ. Previous research have been reported about nanostructured and microstructured YSZ TBCs in the experiment, including the following aspects: (1) the preparation of nanostructured and conventional TBCs, (2) the thermo-physical characterization, such as thermal conductivity or thermal insulation capability, (3) mechanical properties characterization such as residual stress, adhesive strength, thermal shock resistance, high temperature oxidation resistance, and lifetime prediction and so on. Little work has been reported on the microcompression using finite element method about zirconate based TBCs. On the other hand, the microcompression investigation about the LZ TBCs with defects such as pores is nearly a vacancy. Moreover, a new strategy (surface microcompression) about measuring the pore content of coating was proposed for the first time. And it reflects the pore content more truthfully from the whole coating system with three dimensional structure. On the basis of this paper providing us a reliable and effective method, i.e. surface microcompression which can reflect and the pore content of the coating, it can be predicted that the pore content of the coatings will be measured as the development of the microcompression technique and the instrument.

2. Simulation method and procedure

2.1. Model basis for finite element analysis

The plasma spray process usually involves melting of feedstock materials in a plasma plume and rapidly transporting these molten particles to the substrate, where rapid solidification of individual particle occurs upon impingement. Successive build-up of these “splats” results in a layered arrangement in the coating, analogous to a brick-wall-like structure where the splats are entwined in complex arrays [18]. This splat-based layered microstructure leads to an intrinsic anisotropy of the coating in the direction perpendicular to the spray direction. The splats are separated by interlamellar pores resulting from rapid solidification of the lamellae, globular pores formed by incomplete inter-splat contact or around unmelted particles, and intrasplat cracks due to thermal stresses and tensile quenching stress relaxation. This unique microstructural features contributes to a further decrease in thermal conductivity.

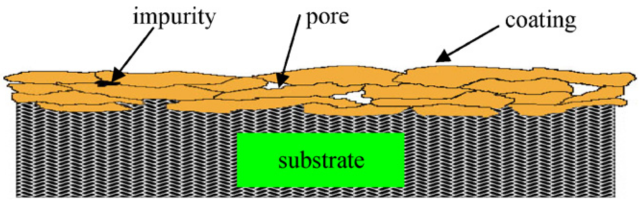

Fig. 1. Typical feature of plasma spray TBCs.

Typical feature of as-sprayed coating is shown in Fig. 1.

2.2. Model description and materials parameters

As the test coating sample is cylinder plate like, an axisymmetry perfect model without pores is established, as shown in Fig. 2. The model only has three layers: DZ125 Ni-based superalloy substrate, NiCoCrAlY bond-coating and ceramic coating. But the ceramic coating has four sub-layers, all the four sublayers are $La_2Zr_2O_7$ (LZ). The properties parameter of each layer came from the reference [19–23]. In the present finite element analysis, the following assumptions were made: (1) the materials properties of $La_2Zr_2O_7$ coatings were considered to be linear elastic; while elastic–plastic responses were included in both the substrate and bond coating; von-Mises yield criterion and bilinear kinematic hardening were assumed to describe the strain-hardening behavior of substrate and bond coating. (2) Although the coating property is different at the spray direction and the interface direction, the micro-defects, such as pores, cracks have no evident direction and the arrangement is irregular, the coating microstructure is not uniform. So the mechanical properties at different directions have little difference, the coating can be viewed as isotropic. The substrates were also isotropic due to that it was polycrystalline material. All the materials were temperature-independent. (3) The creep and oxidation behavior were not included in the models because the microcompression was implemented at room temperature (Table 1).

The thickness of the substrate, bond-coating and top-coating is 6 mm, 100 μm and 400 μm, respectively, and the radius of the cylinder sample is 10 mm.

In the present study, the 2-D axisymmetric case is performed to simulate the elastic–plastic indentation process by the ABAQUS finite element code as the commercial available software package ABAQUS Standard 6.9 version has very high nonlinear solution ability [24]. Nonlinear contact analysis has been implemented in the simulation procedure. The half spherical indenter is used in the model in order to define an axisymmetric model. The specimen is modeled with four-node quadrilateral axisymmetric reduced integration elements (CAX4R element type). In order to study the stress distribution characteristic under the indenter when the load is applied, a fine mesh is used beneath the contact area and near the tip of the indenter which the finest mesh element is the square

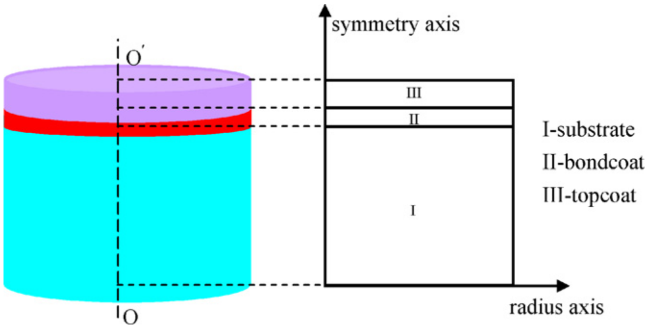

Fig. 2. Model of the sample used in the finite element simulation.