Investigation of Thermal Behaviour of (Steel Alloy (44K2), Titanium Aluminide, SiO₂, Al₂O₃, ZrO₂) Materials on Internal Combustion Engine Valves

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Abstract—The paper aims to study the thermal stresses on an exhaust valve body with and without using the Thermal Barrier Coating technique (TBC) in the valve face region. A 2-dimensional model is created for the numerical analysis. The work is carried out with the aid of the ANSYS- APDL package. The procedure of the numerical analysis is divided into two processes. The first process is the thermal analysis to obtain the temperature values, which are set up as thermal loads for the structural analysis in the second process. The coating of the valve is carried out through three steps of analysis by selecting a single layer of TBC, a double layer of TBC, and a triple layer of TBC. Three types of TBC materials are taken in this work, which are SiO₂, Al₂O₃, and ZrO₂. The location of TBC type for the double and triple cases is taken into consideration, in the steps of analysis of double and triple design of exhaust vale coating is done by changing of the material type of TBC which it is on the upper or lower concerning the valve face. The results showed that using the SiO₂ material as a TBC in the case of single, double, and triple coating of the exhaust valve face gives a low value of thermal deformations and thermal stresses. The stresses in steel alloy in cases without and with TBCs as compared to titanium valve showed a good reduction in thermal stresses for the titanium aluminide exhaust valve.

Index Terms— Thermal Barrier Coating Material, Finite Element Method, Thermal Stresses

I. INTRODUCTION

Improvements in the thermal and mechanical behavior of Internal Combustion (IC) engine components are required to reduce the failure of the engine parts; in particular, moving parts such as piston, rings, connecting rod, crankshaft, camshaft, and both inlet and exhaust valves.

In general, thermal and mechanical stresses are considered to be one of the problems of failure in the IC engine parts when they are subject to high loads and vary in operating conditions in such a way that chemical energy is converted to thermal energy in the combustion chamber (the main thermal source region of the IC engines), and part of the thermal energy is distributed in the exhaust valve body because it is subject to combustion gas flow at high temperatures, and this contributes to the formation of high thermal stress problems in the exhaust valve body.

Therefore, to minimize these stresses it is required to lower the thermal loads. Product gases have high temperatures and lead to create high thermal stresses problem in the exhaust valve body. In general, one of the solutions used to reduce the high thermal stress issue is coating by using layers of insulator materials to the coat valve body acting as a thermal barrier.

Variable operating conditions of the internal combustion engine tend to release some hydrocarbons, carbon monoxide emissions, and fuel soot after combustion, which is why the Thermal Barrier Coating (TBC) materials are used to lower the temperature of the IC engine components and to achieve proper combustion and low emissions Cerit [1]. Thermal barrier coatings are mainly used in high thermal field areas, such as gas turbine blades and internal combustion engine parts, to improve their operating efficiency. Coating affects engine components either by increasing or decreasing when used in any part of the IC engine.

The analysis of the heat transfer for the IC engine is not simple due to the continuous change of boundary conditions within the cylinder and it is not easy to determine the exact value of the temperature and the coefficient of heat transfer, Low thermal conductivity material coating which enhances the piston's performance by lowering the non-inflamed hydrocarbons and heat loses Prasad and Sharma [2]. Every engine is ideal if it can improve its efficiency and reduce its emissions. Researchers have therefore made a great deal of effort to achieve this objective. Gebauer [3] studied the development of valves made of TiAl metallic alloys. As a result, performance is improved and the cost of the internal combustion engine is reduced by Hornik et al [4] when the thermal stress in the exhaust valve was studied using the carbon layer in the turbocharged diesel engine

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Thermal loads in the exhaust valve of the turbocharged diesel engine were determined using the two-zone combustion model and the finite element method.

They also found that the carbon deposit layer had an impact on the increase in the temperature gradient value and thermal stress in the exhaust valve when the valve head surface covered by the carbon film generates additional thermal resistance, the valves become less hot and safer for thermal loads.

In this case, by increasing the thickness of the carbon film, the temperature difference in the valve decreases, while the temperature difference between the center of the valve and the endpoints is 5 °C with a carbon film thickness of 50 μ m and decreases to 1 °C with a carbon film thickness of 0.1 mm. The effect of the carbon film thickness on the exhaust valve was investigated numerically by Karamangil et al. [5] using FEM. They concluded that the stress value of the inertia forces could be reduced by decreasing the mass of the valve.

Cerit and Coban [6] studied the improvement of the diesel engine performance by obtaining temperature and thermal stress distributions on the zirconium-coated aluminum piston crown in a plasma-sprayed magnesia-stabilized case. The investigation was conducted for impacts of the thickness of the coating, which ranged from 0.2 to 1.6 mm, followed by a comparison of the results between the coated and uncoated piston using the finite element method. Maximum combustion chamber temperature was modified using the thermal barrier coating (TBC) to increase the thermal efficiency of the engine.

The thermal performance of the piston is increased by increasing the thickness of the coating material. The analysis indicated that the calculated stress values are lower than the permissible stress values of the materials. The development methods of the finite element method (FEM) models of the surface coating piston were divided in detail into several 2D and 3D FEM models of the coating piston, and the FEM analysis of the models undergoing thermo-mechanical loadings was carried out

The analysis showed that the high efficiency of the coating as a thermal resistance in some parts of the piston using a coating material indicated a massive decrease and 40 percent lower than the temperature for the same piston without a coating Kurowski et al. [7].

Intake and exhaust valves are an important component of internal combustion engines, and their main task is how to control gases as well as control their flow. To protect these valves from the high pressure and temperatures, they are exposed to during the operation of the internal combustion engine. Mahfoudh et al. [8] contributed to predicting the temperature distribution of intake and exhaust valves by using the finite element method for commercial Ansys-CFX. It is found that to avoid overheating of exhaust valves, significant changes in boundary conditions and materials were required.

Satyanarayana et al. [9] are studying the thermal analysis of the IC engine with the help of Catia and ANSYS for the valve modeling under study. The analysis is performed for five different materials: Stainless Steel, Nimonic 80A, Nimonic 105, Aluminium Nit Ride, Silicon, Nitride, and finally, aluminum Nitride material was found to be suitable for exhaust valve due to less stress.

The analysis of thermal and structural of valve with two types of materials (Nimonic 80A and Nimonic 105A) are carried out by Snehal et al. [10] To the engine valve. Nabeel et al. [11] are studying numerical analysis to reduce mechanical loads using the coating technique for the coating of the piston head.

Subodh et al.[12] studied the temperature and thermal loads of a ceramic-coated valve for a diesel engine, where the valve head is coated by plasma-spray zirconia. The thickness of coating valve head which to be investigated was from 0.2 to 1.0 mm, the results indicated that the maximum value of temperature increased up to 33.81% for the 1.0 mm thickness of thermal barrier coating(TBC) with comparing to the valve which is traditional uncoated. Also, the average stress values on the valve with respect to increasing TBC thickness on the valve head surface. Liang Lui et al [13] they have investigated numerically the maps of temperature for the exhaust valves with sodium-cooled for internal combustion engine enhanced with a turbocharger. The valve motion was modeled using a dynamic mesh approach, and sodium sloshing was modeled using a volume of fluid multiphase model to investigate the two-phase flow phenomenon. To extract the temperature map, the average values of these parameters are calculated and incorporated as boundary conditions in a finite element model developed in the commercial code ANSYS. The greatest temperature differences between the simulated and test findings in the axial and radial directions of the valve were 45.5 $\,$ C and 37.2 ℃, respectively. Ziming Yan et al. [14] presented a study of a 0D model for engine thermodynamic coupling with a 1D transient heat transfer model of the coating and pistonThermal barrier coatings (TBCs) on the inside of cylinders reduce heat transfer losses and improve thermal efficiency. Thick TBCs have been proven to have a negative impact on traditional combustion modes, lowering volumetric efficiency and increasing the likelihood of end-gas knock. Due to a reduction in heat transfer during the compression stroke, the volumetric efficiency actually increases by 7.4 percentage points with a thicker coating, allowing for a lower intake temperature required to reach auto-ignition. Arif Taibani et al. [15] researched diesel engine pistons with respect to the performance analysis for the combined combustionconjugate heat transfer. The analysis is done for the design of pistons with partial insulation. For a prototype engine, the full-coverage coated piston technology with 0.5 mm thick Yttria Stabilized Zrconia (YSZ) coating was compared to the non-insulated baseline aluminum piston. When compared to a full-coverage insulated piston with a thermal efficiency of 2.06%, partial coverage insulation demonstrated a 1.98 percent improvement in thermal efficiency.

In this analysis, different combination materials (TBC), four types such as Gd₂Zr₂O₇, MgO-ZrO₂,

 $La_2Zr_2O_7$, and $Sm_2Zr_2O_7$ are used. The analysis is carried out using the Finite Volume Method (FVM) and the governing equation was solved by the multi-physics package COMSOL version 5. The results showed that $La_2Zr_2O_7$ is the best type of combined TBC materials

This paper presents a study of the influence of the thermal barrier material used as thermal insulators in the exhaust valve head surface with respect to the thermal stresses, and its concentration in the valve body, where three types of coating materials are used in the analysis procedure. And investigating the impact of the exhaust material type in the reduction of the thermal stresses.

II. ANALYSIS PROCEDURE AND ASSUMPTIONS

The analysis is divided into two sections. The first section includes a thermal analysis for a two-dimensional model in which the valve is treated with thermal loads. The results of the analysis of the first segment will be taken as loads for the second analysis, i.e. the structural analysis, and the final results will be estimated. Fig. 1 shows the two-dimensional exhaust valve model, all dimensions of the valve in inches.



Figure 1. Exhaust valve dimensions.

The considered assumptions into the current analysis are:

-The case is in a steady state.

-The analysis will be done when the valve is closed (power stroke).

-The thermal loads (boundary condition) are proposed in the previous study Al-Beiruti et al. [16], where the convection heat transfer is applied on the head of the valve, also in the case of the temperature applied to the end of the valve stem as shown in Fig. 2(a), where the temperature load referred to by yellow arrows and convection load by red arrows.

-For structural analysis, the constriction is carried out in X and Y directions in the valve stem groove and the valve seat region as shown in Fig. 2(b) which is referred to by red arrows.



Figure 2. Applying loads in exhaust valve body (a) Thermal loads, (b) Structural loads(displacement).

III. EXHAUST VALVE AND COATING MATERIALS

Titanium Aluminide is chosen for the exhaust valve material. Three types of thermal barrier coating tests are considered where the thermal and mechanical properties are shown in Table I.

The present work consists of three exhaust valve analyses, first with (1 mm) thickness of each of the three TBCs separately, the second with a double coating (0.5 mm) of each, and the third with a triple coating (0.25, 0.5, and 0.25 mm).

Properties	Titanium Aluminide [17]	Steel Alloy	SiO ₂ [18]	Al ₂ O ₃ [19]	ZrO ₂ [18]
ρ	3900	7850	2650	3690	6150
K	28	48.6	1.5	18	2.7
α	12.2 X 10 ⁻⁶	15 X 10 ⁻⁶	0.75 X 10 ⁻⁶	8.1 X 10 ⁻⁶	9.7 X 10 ⁻⁶
Е	170	210	74.8	300	250
P R	0.28	0.3	0.19	0.21	0.32

 TABLE I.
 THERMAL AND MECHANICAL PROPERTIES OF THE

 EXHAUST VALVE AND TBC MATERIALS.
 EXHAUST VALVE

IV. CALCULATION OF THE HEAT TRANSFER COEFFICIENT IN COMBUSTION CHAMBER SPACE

The mathematical expression of the forced gas flow on the cylinder surface is very complex, whereas in the internal combustion engine parts, such as pistons, the impact of the combustion gases on the cylinder surface is complicated, to determine the coefficient of heat transfer on the head surface of the piston, the thermal load is formulated as a heat transfer of forced convection within the combustion chamber. The thermal loads of the combustion products gases are assumed to be as the heat transfer with the turbulent flow of the gases in the engine cylinder as in the below correlation:

$$Nu = C \operatorname{Re}^{m} \operatorname{Pr}^{n} \tag{1}$$

The exponent value (m) is taken as 0.8 for the turbulent flow of fully developed, and 0.4 or 0.3 for the heating or cooling process. The constant (C) is taken from Kays' experimental work [20]. The heat transfer coefficient shall be calculated based on the work of Benson [21], which uses the ratio of the equation (1) to the volume of the cylinder as a function of the piston diameter.

hg=226.6
$$P^{0.8} T^{-0.4} (Vp+1.4)^{0.8}$$
 (2)

Thus, equation (2) is used as the dependent formula for the calculation of the coefficient of heat transfer on the piston crown surface of Al-Beiruti et al.[16]

V. FINITE ELEMENT MODELLING

The longitudinal plane of the exhaust valve was selected as a 3-D symmetry plane in the numerical study. Where the first analysis in this study is performed thermally, where the PLANE77 element is selected for the 2-D design analysis. The PLANE77 has a degree of freedom, temperature, at each node, as shown in Figure 3. Eight-node elements have compatible temperature shapes and are well suited to the curved boundary model.

If the model containing this element is to be structurally analyzed as well, the element should be replaced by an equivalent structural element such as PLANE183 using the option of element change in the ANSYS package software. The PLANE183 element is also a 2-D, 8-node, or 6-node element. The 8-node element is proposed in the present analysis as shown in Fig, 3.



Figure 3. PLANE77 element - PLANE183 element model [22].

Fig. 4 shows the coating layers which are used in this work for the application of the thermal barrier coatings, such as; 1 mm thickness for a single type in the exhaust head, whereas 0.5 mm is used for the double thermal barrier of each type, and the third way is the coating of the exhaust valve with 0.25 mm type 1, 0.5 mm type 2 and 0.25 mm type 3 thermal barriers.



(c) Exhaust valve with a triple coating layer.

Figure 4. Exhaust valve with thermal barrier coating cases of (a) single layer, (b) double layer, and (c) triple layer.

VI. RESULTS AND DISCUSSION

The following results are divided into two parts, the first part dealing with thermal analysis and the second part dealing with structural analysis. By applying the thermal analysis, where the full analysis of this paper is carried out using ANSYS version 14 software. The Titanium Aluminum material exhaust valve is first analyzed before using TBC materials. The thermal analysis is carried out by setting the conditions for the 2-dimensional geometry of the valve body, where a steady-state analysis is studied, the upper end of the valve stem is subjected to a uniform temperature of 60 °C, and the lower side of the valve in the surface is subjected to a convection heat transfer of 334 W/m2 °C and a gas temperature of 925 °C. The results of the thermal analysis, the temperature distribution of the valve body is used as a

boundary condition to obtain thermal stress in the structural analysis, where the stress is based on the equivalent of Von Mises Stresses. The lower side of the valve in the surface is subjected to a convection heat transfer of 334W/m2 °C and a gas temperature of 925 °C. The results of the thermal analysis, the temperature distribution of the valve body, are used as a boundary condition to obtain thermal stress in the structural analysis where the stress is based on the equivalent of Von Mises Stresses. The results are shown in three items depending on the number of coatings on the exhaust valve face with thermal barrier materials as follows:

A. Single Thermal Barrier Coating

Thermal stress values in the distribution of the exhaust valve body are considered in this analysis to be Von Mises Stresses, which is equivalent stress in the calculation of the problem. Maximum stress distribution with the use of thermal barrier coating material shall not be changed, from the results of Fig. 5 it is seen that the maximum stress is 9.46 GPa, for the case without coating with TBC material, and with SiO₂ material, a coating is 9.40 Gpa., whereby coating valve body with Al₂O₃ is 15.8 Gpa and for coating with ZrO₂ Material is about 14.8 Gpa. While the minimum stress distribution involves a change in its distribution in the valve body as shown in Fig. 5.





Figure 5. Thermal stresses in valve (a) without TBC, with TBC (b) SiO₂, (c) Al_2O_3 , (d) ZrO_2 .

B. Double Thermal Barrier Coating

In this analysis, two types of valve face coating with a thickness of 0.5 mm for each of the TBCs are used, taking into account the change of the upper TBC position to the lower TBC with respect to the valve face in the comparison of the results. In this way, six types of coating have occurred and two types are concerning each of the TBCs in the coating valve face, where the coating with SiO_2 and Al_2O_3 type one and the reverse is Al_2O_3 and SiO_2 where the first one means that SiO_2 is on the valve face and the second one is on the coating layer face, And so on for the rest of the double-layer coating. The distribution of thermal stress in the face of the SiO₂ and Al₂O₃ TBC coating materials valve is shown in Fig. (6-a), where the maximum thermal stress value is approximately 9.8Gpa and the minimum is 196 Mpa. The maximum stress is located in the margin region of the valve body, while the minimum stress is located in the valve stem and is approximately 1.26Gpa in contrast to this coating, which is Al₂O₃ and SiO2 TBC as shown in Fig. (6-b), the maximum value is 15.5Gpa and the minimum is between 74.8 Mpa and 1.79 Gpa.



Figure 6. Comparison Thermal stresses in valve (a) with SiO_2 -Al₂O₃ TBC, (b) with Al₂O₃- SiO_2 TBC.

The second configuration of the coating valve face with SiO₂ and ZrO₂ TBC materials shows from Fig. (7-a) that the maximum stress is approximately 9.7 Gpa and the minimum stress ranges between 0.171 Gpa and 1.23 Gpa. While for the reverse of this coating shown in Fig. (7-b), the maximum stress is 14.2 Gpa and the minimum stress value is between 41.3 Mpa and 1.61 Gpa.

Using the Al_2O_3 and ZrO_2 coating valve face as shown in Fig. (8-a), the maximum thermal stress is 17.1 Gpa and the minimum thermal stress values are between 0.744 Gpa and 2.56 Gpa, where the maximum thermal stress value for a reverse coating above is shown in Fig. (8-b) is 15.8 Gpa and the minimum is also between 0.744 Gpa and 2.42 Gpa, and it is shown from the above that the minimum thermal stress is distributed in the valve body rather than other thermal stress distribution values.





Figure 7. Thermal stresses in valve (a) with SiO_2 - ZrO_2 TBC, (b) with ZrO_2 - SiO_2 TBC.



Figure 8. Thermal stresses in valve (a) with $Al_2O_3\text{-}ZrO_2$ TBC, (b) with $ZrO_2\text{-}$ Al_2O_3 TBC.

C. Triple Thermal Barrier Coating

The final analysis in the present work is by using three types of coating with different thicknesses and changing their location with respect to each other. Thermal stress in three TBC-coating materials in the valve face as shown below, where 0.25 mm, 0.5 mm and 0.25 mm are the thickness of each form of TBC-coating concerning the valve face. For this analysis, the results are related to the shift of TBC content in the first and third, whereas the second (medium) is set, and this will be changed to the other steps of the analysis. In SiO₂-Al₂O₃-ZrO₂ coating, the maximum thermal stress is 10.1 GPa and the reverse as the ZrO₂-Al₂O₃-SiO₂ coating, the maximum stress is 16.3 GPa as shown in Fig. 9.



Figure 9. Thermal stresses in valve (a) with SiO₂- Al₂O₃- ZrO₂ TBC, (b) with ZrO₂-Al₂O₃-SiO₂ TBC.

For coating with SiO_2 -Zr O_2 -Al₂ O_3 TBC the maximum stress is the same as in coating with SiO_2 -Al₂ O_3 -Zr O_2 as shown in Fig. (10-a), wherein coating with Al₂ O_3 -Zr O_2 -Si O_2 TBC the maximum is about 17.7 GPa as illustrated in Figure (10-b).

At the end face of the Al_2O_3 -SiO₂-ZrO₂ coating valve and its reverse side as shown below, Fig. 11 shows the maximum thermal stress as 15.7 GPa and the maximum thermal stress for the reverse coating as ZrO_2 -SiO₂-Al₂O₃ is 14.5 GPa.



(a)



Figure 10. Thermal stresses in valve (a) with SiO₂-ZrO₂-Al₂O₃ TBC, (b) with Al₂O₃-ZrO₂-SiO₂ TBC.





Figure 11. Thermal stresses in valve (a) with Al_2O_3 -SiO_2-ZrO_2 TBC, (b) with ZrO_2 -SiO_2-Al_2O_3 TBC.

D. Steel Alloy (44K2) with Three cases of Coating Exhaust Valve Head

In this part of the work, the three cases of coating where selected with using the steel alloy (44K2) as compared to titanium aluminide. Fig. (12-a) shows the

stress distribution in steel alloy exhaust valve without using coatings, and maximum stress is 13.8GPa. Selecting the coating materials and the cases of arrangement for the cases of double and triple coatings where the maximum stresses are achieved for the previous material of the exhaust valve. The single coating is SiO₂ showed that maximum stress of about 13.4GPa in Fig. (12-b), while the double layer of coating (SiO₂-ZrO₂) illustrated in Fig. (12-c) shows maximum stress of 13.1GPa. And the last option of coating is (SiO₂-Al₂O₃-ZrO₂) in Fig. (12-d) the maximum stress is 13.6GPa.











Figure 12. Thermal stresses in valve of steel alloy (44K2) (a) without coating, (b) with SiO₂, (c) with SiO₂-ZrO₂, (d) with SiO₂-Al₂O₃-ZrO₂.

VII. CONCLUSION

From the results of the numerical analysis described above, it is concluded that the distribution of thermal stress in the exhaust valve, there is a shifting in the profile from the minimum to the maximum values for the exhaust valve modeling with coating materials and the arrangement of the coating materials concerning the other double and triple coating designs. If a single TBC is used, the lowest maximum stress value is shown in SiO₂ TBC where the highest stress concentration is concentrated in the valve seat region, while using double TBC materials the lower maximum stress value is seen in SiO₂-ZrO₂ TBC coating. With the use of three TBC coating materials, the average stress is lower in the coating with SiO₂-Al₂O₃-ZrO₂ TBC materials. By using the steel alloy, it is found that there is little impact of the TBCs on stress reduction in the exhaust valve body. Comparing the results of stresses in the valve with respect to material type and the coating cases which mentioned previously, it is found that stress in valve using titanium aluminide without coating is less than of being made by steel alloy as 31%. With regard to coating cases the maximum stress in titanium valve with single layer of SiO₂ TBC is below that of steel alloy by 29.9%, also for double layer coating of valve head with the arrangement of SiO₂-ZrO₂ TBC for titanium valve the maximum thermal stress is lower than of that steel valve with the same arrangement of TBC by 26%. Finally, for the case of the triple layer of TBC, the maximum value of stress for the arrangement of SiO_2 - Al_2O_3 – ZrO_2 with a titanium value is reduced by 25.7% as compared to a steel valve.

CONFLICTS OF INTEREST

The authors declare no conflicts of interest.

AUTHOR CONTRIBUTIONS

Isam E. Yousif wrote and created the valve model using ANSYS package and solved the problem of the research; Tolin S. Othman searched about the materials of thermal barrier coatings; Mohammed Z. Hasan analyzed the data; all authors had approved the final version.

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