International Journal of Heat and Mass Transfer 79 (2014) 954–967

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Effect of interface on the thermal conductivity of thermal barrier coatings: A numerical simulation study

L. Wang [a,b,*], X.H. Zhong [a], Y.X. Zhao [a,c], J.S. Yang [a,c], S.Y. Tao [a], W. Zhang [b], Y. Wang [d], X.G. Sun [d]

[a] Key Laboratory of Inorganic Coating Materials, Chinese Academy of Sciences, Shanghai 201899, PR China
[b] State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, PR China
[c] University of the Chinese Academy of Sciences, Beijing 100039, PR China
[d] Laboratory of Nano Surface Engineering, School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, PR China

ARTICLE INFO

Article history:
Received 20 December 2013
Received in revised form 30 August 2014
Accepted 30 August 2014
Available online 19 September 2014

Keywords:
Thermal barrier coatings
Thermal insulation
Interface
Finite element simulation
Physical mechanism

ABSTRACT

Interface is an important structure in the materials, some rather peculiar physical phenomena can occur at the interface under the application of the exterior physical field. Especially, the grain boundary, phase interface and layer interface are significant factors for improving the thermal insulation behavior of thermal barrier coatings (TBCs). In this paper, finite element method was employed to simulate the heat transfer behavior of TBCs with different interfacial characteristic based on several different interfacial thermal resistance (ITR) models. The simulation results indicate that the heat flux around the interface has exhibited fantastic changing characteristic, the thermal insulation effect of TBCs would be enhanced with the area of the interface increasing. The interface roughness (amplitude) also has a very important effect on the effective thermal conductivity of the as-sprayed TBCs. A novel method, Computational Micromechanics Method (CMM), was utilized to depict the heat transfer behavior of actual coatings with irregular inner interface. The "thermal rectification" mechanism of heat diffusion around the interface make that the heat flux which passes through the interface has exhibited different flow characteristic compared with the positions without interface. In addition, some simple experiments have further verified the existence of the ITR between the bond-coat and top-coat. The investigation results will also provide us a powerful guide to design coating with high thermal insulation property using the physical theory and mechanism of the ITR.

1. Introduction

Thermal barrier coatings (TBCs) are very important structural and functional ceramic coating materials. The aspect of the thermal insulation reflects the functional characteristic. Very complicated physical mechanism exists in the process of heat transfer in the TBCs which should be understood deeply. Generally, the typical TBCs are composed of double layers (metallic layer and ceramic layer). The Y_2O_3 partially stabilized ZrO_2 (YSZ) layer which was usually acted as the thermal insulation layer in the TBCs has low thermal conductivity and plays a key and vital role in protecting the underlying super-alloy substrates, reducing the working temperature and increasing working efficiency of hot section components [1–3]. However, the durability requirements of TBCs for these applications are increasing rapidly with the development of the modern power industry. A higher temperature gradient will also be required. The most direct route to ensure that hot section components coated with TBCs have high Thrust-Weight ratio and a long lifespan is to improve the thermal insulation property. Demand for TBCs with excellent thermal insulation performance is becoming more and more urgent [4].

There are many factors that will affect the effective thermal conductivity of the TBCs, such as the intrinsic thermal conductivity of the ceramic layer of TBCs, the microstructure of the TBCs (architecture of the pores and cracks) and so on. Pores are often beneficial to decrease the thermal conductivity of the TBCs. Some nano-sized pores can also play a special role in changing the thermal shift or heat diffusion behavior in the coatings [5]. Cracks also play an important role in changing the thermal conductivity of the TBCs. Horizontal cracks may be helpful to increase the thermal insulation of the APS-TBCs, but segmentation cracks in the TBCs may be harmful to decrease the thermal insulation, although they can improve the thermal shock life as it can release some stress

* Corresponding author at: Key Laboratory of Inorganic Coating Materials, Chinese Academy of Sciences, Shanghai 201899, PR China. Tel.: +86 021 69906320; fax: +86 021 69906322.
E-mail addresses: L.Wang@mail.sic.ac.cn, glacier_hit@126.com (L. Wang).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2014.08.088
0017-9310/

concentration in the APS TBCs. In addition, the effective thermal conductivity of the gas trapped within the pores is influenced not only by the temperature and pressure, but also by the dimension of the pores at the micro-scale level [6]. This effect depends upon the Knudsen number, and is called Knudsen effect or rarefaction effect. Especially for submicron or nanoscaled pores, the decrease in the thermal conductivity of the trapped gas appears obvious [7,8]. Previous investigations have further shown that pores are of consequences in decreasing the thermal conductivity of materials, and the heat flux around the pores exhibited special flow state compared with the other positions without defects [9,10]. Golosnoy et al. [11] have reviewed the actual physical mechanism of how heat transfer takes place in plasma-sprayed (zirconia-based) TBCs during operation of gas turbines. They thought that the pore architecture (i.e., its morphology, connectivity and scale) has a strong influence on the heat flow. The contributions from convective, conductive and radiative heat transfer are considered under a range of operating conditions. The characteristics are illustrated with experimental data and modeling predictions. But the role of interface role has seemed to be omitted. In fact, interface is a very important phase in the composite system. The physical field in the interface often has the fanciful phenomenon [12,13].

When heat flows across an interface between two different materials (phases) or two adjacent layers, there exists a temperature jump at the interface, then the interfacial thermal resistance (ITR) can be defined as follows:

$$R = \Delta T / J \tag{1}$$

where J is the heat flux density, namely, the heat flow across a unit area in unit time. ΔT is the temperature difference between two sides of the corresponding interface. R is the value of the ITR. This problem was recognized as early as 1941 when Kapitza [14] discovered the temperature jump at an interface between solid and liquid. Generally, as a result of the temperature discontinuity at interfaces, a multi-phase or composite material will exhibit a reduced effective thermal conductivity due to the existence of the ITR.

Computational simulation is an effective routine to solve the ITR and the related heat conduction problems. Usually, two major computational methods have been used, i.e. micro-scale simulation and macro-simulation. Molecular dynamics (MD) simulation is an atomic-level (nano/sub-micro scale) method which has been used to simulate the thermal transport across micro-interfaces. It can describe the physical characteristic of the ITR actually. Generally, in the process of the MD simulation, the positions and momenta of a set of atoms evolve according to Newtonian equations of motion, restricting the validity of the atoms' movement to the classical limit. In this limit, MD simulation is an ideal and effective method for predicting thermal boundary resistance due to that the nature of the phonon scattering are not necessary being considered. The only required input to an MD simulation is the atomic interaction (i.e. potential function) [15]. The computational efficiently will improve as the classical interatomic potentials do not necessary to consider the electronic properties. The details of the thermal transport physics can be studied using lattice dynamics (LD) or non-equilibrium Green's function (NEGF)-based method. The ITR can be predicted and obtained by evaluating a theoretical expressions using the phonon properties which are calculated from these methods [16,17]. The LD and NEGF based methods can be used to obtain phonon properties at temperatures below the Debye temperature where quantum effects are important. The LD method can be also viewed as an equilibrium MD based approach which uses fluctuation dissipation theorem or the Green–Kubo method. It was usually used to calculate the heat flux as the function of the time in a balance system, and the thermal conductivity can be obtained by the Green–Kubo equation eventually. As for the NEGF-based approach, the effects of inelastic scattering can be modeled using this method. And the harmonic approximation is typically applied in order to reduce the computational expense when modeling interfaces [18–20].

Tomar et al. [21] have investigated the correlations between thermal conduction and mechanical strength in ZrB_2/SiC interface. Their analyses indicate that the strength reduction with increase in temperature is strongly correlated to phonon and electron thermal diffusivity change. With increase in temperature, phonon thermal diffusivity increases in the case of ZrB_2 and reduces in the cases of SiC as well as the interface. Tomar et al. [22,23] have also indicated that the thermalmechanical behavior or mechanical strength of the microstructural interface (including the phase interfaces in the multicomponent materials and grain boundary) in the materials can be also calculated by MD, and the classical MD replaces a comprehensive quantum mechanical treatment of interatomic forces with a phenomenological description in the form of an interatomic potential.

Indeed, in the field of the micro-scale heat transfer, the ITR of different material system is the hot topic of the investigation in the current, as the ITR will affect the heat transfer characteristic directly, and thus affect the design of the micro/nano components and the heat optimization.

Besides the MD simulation, finite element simulation (macro-scale simulation) combined with the experimental measurement is also an effective method to investigate the problem of the ITR. Based on the fact that the TBCs must have a certain thermal insulation capability, the typical structural characteristic of TBCs is full of defects (pores, voids and micro-cracks) in the ceramic coating. Some previous work investigated the influence of the interfacial conductance on the thermal conductivity of the TBCs from the experimental methods [24], and some macro-scale numerical (finite difference) and analytical models have been developed for the simulation of heat flow through plasma-sprayed coatings [25]. The effective thermal conductivity of the porous air plasma sprayed TBCs was strongly dependent on its intrinsic structure, such as pores, cracks, pore/coating interface, crack/coating interface, layer interface. Besides the scattering effect at the defects or interfaces, the ITR is another important factor which will affect the eventual effective thermal conductivity of the APS-TBCs. The radiative properties on the effective thermal conductivity of the TBCs has been investigated and extensively developed by Zhao's group [26]. They have developed a Finite-Difference-Time-Domain (FDTD) method which was employed to simulate the radiative heat transfer behaviors of TBCs with different types of microstructures [27]. In this paper, the ITR will be focused on. The current work will try to investigate the influence of the interface on the heat transfer behavior of the TBCs fabricated by APS from both the aspects of finite element simulation and the physical model of heterogeneous material systematically. Especially, the methods of the average t-matrix approximation (ATA) and coherent-potential approximation (CPA) have been used to describe the effective thermal conductivity of the actual TBC model. The "thermal rectification" of heat diffusion around the interface in the TBC has been calculated and discussed in detail based on several different physical models of the ITR.

2. Simulation method and procedure

2.1. Model basis for finite element analysis

Defects (pores, voids and micro-cracks) are usually distributed at random in the as-sprayed TBCs which was coated on the turbine blades (Fig. 1(a)) due to the complicated physical process of