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Effect of anisotropy on thermal radiation transport in porous ceramics

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ABSTRACT

Aiming at promoting the fundamental understanding on relationship between the radiative transfer mechanism and microstructure of thermal barrier coatings (TBCs), here in this study, we numerically demonstrate the anisotropy of radiative properties of air plasma sprayed (APS) TBCs for the first time. The anisotropic microstructures of APS TBCs are quantitatively reconstructed based on Ultra-Small-Angle X-Ray Scattering (USAXS) measurement by the Stony Brook University group (*Li* et al., *J. Amer. Ceram. Soc., 92(2) p. 491–500, 2009*), in which the microscale pores and cracks are treated as oblate spheroids with a preferred distribution of orientations. The anisotropic mesoscopic radiative properties, including scattering coefficient/mean free path and asymmetry factor, are computed using the discrete dipole approximation (DDA) to solve Maxwell's equations. To fully depict the effect of anisotropy on radiative transfer in a macroscopic scale, a random walk scheme is thus proposed to solve the anisotropic radiative transfer problem in such medium, and the macroscopic transport mean free path describing energy diffusion process is derived. Results are further compared with those under isotropic assumption. By considering external blackbody as thermal radiation sources for the coating, we show that anisotropy of radiative properties affects the transmitted radiative heat flux across it considerably, especially at high operating temperatures and for thick coatings. On the other hand, in moderate operating conditions, the simplistic approach can also give an acceptable approximation on heat transfer for the presented particular coating microstructure. The present work provides a fundamental framework for studying radiative transport in anisotropic porous media.

1. Introduction

As one of the key concerns in industrial thermal barrier coating (TBCs) design and applications, thermal conductivity directly determines the thermal insulation performance of TBCs. At high temperature gas-turbine applications, both thermal conduction and radiation contribute to the effective thermal conductivity, and along with the fact that the operating temperature of gas turbines goes higher and higher, the contribution from thermal radiation also becomes prominent. Moreover, ceramic materials used as TBCs are typically transparent in the spectral range where high temperature (~1500 K) thermal radiation concentrates, which actually undermines the radiation insulation capability of TBCs [1–3]. For plasma sprayed TBCs, it is estimated by Golosnoy et al. [4] that at 1500 K, radiative conductivity is around 0.05 W–0.1 $\mathrm{Wm^{-1}\ K^{-1}}$, while at 2000 K it could reach 0.2 $\mathrm{Wm^{-1}\ K^{-1}}$, taking up a 20% proportion of the overall effective thermal conductivity. Unfortunately, although there are many measuring and modeling works on thermal conduction [5–9], few studies are carried out specifically to investigate the mechanism of thermal radiation transport inside TBCs, especially the quantitative analysis on the influence of their complicated microstructures, i.e., the grain boundaries and pore/crack architecture. There still exists a deficiency of a full understanding on microstructural-related thermal radiation transport inside.

The microstructures of TBCs are directly controlled by the fabricating methods and processing parameters. Air plasma sprayed (APS) coatings possess a splat-stacking structure, in which many interlamellar pores and intrasplat cracks exist [10]. In the last several decades, many advanced techniques are employed to study the microstructure of APS coatings, such as X-Ray Computed Micro Tomography (CMT) [11], Scanning Electron Microscopy (SEM) [7], Small Angle Neutron Scattering (SANS) [12] and Ultra-Small-Angle X-Ray Scattering (USAXS) [13], etc., which provide rich microstructural database for further modeling of thermal and mechanical properties. Therefore, it is also very straightforward to adopt the

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available microstructural information to derive the radiative properties of TBCs and deploy a radiative transfer study accordingly. For instance, Dombrovsky et al. [14], Manara et al. [15] and Yang et al. [16] regarded the pores in APS coatings as void spheres in the matrix of YSZ based on SEM images, and used Mie theory [17] to give adequately good predictions on the radiative properties.

However, due to the fabrication procedure of plasma spraying aforementioned, the voids in APS coatings are essentially not spherical, where, specifically, the intrasplat and interlamellar voids actually look like very flat disks, and globular voids are also not perfectly spherical. Many studies have demonstrated that the shape of voids has a great influence on the thermal conductivity and mechanical properties. Thus, the spherical void assumption in the above works on radiative properties is also not appropriate in a similar manner, because the size of the voids is indeed comparable with the wavelength of thermal radiation. In the recent works of our group, Zhang et al. [18] calculated the effective extinction coefficient using the direct numerical electromagnetic method of Finite-Difference Time-Domain (FDTD) and analyzed the effects of size, shape, orientation and space distribution of spheroidal pores and cracks. Wang et al. [19] presented a radiative property correlation model that combined the shape and orientation distributions of pores and cracks into consideration, and a good agreement with experimental data in the literature was achieved.

In addition, a careful observation on microstructure graphs of APS coatings can find that, the intrasplat and interlamellar voids inside all have preferred orientations, i.e., where intrasplat cracks are mostly aligned vertically to the coating surface while interlamellar pores are inclined to spread parallel to the surface. APS coating exhibits a significant anisotropy in thermal and mechanical properties due to this anisotropic alignment, which is confirmed by numerous experimental and numerical works on thermal conductivity and elastic properties [12,20,21]. However, the anisotropy of radiative properties has not been reported and taken into account by any previous studies yet. In fact, the anisotropy of radiative properties is also closely linked to the non-sphericity and specific orientation distribution of the micro pores and cracks, which means that the scattering coefficient and scattering phase function both depend on the direction of thermal radiation transport [22–24].

Traditionally, thermal radiation transport in anisotropic disordered/porous media didn't draw much attention in the heat transfer community, because the effect of anisotropy is usually negligible in terms of radiative heat flux or hard to determine for highly disordered microstructures, and on the other hand, solving the anisotropic radiative transfer problem is also rather troublesome. Nonetheless, in the field of biomedical optics, this problem arises due to the requirement of exact biomedical imaging demand. For example, Kienle et al. [25] examined the anisotropic optical properties of dentin in tooth with aligned cylindrical microstructures. They experimentally and numerically showed that backscattering pattern and time-resolved transmittance of human dentin are heavily affected by this anisotropy, very distinct from the results assuming isotropic optical properties. However, unlike optical imaging, spatial and temporal scattering patterns are not essentially the main concern of radiative heat transfer. Here in this paper, we will, on a macroscopic scale, demonstrate that microscopic anisotropy actually has a significant impact on the macroscopic radiative heat flux as well.

In the present study, the micro pores and cracks are treated as oblate spheroidal scatterers that act as dominating factors that influence radiative properties of APS coatings, and their sizes and aspect ratios as well as orientations are obtained from the USAXS data of Li et al. [13]. Anisotropic mesoscopic radiative properties are calculated by the discrete dipole approximation (DDA) based on microstructures. A random walk approach [26] is developed to trace the radiative "photon" transport process in such anisotropic microstructures, and build up the relationship between microstructures and macroscopic radiative heat transfer quantities. In a word, this work presents the anisotropy of thermal radiation transport in APS TBCs fully in microscopic, mesoscopic and macroscopic scales.

2. Microstructure reconstruction

The microstructures of APS TBCs are the natural consequences of the thermal spraying process, in which the individual molten droplets of the ceramic powder material are accelerated to a high speed and impact on the substrate, followed by a rapid flattening, solidification and cooling procedure, and spread into thin lamellae [27]. Typical SEM images of the cross sections of APS yttria stabilized zirconia (YSZ) coatings are shown in Fig. 1. Generally, there are three types of voids in APS coatings, including interlamellar pores formed by the rapid solidification process, intrasplat cracks due to thermal stresses and tensile quenching stress relaxation, and globular pores resulting from incomplete inter-splat contact or unmelted particles [12]. The interlamellar pores (the long axis) tend to be parallel to the coating surface while the intrasplat cracks prefer a normal orientation.

The actual microstructures, as well as thermal and mechanical properties, vary case by case, heavily depending on processing parameters like ceramic powder characteristics, spraying power, powder feeding rate, spraying distance and substrate temperature [10,28]. Although there are mature techniques to simulate the thermal and mechanical properties directly based on actual SEM images, it is more instructive to derive these properties from simple models based on simplified structures, which is more helpful and valuable for fundamental insights on the underlying physical mechanisms, and can provide guidelines for further design and optimization. For example, Sevostianov et al. [20] treated pores in plasma sprayed coatings as oblate spheroids, and quantitatively investigated the influences of porosity, orientation and aspect ratio of the spheroids on the coating's elastic properties. Lu et al. [29] also constructed a spheroid-pore-based model to study the elastic and thermal conductivity properties for electron beam-physical vapor deposition (EB-PVD) coatings. Therefore, it is urgently necessary to propose a similar modeling framework for radiative property studies.

In this study, a simplified microstructure model is proposed based on the advanced USAXS measurement of Li et al. [13] on yttria stabilized zirconia ceramics (YSZ), which quantified the microstructural information into an unprecedented degree. This model uses oblate spheroids with an aspect ratio of $a/b = 10$ to characterize the intrasplat cracks, oblate spheroids with an aspect ratio of $a/b = 5$ to represent interlamellar pores and spheres for globular voids, where a denotes the semi major axis and b the semi minor axis of the spheroidal void. Instead of adopting the orientation distribution function obtained from the USAXS data, in this model, the major axis of intrasplat cracks is set to be perpendicular to the surface and that of interlamellar pores is set to be parallel to the surface. The sizes and volume fractions (f_v) of these geometries are listed in Table 1, in which the intrasplat cracks have a typical semi-major axis size of 0.27 μm, the interlamellar pores have two typical semi-major axis sizes of 0.525 μm and 1.5 μm to account for the fine and coarse ones respectively, and the radius of globular voids is fixed at 0.94 μm. The chosen sizes and volume fractions of these geometries are confirmed by various SEM images to be adequately representative for the typical microstructures of APS coatings. The cracks, pores and voids are then assumed to be randomly distributed in the entire coating, shown in Fig. 2(a).