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ARTICLE

Thermal-Mechanical Coupling in Plasma-Sprayed Hydroxyapatite Coating on Ti-6Al-4V Substrate

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Abstract: After considering the interactions of the temperature and deformation during plasma spraying, the classical Fourier transient heat conduction equation was modified, and the thermal elastic-plastic nonlinear constitutive equation, suitable for high temperature and high strain rate conditions, was employed. Thus, a thermal-mechanical coupling model was developed according to the special case of plasma-sprayed hydroxyapatite coating on Ti-6Al-4V substrate. Based on the above coupling model, the temperature field and residual stress field were coupling solved by the finite element method. The effect of substrate preheating temperature on residual stress components was also simulated. Moreover, the material removal method was used to evaluate the residual stress of coating near the interface to get a quantitative comparison. The results show that, the calculated result is consistent with the experimental result; obvious stress concentration appears near the interface edge; it is helpful to reduce the residual stress by increasing properly the substrate preheating temperature.

Key words: thermal-mechanical coupling; plasma spraying; hydroxyapatite coating; FEM

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 used as a coating on bone or tooth implants [2], especially 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 often applied 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 measured by these methods may vary at least two orders of magnitude. Besides, some test results are tensile in nature, but others are compressive. These contradictory results are in dispute. There are multiple reasons for these test results inaccurate or conflicting. Firstly, the in-plane stress state or biaxial stress states is often assumed in these test 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 it is not thin when they form a coating/substrate system. Therefore, the above simplified assumption seems to be inappropriate. Secondly, each of the aforesaid techniques has its own advantages and disadvantages. For example, X-ray diffraction is restricted by the shallow penetration of the X-ray beam, so 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, and the result of residual stress might be uncertain. In fact, there is not any unique standard method

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to evaluate the residual stress, and 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 adopting. Up to now, there are few numerical researches undertaken on residual stress of HA coating[8,11,12]. Previous literatures only considered the effect of temperature on deformation, not the effect of deformation on temperature, i.e. without studying the thermo-mechanical coupled effect. In addition, the influence of substrate preheating temperature on residual stress was also rarely simulated. This paper intends to research these .

1 Thermal - Mechanical Coupling Model

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

$$\lambda_t T_{ii} + Q = \rho c_v \dot{T} + (3\lambda + 2\mu)\alpha T_0 \dot{\varepsilon}_{ii} \quad (1)$$

where T is temperature, ε is strain, Q is heat source density, λ_t is thermal conductivity coefficient, ρ is density, c_v is specific heat , α is thermal expansion coefficient, λ and μ are Lame constant. The last item of Eq.(1) shows the coupling between deformation and temperature. Johnson-Cook model[13] is adopted to describe the material constitutive under the high temperature and high strain rate in the paper (seen in Eq.(2)), which considers temperature softening effect, strain hardening effect and strain rate reinforcement effect.

$$\sigma = \left[A + B\left(\varepsilon^{pl}\right)^n\right]\left[1 + C\ln\left(\frac{\dot{\varepsilon}^{pl}}{\dot{\varepsilon}_0}\right)\right]\left[1-\left(\frac{T - T_r}{T_m - T_r}\right)^m\right] \quad (2)$$

where σ is stress, ε^{pl} is plastic strain, T is temperature, T_m is melting point, and 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.

2 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 Fig.1a. The *xoz* plane is the interface between HA coating and Ti-6Al-4V substrate, while the *y* axis is the axis of symmetry. Because the model is symmetrical, only for half a symmetry plane is simulated by FEM, seen in Fig.1b, where *x* and *y* direction is radial and axial direction, respectively. The radius of the sample is 5 mm; the substrate thickness t_s is 3 mm. The initial temperature of HA coating is thought to be its melting point temperature. The substrate material is preheated before HA coating sprayed upon it. In order to study their effects on residual stress, both the coating thickness t_c and the substrate preheating temperature T_s are chosen to be variable parameters.

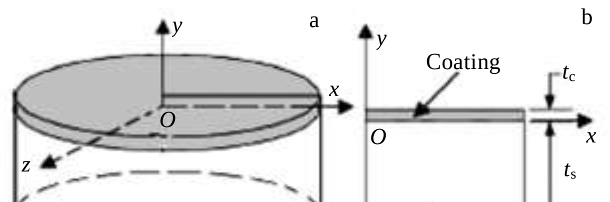

Fig.1 Geometry schematic used in FE simulation

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

3 Results and Discussion

3.1 Temperature field in coating and substrate

The coating thickness t_c and initial substrate preheating temperature T_s are given the following parameter values: t_c=100 μm, T_s=600 ℃.

The transient temperature field and residual stress field are solved by an indirect coupling method. Fig.2 shows the temperature field of entire structure after 250 load steps. It is shown that the obvious thermal gradient exists in coating and substrate. The temperature in the sample, increases along the thickness direction, and decreases along the radial direction. Compared with the usual simplified uniform temperature field in previous studies, the non-uniform temperature field in the present study is closer to the actual working condition. Thus, residual stress based on this non-uniform temperature field will be more accurate and reliable.

Table 1 Material properties

Property	HA	Ti-6Al-4V
Density/g·cm^{-3}	3.1	4.5
Thermal conductivity/W·m^{-1}·K^{-1}	0.72	7.2
Specific heat/J·(kg·K)$^{-1}$	2500	560
Young's modulus/GPa	16	115
Poisson ratio	0.23	0.32
CTE/×10^{-6} K^{-1}	11.5	8.9

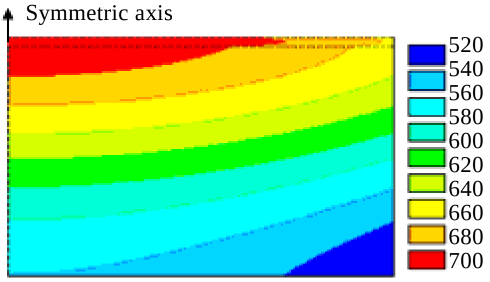

Fig.2 Temperature field after 250 load steps (℃)

3.2 Residual stress field in coating and substrate

Fig.3a and 3b 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. From Fig.3, we can see that von Mises stress in the interface is larger than that in other locations, and obvious stress concentration exists in the edge of the interface. It has also been reported by a direct shear/bending loading that failure often occurs at the HA/substrate interface rather than at HA/bone interface[14]. Accordingly, it can well explain why failure always occurs at the HA/substrate interface during the clinical use of implants[15].

3.3 Effect of substrate preheating temperature

The coating thickness t_c is still 100 μm, 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 2. Fig.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 σ_{x0}, σ_{y0}, τ_{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 σ_{x0}, τ_{xy0}, and Mises_0 decrease obviously. The reason is that

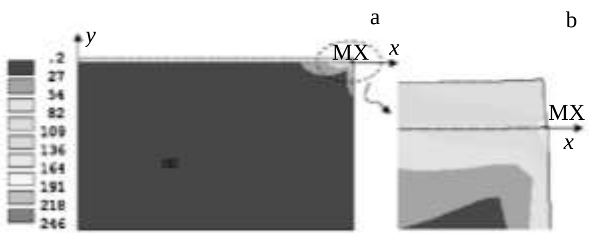

Fig.3 Typical contour of von Mises stress (MPa): (a) the whole region of the sample and (b) the local region near the edge of the coating and substrate interface

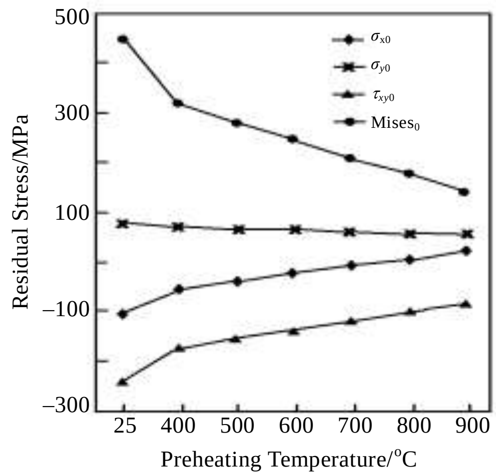

Fig.4 Effect of substrate preheating temperature on residual stresses of coating

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, which makes the residual stress decline. Therefore, the substrate preheating has significant influence on residual stress. It should be noted that σ_{x0} would changes from compressive stress to tensile stress while preheating temperature above 700 ℃, which is more likely to cause coating failure. Therefore, it is advisable that the substrate should be preheated to higher temperature, but not more than 700 ℃.

3.4 Comparison of numerical and experimental results

Fig.5 shows the radial residual stresses of coating at the interface by calculation (denoted as σ_x(Coating)) and by experiment (denoted as σ_x(Coating)(exp)). The latter is measured by the material removal method. From Fig.5, it

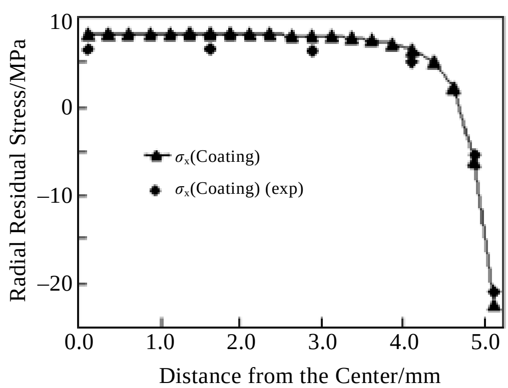

Fig.5 Comparison of numerical and experimental results

can be seen that, the absolute value of the data obtained from experiment is slightly smaller than calculation. The reason may be that 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 coincident.

4 Conclusions

1) There is a remarkable stress concentration near the interface edge.

2) It is helpful to reduce the residual stress by increasing properly the substrate preheating temperature.

3) The residual stress increases with the increase of coating thickness.

4) The calculated result by FEM is consistent with the experimental result.

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Ti-6Al-4V 基体上等离子喷涂羟基磷灰石涂层的热−力耦合

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摘　要：在考虑了温度与变形之间的相互作用后，对经典的 Fourier 瞬态热传导方程进行了修正，并采用适合于高温及高应变率条件下的热弹塑性方程作为本构模型，从而建立了在 Ti-6Al-4V 基体上等离子喷涂羟基磷灰石涂层这一独特条件下的热-力耦合模型。据此，采用有限元方法对温度场和残余应力场进行了耦合求解。模拟了基体预热温度对涂层各个残余应力分量的影响。此外，为了能得到定量的比较，还采用了“材料去除”的实验技术测试了涂层在界面处的残余应力。结果表明：计算结果与实验结果吻合；在界面的边缘处有明显的应力集中；适当提高基体的预热温度对于减少残余应力是有帮助的。

关键词：热−力耦合；等离子喷涂；羟基磷灰石涂层；有限元法

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