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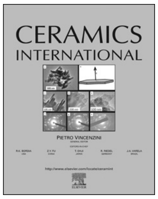

Modeling the thermal radiation properties of thermal barrier coatings based on a random generation algorithm

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A R T I C L E I N F O

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A B S T R A C T

Thermal barrier coatings (TBCs) are porous media in which many different pores and cracks are induced by different manufacturing procedures. Many studies have been conducted to investigate the impact of microstructures of TBCs on thermal conductivity; nevertheless, the influence of microstructures on the radiative properties of TBCs has not drawn significant attention. In addition, the working condition of thermal barrier coatings is at high temperatures at which the contribution of radiative heat transfer plays a very crucial role. Therefore, it is necessary to study the radiative properties of TBCs to characterize their insulation performance. In this work, the microstructures of air-plasma- sprayed (APS) 8 wt% yttria stabilized zirconia (8YSZ) thermal barrier coatings (TBCs) are constructed by the quartet structure generation set (QSGS) algorithm. A finite-difference-time-domain (FDTD) method is carried out to simulate radiative heat transfer through TBCs. Three parameters—average pore size, directional growth probability D_i (especially horizontal growth probability D_{13}) and porosity—have been investigated to study the microstructural effect on the radiative properties of TBCs. The reflectance of freestanding 50-μm-thick thermal barrier coatings is studied using Lumerical FDTD Solutions in the wavelength range from 1 to 6 μm at normal incidence. The absorption and scattering coefficient as a function of wavelength are extracted using the four-flux model. The results will help us to characterize the radiative heat transfer process across the TBCs and provide us with a theoretical guide to design TBCs with a high thermal insulation property.

1. Introduction

A higher operating temperature is required to enhance the operating performance and efficiency of gas turbine engines, which inevitably leads to strong demand for better thermal insulation of the turbine's metallic components. Thermal barrier coatings (TBCs), usually made of yttria partially stabilized zirconia (YSZ), are generally deposited on top of metallic components to shield them from the hot gas steam [1,2]. In the visible and near-infrared wavelength range (~0.4–6 μm), YSZ is semitransparent to radiation, which coincides with the wavelength range (1–6 μm) where turbine engine thermal radiation is concentrated according to Planck's law. It has been recognized that thermal radiation can transport through the coating and reach the metallic components, consequently resulting in the elevation of the surface temperature of superalloy components [3–5]. Hence the radiative heat transfer through TBCs will account for a significant portion of the total heat transfer, and an investigation of the radiative heat transfer mechanism through TBCs is urgently needed.

Thermal barrier coatings are usually fabricated by air plasma spraying (APS) or electron beam physical vapor deposition (EB-PVD). Compared with EB-PVD, APS provides the opportunity to optimize the microstructures of TBCs (pores and cracks) for the purpose of enhancing the backscattering of radiation and thus improving the insulation performance. In the spraying process, the microstructures of TBCs are highly heterogeneous owing to many factors, such as droplet temperature, velocity and substrate temperature [6,7]. The pores and cracks produced by spraying are influential in terms of both thermal conduction and radiation, and the impact of microstructures on thermal conduction has been widely investigated [8–12]. Golosnoy [10] developed numerical and analytical models to study the effect of pore shape on thermal conductivity. Chi and Sampath [11] investigated the correlation between microstructures and thermal conductivity. Their results showed that the interlamellar pores and splat interfaces can significantly influence the thermal conductivity. However, very few studies on the effect of microstructures on the thermal radiation of TBCs have been conducted. Owing to the photon scattering in the defects of TBCs, a minor change in the microstructures may cause a huge difference in the radiative properties of TBCs, so a

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fundamental study of the relationship between microstructures and the radiative properties is essential to optimize the insulation performance of TBCs. Eldridge and Spuckler [13,14] developed a modified four-flux model to study the radiative properties of air-plasma-sprayed (APS) 8 wt% yttria-stabilized zirconia (8YSZ) thermal barrier coatings at room temperature and elevated temperatures. Golosnoy et al. [10] employed the Rosseland diffusion to model the radiative heat transfer through the coating. Because the coating is optically thin, their approximation is not precise. Dombrovsky et al. [15,16] investigated the radiative properties of TBCs with a modified two-flux approximation. In their analysis, they assumed that the scattering in the coating is induced by the isotropic pores, which can be simplified as spherical bubbles, and they determined the radiative properties with the Mie theory. However, the microstructures of TBCs in fact vary with different spraying processes, so it is invalid to study only the scattering caused by isotropic pores. Zhang et al. [17] investigated the relationship between microstructures and the radiative properties of TBCs. Although parameters such as defect size, shape coefficient, porosity and orientation were examined in their work, the absorption coefficient was neglected, and the simulation results did not agree well with the experimental data.

The aim of this work is to study the effect of microstructures on the radiative properties of TBCs and optimize the radiative properties of air-plasma-sprayed (APS) 8 wt% yttria-stabilized zirconia (8YSZ) thermal barrier coatings by modifying the microstructures such that it leads to an increase in the scattering coefficient and hence achieves better insulation performance. The microstructures of TBCs are created and analyzed with an algorithm called the quartet structure generation set (QSGS) [18], which is generally used to construct more realistic microstructures of porous media. This algorithm was used to generate microstructures of TBCs, based on which the effective thermal conductivity was calculated and the results agreed well with experimental data. However, research on the radiative properties of TBCs based on this algorithm has not been conducted. In this paper, the radiative properties of the structures generated by the QSGS algorithm are investigated, and the results are in good agreement with experimental data. The computational method finite-difference-time-domain (FDTD), which has been comprehensively employed to study the radiative properties of nanomaterials [19,20], is applied to study the relationship between microstructures and the reflectance of TBCs. The parameters such as average pore size and shape, porosity and pore orientation with the ratio of horizontal length to vertical length are investigated, and their impact on the radiative properties of TBCs is discussed in detail. In addition, the scattering coefficient and absorption coefficient are obtained using the four-flux model [13]. It is noted that the surface-engineered reflectivity is insignificant because the through-thickness nature of their porosity-engineered reflectance is superior to the surface-engineered reflectivity approaches that are more susceptible to loss by erosion. According to the foregoing discussions, an optimal microstructure is determined to acquire a relatively high reflectance and thus improve the insulation performance of TBCs providing guidance for future research on the optimization of TBCs.

2. Modeling and analysis

2.1. QSGS algorism

The quartet structure generation set (QSGS) algorithm developed by Wang [18] is generally used to construct more realistic microstructures of porous media. Four parameters are defined to control the microstructural characteristics of the generated porous media: core distribution probability (c_d), directional growth probability (D_i), volume fraction (P^n) and phase interaction growth probability ($I_i^{n,m}$). Among the multiphase system of thermal barrier coating, YSZ is defined as a growing phase, and gas remains as a non-growing phase. The initial phase is gas, and the growing process follows the steps below:

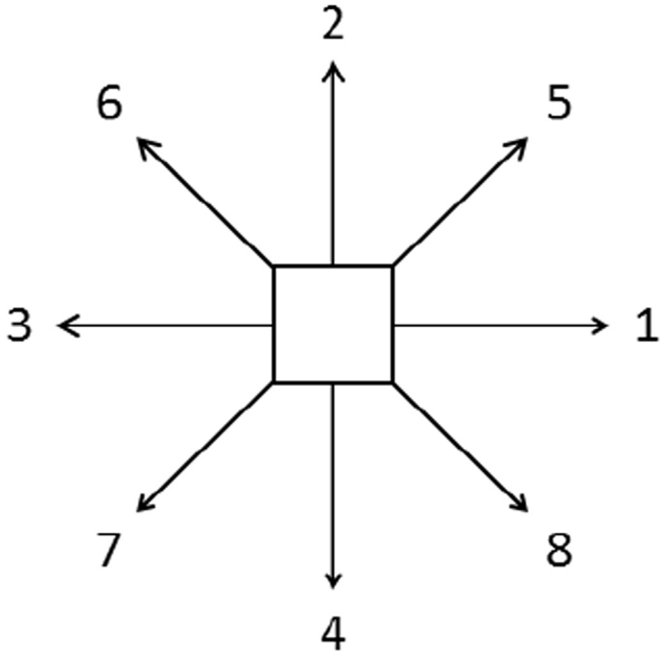

Fig. 1. Growing directions of a cell.

a) Randomly generate the cores of the growing phase over the whole grid system. In each cell of the grid system, a random number is assigned by a uniform distribution function within (0, 1). If the random number is no more than the core distribution probability c_d, whose value must be smaller than the volume fraction P^n, then this cell is chosen to be a core of the growing phase.
b) Every core can grow into its neighboring cells in all directions ruled by each given directional growth probability D_i. In each neighboring cell of the growing elements, a new random number is generated. If the random number is less than D_i, the neighboring cell in direction i will become part of the growing phase. The growing directions are shown in Fig. 1; each cell has eight different directions with different directional growth probabilities (D_i). There are four main directions (1, 2, 3, 4) and four diagonal directions (5, 6, 7, 8). When D_{1-4}: $D_{5-8} = 4$, the generated structure is assumed to be isotropic, which is consistent with the equilibrium density distribution function for isotropic materials [21].
c) Repeat the second step until the volume fraction of the growing phase reaches the given value P^n (porosity is defined as $1 - P^n$).

In this paper, owing to the fact that thermal barrier coating is a two-phase system with one growing phase and one non-growing phase, there is no interaction between these two phases; the parameter $I_i^{n,m}$ can be ignored, and the details about $I_i^{n,m}$ can be found in Wang [18]. The structures generated by QSGS and the real experimental micrograph obtained by scanning electron microscopy (SEM) are shown in Fig. 2. Comparing Fig. 2(a) with (b), under the condition that the ratio of D_{1-4} ($D_1 = D_2 = D_3 = D_4$) to D_{5-8} and the volume fraction P are fixed, the change of c_d can result in a difference in pore size and distribution. The pore size