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Microstructural effect on radiative scattering coefficient and asymmetry factor of anisotropic thermal barrier coatings

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Thermal barrier coatings are common porous materials coated on the surface of devices operating under high temperatures and designed for heat insulation. This study presents a comprehensive investigation on the microstructural effect on radiative scattering coefficient and asymmetry factor of anisotropic thermal barrier coatings. Based on the quartet structure generation set algorithm, the finite-difference-time-domain method is applied to calculate angular scattering intensity distribution of complicated random microstructure, which takes wave nature into account. Combining Monte Carlo method with Particle Swarm Optimization, asymmetry factor, scattering coefficient and absorption coefficient are retrieved simultaneously. The retrieved radiative properties are identified with the angular scattering intensity distribution under different pore shapes, which takes dependent scattering and anisotropic pore shape into account implicitly. It has been found that microstructure significantly affects the radiative properties in thermal barrier coatings. Compared with spherical shape, irregular anisotropic pore shape reduces the forward scattering peak. The method used in this paper can also be applied to other porous media, which designs a frame work for further quantitative study on porous media.

1. Introduction

Owing to the anti-erosion ability, heat insulation and stabilization of TBC, it has become an important component of improving the performance of devices like gas turbines and aero engines [1]. To improve the efficiency of these devices, they are required to work under elevated operating temperature which makes new demands on TBCs [2]. Thermal barrier coatings usually consist of bond coat, mainly metal alloys, and top coat, mainly ceramics containing 6–8 wt% yttrium stabilized zirconia [3]. There are two main approaches fabricating thermal barrier TBCs, including air plasma spraying (APS) and electron beam physical vapor deposition (EB-PVD). We focus on APS considering its wide application, high production efficient, low cost in fabrication and so on. During the fabrication process, defects like pores and cracks are formed in TBCs and play an important role in heat transfer [4]. Although the microstructural effect on heat transfer and mechanical properties in TBCs has been studied extensively in recent years [5–8], most of them paid attention to heat conduction and usually ignored heat radiation for the reason that radiative flux is much less than conductive flux. However, with the increase of operating temperature, heat radiation enhances because the Yttrium-stabilized Zirconia (YSZ) TBCs are intrinsically semitransparent to the wavelength ranging from 0.3 µm-8 µm where over 80% of thermal radiation emitted by objects at 1700–2000 K focuses. Antou et al. [9] investigated air plasma spraying TBCs and found that when the temperature reaches 600 K, thermal conductivity increases sharply due to the fact that the flux of heat radiation is proportional to the four power of temperature. Manara et al. [10] measured transmissivity and emissivity in the wavelength range from 2 µm to 8 µm. It was found that when the temperature is 1150 °C, heat radiation takes up 15%–25% of heat transfer. Actually, heat transfer in the coatings is much more complex with the consideration of the contribution of thermal radiation. Radiative properties are associated with many factors, including micro/nanostructures, materials and temperature. When the maximum linear dimension of pores or cracks is comparable to the radiative wavelength, the interaction between micro/nanostructure and radiation wave is strong. Therefore, it is significant to study the microstructural influence on scattering properties.

Based on the hemispherical reflectance and transmittance of the thermal barrier coatings measured through experiments, Dombrovsky et al. [11,12] gave a semi-empirical formula for absorption coefficient and calculated scattering properties of spherical pores according to Mie theory by assuming that the radiative wave is scattered by spherical pores. However, pore shapes have an obvious influence on thermal or mechanical properties of TBCs [13–

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15]. Many studies treat pore shapes as simple geometries, such as sphere or ellipsoid [6,16,17] which is not agreeable with the actual microstructure of thermal barrier coatings.

Besides, the strong interaction between micro/nanostructure and radiation wave obviously affects radiation transport, including forward scattering interference, coherent backscattering and Anderson localization [18–20]. Therefore, it is necessary to take the wave nature of thermal radiation into account. The radiative transfer theory (RTT) is effective in solving scattering problems and is widely applied in various realistic media, such as atmosphere, biological tissues, porous media and so on [21–23]. The radiative transfer equation (RTE) can be directly derived from the Maxwell equations for sparsely random distributed media under the assumption of independent scattering and the ladder approximation [18,24]. It describes the extinction of coherent light and the multiple scattering of diffuse light [25,26]. Several important optical properties, including reflectance and transmittance, can be obtained through RTE. However, RTE can't consider the forward scattering peak and the coherent backscattering enhancement, which exist in experiments and accurate simulations owing to dependent scattering effect arising from the wave nature of light [27,28]. In practical applications, the form of RTE can still be retained to describe the transport of diffusive radiation intensity, especially for highly scattering and optically thick random media where coherent intensity is strongly attenuated and diffusive intensity dominates. This treatment is widely applicable in many dense media radiative transfer problems with strong interference effects and has been validated by many authors in the field of radiation heat transfer [16,29,30], remote sensing [31] etc. In this condition, the radiative properties should be modified from independent scattering approximation to consider the dependent scattering effect [32,33]. In this paper, due to the complicated microstructure, direct theoretical modeling of radiative properties is impossible. The inverse process provides a convenient way to retrieve radiative properties with the consideration of wave interference instead of direct theoretical modeling based on Maxwell equations. Using the inverse method, we retrieve the radiative properties from numerically exact FDTD simulation directly based on different microstructures. This simulation can be regarded as a virtual experiment if high numerical accuracy is achieved, which avoids establishing complicated theoretical models as well as carrying out real experiments [18,19,25]. Then the inverse problem can be seen as the process that the radiative properties are retrieved based on the real experiment. This treatment enables us to build controllable microstructures for deeply studying microstructural influence on scattering. Thanks to the computation capability, the retrieved radiative properties are identified with the angular scattering intensity distribution obtained by FDTD method under different pore shape, which takes dependent scattering and anisotropic pore shape into account implicitly, so that the retrieved radiative properties can partly reproduce the simulation results.

Based on the previous researches, we have employed the finite-difference-time-domain method to study the microstructural effect on the radiative properties of TBCs quantitatively and calculated the total reflectance, transmittance and scattering coefficient [34–36]. However, absorption coefficient, scattering coefficient and phase function, which are intrinsically bound up with light scattering in TBCs, are seldom studied and the microstructural effect is usually ignored. According to our previous study, it has been found that the effects of anisotropy of radiative properties of TBCs on heat flux and transmittance are insignificant [37]. Similarly, owing to moderate refractive index of thermal barrier coatings, applying anisotropic radiative properties or averaged ones makes a little difference. The averaged radiative properties can also give an acceptable approximation for the presented particular coating microstructure. Therefore, to some extent, the averaged radiative properties can well describe the scattering in TBCs. Furthermore, it is more convenient to use averaged radiative properties in practical applications.

As a result, this paper aims to study the effect of anisotropic microstructure on radiative properties with the consideration of wave effect. The rest of this article is organized as follows. In Section 2 the microstructures of thermal barrier coatings are constructed based on the quartet structure generation set (QSGS) algorithm and the scattering intensity distribution of these anisotropic structures are calculated with the finite-difference-time-domain (FDTD) method. Then the asymmetry factor, scattering coefficient and absorption coefficient are retrieved simultaneously based on radiative transfer equation by combining Monte Carlo method with Particle Swarm Optimization. In Section 3, angular scattering intensity distribution and the retrieved scattering properties with different thicknesses, porosities, pore sizes and pore shapes are compared. And then we discuss the microstructural effect on radiative properties. Finally, conclusions about the scattering intensity distribution in the microstructures of TBCs are drawn. It has been found that microstructure plays an important role in radiative scattering in thermal barrier coatings.

2. Methodology

2.1. Assumptions and modeling

As for the calculation of the near-infrared radiative properties of TBCs, several simplifications are made as following:

(1) The complex refractive index of YSZ TBCs is determined from literature, shown in Fig. 2. The real part of refractive index n can be calculated in a three-term Sellmeier equation [38]

$$n^2 - 1 = \frac{2.117788\lambda^2}{\lambda^2 - 0.166739^2} + \frac{1.347091\lambda^2}{\lambda^2 - 0.062543^2} + \frac{9.452943\lambda^2}{\lambda^2 - 24.320570^2} \tag{1}$$

which is valid in the wavelength range up to 9 µm. The imaginary part κ can be calculated with the data from Dombrovsky et al. [11]. Considering that absorption and scattering characteristics of YSZ material are insensitive to small uncertainties of refractive index [39], it is reasonable to apply these data.

(2) The pores are separated widely enough that the each of them is located in the far field zones of other pores. The porosity studied in this paper is below 20% and the pore diameter is less than 4 µm. And the linear dimension of the structure is several hundred microns, much larger than the pore size and wavelength, which makes it reasonable to make this assumption.

(3) In order to save the computation time, two-dimensional model with randomly distributed pores (as illustrated in Fig. 1) is simulated in the present paper. Key microstructural parameters, including the pore size, pore shape and porosity, are considered.

This paper aims to study the effect of anisotropic microstructure on radiative properties with the consideration of wave effect in practical applications. Both three-dimensional model and two-dimensional model are of vital importance in the study of the microstructural effect. Considering that hundreds of cases need to be calculated in this work and it takes too much time and internal memory, it is unpractical to simulate realistic three-dimensional models through FDTD method in the present case. In addition, the two-dimensional model constructed in this paper can still represent the real sample to a certain extent and capture the main physical mechanisms. It also has profound implications in both theory and applications in other porous media like fiber [40–42].

In general, the microstructure of porous media is usually described with some statistical information like average porosity and