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Effect of substrate preheating temperature and coating thickness on residual stress in plasma sprayed hydroxyapatite coating

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Abstract. A thermal-mechanical coupling model was developed based on thermal-elastic-plastic theory according the special process of plasma spraying Hydroxyapatite (HA) coating upon Ti-6Al-4V substrate. On the one hand, the classical Fourier transient heat conduction equation was modified by introducing the effect item of deformation on temperature, on the other hand, the Johnson-Cook model, suitable for high temperature and high strain rate conditions, was used as constitutive equation after considering temperature softening effect, strain hardening effect and strain rate reinforcement effect. Based on the above coupling model, the residual stress field within the HA coating was simulated by using finite element method (FEM). Meanwhile, the substrate preheating temperature and coating thickness on the influence of residual stress components were calculated, respectively. The failure modes of coating were also preliminary analyzed. In addition, in order to verify the reliability of calculation, the material removal measurement technique was applied to determine the residual stress of HA coating near the interface. Some important conclusions are obtained.

1. Introduction
Hydroxyapatite (HA) is a biological active material with nearly the same chemical composition as natural bone, and can be used to guide bone regeneration [1]. One of the most important clinical applications of HA is as a coating on bone or tooth implants [2], especially plasma sprayed HA coating applied on Ti-6Al-4V substrate. These implants combine the mechanical advantages of substrate with the excellent biocompatibility and bioactivity of HA. However, It has been reported that failure often occurs at the HA/substrate interface during the surgery or after implantation [3]. One of the major causes of failure is the existence of high residual stresses within the implant. Therefore, the overall understanding of the residual stress is crucial in failure analysis of these composite materials. Moreover, modeling and simulation of the residual stress field will be also useful for guiding the design process of HA coating.

Several techniques are usually employed for the measurement of residual stress in HA coating. These include specimen curvature [4], Raman spectroscopy [5], X ray diffraction [6], nanoindentation [7], high-energy synchrotron [8], and material removal method [9]. Unfortunately, the residual stress

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measured by these methods may vary over at least two orders of magnitude. Besides, some test results are tensile in nature, but others are compressive in nature. These contradictory results are in dispute. There are multiple reasons causing these test results inaccurate or conflicting. Firstly, the in-plane stress state or biaxial stress state is often assumed in these tests techniques [10], i.e. the stress component perpendicular to interface and the shear stress are ignored. The thickness of coating is thinner than that of substrate, but the thickness of the coating/substrate system is not thin. Therefore, the above simplified assumption seems to be inappropriate. Secondly, each of the aforesaid techniques has its own advantages and disadvantages. For example, The X-ray diffraction is limited by the shallow penetration of the X-ray beam, therefore only the top surface average residual stress can be obtained; the accuracy of Raman spectroscopy depends on the resolution of Raman frequency shift, since this shift is apparently small, uncertainty of residual stress result might be incurred. In fact, there is not any unique standard method for evaluation of residual stress, it is nearly impossible to compare one reported data with another.

In order to obtain the complete and accurate value and state of the residual stress, numerical simulation technology is worth to adopt. Up to now, there are few numerical researches undertaken on residual stress of HA coating [8, 11]. Previous investigations only considered the effect of temperature on deformation, not considered the influence of reverse, i.e. without studied the thermo-mechanical coupled effect. In addition, the influences of substrate preheating temperature and coating thickness on residual stress were also less simulated. This paper intends to continue these work.

2. Thermal-mechanical coupling model

It is well known that the classical Fourier heat conduction equation is derived under the assumption of “unit volume constant”, which ignores the effect of strain field on the temperature field. However, in plasma spraying process, the change of temperature is sudden, and its change rate is great, volume change caused by the sudden deformation would affect the heat transfer. Therefore, Fourier heat conduction equation need to be modified in order to reflect the influence of deformation on temperature. The modified Fourier heat conduction equation according to the first law of thermodynamics is as follows:

$$\lambda_i T_{,ii} + Q = \rho c_v T_0 \varepsilon + (3 \lambda + 2 \mu) \alpha T_0 \varepsilon$$  \hspace{1cm} (1)

Where $T$ is temperature, $\varepsilon$ is strain, $Q$ is heat source density, $\lambda$ is thermal conductivity coefficient, $\rho$ is density, $c_v$ is specific heat, $\alpha$ is thermal expansion coefficient, $\lambda$ and $\mu$ are Lame constant. The last item of equation (1) shows the coupling between deformation and temperature.

Johnson-Cook model [12] is adopted to describe the material constitutive under the high temperature and high strain rate in the paper (seen in equation (2)), which considers temperature softening effect, strain hardening effect and strain rate reinforcement effect.

$$\sigma = [A + B (\varepsilon^p)^m] \left[1 + C \ln \left(\frac{\varepsilon^p}{\varepsilon_0}\right) \right] \left[1 - \left(\frac{T - T_r}{T_m - T_r}\right)^n \right]$$  \hspace{1cm} (2)

Where $\sigma$ is stress, $\varepsilon^p$ is plastic strain, $T$ is temperature, $T_m$ is melting point, $T_r$ is room temperature. Five Johnson-Cook model constants by compression experiment are as follows: $A=1000$MPa, $B=780$ MPa, $C=0.033$, $m=1.02$ and $n=0.47$.

3. Finite element simulation

A simple cylindrical Ti-6Al-4V substrate with HA coating on top surface of the sample is selected as the calculating geometry model, shown in figure 1(a). The $xoz$ plane is the interface between HA coating and Ti-6Al-4V substrate, the $y$ axis is the axis of symmetry. Because the model is symmetrical, so only for half a symmetry plane is simulated by FEM, seen in figure 1(b), $x$ and $y$ directions are radial and axial direction, respectively. The radius of the sample is 5 mm; the substrate thickness $t_s$ is 3
The initial temperature of HA coating is considered to be its melting point temperature. The substrate material is preheated before HA coating sprayed upon it. Both the coating thickness $t_c$ and the substrate preheating temperature $T_s$ are chosen as variable parameters, in order to study their effects on residual stress.

![Figure 1. Geometry schematic used in FE simulation.](image1.png)

After the deposition process, heats are lost from every surface of the coating and substrate to the ambient air by convection. The heat transfer coefficient is 16 W/(m$^2$•K). Materials’ properties used in simulation are summarized in Table 1.

<table>
<thead>
<tr>
<th>Properties</th>
<th>HA</th>
<th>Ti-6Al-4V</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg·m$^{-3}$)</td>
<td>3100</td>
<td>4500</td>
</tr>
<tr>
<td>Thermal Conductivity (W·m$^{-1}$·K$^{-1}$)</td>
<td>0.72</td>
<td>7.2</td>
</tr>
<tr>
<td>Specific Heat (J·(kg·K)$^{-1}$)</td>
<td>2500</td>
<td>560</td>
</tr>
<tr>
<td>Young’s Modulus (GPa)</td>
<td>16</td>
<td>115</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.23</td>
<td>0.32</td>
</tr>
<tr>
<td>CTE (×10$^{-6}$K$^{-1}$)</td>
<td>11.5</td>
<td>8.9</td>
</tr>
</tbody>
</table>

4. Results and discussion

4.1. Fundamental analysis of residual stress field

In this section, the coating thickness $t_c$ and initial substrate preheating temperature $T_s$ are given the following parameter values respectively: $t_c=100$ μm, $T_s=600$ °C. Figures 2(a) and 2(b) show the typical contour of von Mises residual stress in the whole region of the sample and in the local region around the free edge of coating and substrate interface, respectively. For all specimens (including other thickness, other preheating temperature, etc), modeling result shows that, von Mises stress in the interface is larger than in other locations, and there is a significant stress concentration near the free edge.

![Figure 2. Typical contour of von Mises stress (MPa): (a) the whole region of the sample; (b) the local region near the edge of the coating and substrate interface.](image2.png)
edge of the interface. It has also been reported that failure often occurs at the HA/substrate interface rather than at HA/bone interface from a direct shear/bending loading [13]. Accordingly, it can well explain why failure always occurs at the HA/substrate interface during the clinical use of implants [14].

Figures 3(a)–3(d) shows the distributions of radial residual stress, axial residual stress, shear residual stress, and von Mises residual stress of the coating and substrate at the interface respectively. From figure 3(a), it can be seen that, for the most part locations in far away from the interface edge, the radial residual stress of coating (denoted as $\sigma_r^{(Coating)}$) is tensile stress, the radial residual stress of substrate (denoted as $\sigma_r^{(Substrate)}$) is compressive stress, and they does not change significantly in these locations. However, in the local positions near the interface edge, there is an obvious stress concentration. Figure 3(b) shows that, for the most part locations in far away from the interface edge, the axial residual stress of coating is not large, and the axial residual stress of substrate is compressive stress, however, near the interface edge, the axial residual stresses of coating and substrate change from compressive stress to tensile stress, and there is a remarkable stress concentration. The tensile axial stress, acting in the direction normal to the interface, may likely tear the coating apart from the substrate. In places far from interface edge, shear residual stresses (seen in figure 3(c)) of coating and substrate are fairly small, but near the interface edge, both the absolute value of them increase abruptly, they are easy to cause coating delamination or dislocation. It is also shown from von Mises residual stresses (seen in figure 3(d)) that, a remarkable stress concentration exists at the edge of the interface, and it may cause the spallation or crack of the coating.

Figure 3. The distributions of residual stress components of coating and substrate at the interface respectively.
4.2. Effect of substrate preheating temperature

In this section, the coating thickness $t_c$ is still 100μm, but the initial substrate preheating temperature $T_s$ is used as a variable parameter between 25 to 900℃. The rest of parameters are the same as the section 3. Figure 4 shows the effect of substrate preheating temperature on the maximum of single residual stress component in stress concentration area of interface, i.e. the maximum of radial residual stress, the maximum of axial residual stress, the maximum of shear residual stress, and the maximum of Mises residual stress, denoted as $\sigma_{x0}$, $\sigma_{y0}$, $\tau_{xy0}$, and Mises$0$, respectively. It can be seen that, all absolute values of these stress components decrease with the rise of preheating temperature, especially the decreases of $\sigma_{x0}$, $\tau_{xy0}$, and Mises$0$ are most obvious. The reason is that, the temperature difference between coating and substrate is reduced if the substrate has been preheated to higher temperature before the HA coating sprayed upon it. Therefore, the substrate preheating has significant influence on residual stress. It should be noted that $\sigma_{x0}$ would changes from compressive stress to tensile stress while preheating temperature over 700℃, which perhaps more likely to cause coating failure. Therefore, it is important to advice that the substrate is preheated to higher temperature, but not more than 700℃.

![Figure 4. Effect of substrate preheating temperature on residual stresses of coating.](image)

4.3. Effect of coating thickness

In this section, the initial substrate preheating temperature $T_s$=600℃, the coating thickness $t_c$ is used as a variable parameter between 40 to 160μm. The rest of parameters are the same as the section 3. Figure 5 shows the effect of coating thickness on $\sigma_{x0}$, $\sigma_{y0}$, $\tau_{xy0}$, and Mises$0$. It can be seen that, in addition to the changes of $\sigma_{x0}$ and $\tau_{xy0}$ are not obvious, both $\sigma_{y0}$ and Mises$0$ increase with the increasing of coating thickness. So, in order to decrease the level of residual stresses and control the stress concentration in critical regions, the coating should not be very thick.

![Figure 5. Effect of coating thickness on residual stresses of coating.](image)

4.4. Comparison of experimental and numerical results

Figure 3(a) shows the radial residual stresses of coating at the interface by calculation (denoted as $\sigma_c$ (Coating)) and by experiment (denoted as $\sigma_c$ (Coating)(exp)). The latter is measured by using the material removal method. From figure 3(a), it can be seen that, the absolute value of the data by experiment is smaller than by calculation, which may be due to a small part of the residual stress in coating has been released after removing the constraint of substrate. The distribution trend of them is the same, so the calculation result and experimental result is basically coincident.
5. Conclusion
There is a remarkable stress concentration near the interface edge. It is helpful to reduce the residual stress by increasing properly the substrate preheating temperature. The residual stress increases with the increasing of coating thickness. The calculated result by FEM is consistent with the experimental result.

References