

Design of Highly Reflective TBC System for Gas Turbine Application

Dongmie Wang and Xiao Huang Dept. of Mechanical and Aerospace Engineering, Carleton University, Canada Tel: (613) 520 2600 x 5707 Email: xhuang@mae.carleton.ca

> Prakash Patnaik Structures, Materials and Propulsion Laboratory Institute for Aerospace Research, National Research Council Tel: (613) 991 6815 Email: prakash.patnaik@nrc.ca

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Abstract

Ceramic thermal barrier coatings (TBCs) are playing an increasingly role in advanced gas turbine engines due to their ability to sustain further increases in operating temperatures. Higher operating temperature has resulted in increased radiation in the combustion chamber and turbine section. As reported, radiation within the wavelength range of $0.3 \sim 10 \,\mu\text{m}$ can transmit directly through zirconia based TBCs to the metal substrate, thereby causing the temperature to increase substantially on the metallic substrate. In order to effectively reduce thermal radiation transport through TBC systems, a ceramic based multiple layered TBC system was specifically designed in this research. This multiple layered TBC system has high reflectance to radiation in the wavelength range of $0.3 \sim 5.3 \,\mu\text{m}$ within which more than 90% of the radiation from typical gas turbine engine falls.

The multiple layered TBC system consists of a single layer ceramic material with low thermal conductivity and low refractive index, and several high reflectance multiple layered ceramic stacks, each stack designed specifically to reflect a targeted range of wavelength. A broadband reflection for the required wavelength range can be obtained using sufficient number of stacks. To achieve a high reflectance for each wavelength range, each stack must have multiple layers of at least two ceramic materials with alternating high and low refractive indices and the optical thickness of each layer is equal to a quarter wavelength in order to meet the condition of multiple-beam interference. The physical thicknesses of the high reflectance multiple layered structures in the present design can be tailored for different wavelength ranges so that a wide range of thermal radiation can be reflected, achieving more effective thermal radiation reduction.

A one-dimensional heat transfer model has been established by the authors and radiation transfer equations are used to compute the steady state heat transfer through the designed multiple layered TBC system. Using the established model and software developed, various coating material properties and thicknesses are used as input to this model and temperature distributions within the TBC system are then computed. The temperature reduction on the metal surface was estimated to be close to 90°C when multiple layered coating system is used. Further, substantial temperature reduction on the coating surface can also result.

1. Introduction

Thermal barrier coatings (TBCs) have played important roles in protecting superalloy substrate components in gas turbine engines from reaching excessive temperatures. Further increase in turbine inlet temperatures (TIT) for improved efficiency of gas turbines requires continuous development of new superalloys, better cooling schemes, and more importantly, superior thermal barrier coating systems. These new thermal barrier systems are comprised of coating materials, novel coating new microstructures and state-of-the-art coating deposition technologies. Currently, the most widely used ceramic material for thermal barrier applications is yttria stabilized zirconia (YSZ). In general, it has lower thermal conductivity, higher thermal expansion coefficient and superior high temperature performance than other traditional ceramic materials. As such, zirconia based ceramic material has been the material of choice for TBC applications in gas turbine engines.

The performance of TBCs is dependant on the coating deposition process. The commonly used deposition processes for the application of TBCs are plasma spraying (PS or VPS) and electron beam physical-vapor-deposition (EB-PVD). The TBCs produced by the PS process have lower thermal conductivity than those of the same compositions applied by EB-PVD, but are less strain compliant due to their laminar microstructure characterized by the existence of inter-splat pores and cracks parallel to the coating surfaces. Therefore, plasma sprayed coatings experience shorter thermal fatigue life and are mostly used on non-rotational components, such as combustion chambers and vanes, in gas turbine engines. On the other hand, TBCs produced by EB-PVD exhibit better strain tolerance and improved erosion resistance as a result of their columnar microstructure with elongated grains and pores aligned perpendicular to the coating surface. These characteristics make the TBCs applied by EB-PVD suitable for more demanding applications where higher thermal and mechanical loads are seen, as for example, turbine blades are coated with TBCs applied by EB-PVD process [1]. However, EB-PVD applied coatings exhibit higher thermal conductivities in comparison to that of plasma sprayed coatings due to the columnar structure and the inter-columnar pores, thereby limiting their use on combustion components which experience the hottest temperatures [2]. In order to fully exploit the advantages of EB-PVD coatings, extensive research on the reduction of thermal conductivity of EB-PVD coatings has been carried out worldwide, with primary focus on the modification of the chemical composition of the TBC materials as well as the coating's microstructure [3, 4].

Current materials used for thermal barrier coating applications are usually transparent or translucent to radiation in a certain wavelength range. Heat is transferred in ceramic materials via two mechanisms, namely thermal conduction and thermal radiation. Historically, most of the research effect has focused on reducing the thermal conductivity of the ceramic materials by means of modifying the compositions of the ceramic materials, improving the deposition processes, and developing completely new families of TBC materials. Research endeavour in reducing thermal radiation transport has been limited, in part, due to the fact that the thermal conduction dominates heat transport at lower gas temperatures. However, at higher temperatures radiation emitted from the hot gas shifts to a shorter wavelength range and falls within the transparent region for zirconia based ceramic materials. Under such service conditions, the temperature increase on the metallic substrate as a result of thermal radiation becomes significant. This effect has been observed by several researchers [2, 5 and 6].

According to thermal conductivity theory [7], the intrinsic thermal conductivity of ceramic coatings has an inverse dependence on temperature. However, the measured values of thermal conductivities have been found to conflict with this trend. Specifically, increasing thermal conductivity with rising temperatures has been observed. This increase in thermal conductivities is attributed to thermal radiation since the TBC materials are partially or fully transparent to thermal radiation at higher operating temperatures.

The temperature increase within a TBC system as a result of thermal radiation was evaluated by Siegel and Spuckler [8]. In this analysis, the effect of thermal radiation on the temperature profile of a TBC system operating in a gas turbine combustion environment was computed. The temperature increase on the metallic substrate due to the radiation effects was predicted to be as high as 50° C (Fig. 1) when compared to that of an opaque coating. Thus, an effective reduction of thermal radiation heat transfer could play a crucial role in offering improved thermal insulation to the gas turbine components.



Fig. 1. Temperature Distributions in Zirconia Thermal Barrier Coating on the Wall of a Combustor Compared With an Opaque Thermal Barrier Coating [8]

To effectively reduce the thermal radiation transport through TBC systems, some experimental studies have been carried out with an emphasis on increasing photon scattering within the coating as well as enhancing the coating's reflectivity. For example, increasing scattering defects such as microcracks and pores within the coating has been reported to be an efficient approach to reduce thermal radiation [4, 9]. In another study, a multiple layered coating structure [10] was designed to contain highly reflective metallic layers within the ceramic coatings as a means to reduce the radiation heat transport.

More recently, a new layered EB-PVD coating structure, with short range alternating layers of 8YSZ with high and low densities, was created by periodically interrupting incoming vapor flux during the PVD deposition process [11]. The variation in density resulted in a difference in the refractive indices of the alternating layers. The reflectance to the radiation with 1 μ m wavelength was increased from 35% for single layered coating to 45% for coating with 20 To further increase the coating's layers. reflectance, materials with different chemical compositions were used to produce multiple layered coatings. Preliminary experiments with alternating layers of 8YSZ (high refractive index) and Al₂O₃ (low refractive index) showed a further increase in the reflectance (Fig. 2) for coatings with both fixed and variable spacing. These multiple layered coatings were not, however, specifically designed to reflect broad band radiation as can be observed from the variation in reflectance with wavelength.



Fig. 2. Reflectance of Multiple Layered TBC with Fixed and Variable Layer Spacings [11]

Since the operating temperature in a gas turbine varies from component to component and during operation, it is therefore critical to design a coating structure that could cover a broad band radiation with increased reflectivity over a wider temperature range. In this paper, a highly reflective multiple layered TBC structure capable of covering a broad band radiation is presented.

2. Radiation Transport through Zirconia Based Ceramic Coatings

Within ceramic coatings, heat is transferred via two means: the thermal conduction which transfers heat from the hot coating surface to the metal substrate by phonon vibration; and the thermal radiation which includes both internal radiation emitted by the hot coatings themselves and external radiation emitted by hot gases and transmitted into the coatings by photons. Radiation within the transparent wavelength range for ceramic coatings, if not reflected, will be transmitted directly through the coatings to the metal substrate with little or no absorption. Radiation beyond the transparent wavelength range will be absorbed, and the absorbed radiation being re-emitted by the ceramic coatings.

The optical properties of YSZ were evaluated extensively [12]. The spectral hemispherical transmittance, reflectance and emittance of single crystal 13.5YSZ specimens with varying thicknesses were measured at room temperature. Thermal radiation can either be transmitted directly through the zirconia based material to the metal substrate, or be absorbed and reemitted depending on the wavelength of the radiation. A high transmittance and low absorption within the radiation wavelength range of 0.3~5.3 µm were observed as shown in Fig. 3. For radiation beyond 10 µm, YSZ is nearly opaque and as such the radiation is absorbed and subsequently re-emitted. For radiation within wavelengths of $5.3 - 10 \mu m$, it is partially transmitted and absorbed. Under a black body assumption, 80% of the radiation flux emitted from the hot gases within the temperature range of 1700-2000K, typical of a combustion environment, falls within the transparent wavelength range for YSZ. The design of the multiple layered coating structures covered in this paper will focus primarily on this transparent wavelength range.



Fig. 3. Room-Temperature Hemispherical Transmittance and Emittance /Absorption along the (100) Direction of Single Crystal 13.5 YSZ Specimens with Various Thicknesses [12]

Radiation transport through ceramic coatings can be evaluated using radiation transfer theory [13]. Using this theory, the radiation intensity i_{λ} along a path x within a medium that can be absorbing, emitting, and scattering are expressed as:

$$\frac{di_{\lambda}}{d\kappa_{\lambda}} + i_{\lambda}(\kappa_{\lambda}) = I_{\lambda}(\kappa_{\lambda}, \omega)$$
(1)

 $I_{\lambda}(\kappa_{\lambda}, \omega)$ in (1) is the source function, representing the sum of the gain by local blackbody emission $i_{\lambda b}(\kappa_{\lambda})$ and the gain by scattering into *x* direction. $I_{\lambda}(\kappa_{\lambda}, \omega)$ is expressed as:

$$I_{\lambda}(\kappa_{\lambda},\omega) = (1 - \Omega_{\lambda}(\kappa_{\lambda})) \cdot i_{\lambda b}(\kappa_{\lambda}) + \frac{\Omega_{\lambda}(\kappa_{\lambda})}{4\pi} \int_{\omega_{i}=0}^{4\pi} i_{\lambda}(\kappa_{\lambda},\omega_{i}) \Phi_{\lambda}(\omega,\omega_{i}) d\omega_{i}$$

$$(2)$$

where $\Phi_{\lambda}(\omega, \omega_{l})$ is the phase function and κ_{λ} , as a function of *x*, is the optical depth which is defined as:

(3)

$$\kappa_{\lambda}(x) = \int_0^x [\alpha_{\lambda}(x^*) + \sigma_{s\lambda}(x^*)] dx^*$$

where $\alpha_{\lambda}(x)$ and $\sigma_{s\lambda}(x)$ are the absorption coefficient and scattering coefficient, respectively. $\Omega_{\lambda}(x)$ is called the albedo and is defined as:

$$\Omega_{\lambda}(x) = \frac{\sigma_{s\lambda}(x)}{\alpha_{\lambda}(x) + \sigma_{s\lambda}(x)}$$
⁽⁴⁾

For one dimensional heat transfer analysis where the positive direction *x* points from the coating surface to the metal substrate, the radiation intensity of wavelength λ at position *x* is denoted as $i_{\lambda}^+(x,\mu)$, and the intensity in the opposite direction at position *x* as $i_{\lambda}(x,\mu)$ where $\mu = \cos\theta$ and θ is the incident angle of radiation onto the coating surface. The spectral radiation flux through the coating can be evaluated by integrating the intensity of radiation from both directions over 90 degrees:

$$q_{r\lambda}(x)d\lambda = 2\pi d\lambda \int_{\mu=0}^{1} \left[i_{\lambda}^{+}(x,\mu) - i_{\lambda}^{-}(x,-\mu) \right] \mu d\mu$$
(5)

As seen from equation (5), the value for the $[i_{\lambda}^{+}(x,\mu)-i_{\lambda}(x,-\mu)]$ term should be kept as low as possible in order to reduce the total radiation flux through the TBC system. This can be achieved by either increasing the reflected radiation, i.e., maximizing $i_{\lambda}(x,\mu)$. One effective method to increase reflected radiation is to use multiple layered coatings with alternating layers of high and low refractive indices. Unlike that in a single crystal, thermal radiation transferred through YSZ thermal barrier coatings deposited by either plasma spray or EB-PVD processes will experience scattering caused by pores and other defects existing in the coatings. The effect of scattering is currently being studied by the authors and will be reported at a future venue.

3. Design of High Reflectance Multiple Layered Coating Structures

The concept of multiple layered coatings containing stacks is proposed in this study. The purpose of this design is to effectively reflect the radiation within a wavelength range of 0.3~5.3 µm. This structure consists of several sets of highly reflective multiple layered stacks, with each stack being specifically designed to reflect a target range of wavelength. A broadband reflection of the required wavelength is realized by using a sufficient number of stacks. To achieve a high reflectance, each stack will include several alternating layers of ceramic materials with high and low refractive indices n_H and n_L , as shown in Fig.4.

The multiple layered stacks can be designed by calculating the physical thickness of each layer in the stack using [14]:



Fig.4. Schematic Diagram of High Reflectance Multiple Layered TBC Structure

Where d_H and d_L represent the thicknesses of the alternating layers within one stack, and n_H and n_L are the refractive indices of the alternating layers. H denotes layer with high refractive index and L denotes layer with low refractive index. λ is the radiation wavelength.

Assuming that the absorption of and scattering of the radiation in the high reflectance stacks are negligible in this study; the reflectance R for one wavelength range can be calculated as follows:

$$R = \left(\frac{\eta_0 B - C}{\eta_0 B + C}\right) \left(\frac{\eta_0 B - C}{\eta_0 B + C}\right)$$

$$\begin{bmatrix} B\\C \end{bmatrix} = \left(\prod_{r=1}^q \left[\frac{\cos \delta_r}{i\eta_r \sin \delta_r} \frac{(i \sin \delta_r)/\eta_r}{\cos \delta_r}\right]\right) \begin{bmatrix} 1\\\eta_m \end{bmatrix}$$

$$\delta_r = 2\pi n_r d_r \cos \theta_r / \lambda$$
(8)

(9)

(10)

(11)

where η_0 , η_r and η_m are the optical admittances for incident medium, high reflectance multiple layers and metal matrix, respectively. θ_r is the incident angle, d_r is the layer thickness of layer r, n_r is the refractive index of layer r, r is the layer number and q is the total number of layers within a stack.

For p-wave, $\eta_p = \frac{2.6544 \times 10^{-3} n}{\cos \theta}$; and for s-wave, $\eta_s = 2.6544 \times 10^{-3} n \cos \theta$.

Under normal incidence conditions, the reflectance in air or free space for one wavelength range can be simplified as:

$$R \approx 1 - 4\left(\frac{n_L}{n_H}\right)^{2q} \frac{n_m}{n_H^2}$$

The width of the wavelength is given as:

$$\Delta \lambda = \frac{2\lambda}{\pi} \sin^{-1} \left(\frac{n_H - n_L}{n_H + n_L} \right)$$

where n_m is the refractive index of the metal substrate and in the current study the optical property of metal substrate is considered to be that of TGO. Assuming $n_L = 1.5$, $n_m = 2.2$, and $n_H = 2.2$, the number of stacks and layers as well as the physical thickness of each layer can be calculated. Based on this design, the hemispherical reflectance of the multiple layered coatings with a total of 12 stacks, each stack containing 12 layers, is computed and shown in Fig. 5. The total physical thickness of the 12 multiple layered stacks is 44.9 µm. From this figure, it is seen that about 90% reflectance can be achieved under normal incidence, and this ensures a hemispherical reflectance of greater than 50% within the wavelength range of 0.3~5.3 µm.



Fig. 5. Calculated Reflectance of Multiple Layered Structure with 144 layers Under Normal Incident Condition

Based on the above calculation, it is seen that a total coating thickness of 45 µm is sufficient to reflect more than 50% of the radiation in a typical gas turbine environment. Further increase in the thickness of the multiple layers will not significantly increase the reflectance; rather, the thermal insulation capability of the overall TBC may be compromised due to the use of two different ceramic materials with high and low refractive indices. Since it is not possible to select both materials with the lowest thermal conductivity, it is determined that the multiple layered coating structures are best used in combination with single layered ceramic material. In the following section this design methodology is further described.

In this new multiple layered high reflective coating system, the multi-layered TBC system consists of a number of high reflectance multilayered ceramic stacks, a single ceramic layer, a bond coat and the metal substrate as illustrated in Fig. 6. There are four components to the TBC system: the multiple layered stacks incorporated in these systems to reflect thermal radiation in the wavelength range of $0.3 \sim 5.3 \mu m$; the single ceramic layer to provide reduced total heat transfer with its lower thermal conductivity; the bond coat to impart oxidation protection to substrate and bonding between metal substrate and TBC; and finally the substrate which constitutes load bearing functions.

Considering that the radiation with shorter wavelengths will be scattered more strongly, the sequence of the stacks in the multiple layers should be arranged in such a way to have the stack reflecting shortest wavelength range on the outer layer and the stack reflecting longest wavelength range in the inner layer.



Fig. 6. Schematic Representation of the Multiple Layered High Reflectance TBC Structures

There are two configurations for the multiple layered coating structure design. If the single layer is designed to be placed on top of the multiple layered stacks, it is required to have low scattering coefficient and low refractive index while having a low thermal conductivity at the same time. This low refractive index ensures a decreased internal reflection at the coating interface and a minimum internal radiation emissive in this layer [13]. The selection of the low scattering coefficient is to make certain that the reflected radiation from high reflectance multiple layers will not be scattered back. In addition, the single ceramic layer, when placed on the top of the multiple layered stacks, is directly exposed to the hottest environment. The phase stability is very critical for the performance of TBC system. A zirconate ceramic material with pyrochlore based structure is potentially the best choice for the single layer. On the other hand, if the single ceramic layer is placed between the multiple layered stacks and the bond coat, zirconates may not be the suitable materials since they may not be thermodynamically compatible with current MCrAlY bond coat and excessive thermal stresses may arise due to the mismatch in the coefficient of thermal expansion between zirconates and MCrAlY. The doped 7YSZ may provide a suitable option. Overall, the selection of materials and the related physical and optical properties have to be optimized systematically based on the service environment.

4. Computational Analysis of the Multiple Layered Coating Structures

Consider a multiple layered thermal barrier coating system in the environment of a gas turbine engine. The ceramic coating surface is exposed to the hot gases and heated by convection that results in a temperature increase on the coating surfaces. Assume that the heat transfer has reached a steady state, and there is no other heat source inside the system. The total heat flux reaches a constant. Within the single ceramic layer and multiple layered stacks, the heat is transferred by both thermal conduction and thermal radiation.

Additional assumptions are also made for the computation:

- 1. The absorption & scattering coefficients of single layer and multiple layered high-reflectance stacks are assumed to be the same as that of pure zirconia [8].
- 2. The refractive index does not change with wavelength.
- 3. The gray layer assumption is assumed.
- 4. The multiple layered stacks will be considered as a highly reflective single layer with an effective hemispherical reflectance of 50%.
- 5. The thermal conductivity of multiple

layered stacks is calculated using $l/k_j = l/k_H + l/k_L$.

- 6. The multiple layered stacks assume an overall refractive index of 2.2 [8].
- 7. The gas turbine hot gas is assumed to be a black body.

For a one dimensional heat transfer condition, the energy equation can be expressed as:

$$Q_{tot} = -k_j \frac{dT_j(x_j)}{dx_j} + q_{rj}(x_j)$$

$$j = \begin{cases} S \\ 1, 2, \dots, q \end{cases}$$
(12)

Where *S* is the subscript index for single ceramic layer, *q* is the number of coating layers. Q_{tot} is the total heat flux within the coatings, $q_{rj}(x_j)$ is the radiation flux at position *x* of the *j*th layer of the coatings along the *x* direction, k_j is thermal conductivity of the *j*th layer and $T_j(x_j)$ is the temperature at position *x* of the *j*th layer.

Within the metal substrate, the radiation flux has been totally absorbed and converted into heat due to the opaque characteristics of metallic materials, and only thermal conduction operates. Thus we have:

$$Q_{tot} = -k_m \frac{dT_m(x_m)}{dx_m}$$
(14)

Where k_m is the thermal conductivity of metal substrate and $T_m(x_m)$ is the temperature at position x_m within the substrate. Here the bond coat is assumed to be thin enough that the temperature difference between the bond coat and metal substrate is negligible. Detailed procedures used to solve the above energy equations were reported in [15]. Two structures illustrated in Fig. 6 (A) and (B) are simulated in this study. In the computational analysis presented in the following section, both Al₂O₃ and 7YSZ were selected as the materials for alternating layers in the multiple stacks. The selected properties of these two materials are given in Table 1.

Table 1 Selected Properties for Al₂O₃ and 7YSZ [8, [12]

	Refractive index	Thermal conductivity
Al ₂ O ₃	$n_L = 1.5$	$k_L = 2.4 \text{ Wm}^{-1}\text{K}^{-1}$
7YSZ	$n_{H} = 2.1$	$k_H = 0.8 \text{ Wm}^{-1}\text{K}^{-1}$

4. Results and Discussion

The temperature distributions within the coatings and the total heat flux through the TBC system for these two structures are calculated by solving radiation transfer equations and heat transfer equations using methods detailed in [15]. The total thickness of the multiple layered coating, including single layer and multiple layered stacks, is first assumed to be 250 µm whereas the thickness of the high reflectance multiple layered stacks is 45 µm. For comparison purposes, a coating containing a single layer of 7YSZ of the same total thickness was used as the base line in the computational analysis. The calculated temperature distributions for structures A and B are shown in Fig. 7.

It is found from these results that the structure B can achieve the most significant temperature reduction on the metal substrate. At an assumed environment temperature of 1727°C (2000 K), temperature reduction of $90^{\circ}C$ (K) can be achieved on the metal surface when structure B is used in place of a single layer 7YSZ of the same thickness. When structure A, where multiple layered stacks placed on top of the single layer, is used a temperature reduction of 46° C can be realized on the metal surface when compared to that of 7YSZ of the same thickness. It is clear that the high reflectance multiple layered coating systems, irrespective of the layer arrangement, can effectively reduce the temperature on the metal surface by reducing the radiation entering into the coating system.

Comparing the temperatures given in Fig. 7, it is found that in addition to the observed temperature decreases on the metal surface, the temperature on the coating surface can also be significantly reduced when structures A and B are used. In contrast to the temperature on the coating surface of mono-layered structure, structures A and B achieved further surface temperature reductions of 46° C (K) and 86° C (K), respectively. This is attributed again to the effective reduction of radiation entering the coating system. This reduction in coating surface temperature could play a significant role in extending coating's useful life.



Fig. 7. Temperature Distributions for a $250 \mu m$ Thick Multiple Layered Coating

Further analysis is carried out to compute the temperature distributions within the coating system with increasing total thicknesses from 250 μ m to 1000 μ m. In this simulation, the thickness for multiple layered stacks is kept to a constant value of 45 μ m. The temperature reduction is plotted using the difference in metal surface temperatures - as a result of using multiple layered coating and single layer 7YSZ of the same thickness - against the total coating thickness.

It can be seen from Fig. 8 that when coating structure B is used, the temperature on the metal substrate is consistently lower than that when structure A of the same thickness is used. This could be interpreted by the fact that both internal and external radiations are more effectively reflected in structure B since it is placed below the single layer. On the other hand, the structure A can only reflect the external radiation and as such a higher metal surface is seen due to the inability to reflect the internal emitted radiation. However, our most recent study has shown that this trend is significantly dependent upon the selection of materials and consideration of the scattering effect. The best design structure is to include two multiple layered stacks with single layer sandwiched in between.

The reduction in temperatures on the metal surface for both structures is less pronounced when the total coating thickness is further increased. This indicates that the multiple layered structure is more effective when used in thinner coatings.



Total Coating Thickness (micron)

Fig. 8. Temperature Reduction for Multiple Layered Coatings with Varying Total Thickness

In the simulation described above, the effect of grain and layer boundaries on the thermal conductivity has not been considered. However, from the theory of grain boundary phonon transport, the phonon mean free path is governed by the layer thickness. The thinner the coating layer thickness, the shorter the phonon mean free path. Consequently, the effective thermal conductivity of the high reflectance multiply layered stacks may be reduced due to the existence of nanodimensional grains or layers. It is anticipated that the high reflectance multiple layered coating system could contribute to reduced photon and phonon transports through the TBC system.

5. Conclusion

In this study, two multiple layered TBC coating structures have been designed. A computational analysis was carried out to predict the temperature distribution on the metal surface as a result of applying the multiple layered coatings. Based on the simulation results, it is concluded that the multiple layered TBC system can provide further protection to the gas turbine components used in hot sections by reducing metal surface temperature up to $90^{\circ}C$ (K).

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