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Effect of C/Mo Duplex-coating on Thermal Residual Stresses in SiC_f/Ti_2AlNb Composites

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Abstract: Three-dimensional finite element physical models considering the layered distribution of materials at the interface were developed to study the effect of the coating system on distributions of thermal residual stresses in SiC_f/Ti_2AlNb composites. Two coating systems were comparatively studied, namely C coating and C/Mo duplex-coating. The thermal residual stresses after 1 080 ℃/1 h solution treatment and 800 ℃/20 h ageing treatment in the composites were also analyzed. The experimental results show that Mo coating can decrease thermal residual stress magnitude in the matrix. However, it would increase the thermal residual stresses in the interfacial reaction layer of TiC. The change of radial thermal residual stress in TiC layer is inconspicuous after solid solution and ageing treatment, but the hoop and axial thermal residual stresses increase obviously. However, the heat treatment can obviously reduce hoop and axial thermal residual stresses of the matrix, which is benefit to restrain the initiation and propagation of cracks in the matrix.

Key words: finite element simulation; titanium matrix composite; SiC fiber; thermal residual stress

1 Introduction

Continuous SiC fiber-reinforced titanium alloy-matrix composites (TMCs) can not only meet the needs of weight reduction and strength improvement, but also possess excellent high-temperature mechanical performance, such as high creep and fatigue resistance. Hence, TMCs are particularly suitable for the manufacture of components in the aero-engine field and skins for hypersonic transport aircraft and aerospace aircraft[1,2]. However, thermal residual stresses caused by the mismatch in the coefficients of thermal expansion (CTEs) between Ti alloy matrix and SiC fiber reinforcement during the cooling from consolidation temperature or high service temperature would influence the overall mechanical properties of the composites, such as the formation and propagation of fatigue crack, yield strength and interfacial shear strength[3-5]. Therefore, knowing thermal residual stresses is of great significance for the preparation and application of high performance SiC fiber-reinforced TMCs.

At the same time, in the composites, there is an interfacial region (*i e*, an interface coating or an interfacial reaction layer) between the fiber and matrix with a finite thickness[6-9]. Thermal residual stresses in interfacial region have a significant influence on the properties of composites[10-14]. Consequently, more attentions have been focused on thermal residual stresses near the interfacial region in TMCs. At present, experimental technologies of measuring residual stresses have made great progress. The main experimental methods for measuring residual stresses include X-ray diffraction, neutron diffraction, laser Raman spectroscopy, electron Moire wave and ejection test, peeling method, substrate bending method, selective matrix corrosion method and so on[15]. However, the thermal residual stresses of composites measured by these test methods are just the average thermal residual stresses within a certain scale range, and their fatal weakness is that they can not reflect the complex stress changes at and near the composite interface[16]. However, the thermal residual stresses calculated by finite element simulation can

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fundamentally overcome this drawback. So, many studies concerning the interfacial thermal residual stresses of composites have been studied by finite element analysis method.

For example, Shaw and Miracle[10] studied the effect of interfacial region on the transverse mechanical behavior of metal-matrix composites using finite element analysis (FEA). In their model, the interface was treated as a thin layer with a finite thickness between the fiber and matrix. Three separate interfacial conditions (*i e*, a graded carbon coating, an Y_2O_3 coating and an uncoated interface) have been considered to evaluate their influence on the (independent) thermal and mechanical properties of the interfacial region. Their results show that the thermal residual stresses in the interfacial region strongly depend on the properties of the interfacial region, while the residual stresses in the matrix and fiber are not significantly affected by these properties. And they believed the thickness of the coating has little influence on the thermal residual stresses. Haque and Choy[11] investigated the effect of the coating on thermal residual stresses generated at the fiber/matrix interface due to differences in the CTE mismatch between the various materials within the coating system. Their results show that the functionally-graded coating can reduce residual stresses generated due to CTE mismatch. Xia *et al*[12] investigated the axial stresses in TMC composites by using a three-dimension (3D) finite element model with concerning the interfacial reaction layer thickness. Lou and co-authors[13] investigated the effects of fiber volume fraction on transverse tensile properties of SiC_f/Ti-6Al-4V composites. Their results indicate that the applied stresses required to cause interfacial debonding (corresponding to strain jumps in stress-strain curves) are mainly affected by interfacial residual radial stresses at $\theta=0°$ under fixed interfacial bonding strength. Huang *et al*[14] also studied the effect of interfacial reaction layer thickness on the thermal residual stresses in SiC_f/Ti-6Al-4V composites. Their results show that for the interfacial region with thickness from 1 μm to 3 μm, a thicker interfacial region can reduce most of the thermal residual stresses in composites and can improve the axial tensile strength of the composites.

In this work, the attention was focused on simulating the thermal residual stresses in SiC_f/Ti_2AlNb composite system by using a three-dimension (3D) model with concerning the different coating systems and reaction layers, which would help to understand and optimize the mechanical properties of the composite with C coating and Mo coating.

2 Finite element analysis

2.1 Properties of the composite constituents

The composite system consists of a titanium alloy matrix, Ti_2AlNb, reinforced by SiC fibers with a volume fraction of 35% and an interfacial region. In the system, SiC fiber was treated as elastic substance (Table 1), whereas temperature dependent elastic-plastic behavior was considered to describe the isotropic Ti_2AlNb matrix. Fig.1 shows the main mechanical properties of Ti_2AlNb matrix as a function of temperature used in the models[17].

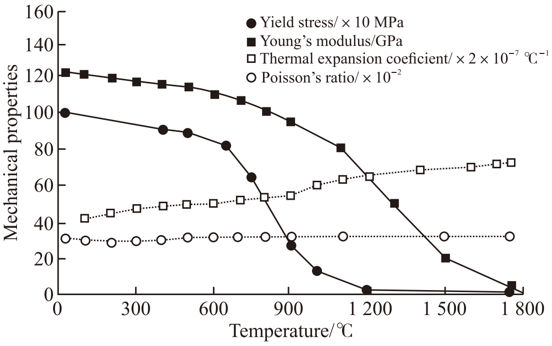


Fig.1 Mechanical properties of Ti_2AlNb matrix as a function of temperatures[17]

In our earlier work, C/Mo duplex-coating-coated SiC fiber-reinforced Ti_2AlNb-matrix composites have been studied by experiments[18,19]. The C coating and C/Mo duplex-coating were mostly investigated in these literatures. The C coating can prevent the direct chemical reaction between SiC and matrix and produce brittle TiC between C coating and matrix. Therefore, the interfacial region can be simulated as C/TiC in case of C coating. For the as-prepared $SiC_f/C/Mo/Ti_2AlNb$

Table 1 The main properties of SiC fiber and other interfacial materials

Material	Temperature/℃	Yong's modulus/GPa	Poisson ratio	Coefficient of thermal expansion/(10^{-6}/℃)
TiC	All temperatures	440.00	0.20	7.60
C	All temperatures	160.00	0.23	10.00
SiC	All temperatures	413.70	0.33	4.86

Table 2 The main properties of Mo coating used in the models

Temperature/℃	Young's modulus/GPa	Poisson's ratio	Yield stress/MPa	Shear modulus/GPa	Coefficient of thermal expansion /(10^{-6}/℃)
25	335.71	0.324	550	20	5.8-6.2
100	322.38	0.324	478	20	
200	326.19	0.324	370	20	
300	322.86	0.324	320	20	
400	318.10	0.324	278	20	
500	307.39	0.324	240	20	
600	307.14	0.324	218	20	
700	302.38	0.324	208	20	

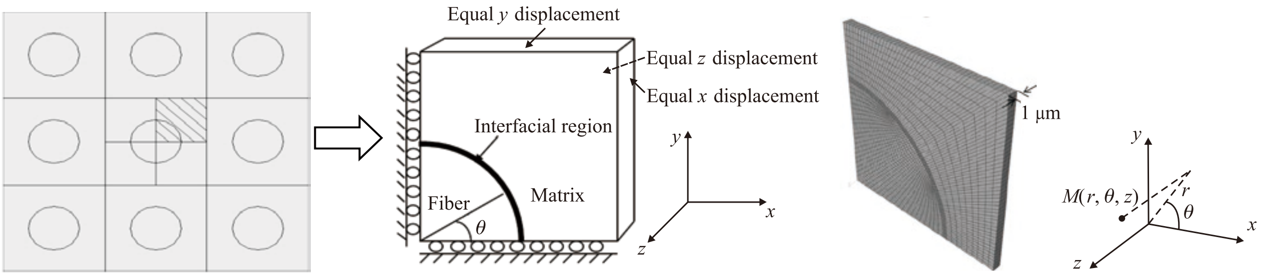
Table 3 The main properties of B2 used in the models

Temperature/℃	Young's modulus/GPa	Poisson's ratio	Yield stress/MPa	Shear modulus/GPa	Coefficient of thermal expansion /(10^{-6}/ ℃)
20	105.4	0.31	600	40.98	8.6
100	104.4	0.31	600	40.26	8.7
200	102.025	0.31	600	39.33	9.14
300	97.575	0.31	600	38.16	9.32
400	94.825	0.31	600	37.06	9.61
500	92	0.31	600	36.74	9.79
600	86	0.31	600	32	10.24
700	77	0.31	600	29	10.24

composite, there exists a uniform C coating on the surface of the SiC fiber, then Mo coating next to the C coating, and there is a transition zone between the Mo coating and the normal matrix, which is affected by the diffusion of Mo atoms. Mo element is a B2 phase stabilizer for Ti_2AlNb alloy[20], so the transition zone should be mainly B2 phase. Our earlier work had reported that B2 phase is a type of plastic phase[19], which could effectively accommodate the interfacial thermal residual stresses of the composites[21]. As described above, the interfacial regions can be modelled as C/TiC in case of C coating and C/Mo/TiC/B2 in case of C/Mo duplex coating, respectively. C and TiC were treated to be elastic and isotropic substances. Their thermal and mechanical properties are shown in Table 1. Mo and B2 were treated to be elastic-plastic substance. Their thermal and mechanical properties are shown in Tables 2 and 3, respectively.

2.2 3D finite element model

Finite element analysis was implemented using the ABAQUS code. A 3D model with a square fiber array pattern includes three main phases, *i e*, the SiC fiber, interfacial region and the matrix. As shown in Fig.2(a), a representative volume element (RVE) was selected to calculate thermal residual stresses in SiC_f/Ti_2AlNb composite. The whole behavior of the composite was assumed to be the same as that of the RVE. The diameter of SiC fiber is 140 mm. Along the fiber axis, the model thickness is 1 µm. We set the following boundary conditions (Fig.2(b)): the nodes on the bottom face of the model (*i e*, the x-z plane at $y = 0$) were not allowed to move in the y-direction, while the nodes on the top face of the model were coupled together to shift an equal amount of displacement in the y-direction. Similarly, the nodes on the front face of the model (*i e*, the y-z plane at $x = 0$) and on the left face of the model (*i e*, the x-y plane at $z = 0$) were not allowed to move in the x-direction and z-direction, respectively, while the nodes on the back and right faces of the model were coupled together to shift an equal amount of displacement in the x-direction and z-direction, respectively. Furthermore, the node at the origin of the model was not allowed to move in any directions to prevent rigid body displacement. All interfaces in the composites were assumed to be perfectly bonded. Fig.2(c) shows the complete geometry of the model and the finite element mesh. Meshing is an important step for finite element simulation. The quality of meshing often affects the accuracy of calculation results and the convergence of calculations. Therefore, cell type and meshing should be carefully selected when meshing. Since the stress magnitude and distribution at the



(a) (b) (c)

Fig.2 The finite element models: (a) Square fiber geometry model; (b) Selected 1/4 fiber model as RVE and the boundary conditions; (c) Finite element mesh of the RVE and the relationships between the cylindrical coordinate used in the model and the Cartesian coordinate for the composites

interface would be mainly concerned, the mesh near the interface was specially refined, as shown in Fig.2(c). It should be pointed out that, according to the simulation results of different mesh sizes, no matter how fine the mesh is, it will only affect the decimal value of the simulation results. Therefore, as long as the mesh division is relatively small, it is reasonable.

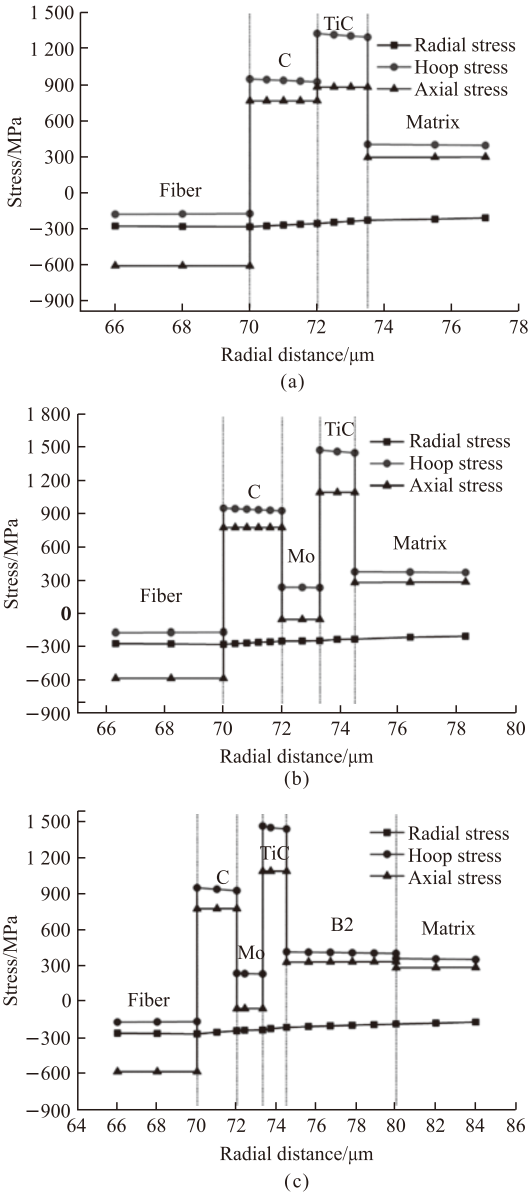
In this paper, the C3D20R hexahedral meshing unit was used, and the meshing method was structural meshing. The total number of grids in the whole model was about 12 500. We chose 980 ℃ as the reference temperature, which is a hot-pressing temperature for SiC_f/Ti_2AlNb composites[19]. So the simulation of thermal residual stresses was from the high temperature of 980 ℃ to the room temperature of 25 ℃.

As mentioned before, in case of C coating, the interfacial region can be modelled as C/TiC. According to our previous studies[19], the thicknesses of C and TiC layers were 2 μm and 1.5 μm, respectively. Similarly, in case of C/Mo duplex coating, the thicknesses of C, Mo, TiC and B2 layers were 2 μm, 1.3 μm, 1.2 μm, and 5.5 μm, respectively. In addition, the effect of solution and aging treatment on the thermal residual stresses was studied. According to our earlier work[18], in case of C single coating, after 1 080 ℃/1 h solution treatment and 800 ℃/20 h aging treatment, the C coating had been exhausted and SiC fiber had reacted with the matrix directly, so the thickness of the reaction layer increased up to 2.8 μm. TiC was the main interfacial reaction product, so the composition of the interfacial region was treated as TiC in this work.

3 Results and discussion

3.1 The influence of different interfacial regions on thermal residual stresses

Fig.3 shows the distributions of thermal residual stresses along radial direction at θ=0° on z=0 plane



(a)

(b)

(c)

Fig.3 Distributions of the thermal residual stresses along radial direction at θ=0° on z=0 plane in the as-prepared Ti_2AlNb-matrix composite when different coating systems are applied: (a) C coating; (b) C/Mo duplex-coating; (c) C/Mo(B2) coating in the as-prepared Ti_2AlNb-matrix composite when different coating systems are applied. As can be seen, in the interfacial region, the radial stress is compressive in all constituents and the value changes brightly along the radial direction. The hoop stress and axial stress are compressive ones in the fiber but tensile ones in other constituents. However, the values of hoop stress and axial stress differ greatly. Both in case of C coating and C/Mo duplex-coating, the maximum hoop stress exists in TiC layer of the interfacial region. So more attention should be paid to the thermal residual stress near the interface between the reaction layer and the matrix where microcracks appear easily.

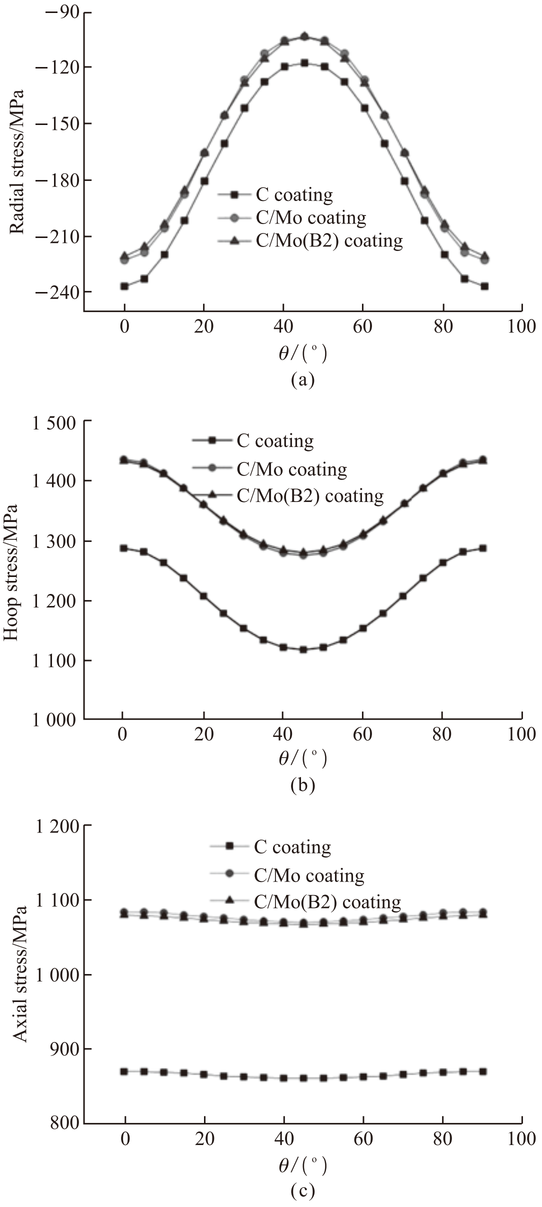


Fig.4 Distributions of thermal residual stresses in the TiC layer adjacent to the matrix at θ=0-90° on z=0 plane when different coating systems are applied: (a) Radial stress; (b) Hoop stress; (c) Axial stress

Fig.4 shows the distributions of thermal residual stresses in the TiC layer adjacent to the matrix at θ=0-90° on z=0 plane when different coating systems are applied. As can be seen, the coating system has a significant influence on the hoop stresses and axial stresses (Figs.4(b-c)). Compared with C single coating, the stresses of C/Mo duplex-coating increase significantly no matter considering the B2 phase or not. Especially for the axial stress, the value increases by 200 MPa. In addition, the value of the hoop stresses is very high in TiC adjacent to the matrix, even close to 1 500 MPa. The high hoop stresses generally make the cracks generate easily perpendicular to the hoop direction in this zone during the fabrication process of the composite. In contrary, the radial stresses in the interfacial region reduce slightly when using C/Mo duplex-coating (Fig.4(a)).

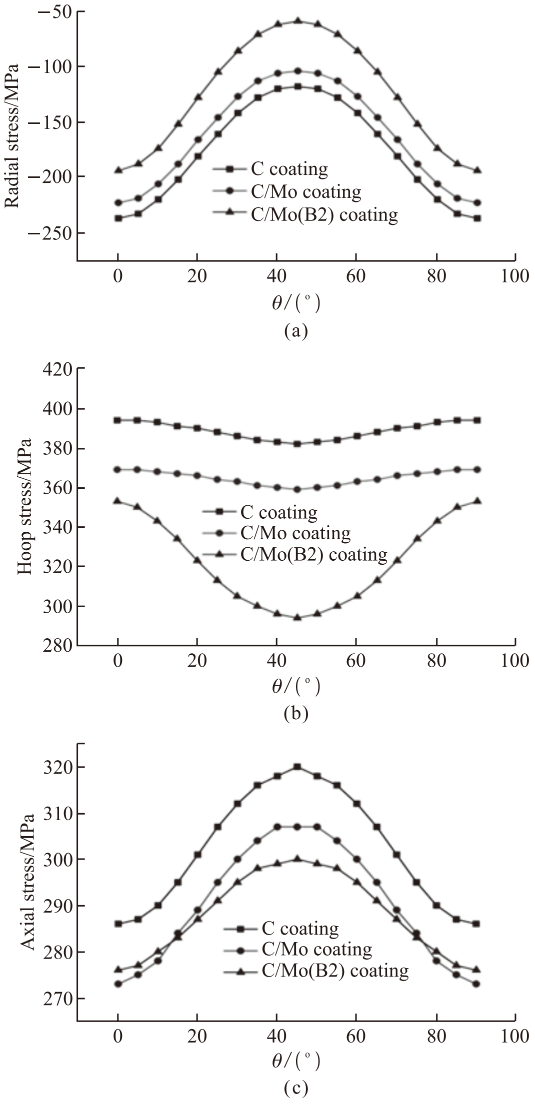


Fig.5 Distributions of the thermal residual stresses in the matrix adjacent to TiC layer at θ=0-90° on z=0 plane when different coating systems are applied: (a) Radial stress; (b) Hoop stress; (c) Axial stress

Fig.5 shows the distributions of thermal residual stresses in the matrix adjacent to TiC layer at θ=0-90° on z=0 plane when different coating systems are applied. As can be seen, compared with C single coating, the stresses for C/Mo duplex coating decrease to varied extents. The Mo coating does not change the uniformity of the stress distribution when B2 phase was not considered. However, the hoop stress gradient was increased among θ=0-90° when B2 phase was considered. As shown in Fig.5(b), the hoop stress value decreased by almost 100 MPa at θ=45° for C/Mo(B2) coating. Although the bigger gradient is not an ideal result, the stress value decreases. Lower tensile stress can reduce the initiation and propagation of cracks[18]. The above results indicate that Mo coating can significantly reduce the stress magnitude in the matrix. However, it would increase the stress in the TiC reaction layer.

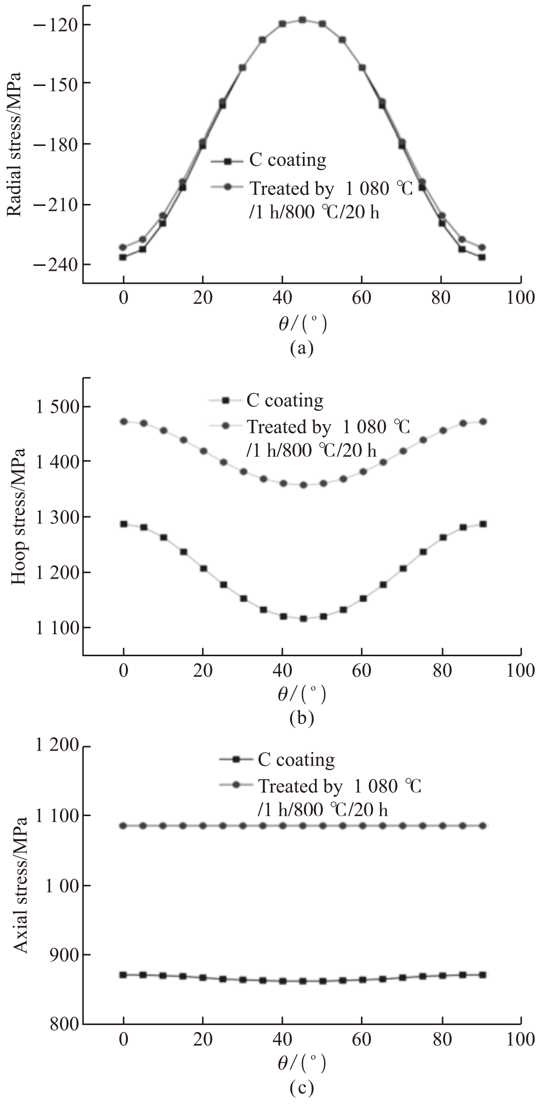


Fig.6 Distributions of the thermal residual stresses in TiC layer adjacent to the matrix at θ=0-90° on z=0 plane before and after treated by 1 080 ℃/1 h/800 ℃/20 h: (a) Radial stress; (b) Hoop stress; (c) Axial stress

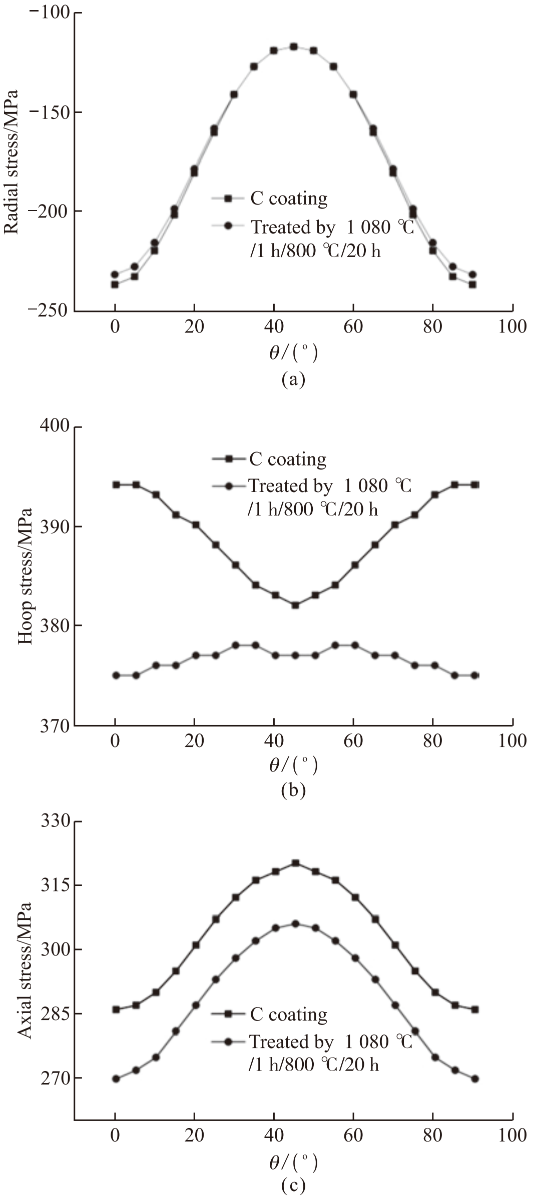


Fig.7 Distributions of the thermal residual stresses in the matrix adjacent to TiC at θ=0-90° on z=0 plane before and after 1 080 ℃/1 h+800 ℃/20 h heat treatment: (a) Radial stress; (b) Hoop stress; (c) Axial stress

Generally, the larger CTE mismatch between components is, the higher the thermal residual stresses are in composites. As shown in Tables 1-3, the CTE mismatch degree between TiC and the matrix is smaller than that between Mo and the matrix, whereas the Young's modulus mismatch degree between TiC and the matrix is higher than that between Mo and the matrix. In fact, in Figs.4(b) and 4(c), the hoop stress and axial stress in TiC are higher in case of C/Mo duplex coating than in case of C single coating, while in Figs.5(b) and 5(c), the hoop stress and axial stress in the matrix are higher in case of C coating than in case of C/Mo duplex coating. Therefore, the hoop and axial stresses in the reaction layer are mostly dependent upon the CTE mismatch rather than Young's modulus mismatch between the components. However, the hoop and axial stresses in the matrix are mostly dependent upon the Young's modulus mismatch rather than CTE mismatch between the components.

3.2 Effect of solution and aging treatment on residual thermal stresses

Fig.6 shows the thermal residual stresses in TiC adjacent to the matrix as a function of the angle before and after 1 080 ℃/1 h solid solution and 800 ℃/20 h ageing treatment. It can be seen that the change of the radial stresses in TiC is inconspicuous after the solution and aging treatment (Fig.6(a)). However, the heat treatment has an outstanding influence on the hoop and axial stresses in TiC: the hoop and axial stresses increase obviously (Figs.6(b-c)). This result can be mostly contributed to the reduction of C layer and the increase of TiC layer. The Young's modulus of TiC is significantly larger than that of C layer, therefore it is easier to have stress concentration.

Fig.7 shows the thermal residual stresses in the matrix adjacent to the TiC layer before and after 1 080 ℃/1 h solid solution and 800 ℃/20 h ageing treatment as a function of the angle. It shows that the heat treatment can significantly reduce the hoop and axial thermal residual stresses. The reduced hoop and axial residual stresses are benefit to restrain the initiation and propagation of cracks in the matrix when the composite is subjected to external tension, thus the tensile performance of the matrix can be improved.

4 Conclusions

C/Mo duplex coating can improve interfacial compatibility of the SiC$_f$/Ti$_2$AlNb composites. Mo coating has a significant influence on thermal residual stresses in TiC layer formed during the interfacial reaction, especially on the hoop and axial thermal residual stresses. Mo coating can reduce the stress magnitude in the matrix, however, it would increase the stresses in TiC layer. After 1 080 ℃/1 h solution treatment and 800 ℃/20 h aging treatment, the change of the radial stresses in TiC is inconspicuous, however, the hoop and axial stresses increase obviously. The solution and ageing treatment can significantly reduce the hoop and axial stress of the matrix, which can improve the mechanical properties of the matrix.

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