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Thermal stress analysis on chemical vapor deposition tungsten coating as plasma facing material for EAST

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ABSTRACT

Chemical vapor deposition-tungsten (CVD-W) coating on CuCrZr surface forming a flat-type structure is likely to be used as the vacuum wall materials except the divertor areas in EAST during its up-grade phase. This paper describes the residual thermal stress distribution in CVD-W coating substrate system using finite element analysis method (ANSYS code). Especially, the influence of interlayers, i.e. oxygen-free Cu (OFC) and W/Cu functionally gradient materials (FGMs) interlayer have been investigated in view of stress alleviation. Both the OFC and W/Cu FGMs interlayer can reduce the residual thermal stress, in which the OFC shows better interface and surface stress distribution than W/Cu FGMs, and is a preferred interlayer for CVD-W coating processing.

1. Introduction

In the coming up-grade phase of EAST, the current carbon based plasma facing component will be gradually switched to full tungsten (W) coated wall [1], because of the high melting point, low tritium retention and low sputtering yield of W which is foreseen as the ITER plasma facing material for divertor and currently the first candidate for DEMO first wall [2]. And, chemical vapor deposition-W (CVD-W) coating with several millimeters covering on the surface of CuCrZr heat sink is likely to be used as plasma facing material for primary first wall area [1]. The advantages of CVD-W coating are the high purity, high density, high thermal conductivity and possibility of in-situ repair [3,4], etc. The coating design, preparation and properties test are now performing in Institute of Plasma Physics, Chinese Academic of Sciences (ASIPP) in collaboration with Xiamen Honglu Tungsten Molybdenum Industry Co. Ltd.

The properties of CVD-W coating, to some extent, depends largely upon the residual thermal stress which is very common in coating deposition technology and originates from the mismatch of coefficient of thermal expansion (CTE) between coating and substrate materials when coating substrate system is cooled down to room temperature from deposition temperature [5,6]. Furthermore, the residual thermal stress in CVD-W coating-system would be superposed by the operational thermal stress caused by the cyclic heat deposition during operation. In general, the concentration of thermal stress in coating substrate system develops at the interface corner where the failures such as crack or exfoliation often originate [6,7]. Large residual thermal stress generated in CVD-W coating-substrate system may lead to the poor adhesion between substrate and coating and also the coating properties. As a result, the detaching and exfoliation of the coating would occur easily [7]. Indeed, the experiment that CVD-W coating on Cu substrate forming a W/Cu plasma facing block was exposed to the edge plasma in TEXTOR tokamak shows that the failure behavior of the coating is attributed to the large mismatch of the coefficient of thermal expansion (CTE), thus implying that deposition of W coating directly on heat sink material is not idealistic [4]. In addition, the deposition of W coating directly on CuCrZr at 500 °C shows severe cracking at surface, as reported in Ref. [1]. To mitigate the thermal mismatch, two kinds of interlayer, i.e. oxygen-free Cu (OFC) and functionally gradient materials (FGMs) have been designed as a transition interlayer inserting between the surface CVD-W coating and CuCrZr in plasma facing components [1,8]. Therefore, evaluation of residual thermal stress is an essential aspect of coating design strongly influencing the CVD-W coating properties.

In this paper, residual thermal stress in a 3D cylindrical CVD-W coating substrate system was successfully simulated using a finite element method (ANSYS code), and the interlayer effect was analyzed with respect to the stress alleviation. This work aims to achieve the distribution of residual thermal stress in CVD-W coating substrate system with different interlayer architectures and to choose a proper interlayer for the processing of CVD-W coating substrate system.

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2. Model and materials

To simulate the residual thermal stress in CVD-W coating-substrate system, a 3D cylindrical solid model with axis-symmetry option was considered, as shown in Fig. 1a. The diameter and thickness of the cylindrical coating substrate system are 20 mm and 8 mm, respectively, and the coating thickness is fixed as 2 mm. Such coating thickness is larger than that reported in the similar work [7,9], because the engineering requirement for PFMs needs appropriate thickness to withstand the cyclic plasma erosion for essential lifetime. A twenty-node hex/wedge solid 186 element was used to model such CVD-W coating-substrate system. The 3D 1/4 analytical model was meshed for FEA model with sweep meshing using the hex/wedge elements, which is shown in Fig. 1b. Especially, the meshing size near the edges was finer than that near center because these areas were under very high stress concentration. The horizontal displacement was applied on the symmetrical structure (in the *xoz* coordinate plane, Uy = 0, and in the *yoz* coordinate plane, Ux = 0), and the vertical displacement was constrained in the coordinate origin ($x = 0$, $y = 0$, $z = 0$, Uy = 0). All other sides were free so that bending was permitted during the cooling process. The residual thermal stress in the entire coating-substrate system would be produced by loading the uniform deposition temperature assuming 400 °C as initial temperature and room temperature as final temperature on the FEA model. It is assumed: (a) that the coating, interlayer and substrate were perfectly bonded at the interface; (b) that a uniform temperature was established in the FEA model before and after cooling without any transient effects; and (c) that the coating substrate system was in a stress free state at the deposition temperature.

The mechanical temperature-dependent properties of the W, CuCrZr and OFC for finite element analysis (FEA) are listed in Table 1, referencing from the similar work [10–12]. All the materials exhibit elastic–plastic behaviors. In particular, the layer number of the FGMs interlayer is fixed as 4, and the spatial composition of FGMs interlayer varies step-wisely and obeys an exponential function distribution [13]. And, the Kerner rules are used to calculate the properties of W/Cu mixed composite layers [14]. Three kinds of distribution, i.e. liner, W rich and Cu rich FGMs interlayer and OFC interlayer were analyzed and their architectures as well as the thickness were described in Fig. 1**c**.

3. Results and discussions

The distribution of stress and strain in coating-substrate system is not well-proportioned, but shows same at each radial–poloidal profile through the toroidal direction which is in good accordance with the axi-symmetry model option. For the sharp joint, the maximum von mises stress is as high as 1270 MPa, which is found in CVD-W coating at the corner where the stress singularities often occur, while the maximum von mises plastic strain of 1.47% occurs at CuCrZr substrate, as shown in Fig. 2a and b, respectively.

Table 2 shows the compare of the stress and plastic strain distribution with different interlayer architectures. For the architecture with OFC interlayer, the maximum von mises stress decreases to 612 MPa and is also found in CVD-W coating, however, the maximum von mises plastic strain increases to 2.4% and occurs at OFC interlayer while disappears at CuCrZr. The reduction of the maximum von mises stress can reach up to 51.8% if the 1 mm OFC interlayer is used. The stress alleviation mechanism may be attributed to the high plastic behavior of the OFC. While for the models with 4 mm Cu rich, liner and W rich FGMs interlayer, the maximum von mises stresses are 658, 467 and 615 MPa, respectively, illustrating that the component

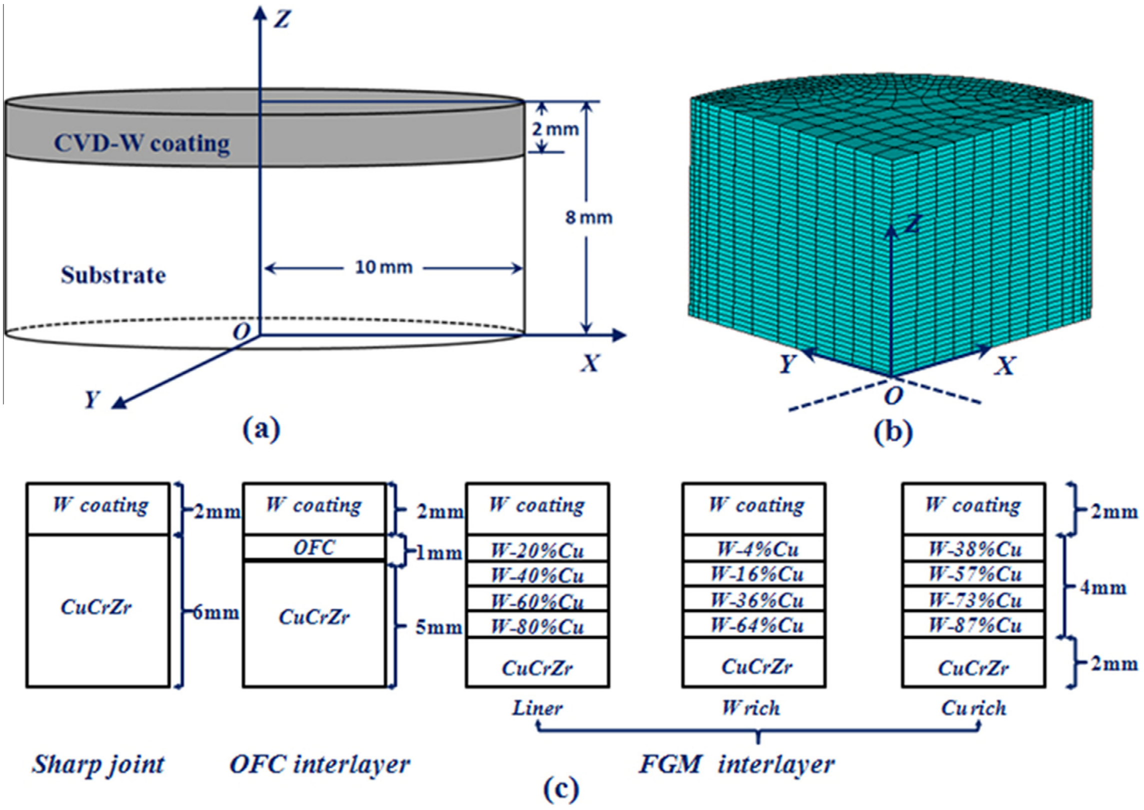

Fig. 1. Solid model and finite element model for the finite element analysis: (a) 3D cylindrical solid model as well as the dimension; (b) 3D 1/4 symmetry finite element model; and (c) different architectures of interlayer, i.e. OFC and liner, W rich and Cu rich FGMs interlayer.

Table 1
Temperature-dependent properties of the W, CuCrZr and OFC for FEA .

Materials	Temperature (°C)	CTE (10^{-6} K^{-1})	Elastic modulus (GPa)	Yield stress (MPa)	Tangent modulus (GPa)
W	20	3.93	398	1360	1.3
	500	4.21	390	854	1.0
CuCrZr	20	15.7	128	293	0.9
	250	17.3	118	257	0.7
	500	18.6	102	194	0.6
OFC	20	16.7	125	69	1.5
	400	17.8	100	45	0.9

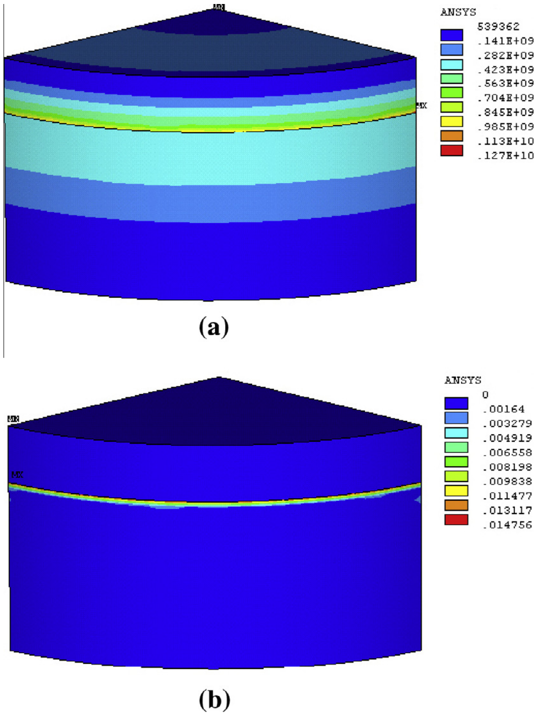

Fig. 2. Residual thermal stress and plastic strain distribution in CVD-W coating-substrate system ~~with and~~ without ~~OFC~~ interlayer.

Table 2
Compare of stress and plastic strain in coating substrate system with different architectures.

Architecture	Sharp joint	OFC	FGMs		
			Cu rich	Liner	W rich
σ (MPa)	1270	612	658	467	548
ε (%)					
Interlayer	0	2.41	0	0	0
CuCrZr	1.48	0	0	0	0.35

distribution in FGMs interlayer is a critical aspect influencing the stress alleviation and also distribution. It also implies that the optimized FGM interlayer can decrease the thermal stress to a level even below the OFC interlayer. Since the residual stress is caused due to the large thermal mismatch especially the coefficient of thermal expansion (CTE) between W coating and CuCrZr material, the FGMs leading the resultant smooth transition of the CTE from the copper substrate to the W coating can be considered as the possible reason for the reduction of the residual thermal stress. Meanwhile, the plastic strain disappear in the cases with Cu rich and liner FGMs interlayer, and it was only found in the case with W rich, which is smaller than that in sharp joint and with OFC interlayer.

At the edge line through thickness, the axial stress is larger than the other stress component, i.e. radial stress and shear stress etc., and is chose as a criterion to evaluate their interface performance. The distribution of the axial stress component through the thickness from substrate to coating with and without interlayers is presented in Fig. 3. The axial stress exhibits tensile stress at W coating and compressive stress at CuCrZr, and significant singularity at interface. These stress distribution may lead to the dominantly separate cracking at interface and can be effectively mitigated by introducing the OFC or three kinds of FGMs interlayer, in which the case with OFC showing lowest tensile stress is better than that case with FGMs interlayer. Therefore, the reduction of the tensile stress at the coating acts to enhance adhesion between the coating and substrate. Mechanically, the OFC interlayer acting as a soft flexible interlayer stops the propagation of cracks at the interface.

It is well known that the CVD-W coating shows columnar crystal and the grain boundary is weakly of which the reason is that the crack failure often occur at coating surface [1,3]. Thus the surface stress distribution which needs to be accessed is a critical aspect related to the coating properties after deposition. The radial stress distribution through surface from center to edge with and without interlayer is shown in Fig. 4. It is visible that the radial stress shows nearly tensile stress at surface, which causes the surface cracking. Without any interlayer, the maximum radial stress is found approaching edge side. While with both OFC and FGMs interlayer, the maximum radial stress is found in center. However, the OFC reduce the maximum radial stress, while all the three kinds of FGMs interlayer increase the maximum radial stress. In the case with OFC, the maximum surface tensile stress is 125 MPa which is 46% lower than that without any interlayer. While in the case with FGMs interlayer, the maximum surface tensile stress can reach up to 549 MPa. The reason may be that the high plastic strain in OFC decreases the total radial strain (0.23%) in W coating layer compare to that (0.54%) with sharp joint, while the decrease of

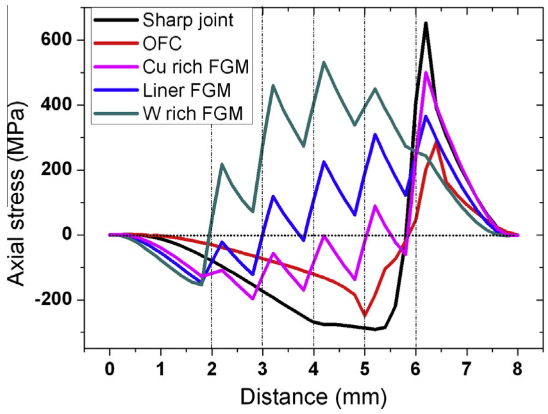

Fig. 3. Axial stress distribution through edge line from substrate to coating with and without interlayer.

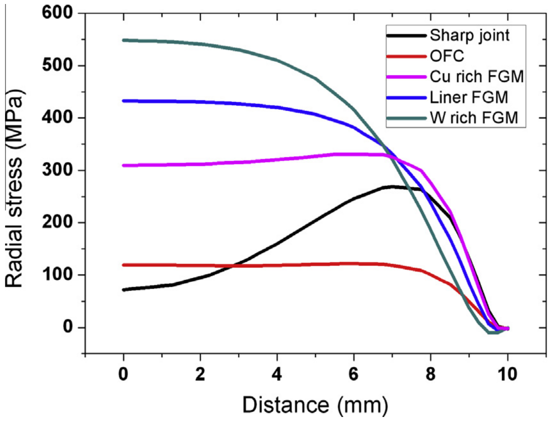

Fig. 4. Radial stress distribution through surface from center to edge with and without interlayer.

the plastic strain in CuCrZr in case of FGMs interlayer joint increase the radial strain (0.78%, 0.61% and 0.99% for Cu rich, liner and W rich cases, respectively) in W coating layer. The high tensile radial stress existing in coating surface means that the surface cracking easily occurs, especially for the CVD-W coating with columnar crystal posing a weak strength at radial direction. The former can be identified by the experiment result that the CVD-W coating on CuCrZr shows no crack at surface if the OFC interlayer is inserted between them [1], while the later is lack of the direct evidence which need the further efforts. That is to say, smaller radial stress within CVD-W coating surface can be obtained using OFC interlayer.

Altogether the FGMs interlayer can decrease the thermal stress even lower down the OFC interlayer. However, the better stress distribution at interface and especially at surface exists in CVD-W coating substrate system with OFC than that with FGMs interlayer. Therefore, one can conclude that the OFC is more preferred compared to the FGMs interlayer for CVD-W coating processing in view of the stress alleviation and also coating properties.

4. Conclusions

Residual thermal stress in CVD-W coating-substrate system was successfully simulated using finite element method (ANSYS code). In particular, the influence of the interlayer, i.e. OFC and W/Cu FGMs interlayer on the generation of residual thermal stress in CVD-W coating was discussed as regards interface and surface performance. Both the OFC and W/Cu FGMs interlayer can reduce the residual thermal stress, in which the OFC shows the better interface and surface stress distribution than W/Cu FGMs, and is a preferred interlayer for CVD-W coated plasma facing component. The future work will focus on the OFC interlayer thickness optimization taking into account a tile-sized model and combining the operational thermal stress analysis.

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