Numerical Analysis of Composite Coating (\(\text{Al}_2\text{O}_3+\text{ZrO}_2\cdot5\text{CaO}\)) applied on Cast Iron

Abhinav1, Bal Sasmita2 and K Kapilesh3
Alliance College of Engineering and Design, Alliance University, Bangalore-106

Email: abhinavtechno5@gmail.com & sasmitabal@gmail.com

Abstract. A new method, the rule of the mixture is developed for the determination of thermal conductivity (K), allied properties viz. density and the volume of the individual composite coating powders. Optimum coating thickness through steady-state thermal analysis of composite coating (\(\text{Al}_2\text{O}_3+\text{ZrO}_2\cdot5\text{CaO}\)) applied on cast iron surface is carried out. Also, the thermodynamic behaviour of TGO and bond coat were simulated. The thickness of the topcoat, TGO, and the bond coat was varied independently in the range of 0.1 to 0.04 mm. Results show that topcoat thickness doesn’t have much influence on the heat transfer. However, TGO and the bond coat plays a crucial role in heat transfer study. Maximum heat resistance, 171.47 °C observed at 1 mm TGO thickness, compared to 88.94 °C in case of bond coat for the same coating thickness. It is also understood that 1 mm of optimal TGO thickness may be beneficial in the design of thermal barrier composite coating systems.

1. Introduction
Thermomechanical analysis is a well-known finite element technique to predict the residual stresses in the coating systems [1]. The residual stress induced in the thermally grown oxide (TGO) may lead to early spallation of the topcoat. Studies have been carried out to examine the stress built up at the interface of the topcoat and TGO and also between TGO and bond coat and found that TGO thickness and radii of curvature significantly affects the life of the coating systems. It has been also, found that at a higher thickness of TGO yields a high concentration of residual stress that may lead to early spallation of the topcoat [2]. A dual model based on a 2D wave profile was developed to visualize the attributes in the interface. In his study diffusion model was utilized to determine TGO growth [3, 4]. TGO growth behavior found to be one of the vital parameter affecting stress development. Extensive work has been carried out using a 2-D profile in this area [5]. Attempts have been made by many researchers to detect TGO profile but it was found that experimental methods for this purpose are very challenging [6, 7]. For this reason modeling of TGO will be more effective than conducting an experiment. A model based on the Finite element method (FEM) was proposed to find conductivity of Thermal barrier coating (TBC) made by EB-PVD [8]. A numerical model was developed to determine TGO growth and to study the strength of the topcoat which affects the life span of a TBC system [9]. In another investigation carried out on graded coating system and found that that presence of TGO with a thickness of 2-3 μm has a positive effect on the resistance against thermal shock [10]. In the present work mathematical model has been developed for the determination of thermal conductivity (K) using the rule of the mixture and also Optimum coating thickness through steady-state thermal analysis is carried out for the design of improved thermal barrier coating systems. The thickness of the topcoat, TGO, and the bond coat was
varied independently in the range of 0.1 to 0.04 mm and results are presented in terms of temperature drop and heat flux.

2. Mathematical Formulation - Rule of Mixture

A new mathematical model has been developed for the determination of thermal conductivity (K) using the rule of mixture. The conductivity “K” considered an inertial property. The effective conductivity, effective density and the total mass of the composite coatings include a topcoat (Al₂O₃+ZrO₂∙5CaO) and bond coat (Fe₃Ni₁₀Al) were calculated using the empirical relation shown in Equation 1, 2 and 3. The topcoat comprises of 50 wt. % Alumina, 45 wt. % Zirconia dioxide and 5 wt. % Calcia Oxide, similarly the bond coat contains 52 wt. % Fe 38 wt. % Ni and 10 wt. % Al. Their masses were calculated along with the density shown in Table 1. The K_eff of the topcoat and bond coat were found to be 6.8329 W/m²k and 69.99 W/m²k respectively at ambient temperature. The total mass of the coating can be calculated by multiplying effective density (ρ_eff) with total volume (V total) and the total volume is based on the available area and thickness of the coatings which is in the present case (10mm×10mm×5mm). The K_eff of TGO (7 W/m²k) obtained from the previously published literature [11].

\[
K_{eff} = \left( m_1/Mc \right) K_1 + \left( m_2/Mc \right) K_2 + \left( m_3/Mc \right) K_3
\]

(1)

\[
\rho_{eff} = 0.5\rho_1 + 0.45\rho_2 + 0.05\rho_3
\]

(2)

\[
M_c = \rho_{eff} \times V_{total}
\]

(3)

where m_1, m_2, m_3 are Individual mass, ρ_1, ρ_2, ρ_3 are individual density, K_1, K_2, K_3 are Individual thermal conductivity of the powders respectively and M_c is the total mass of the composite powder, ρ_eff, K_eff, \rho_{eff}, V_{total}. Total Effective density, thermal conductivity and Volume of the coatings respectively.

| Topcoat Powders | Al₂O₃ | ZrO₂ | CaO |
|-----------------|-------|------|-----|
| Mass, (m= wt.% ×Mc), (g) | 117.46 | 105.71 | 11.74 |
| Density(g/cm³) | 3.95 | 5.68 | 3.35 |

| Bond Coat Powders | Fe | Ni | Al |
|-------------------|----|----|----|
| Mass (wt.% ×Mc), (g) | 201.29 | 147.09 | 38.71 |
| Density(g/cm³) | 4.09 | 3.38 | 0.27 |

3. Methodology

A two-dimensional a physical model developed using commercial software (Ansys 15). A steady-state heat transfer analysis carried on the topcoat, TGO, BC whose thickness individually varies from 1mm to 0.04 mm. The heat is applied from the topcoat side (Al₂O₃+ZrO₂∙5CaO) considered as a heat source and a substrate end considered as a sink in the present model. The lateral side of the topcoat subjected to 375 ºC and the remaining sides were kept at the ambient temperature of 22 ºC. The selection of the temperature is based on approximate temperature commonly observed in the case of internal combustion engines (diesel engines). A perfect bonding established at the interfaces of the graded coatings. The physical model along with boundary conditions is shown in Fig. 1(a) & (b). The thermal conductivity of the topcoat and bond coat calculated using the rule of mixture discussed and obtained in section 2. A quadratic element was used to mesh the model. The total number of nodes and elements developed in the 2D model is approximately 17980 and 17280 respectively.
Figure 1. 2D physical model with (a) applied boundary condition (b) applied bonded contact relation at the interfaces

4. Results and Discussion

The thermal conductivity ($K_{eff}$) of Fe$_3$Ni$_{10}$Al (BC) and Al$_2$O$_3$+ZrO$_2$·5CaO (TC) was found to be 69.99 W/m$^2$k and 6.8329 W/m$^2$k respectively. Figures 2(a),(b),(c),(d),(e) & 3(a),(b),&( c) respectively show temperature and heat flux variation in topcoat, thermally grown oxide, bond coat, the substrate (CI) and composite systems. In the topcoat, no significant change in temperature drop noticed when the coating thickness varies from 1 to 0.04 mm refer Fig 2(a). It is understood that if the coating thickness varies in this range, temperature drop can be arrested. Also, one of the apparent reasons may be attributed to a very low thermal conductivity value, 6.893 W/m$^2$k obtained for the topcoat (Al$_2$O$_3$+ZrO$_2$·5CaO) mixture. However, temperature gradient (temperature drop) observed at all the thickness in the graded coating systems. In the case of TGO, BC, and substrate as the coating thickness change from 1 to 0.04 mm, a significant amount of temperature drop observed refer Fig.2 & 4. The reason for significant change attributed to the comparatively large magnitude of $K_{eff}$ in case of BC (69.99 W/m$^2$k) Fe$_3$Ni$_{10}$Al whereas in case of TGO ($K_{eff}$=7 W/m$^2$k) drop in temperature observed less compared to BC. The temperature distribution at TC, TGO, BC, substrate & on overall coating systems is shown in Fig.2 (a), (b), (c), (d) and (e) respectively. From the Fig.4 a constant decrease in temperature understood when the thickness of the coatings (BC, TGO & Substrate) varied from 0.04 to 0.09 and the rectangular parabolic trend observed when the thickness changes from 0.1 to 1 mm. The effect of thickness of TGO has an important significance in the design of graded coating systems [12]. In the heat transfer analysis, the heat flux behavior was also examined and found that the concentration of heat flux is more at the free edge compared to the coatings in contact. Also, an abrupt change in heat flux noticed when thickness varies in the range of 0.04 to 0.1 mm refer Fig.5. The reason attributed to an abrupt change in temperature over a small area where the heat couldn’t able to transfer the heat due to direct exposition to ambient temperature, however, the dissemination of heat flow found easily as heat flows from the free edge refer to Fig.3.
Figure 2. Schematic of temperature drop in (a) TC, (b) TGO, (c) BC, (d) Substrate (Cl), (e) In composite systems

Figure 3. Schematic of change in Heat flux at the interfaces of (a) TGO and TC, (b) TGO and BC, (c) BC and substrate
5. Conclusions

1. In the present graded coating system (\(\text{Al}_2\text{O}_3\+\text{ZrO}_2\cdot5\text{CaO}\)) an optimal coating thickness below 1 mm is recommended for extended life span.

2. Linear and Non-linear parabolic temperature signature examined at the thickness of 0.04 to 0.09 mm and 0.1 to 1 mm respectively irrespective of TC, BC, and TGO. However, change in heat flux shows a parabolic signature at above thicknesses.

3. Optimization results revealed that the concentration of heat flux was found to be more at the free end compared to the coatings in contact.

4. Since the conductivity of the bond coat is more compared to TGO, significant temperature drop observed in the bond coat compared to TGO. Therefore, from the above studies, it can be anticipated higher the bond coat thickness lesser will be the temperature drop.
References

[1] Kski K., Arthur, J., 2013, Predicting failure within TBC system: Finite element simulation of Stress within TBC system as affected by sintering of APS TBC, geometry of substrate and creep of TGO. Engineering Failure Analysis, Vol. 27, pp 150-164.

[2] T.-J. Chuang, E. R. Fulle Jr., 2002, Analysis of Residual Stress State in Thermal Barrier Coatings. Fracture Mechanics of Ceramics, Vol. 13, pp 169-178.

[3] Hermosilla, U., Karunaratne, M. S. A., Jones, I. A., Hyde, T. H., & Thomson, R. C., 2009, Modelling the high temperature behaviour of TBCs using sequentially coupled microstructural–mechanical FE analyses. Materials Science and Engineering: A, Vol. 513, pp 302-310.

[4] Busso, E. P., Lin, J., Sakurai, S., & Nakayama, M. 2001, A mechanistic study of oxidation-induced degradation in a plasma-sprayed thermal barrier coating system: Part I: model formulation. Acta materialia, Vol. 49(9), pp 1515-1528.

[5] Bednarz, P, 2006, Finite element simulation of stress evolution in thermal barrier coating systems Ph.D. thesis, Forschungszentrum Julich GmbH, Julich.

[6] Schweda, M., Beck, T., & Singheiser, L., 2012, Thermal cycling damage evolution of a thermal barrier coating and the influence of substrate creep, interface roughness and pre-oxidation. International Journal of Materials Research, Vol. 103(1), pp 40-49.

[7] Czech, N., Juez-Lorenzo, M., Kolarik, V., & Stamm, W., 1998, Influence of the surface roughness on the oxide scale formation on MCrAlY coatings studied in situ by high temperature X-ray diffraction. Surface and Coatings Technology, Vol. 108, pp 36-42.

[8] Lu, T. J., Levi, C. G., Wadley, H. N., & Evans, A. G., 2001, Distributed porosity as a control parameter for oxide thermal barriers made by physical vapor deposition, Journal of the American Ceramic Society, Vol. 84(12), pp 2937-2946.

[9] Hille, T. S., Turteltaub, S., & Suiker, A. S. J., 2011, Oxide growth and damage evolution in thermal barrier coatings. Engineering Fracture Mechanics, Vol. 78(10), pp 2139-2152.

[10] Kaveh Torkashvand et al., June 2018, Effect of TGO thickness on the Thermal Barrier Coatings Life under Thermal Shock and Thermal Cycle Loading, Ceramic International, Vol. 44(8), pp 9283-9293.

[11] Vaben, R., Giesen, S. and Stöver, D., 2009, Lifetime of Plasma-Sprayed Thermal Barrier Coatings: Comparison of Numerical and Experimental Results. J. Therm. Spray Technol., Vol. 18(5-6), pp 835-845.

[12] Kaveh Torkashvand et al., September 2018, Effect of temperature and ceramic bonding on BC oxidation behavior in plasma-sprayed thermal barrier coatings, Surface & Coatings Technology, Vol. 349, pp 177-185.