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Coating thickness and roughness effect on stress distribution of A356.0 under thermo-mechanical loadings

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Abstract

Cast aluminium-silicon alloy, A356.0, is widely used in automotive components such as diesel engine cylinder heads and also in aerospace industries because of its outstanding mechanical, physical, and casting properties. Thermal barrier coatings are applied to combustion chamber in order to reduce fuel consumption and pollutions and also improve fatigue life of components. However, studies on behaviour of A356.0 with thermal barrier coating are still rare.

The purpose of the present work is to simulate stress distribution of A356.0 under thermo-mechanical cyclic loadings, using a two-layer elastic-visco-plastic model of ABAQUS software. The results of stress-strain hysteresis loop are validated by an out of phase thermo-mechanical fatigue test. Then, ceramic coating thickness effect on stress distribution of test specimens is investigated. Different thicknesses from 300 to 800 microns of top coat and also roughness of the interfaces are simulated to get best stress gradient which can cause an improvement of fatigue life. Studying realistic interface roughness shows the critical area of tensile stress which results in crack initiation. Furthermore increasing TC thickness results in stress growth.

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1. Introduction

Thermal Barrier Coatings (TBCs) can be applied to the combustion chamber of diesel engines in order to allow higher combustion temperatures which increase the thermal efficiency or to achieve lower base
metal temperatures. This can cause an increase in fatigue life of high temperature components and also reduction in fuel consumption and some emissions such as hydrocarbons [1-4]. A TBC consists of two-layer systems which are a heat-resistant ceramic top coat (TC), mostly Yttrium stabilized Zirconium (YSZ) with typical composition ZrO2-8%Y2O3 and also a metallic bond coat (BC), mostly made of Ni-Cr-Al-Y. These layers were applied by Air Plasma Spraying (APS) to the substrates.

Aluminum alloy cylinder heads, as a part of combustion chamber, are required to meet two essential material requirements including the resistance to deformation under combustion pressure and assembly loads and also the toughness at high temperatures of flame to prevent cracking [5]. These thermo-mechanical loading conditions can only be handled by a combination of modern cooling methods or protective coatings such as TBCs which leads to lower thermal stresses due to lower temperature gradient. The TBC provides a temperature drop of 100-200°C due to its low thermal conductivity [6].

The different aspects of exposure conditions and failure mechanisms of TBC systems must be considered in order to model and predict the fatigue life. A major weakness is the interfaces between the bond coat and the substrate and also between the bond coat and the top ceramic coat. These interface regions undergo high stresses due to the mismatch of thermal expansion between materials and due to interface roughness [6]. Another failure mechanism is the development of thermally grown oxide (TGO) at the interface formed as a result of bond coat oxidation at about 900°C [7].

One of the key issues of the present paper is to investigate the influence of top coat thickness and the interface roughness effect on stress distribution by using finite element (FE) modeling of TBC systems. FE simulation of TBC systems on aluminum alloys is rare and most researches were about modeling of coating on super alloys. Finite element analysis for the development of residual stresses during spraying of zirconia-based thermal barrier coatings is presented by Bengtsson and Persson [8] and also Widjaja et al. [9]. To simplify the approach, a flat interfaces hypothesis is assumed between dissimilar materials. The time-dependent model of CMSX-4 is presented by Schubert et al. [10]. The oxidation process has been simulated by growth the thickness of TGO elements. The development of cracks at the TGO/BC interface has been simulated using cohesive zone elements. Hsueh and Fuller [11] examined the effect of curvature and height of the interface asperity on stresses formation during the service.

Bialas [6], Ranjbar-Far et al. [7] and Sfar et al. [12] modeled the top coat and bond coat interface roughness, the volume growth of the oxide layer, the cyclic loading and the creep relaxation to predict their effects on the stress distribution by considering a homogenous type for the temperature distribution. Liu et al. [13] performed experimental and numerical life prediction of thermally cycled thermal barrier coatings by considering different thicknesses for top coat. Bialas [6] performed a numerical simulation of crack development within APS TBC systems. The TGO thickening and creep deformation of all system constituents is modeled. Two dimensional periodic unit cell is used to examine the effect of interfacial asperity on stress distribution and subsequent delamination of APS TBC. The finite element analysis shows that the development of the interfacial crack allows for a micro-crack formation within APS TBC. In another paper, Ranjbar-Far et al. [14] presented a new step in the objective to continue the development of the TBCs performance by considering a non-homogenous temperature model and using the finite element code ABAQUS to study the thermo-mechanical behavior of the thermal barrier coating systems. The results show that the oxide formed on rough TC/BC interface during service has an intrinsically different morphology and different growth rate compared to those formed when considering a homogenous temperature.

In the present paper, coating thickness effect on stress distribution of A356.0 is performed under thermo-mechanical loadings. The development of TGO is neglected due to temperature range below 500°C, but the surface roughness of the interfaces between substrate and BC and also between BC and TC layers is considered. As a result, thermo-mechanical stress distributions for different top coat thicknesses are drawn in the figures.

2. Finite Element Simulation Scheme
FE simulation has taken into account to study stress distribution in TBCs and thus evaluating the optimized thickness. Many efforts have been done to numerically investigate stress development in TBC systems. Often times a two dimensional unit cell symbolizing a single asperity has been used to be representative for the entire surface area stress field [6]. For the reason that interface profile between substrate/BC and BC/TC has a random nature, the idealized simulating of a single asperity cannot predict the real behavior of TBC system. Furthermore, the substrate/BC roughness has not been considered in former simulations. The reason is that in gas turbine application for TBC systems, temperature ranges are high and predominant failure mechanism is the development of TGO at about 900°C in BC/TC interface [7]. In the present paper, the cylinder heads application for TBC system is studied where the working temperature is below 500°C and therefore TGO growth is not taken into account. A thermal shock test has been performed on 3 different thicknesses of TC. This experiment was carried out by repeating flame heating of the specimens to a specific temperature and abruptly quenching in 40°C water. Failure analysis shows that coating layers including both BC and TC were separated from based material (Figure 1). On one of the specimens with thinner TC thickness, some parts of BC layer was observed. This is the reason for consideration the roughness of substrate/BC interface.

To improve modeling of a multi layer system, a picture of an optic metallographic microscope is taken from a sample which is shown in Figure 2 (a). Then, the profile between substrate/BC and BC/TC interface is extracted by the aid of image processing. This profile is used instead of a single asperity for modeling. Based on the above discussion, a two dimensional axisymmetric model of the specimen is created in ABAQUS finite element simulation package. The FE model is shown in Figure 2 (b) where axisymmetric condition is considered for A-face. The transient de-coupled temperature-displacement analysis is used in present investigation. A finer mesh was used for interface layers where excessive gradient of temperature and stress may occur.

![Fig. 1. The specimens after separation of coating layers from substrate in thermal shock test](image)

![Fig. 2. (a) An optic metallographic microscopic picture for coated sample; (b) FE model of the specimen with meshed TBC system](image)

The TBC system is composed of A356.0 substrate, Ni-Cr-Al-Y bond-coat and ceramic top-coat (ZrO$_2$-8%Y$_2$O$_3$). For material properties, the cyclic hardening characteristic is expressed by the isotropic hardening law. The non-linear kinematic hardening component describes Bauschinger effect by explaining the translation of the yield surface in stress space through the back-stress. This law is defined
as a supplement combination of a linear term and a relaxation term, which presents the non-linearity (See [15] for complemented data). Other material parameters are considered as [7, 14].

The load cycle is composed of thermal and mechanical cycling in synchronized out-of-phase (OP) triangular waves. The temperature range is from 100 to 250°C in 10 minutes which is applied on D-face of the specimen in Figure 2 (b). The mechanical strain amplitude varies in a range between ± 0.5 % which is applied on B and C-faces of the specimen in Figure 2 (b). The OP thermo-mechanical loading is shown in Figure 3 (a). The mentioned loading simulates cylinder heads at the severest engine condition [5]. For models considering the absence of crack propagation, the influence of the thermal cyclic loading on stress distribution is not important [7], therefore, a single cycle is considered.

To ensure that the model is working properly based on material data, a comparison between experimental data of A356.0 without coating layers under thermo-mechanical loading has been considered. The comparison of hysteresis loop is shown in Figure 3 (b). As it can be seen, the simulation is in good agreement with experimental data especially in tension, which is our area of concern.

3. Results and discussion

Thermo-mechanical stresses in y-direction and along the interfaces of substrate/BC and BC/TC are shown in Figures 4-5 for different thickness of TC layer from 300 to 800 (micron). The thinner thickness, about 250 (micron) of TC layer is proper for wear applications and has less fatigue life [1] and thus, the thickness less than 300 (micron) is not considered in this study.

As it can be seen in figures, the stress range in BC layer is more than substrate and TC. Also, in the BC/TC interface, most stresses are compressive at BC side and the stress rang in TC layer is less than anywhere else. Values of yield strength for TBC vary from 10 to 100 MPa and for BC is equal to 270 MPa, respectively [7,14]. Although yield stress of BC layer is more than TC, but still the ratio of developed stress to yield stress is higher in BC layer. Excessive stress in BC compare to other layers can be a reason for the separation of BC from based material as a failure mechanism in TBC system.

We have studied a large and realistic spectrum of interfaces waves and their bilateral influence which has not been done before. In Figure 2 (a), near X = 0.9 (mm), the roughness of both substrate/BC and BC/TC interfaces has the same wave in an in-phase situation. In this location, shown in the circles on Figures 4-5, the maximum stress is occurred. Stresses in BC/TC and substrate/BC in BC side are both tensile in this region. This can be due to the existence of the thinnest thickness of BC layer which can cause combination of stress fields of asperities in either interface and also can be assignable to sever undulations(high amplitude in short wavelength). In Figure 5 (b), although the maximum stress is happened at difference places but also at X = 0.85 (mm) the magnitude of the stress is almost high as the maximum stress. Moreover in fig.4-b, X=0.35 has also great tensile stress but in figure 5-a, this region hasn’t a considerable stress. This region has severed undulation but the thickness of BC is approximately high.

![Fig. 3. (a)Thermal and mechanical loadings applied to the specimen; (b) Verification of stress-strain behaviour of A356.0](image-url)
Figure 4 shows that Sy component of stress at substrate/BC interface is maximum in BC side. Max tensile stresses occur in this region and near the peak of the rough bond coat, at about X = 0.9 (mm). Thus, this is the most probable area of failure which produces delamination cracks parallel to the interface and Sy component of stress lead to the much more likely mode-I fracture. So detached of the TBC system from substrate (in cylinder heads application) is more probable than separation of BC and TC (which is more probable in gas turbines application).

As another result, the stress for 800 (micron) thickness of TC layer is more than the other thicknesses. In other words, increasing the thickness results in stresses growth. In the region of maximum stress, the stress amplitude of the thicker TC layer is more than the thinner TC layer. Thus, thinner thicknesses have better fatigue lives due to less stresses. This is also observed in thermal shock test where failure (separation of BC layer from based material) occurred after 333 cycles for 300 (micron) thickness of TC layer however for the thicker TC, the fatigue life was about 305 cycles.

Stresses in the ceramic layer at the peaks of BC profile, are roughly two orders of magnitude higher than expected at smoother interface. Thus, the rough interface of TBC system, not only increases initial adherence with the coating layers through mechanical interlocking but also drives its delamination and reduction in life [16]. The critical area in the present investigation, in Figure (a), at about X = 0.9 (mm), in realistic condition, is a place where is not covered by sand blast process and thus a peak in roughness is seen there. This area is more likely to crack comparing to a region where is over blast and valley occurs. Therefore, to improve the TBC life, sandblast should be used with full coverage of the surface.

![Fig. 4. Thermo-mechanical stresses for different TC thicknesses, Sy in substrate/BC interface, (a) substrate side; (b) BC side](image)

![Fig. 5. Thermo-mechanical stresses for different TC thicknesses, Sy in BC/TC interface, (a) BC side; (b) TC side](image)
4. conclusion

Thermo-mechanical stress analysis of a realistic rough interface of a Plasma sprayed TBC systems is performed using FE method in ABAQUS software. As a result, stresses in the ceramic layer at the peaks of BC profile, are roughly two orders of magnitude higher than expected at smoother interface. Although the rough interface of TBC system increases initial adherence with the coating layers, but it also causes decrease in fatigue life. Studying the thickness effect of TC layer shows that increasing TC thickness results in stress growth. Thus, thinner thickness of coating has better fatigue life, as it was also observed in thermal shock test.

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