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RESEARCH ARTICLE

Experimental and Numerical Investigation of Heat Transfer of TiN/TiCN/TiC Deposited on Cp-Ti and Ti6Al4V Substrate Materials

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HIGHLIGHTS

> A multilayer heat conduction problem which is exposed to Cp-Ti and Ti6Al4V heat flux with TiN / TiCN / TiC coating and different base material has been solved analytically.

> A theoretical model based on some basic assumptions has been developed. The experimental results were observed with very good results.

> In addition, all multilayer solid assemblies, finite element method, first multi-layer, then the amount of heat passing directly to the base material and heat dissipation to describe and numerical analysis, we have proved to match the experimental results.

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ABSTRACT

Experimental and numerical analysis on heat transfer characteristics of TiN/TiCN/TiC coating was investigated in this study. The TiN/TiCN/TiC coating was deposited on commercially pure Titanium (Cp-Ti) and Ti6Al4V substrates using a magnetron sputtering technique. The structural and chemical characterization of the coating was analyzed by X-ray diffraction (XRD). Results of the XRD analysis showed reflections corresponded to cubic and polycrystalline structure for TiN/TiCN/TiC films. Test specimens were placed in the heat conduction equipment and heat analyzes were performed experimentally. In addition to experimental investigation, numerical studies of coated substrate materials have been performed under the same experimental conditions with the ANSYS Fluent program.

Contents

1. Introduction

Titanium and its alloys are widely used in aerospace, automotive, dentistry, and medical industries because of their low density and modulus of elasticity, high corrosion resistance, and long fatigue life. Titanium is increasingly used in dental applications due to its excellent biocompatibility [1], high corrosion resistance, low density, high strength to weight ratio, low thermal conductivity and sufficient mechanical properties [2–5].

The most widely used titanium alloy is Ti6Al4V [6, 7] because of its most suitable mechanical properties. Titanium

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has a much lower density (4.2 g / cm3) than conventional alloys such as cobalt-chromium (8.9 g / cm3) and gold (19.3 g / cm3).

The low density associated with the high chemical reactivity of titanium with high melting point (commercially pure titanium - about 1720ºC for CP-Ti) and elements [3, 8] in investment requires special casting machines [4, 9]. At room temperature, Cp-Ti has a hexagonal close-closed crystal structure, called the (alpha) phase.

At 883ºC, this structure (beta) transforms into a body-centered cubic crystal structure called a phase. These phase changes can directly affect the properties of titanium.

Due to the high melting point of titanium and the investment pattern with exhaustion temperatures below 800°C, the large heat gradient that titanium has to pass can cause a major change in its mechanical properties [10].

The aim of this study is to evaluate the effect of heat treatments on the thermal properties of TiN/TiCN/TiC coated on CP-Ti and Ti6Al4V. In this study, the geometric dimensioning was shown by taking the three-dimensional geometric model and the geometric model was arranged according to the data from the previous studies and observations [11]. A linear dimensional heat conduction solution was realized by using the data in the direction of conducting heat transmission via the geometric model.

2. Material and Methods

High strength, toughness, low density and good corrosion resistance of various titanium alloys from very high to very low temperatures allow great weight savings in space and aerospace industry and other high-performance applications.

The atomic mass of titanium is 47.88. Titanium is light, strong, resistant to corrosion, but it is an element which is quite present in nature. Titanium and its alloys have a tensile strength of 30,000 - 200,000 psi (210-1380 MPa). Most of these values cannot be achieved in the equivalent steel alloy.

Titanium is a low-density element (approximately as low as 60% of iron) and can be reinforced by deformation processes with the alloy. Coefficient of thermal expansion is less than half of steel and aluminum alloys. Experimental parameters of TiN/TiCN/TiC coating are shown in Table 1.

Table 1 The TiN/TiCN/TiC multilayer thin film obtained by N2 and CH4 flow rate.

Phase	Ion cleaning	Ti (interlayer)	TiN	TiCN	TiC
Ar flow rate (%)	100	100	40	25	75
N_2 flow rate (%)	0	0	60	5	0
C_2H_2 flow rate (%)	0	0	0	70	25
Ti target current (A)	0	6	6	6	6
Treatment time (min)	20	2	10	45	15

The crystalline structure of the TiN/TiCN/TiC multilayer film was investigated by the GNR X-Ray Explorer diffractometer using CuKα radiation (λ=1.5406 Å) with a Bragg-Brentano configuration (θ/2θ) and the scan range was from 20° to 90° at a scan speed of 2°/min.

XRD reflections were determined by comparing their peak lists and literature with JCPDS (Joint Committee on Powder Diffraction Standards).

The XRD pattern of TiN/TiCN/TiC multilayer film coated on silicon is given in Figure 1. According to XRD pattern all peaks related to the (111), (220) and (222) plane of the cubic TiCN phases, (111) and (200) planes of the TiC phases and TiN (311) phase have been found in TiN/TiCN/TiC multilayer coating. The Ti peak (101) which has been applied as Ti interlayer for an increase in adhesive properties between coating and substrate also has been found in multilayer coating [11–13].

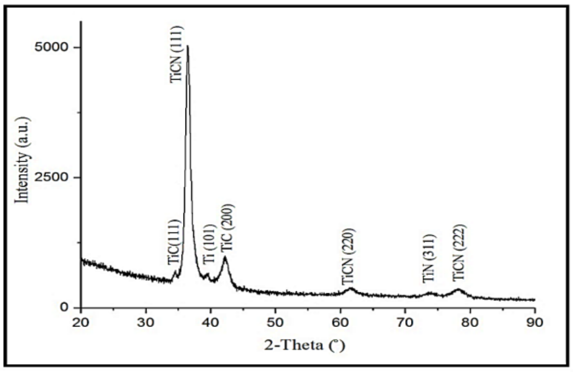

Figure 1 XRD patterns of TiN/TiCN/TiC coating coated on silicon

One of the most important properties of titanium is that the melting point is quite high; 3135 DEG F. (1725 DEG C). This melting point is about 400 °F for steel and over 2000 °F for aluminum.

Titanium can be passivated and highly resistant to most acid minerals and chlorides. Titanium is non-toxic (non-toxic) and can generally adapt to human bone and tissue. It has excellent corrosion resistance and is used in chemical, petrochemical, marine and biomaterial applications thanks to its harmony with nature. In Figure 2, we have shown each layer schematically (x1, x2, x3, x4) as shown, and we have shown the base material x5.

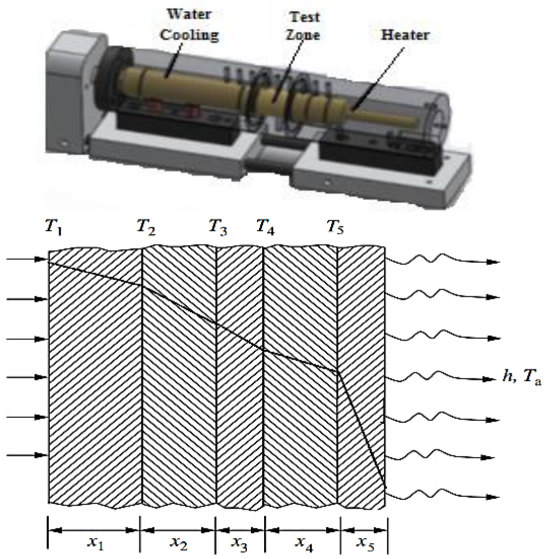

Figure 2 Linear heat conduction measurement system

2.1. Thermal Conductivity Measurement Methods

In nature and in various engineering applications, composite materials and/or porous media are encountered. The active thermal conductivity of this environment, insulation operations, drying processes, cooling operations, etc. is seen as an important feature in the areas. In addition, its thermal conductivity is important for thermal design and numerical simulations of such materials.

In addition to experimental data, it also uses analytical data in practical applications. Analytical solutions are based on mathematical models derived using physical laws with a limited number of parameters. The accuracy of any model depends on the accuracy of the physical properties dealt with assumptions, parameters, and other factors. To be costly, the experimental data related to materials are difficulties in terms of ease of application required and that the need to bond to give different parameters depending on the thermal conductivity and to this end work is done.

In general, thermal conductivity is defined by the following correlation;

$$K = \frac{Q/_{A}}{\Delta T/_{\Delta L}} \tag{1}$$

The thermal power passing through section Q and A is the temperature difference between the thickness of ΔT and ΔL. (Q / A) is the heat flux generated by the ΔT / ΔL temperature gradient.

The thermal conductivity measurement therefore always includes the measurement of heat flux and temperature difference. The measurement difficulty is always related to heat flow measurement. The measurement is called absolute when the measurement of the heat flux (for example, by the electric power measurement to the heater) is done directly. Where the measurement of flux is carried out indirectly (by way of comparison), this is called the comparative method.

In addition to these two basic methods, other secondary methods, which are generally temporary in nature, can also give thermal conductivity.

In all cases, the total heat flux of the sample (and references, as a comparative example), must be uniaxial. Simple solutions such as this can be accomplished to a degree with a "protection" installation with insulation material around the sample. The protection of the sample is controlled for the same temperature difference. The thermal conductivity in a given measurement system and configuration is significantly affected by the sample size. When the thermal conductivity is high, samples (eg cylindrical) are generally selected as "long". When the conductivity is low, samples (for example, in the form of plates or discs) are generally selected as "flats".

Axial flow methods have been carried out for many years and have achieved the most sensitive and reliable results in the literature. This is a preferred method at very low temperatures. These losses are very low at low temperatures. As the temperature of the sample moves above room temperature, the control of heat losses becomes more difficult.

In practice, however, cylindrical symmetry heat transfer is used. In addition to the protected and unprotected solution, other categories are also separated: The absolute axial heat flow is often used in sub-environments. Such systems require very precise information to adjust the heater electrical power. As a result, hot heater surfaces play an important role in losses. This is perhaps the most widely used method for testing axial thermal conductivity. This is done in the measurement principle by comparison with a known example of a thermal temperature gradient and an unknown sample. Rather, the sample is compressed between two known "references" for smaller heat losses which are very difficult to eliminate the unknown (Figure 3) element.

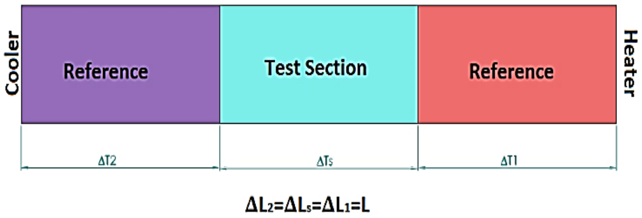

Figure 3 Schematic gradient of temperature distribution

K_R is the reference to thermal conductivity. Here, the thermal conductivity K_S of an unknown sample can be obtained from the following equation:

$$\frac{Q}{A} = K_S \frac{\Delta T_S}{L} = K_R \frac{\Delta T_1 + \Delta T_2}{2} \frac{1}{L} \tag{2}$$

Fourier's law is a vector expression used to express the heat flux perpendicular to the temperature curve (isotherm) which is the basis for the heat transfer by the transmission based on the generalization of experimental findings and the temperature drop in this flux direction. The transmission heat transfer is based on the Fourier Act and the general expression of the heat transfer rate (heat flux) equation is written as follows.

Figure 4 Heat conduction unit used in numerical calculations and experiments

This test has a solid brass bar with a round cross-section, consisting of two sections with an interchangeable central section. The test plate is assembled in Figure 4, to the base plate with an open scheme. The first brass section has two thermocouples and electric heat source. The second brass part has a small water-cooled, heat sink and two more thermocouples. The exchangeable middle sections were made of metals composed of different aluminum copper or brass metals.

Plot the temperature versus distance over the sample from the results obtained for each power setting with the aid of the first thermocouple (See Figure 5). You should be able to draw a good graph in response to your results.

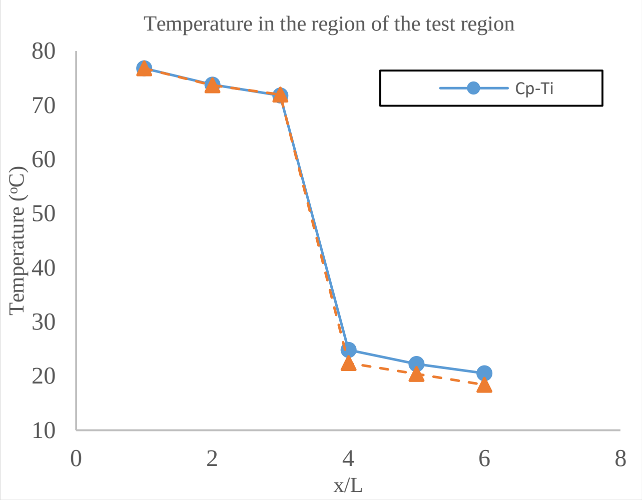

Figure 5 Graphing for standard material testing

In the diagram shown in Figure 3 and Figure 5, (x / L) is any x point in length L. This power was used for the calculation of the heat conduction coefficient because of the 20 W power input for the constant heat output. The data was transferred in detail. To find the thermal conductivity of the sample, find the distance, heater power and sample space of the T1 and T6 measurements at the extreme points by using the following equation. With the results we obtained, the known values of both materials can be compared.

2.2. Numerical Examination

2.2.1. Mesh Validation

Mesh quality correction and mesh production are a very important problem for numerical simulations. The elements on the shape, size, number and area boundaries of the used element are the most important factors that determine the mesh quality, and the proper selection of these properties positively affects both the accuracy of the solution and the time to be used for the solution time. The approaches developed for correct mesh production in complex and large geometries and the problems solved will provide great savings in the solution of later problems both in terms of time and effort. While increasing the cost and time in the industrial sense, increasing the quality is one of the most interesting subjects in engineering design. Thus, finite element analysis is widely used as an auxiliary tool in product design in order to make the best possible decision regarding product specifications.

The finite element method is a numerical process that can result in a wide variety of engineering problems. Stress analysis, stress analysis, heat transfer analysis, fluid mechanics analysis and analysis of electromagnetism problems can be done with finite element method.

When modeling parts with the Finite Element method, the model is divided into basic elements consisting of small parts. Each element has nodes in the corners. Calculations are performed on these nodes. The physical environment is then divided into elements (element) and the corner points of the elements become the space of the points representing the physical environment. The results obtained are the values above these points.

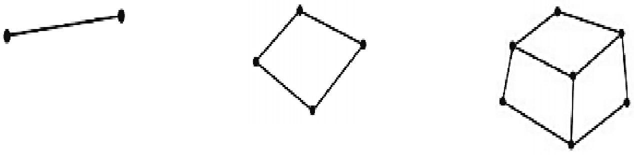

Figure 6 Element (element) types: 1-dimensional linear element 2-dimensional planar element 3-dimensional solid element

When the calculations are performed on nodes, the equations on these nodes are created. Thousands of equations are obtained according to the magnitude of the problem. The solution of this equation set is made possible by the computer. Values found on the nodes are the values found on the nodes (show in Figure 7). Therefore, for a good calculation, first of all, a good element structure and its structure are important.

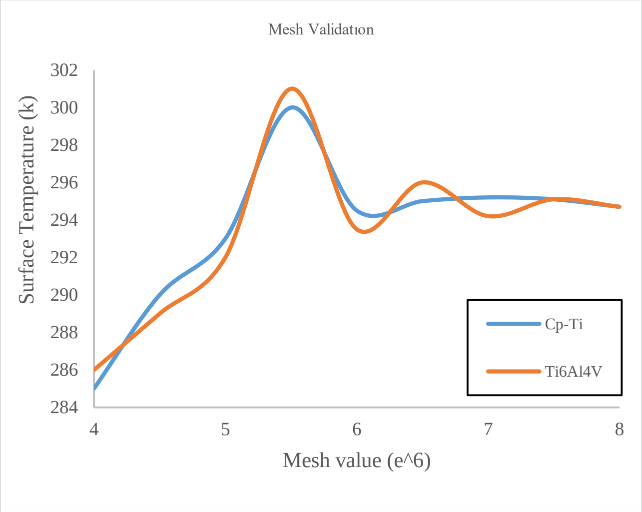

Figure 7 temperature value through TiN / TiCN / TiC and base Cp-Ti, Ti6Al4V base materials for verification of mesh validation

In the numerical study, the geometric measures required to identify the problem and the boundary conditions that should be given for the purpose of verifying the experimental study were taken from the experimental study. While calculating the numerical model, the convection coefficient calculated in the refrigerant fraction modeling was taken into consideration. The erosion surface area was simply modeled for simplicity in the solution phase, and the numerical solution was made using the Ansys-Workbench finite element code.

3. Results

The aim of this study is to investigate the machinability of titanium and its alloys, which are increasing day by day. As a result of the numerical study, it was observed that both models for Cp-Titanium and Ti6Al4V substrate material produced approximately accurate data but a better thermal conductivity approach was obtained in case of internal cooling modeling.

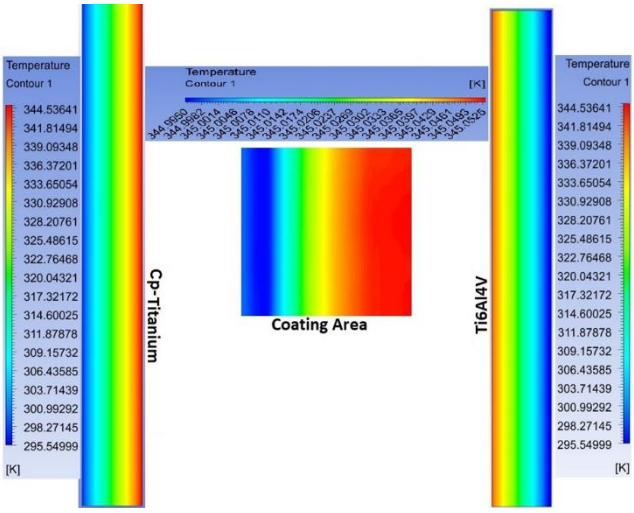

Figure 8 Thermal analysis of the model at Ansys Fluent-16

The numerical study of the experimental data was examined both in terms of self and comparatively. Results obtained from the obtained data: The validity of the numerical approach to the experimental study is quite high. In the experimental study, the constant heat flux applied to keep the resistance temperature at a certain value, and in this case, the results can be taken with the acceptance of constant resistance temperature in the digital model.

4. Conclusions

In the results section and in Figure 8 and Figure 5, detailed results are explained experimentally and quantitatively. The overall results are summarized as follows. The multilayer TiN/TiCN/TiC coating is a good structure to dissolve the heat transfer factor. The Ti interlayer in the multi-layer TiN/TiCN/TiC coating can effectively suppress the heat transfer event. Multilayer TiN/TiCN/TiC is a good structure that can increase corrosion resistance and ductility in coatings other than heat transfer. Nano-crystalline materials with particle sizes have properties that exceed those of coarse grains. In the future, a multilayered structure may be designed, such as 100 layers or more (to keep the thickness of the Ti multilayers), to make the Ti crystal lower in nano-crystalline form.

Nomenclature

k: Heat conduction coefficient [W / mK]

Q: Thermal energy (heat/time) [W]

dx: Heat transfer length (0.02 m)

dT: Temperature difference [° C]

A: The heat transfer area (7,065x10-4 m2)

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