Thermal Stress Analysis of W/Cu Functionally Graded Materials by Using Finite Element Method

Zhenxiao Yang\textsuperscript{1,2,*}, Min Liu\textsuperscript{2}, Chunming Deng\textsuperscript{2}, Xiaofeng Zhang\textsuperscript{1,2}, Changguang Deng\textsuperscript{2}

\textsuperscript{1}School of Materials Science and Engineering, South China University of Technology, Guangzhou, 510640, China
\textsuperscript{2}Guangzhou Research Institute of Nonferrous Metals, Guangzhou 510651, China

E-mail: yangzhenxiao@163.com

Abstract: Copper alloys with tungsten coating shows an excellent plasma irradiation resistance, however, the difference of coefficient thermal expansion between W and Cu makes it really a difficult job to prepare over 1 mm W coating with high adhesive strength. Functionally graded material (FGM) seems to be an effective method to improve the adhesive strength of thick W coating. This paper focused on the finite element simulation on thermal stress for W/Cu FGM with different graded layers, composition and thicknesses. In addition, the variance of stresses for functionally graded coatings with the steady state heat flux were simulated by finite element analysis (ANSYS Workbench). The results showed that the W/Cu FGM was effectively beneficial for the stress relief of W coating. Meanwhile, the maximum von mises stress decreased approximately by 52.8\% compared to monolithic W plasma facing material. And the four-layer FGM with a compositional exponent of 2 was optimum for 1.5 mm W coating.

1 Introduction

Tungsten is regarded as promising plasma facing material (PFM) for the nuclear fusion. Tungsten not only has the highest melting point among metals and low sputtering yields, but also owns low tritium retention and low erosion rate under plasma loading [1-2]. Copper and its alloys are being developed as heat sink materials due to their prominent thermal conductivity [3-4]. Low pressure plasma spraying (LPPS) offers the ability to coat large area, complex shapes coating and in-situ repair of the damaged coating [5]. But it is a challenge to deposit tungsten coating on CuCrZr for the larger mismatch of physical properties, which will cause thermal stress concentration on the W/Cu interface and lead to failure modes such as cracking or W coatings spalling when W/Cu exposing to severe thermal loading. The studies show that the introduction of W/Cu functionally graded materials (FGMs) can effectively alleviate the stress concentration on the W/Cu interface, release residual stress and improve the adhesive properties [6-8].

In this paper, the thermal stresses of W/Cu FGMs with different graded layers, different compositional exponent and different thicknesses, as well as the changes of stresses under the steady heat flux were simulated by finite element ANSYS Workbench code.

2 Establishment of finite element model

\* Corresponding author. Tel.: +86-20-37238263; Fax: +86-20-37238531.
Email: yangzhenxiao@163.com.
2.1 Geometric model and finite element model

Figure 1(b) shows the geometric model of the W/Cu plasma facing component (PFC) and the design scheme of functionally graded coatings. The size of CuCrZr substrate is 30×40×25 mm, a straight tube with diameter of 10 mm, an average temperature of 30°C and a convection exchange coefficient of 5 MW/(m²·K) was assumed on substrate. Meanwhile, the steady state heat flux of 8 MW/m² was loaded on the top surface of W/Cu, the thickness of W coating was set for 1.5 mm and W/Cu graded layers were designed for 0.2~5.0 mm, the number of layers ranged from 1~10. The compositional distribution was using the exponential function: \( f_{Cu} = (Z/t_{FGM})^p \), where \( f_{Cu} \) is the volume content of Cu, \( p \) is a compositional exponent. Different \( p \) represents different composition distribution discipline. When \( p<1 \), which means whole graded layers owns more volume content of Cu; when \( p>1 \), the volume content of W is more; \( p = 1 \), the volume content of W and Cu shows a linear distribution.

The calculation was performed on ANSYS Workbench station, hexahedral eight-node elements (SOLID5) were selected as the thermal-structure model. The coating and substrate were assumed to be isotropic for simplicity in this study. The analytical model was perfect elastic body without plastic deformation. Thermal radiation and phase transformation were not considered in the calculation. The modeling consisted of two steps. Firstly, a thermal model was used to determine the temperature through the specimen during heat loading. Secondly, the resulting thermal histories were transferred to a mechanical model to compute the thermal stresses both coating and substrate. A fine mesh is introduced to model including substrate, graded layer and W coating, seen in Figure 1(a).

![Geometry model (a) and finite element analysis model (b) of W/Cu PFC](image)

2.2 Physical properties model

Table 1 lists the materials properties used in the simulation. Physical properties for different graded layers were calculated by the rules of mixture called Kern, which can be assumed from the following equations [9].

\[
C = \frac{v_{Cu}c_{Cu} + v_{W}c_{W}}{v_{Cu} + v_{W}} \frac{3c_{Cu}}{2c_{Cu} + c_{W}}
\]

\[
\alpha = v_{Cu}\alpha_{Cu} + v_{W}\alpha_{W} + \frac{4G_{Cu}(K-K_{Cu})(c_{Cu} - c_{W})v_{W}}{K} \frac{4G_{Cu} + 3K_{W}}{G_{Cu} + 3K_{W}}
\]

Where \( v, v_{Cu}, v_{W} \) is volume fraction respectively; \( C, c_{Cu}, c_{W} \) is thermal conductivity; \( \alpha, \alpha_{Cu}, \alpha_{W} \) is coefficient of thermal expansion and \( K, K_{Cu}, K_{W} \) is bulk modulus of graded layer, Cu and W. Young's modulus \( E \), Posison's ratios \( \gamma \) were calculated by average field theory [10], shown as
follow.

\[ K = K_{Cu} + \frac{v_{W}}{3K_{Cu} + 4G_{Cu}} \]  
\[ G = G_{Cu} + \frac{v_{W}}{6G_{Cu}(3K_{Cu} + 4G_{Cu})} \]  
\[ \gamma = \frac{3K - 2G}{6K + 2G} \]  
\[ E = 2G(1 + \nu) \]

Where \( G, G_{Cu}, G_{W} \) is the shear modulus of graded layer, W and Cu, respectively. Specific heat \( \lambda, \) Density \( \rho, \) were determined by (7) and (8).

\[ \rho = \rho_{Cu}v_{Cu} + \rho_{W}v_{W} \]
\[ \lambda \approx \lambda_{Cu}v_{Cu} + \lambda_{W}v_{W} \]

Where \( \rho, \rho_{Cu}, \rho_{W} \) is the density. \( \lambda, \lambda_{Cu}, \lambda_{W} \) is specific heat of graded layer, W and Cu, respectively.

**Table 1.** Physical properties of W, Cu, and different W/Cu graded layers

| Name     | Density (g/cm³) | Thermal conductivity (W·m⁻¹·K⁻¹) | Specific heat (J·kg⁻¹·K⁻¹) | Coefficient of thermal expansion (10⁻⁶K⁻¹) | Poisson's ratios | Young's modulus (GPa) |
|----------|-----------------|----------------------------------|------------------------------|------------------------------------------|-----------------|----------------------|
| CuCrZr   | 8.96            | 397                              | 386                          | 17                                       | 0.34            | 128                  |
| W        | 19.32           | 174                              | 138                          | 4.5                                      | 0.28            | 410                  |

**3 Results and discussion**

**3.1 Effect of number of graded layers on thermal stress**

Figure 2 shows the influence of layer number on the von mises stress, surface temperature with the compositional exponent of Cu volume content is 1. It can be seen that the maximum surface temperature changed slightly with the increase of number of graded layers, nearly as a straight line, which caused by reduction of the overall thermal conductivity and modest graded layers. Further, the von mises stress decreased to 756 MPa at the joint of five-layer system, which reduced by 22.7 % in contrast to single-layer system, while its temperature increased with only 6 °C. Additionally, the von mises stress changed within a wavy motion after the graded layers over five. The reason for this behavior that the coefficient of thermal expansion between each graded

![Figure 2](image-url)
layer reduced, which is conducive to reduce thermal stress. Moreover, the stress caused by temperature increased with increase of the surface temperature, which caused the von mises stress showing such trends.

3.2 Effect of compositional exponent on thermal stress
The thermal stress evolution is strongly influenced by compositional exponent of Cu volume content (p), shown in Figure 3. It can be observed that the surface temperature gradually increased with increase of the value of p, which is related to reduced Cu content of graded layers and increased W-content. With the increase of p-value, the von mises stress firstly decreased sharply. And then no remarkable change was observed when it increased to 10, reflecting physical properties of the changed graded layers. This shows that a reduction depends on the composition of the graded interface and significantly enhanced by the use of a partial graded with a high W-content. For five-layer system, when 0< p <1.6, the von mises stress reduced evidently, but the effect of p-value to stress was little when 1.6< p <10. The increase of surface temperature was slow with the increase of p-value.

3.3 Effect of graded thickness on thermal stress
To optimize the thickness of W/Cu graded layers, the compositional exponent p-value of 2 and four-layer system was used. The surface temperature, von mises stress versus graded layer thickness is shown in Figure 4. The surface temperature gradually increased along with the increment of graded layer thickness. In contrast to monolithic tungsten coating without FGM model, the temperature of 5.0 mm thickness system raised nearly 170°C. However, the von mises stress rapidly reduced to 474.39 MPa from 1006.2 MPa at 5.0 mm. The reason is that with the increase of graded layer thickness, which offered a wider adjustment space for the coefficient of thermal expansion and the elastic modulus of each graded layer, and thereby achieved a more uniform distribution of the internal stress. Therefore, in order to achieve an optimum stress relaxation, the thickness can be selected larger appropriately, but surface temperature rose. Further analysis, just for the purpose of stress reduction, the thicker graded layers is a better choice. But from another perspective, with the graded layer thickness increasing, the tungsten surface will be farther away from the location of the cooling water tube, the surface temperature will rapidly rise. When the graded layer thickness reaches a certain value, the temperature may reach the melting point of Cu and then lead to Cu melting, which is bound to reduce the ability of whole layers to conduct heat. Meanwhile, it will bring the newborn holes to composite material, causing W/Cu
plasma facing component to fail.

3.4 Simulation results of 4.0 mm W/Cu graded layer model

Figure 5 is the temperature and the thermal stress distribution of 4.0 mm W/Cu graded layer model when compositional exponent \( p \) is 2. As shown in Figure 5(b), an obvious deformation and stress concentration phenomenon occurred at the edges of the coating. The reason for the edge effect is that stress singularities occur at the outer surface, which characterized by element sizes. So the comparison of stresses was done at the symmetry axis (Y-axis), starting from the top of the cooling water tube to W outer surface. The von mises stress distribution of designed path (1 → 2) along the Y-axis is shown in Figure 5(d), and the maximum stress reduced by 48.8\% lower than that of monolithic tungsten coating without FGM model. The stress at the interface between the graded layer and the copper substrate is almost the same, but with the increase of the graded layer thickness, the stress at the interface between the graded layer and W coating reduced significantly. Although the stress relaxation is very obvious, the maximum surface temperature increased by 134.26°C.
4 Conclusions

The introduction of W/Cu FGM effectively alleviates the stress concentration. Four-layer model with compositional exponent of 2 was optimum for 1.5 mm W coating, which induced a 23 % reduction of the maximum stress compared to the monolithic W as PFM. Meanwhile, the von mises stress was decreased with the increase in the number graded layers firstly, and then changed within a wavy motion after the graded layers beyond five. Besides, with the increase of compositional exponent, the von mises stress firstly decrease sharply, no remarkable change was observed though it increased to 10. Results also showed that the von mises stress decreased with increase of the FGM thickness.

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