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Modeling radiative properties of air plasma sprayed thermal barrier coatings in the dependent scattering regime

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A R T I C L E I N F O

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A theoretical model on radiative properties of air plasma-sprayed (APS) 8 wt% yttria stabilized zirconia (8YSZ) thermal barrier coatings (TBCs) is proposed and validated. Starting from analysis of microstructures, pores inside the coating are regarded as scatterers. Dependent scattering effects among scatterers are thoroughly considered in the framework of quasicrystalline approximation (QCA) and Percus–Yevick (P–Y) pair distribution function for sticky hard spherical particles, in which large nonspherical pores are treated as clusters of the elemental pores. Afterwards, the Monte Carlo (MC) method is used to solve the radiative transfer problem inside TBCs based on the radiative properties. The predicted optical responses including reflectance, transmittance and absorptance of TBC slabs with different thicknesses agree well with the experimental data. The widely used independent scattering assumption in conventional studies is also investigated and examined to be inapplicable in the semitransparent spectral region of TBCs, especially between around 3.2 and 5.6 μm. This study provides a simple and physically robust direct prediction on radiative properties of TBCs solely based on their microstructures and bulk optical properties of the material. Moreover, the present method can be easily applied to the studies on radiative properties of other semitransparent porous media.

1. Introduction

In order to improve the operating performance and efficiency of gas turbine engines, a higher inlet gas temperature is demanded, which stimulates the application of thermal barrier coatings (TBCs) to provide thermal insulation for the superalloy components [1,2]. As the gas temperature rises, its thermal radiation energy will contribute to the total heat flux substantially, and moreover, according to Planck's law, concentrate in the wavelength range of 1–6 μm, which is also the theoretically semitransparent spectral range of ceramic thermal barrier coating materials [3,4]. This means that much thermal radiation will be able to transport across the coating and consequently elevate the surface temperature of superalloy components. Hence a full understanding on the radiative transfer mechanism in TBCs is urgently required for the state-of-the-art TBC heat transfer analysis and design.

Early in the 1990s, Siegel and Spuckler [5–7] carried out a series of parametric studies on the influencing factors of thermal radiation transport inside semitransparent layers, like TBCs, using a two-flux method to solve the radiative transfer equation (RTE) approximately. They showed that radiative properties of the semitransparent layer, including refractive index, scattering coefficients and absorption coefficients (or the albedo), can affect the internal temperature distribution dramatically. However, radiative properties used in their studies were adjustable parameters, which were not derived from actual TBCs. For a more practical prediction of radiative heat transfer across TBCs, many researchers measured the spectral reflectance and transmittance of various TBC samples and subsequently retrieved their radiative properties based on different inverse methods for RTE. For instance, Eldridge and Spuckler [8,9] implemented a modified four-flux model to obtain the radiative properties of air plasma sprayed (APS) 8 wt% yttria-stabilized zirconia (8YSZ) thermal barrier coatings at room temperature and elevated temperatures. Dombrovsky et al. [10] identified the transport scattering coefficients and absorption coefficients of solution-precursor plasma-sprayed (SPPS) 7YSZ thermal barrier coatings in the wavelength range of 2.5–9 μm using a modified two-flux method. Wang et al. [11] also used the modified four-flux method to extract radiative properties of APS $Gd_2Zr_2O_7$ TBCs. Simple and efficient, these inverse methods remain as the main technique to recognize thermal radiative properties of TBCs.

Although those inverse methods can fit the experimental data well, they are just a kind of *ad hoc* techniques for the specific set of samples under particular experimental investigations.

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Moreover, the inherently ill-conditioned inverse techniques are very sensitive to experimental uncertainties and the choice of the form of phase functions [12–14], and they cannot provide any in-depth understanding of the micro-scale radiative transfer mechanism. Therefore, more general methods should be proposed to give a direct prediction of radiative properties of the TBCs solely based on the bulk material optical properties and their microstructures, which were already intensively developed in other kinds of porous media [15–17].

Trials have been made by many researchers. Dombrovsky et al. [10] used the Mie theory [18] of small bubbles to predict the transport scattering coefficients of 7YSZ, resulting in a qualitative agreement with retrieved values from experiments. Manara et al. [19–21] modeled the effective scattering coefficients of high porosity ceramics (up to around 40%) with the Mie theory. Recently, our group also made predictions for radiative properties of APS TBCs using the Mie theory for small pores, but good agreement with experimental data was achieved only when the porosity was very low (around 5%) [4]. Note that, all these predictions were based on the assumption that the scatterers (i.e., pores in their studies) in the host medium scatter light independently, which implies that those scatterers scatter light in the same manner as if other scatterers do not exist [22]. Unfortunately, this assumption is violated when those scatterers occupy a considerable volume fraction (typically larger than 10%, yet heavily depending on scatterer size, light wavelength and scatterer clearance) [23], where the correlation between scatterers becomes important and the coherent interaction effect of light must be taken into account. This phenomenon has been reported and confirmed by several well-controlled laboratory experiments [24,25] and this sort of media is termed as “densely packed (random) particulate media” [26,27]. In the present case of APS TBCs with a typical porosity in the range of 10–20%, the pore size is usually around 1 μm, and the pore clearance is around 1∼10 μm, which are both in the same order with the wavelength of thermal radiation (1–6 μm). This implies the existence of strong collaborative scattering effects of neighboring pores, including the deformation of electromagnetic fields impinging on pore surfaces and the interference of scattered waves, etc.

In the dependent scattering regime, the classical radiative transfer theory presupposing independent scattering is no longer valid [28], but the form of radiative transfer equation (RTE) can be still retained, in which the extinction coefficient and phase function should be substantially modified by considering correlation effects [29]. This means that traditional techniques to solve RTE are still applicable and the main concern turns out to be deducing effective extinction coefficients and phase functions from actual microstructures of those densely distributed scatterers. Note that unlike the heuristic origin of classical radiative transfer equation, the equivalent radiative transfer equation for dense media is derived rigorously from analytic wave theory through the ladder approximation of the Bethe–Salpeter equation for the second moment of the field [30].

Various approximate methods are developed to combine the statistical distribution and coherent scattering effects of scatterers to gain effective radiative properties in the dependent scattering regime, such as the interference approximation (ITA) under Rayleigh–Gans approximation [31], the quasi-crystalline approximation (QCA) and the quasi-crystalline approximation with coherent field (QCA-CP) [30,32]. In the meanwhile, direct numerical simulations of the light extinction rate of a large group of particles are also feasible but still very time-consuming, which thus are not recommended here [33–35].

In this paper, QCA for moderate-size (i.e., size parameter $ka \sim 1$) spherical particles[30] is implemented to model the effective radiative properties of densely distributed pores in air plasma sprayed 8YSZ TBCs in the dependent scattering regime. The effective radiative properties are then substituted into RTE to derive the hemisphere reflectance and transmittance of slabs of 8YSZ TBCs, by means of the Monte Carlo method [36]. The computed hemisphere reflectance and transmittance are validated by our measured results. In the meanwhile, the applicability of the conventional radiative transfer model under independent scattering assumption is discussed. The main objective of this work is to provide a fast and physically reasonable direct prediction framework for radiative properties of TBCs and other porous ceramics, solely based on their microstructures and optical properties of the bulk material, giving a full understanding of the internal micro-scale radiative transfer mechanism.

2. Theory and modeling

2.1. Size distribution and pair distribution function of pores

In this study, several air plasma sprayed 8 wt% yttria stabilized zirconia TBC samples with different thicknesses are prepared. The porosity of these samples is evaluated by density measurements to be 15% with a deviation of ±1%. A SEM analysis (FEI-Sirion 200 at IAC of SJTU) is carried out to study their microstructures, and the cross section images of a 200 μm thick sample are shown in Fig. 1. Typical features of the microstructures of APS TBCs, which originate from the thermal spraying process, can be recognized in Fig. 1a and 1b. Firstly, the typical lamellar structure formed by stacking splats with very thin inter-lamellar cracks parallel to the coating surface can be observed, while intra-splat cracks due to thermal stresses and tensile quenching stress relaxation are also very common. Secondly, there are also many globular and irregular pores (or voids) owing to imperfect contact and partially molten YSZ particles [37]. Thirdly, those pores distribute in a very nonuniform manner in short range (∼50 μm).

By directly mapping the pores in the SEM-EBSD images of cross section with equivalent spheres, and ignoring inter-lamellar and intra-splat cracks that are very thin (Fig. 1(c)), the size distribution of the spherical pores is obtained in Fig. 2 and the number probability density function is fitted with a log-normal distribution function by the least-square minimization technique as:

$$f(D) = \frac{1}{\sqrt{2\pi}D\sigma}\exp\left(-\frac{\ln(D/D_c)}{2\sigma^2}\right) \quad (1)$$

where $\sigma = 0.32$ is the standard deviation and $D_c = 0.58$ μm is the median size.

The obtained size distribution function is crucial for conventional independent scattering modeling using Mie theory. However, in the present dependent scattering modeling, it is too coarse to use, and a finer mapping method is proposed here.

Since the cross section images are two-dimensional, the number of small pores (smaller than the median size D_c) would be overestimated (because the pore size in the third dimension is unknown). Hence in the first step, the small globular pores are all replaced by median-size pores. Furthermore, to consider the nonsphericity of large irregular pores and inter-lamellar cracks, they are treated as *clusters* of the median-size pores. The TBC slab is then simplified into a *monodispersed* system of spherical pores with a diameter equal to 0.58 μm in the host medium YSZ, shown in Fig. 1(d). Note that, although some inter-lamellar cracks are partitioned into small pores, other inter-lamellar cracks are still too thin to be correctly resolved or even recognized. After that, to further investigate the correlation between the “elemental” pores, especially incorporating the existence of pore aggregates, the pair distribution function (PDF) of spherical pores is introduced. The