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Optimization design and residual thermal stress analysis of PDC functionally graded materials*

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Abstract: The distribution of thermal stresses in functionally graded polycrystalline diamond compact (PDC) and in single coating of PDC are analyzed respectively by thermo-mechanical finite element analysis (FEA). It is shown that they each have a remarkable stress concentration at the edge of the interfaces. The diamond coatings usually suffer premature failure because of spallation, distortion or defects such as cracks near the interface due to these excessive residual stresses. Results showed that the axial tensile stress in FGM coating is reduced from 840 MPa to 229 MPa compared with single coating, and that the shear stress is reduced from 671 MPa to 471 MPa. Therefore, the single coating is more prone to spallation and cracking than the FGM coating. The effects of the volume compositional distribution factor (n) and the number of the graded layers (L) on the thermal stresses in FGM coating are also discussed respectively. Modelling results showed that the optimum value of the compositional distribution factor is 1.2, and that the best number of the graded layers is 6.

Key words: Functionally graded materials (FGM), Optimum design, Polycrystalline diamond compact (PDC), Residual thermal stress, Finite element method (FEM)
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INTRODUCTION

Polycrystalline diamond compacts (PDC), consisting of a polycrystalline diamond (PCD) layer on a WC-Co substrate, and having high hardness and abrasive resistance, are used in a variety of drilling and machining applications (Farhad, 2001; Sadi and Muzaffer, 2001). However, due to differences of thermal and mechanical properties in diamond and WC-Co substrate, residual thermal stresses develop in regions near the interfaces during fabrication. The diamond coating exhibits a smaller coefficient of thermal expansion than the substrate, resulting in the development of residual thermal stresses during cooling from the sintering temperature. Therefore, polycrystalline diamond coatings usually suffer premature failure because of spallation during cooling due to excessive residual stresses generated near the interface and poor bond strength between the coating and the substrate (Jia and Wang, 2005; Paggett *et al*., 2002; Amirhaghi *et al*., 1999). Cracking and spallation usually occur at the interface of coatings. These residual stresses affect the lifetime and performance of PDC such as bond strength, thermal cycling, etc.

In an effort to reduce the residual stress and improve the properties of polycrystalline diamond coatings, functionally graded material (FGM) with a graded composition from the top coat to the bond coat were designed in order to reduce thermal expansion mismatch among the different coating layers and substrate (Carpinteri and Pugno, 2006).

However, up to now, there have been few investigations on the effectiveness of FGM coatings in

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the reduction of thermal stresses and improvement of the properties, and as we know, the poor bond strength between the coating and substrate of PDC is always a problem when these coatings are subjected to mechanical and thermal stresses (Krawitz *et al.*, 1999). In this paper, residual stresses are calculated by non-linear thermo-mechanical FEA using finite element software ANSYS9.0. At the same time, the influence of the volume composition distribution factor and the number of the graded layers on the maximum stress is analyzed. For contrast, the residual stresses in single coating are also calculated using FEA method.

THERMAL STRESS ANALYSIS OF SINGLE LAYER PDC

Analytical models

The specimen consists of diamond-coated cylindrical substrates with a diameter of 13 mm. The thickness of the diamond layer is 1.2 mm. The PCD layer consists of 6% (wt%) Co cemented carbide, and the substrate consists of WC-15% Co (wt%) cemented carbide. The density, thermal expansion coefficient, thermal conductivity coefficient, Young's modulus and Poisson's ratio of these materials are given in Table 1.

Table 1 Physical properties of PCD and substrate

Parameter	PCD	Substrate
Density (kg/m^3)	3830	13950
Conduction coefficient (W/(m·K))	560	80
Expansion coefficient ($\times10^{-6}$ K^{-1})	2.6	5.4
Young's modulus ($\times10^9$ Pa)	890	580
Poisson's ratio	0.07	0.22

The residual stresses of PDC are analyzed by the finite element method (FEM, ANSYS9.0). The coating and substrate are assumed to be isotropic for simplicity in this study. The analytical model is a perfect elastic body without plastic deformation. It is assumed that the specimen was fabricated at a temperature of 1320 °C and cooled to room temperature (20 °C). Cooling is assumed to be uniform throughout the specimen, and the effect of time-dependent materials evolution processes such as creep is ignored (Li and Dong, 2001). An axial symmetric model is chosen in order to reduce computer costs and data manipulation time. A fine mesh is introduced to model both the coating and the substrate. The thermal-structure element Plane13 is selected. The geometrical and the analytical models are given in Fig.1.

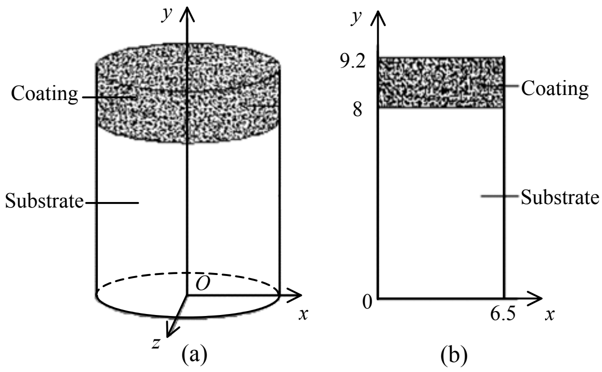

Fig.1 Typical model of PDC. (a) Geometrical model; (b) Analytical model

Contour plot of residual stress distribution of single coating PDC

Results for the single coating showed that there is a large stress concentration near the edge of the substrate and the coating interface, as shown in Fig.2. Radial stress is usually tensile in substrate because the thermal coefficient expansion of substrate is larger than that of the diamond coating. The largest tensile stress (1290 MPa) is generated at the interface of the specimen.

Fig.2b shows a contour plot of axial stress distribution of the single coating. Near the free edge of the specimen, the axial stress is tensile in the whole diamond coating. The largest stress (840 MPa) occurs near the specimen interface, and may cause the spallation of the coating.

There is a remarkable shear stress concentration at or close to the edge of the specimen, as can be seen from Fig.2c. The shear stress concentration near the edge is related to the interface crack (Zhang *et al.*, 2006).

THERMAL STRESS ANALYSIS OF FGM PDC

Models and materials

The diameter of the FGM PDC is 13 mm. The diamond layer thickness is 0.2 mm, and the thickness of the FGM layer is 1 mm. The overall thickness of

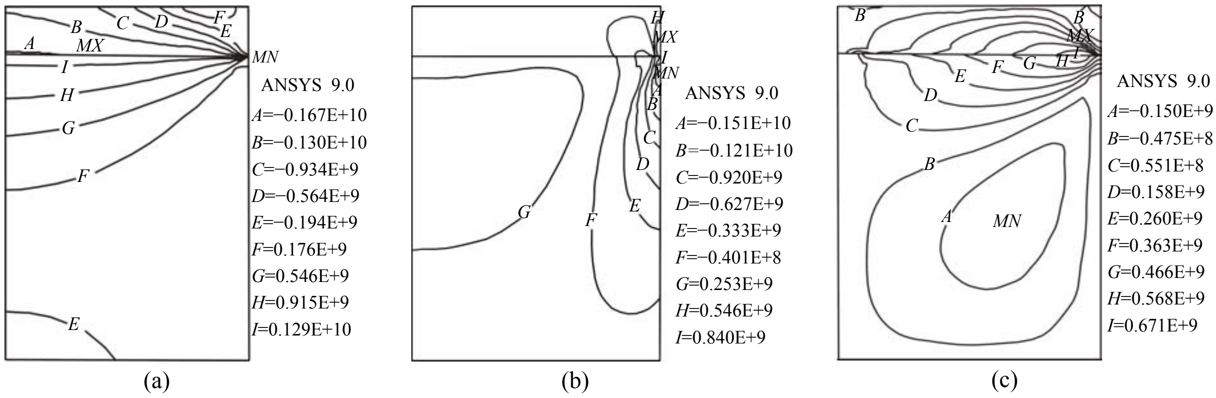

Fig.2 Contour plot of residual stresses distribution of single coating. (a) Radial stress; (b) Axial stress; (c) Shear stress

the PDC is 9.2 mm. The geometrical model is shown in Fig.3. The materials of PCD layer and the substrate are the same as that of the single layer PDC specimen.

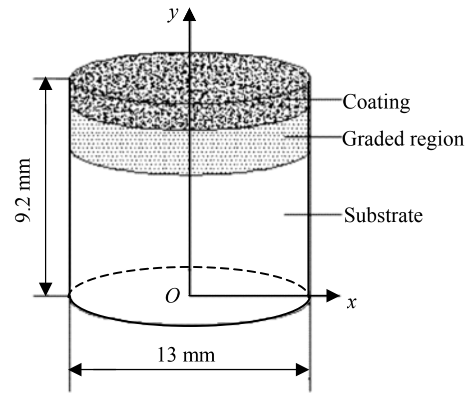

Fig.3 Geometrical model of FGM PDC

The volume fraction of each graded layer is determined by the following function:

$$f(y)=\begin{cases} 0, & 0\le y\le 8, \\ \left(\dfrac{y-8}{H}\right)^n, & 8<y\le 9, \\ 1, & 9<y\le 9.2, \end{cases}$$

in which $f(y)$ is the PCD volume fraction of each graded layer, y is the distance from the bottom (substrate) layer to the graded layer, and H is the thickness of the graded region (1 mm in the present case), n is the compositional distribution factor. Variations of the volume fraction of PCD throughout the graded regions with variations of n values are shown in Fig.4.

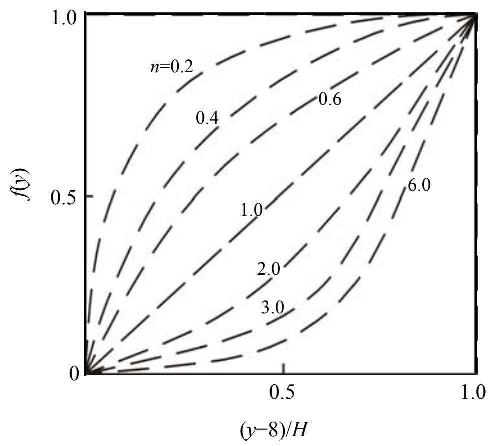

Fig.4 Variations of the volume fraction of PCD for several values of the exponent *n*

Each graded layer is assumed to be isotropic and elastic. Thermal expansion coefficient, thermal conduction coefficient, density, Poisson's ratio and Young's modulus of each graded layer are assumed to be independent to temperature for simplicity. Thermal conduction coefficient is calculated from the Maxwell equation:

$$\lambda=\lambda_1\times\frac{3\lambda_2+2(1-f_2)(\lambda_1-\lambda_2)}{3\lambda_1-(1-f_2)(\lambda_1-\lambda_2)}, \tag{1}$$

in which λ, λ_1 and λ_2 are the thermal conduction coefficient of graded layers, substrate and PCD, respectively. f_2 is the volume faction of PCD.

Thermal expansion coefficient of graded layer is calculated from the Kerner equation (Xu and Wei, 2000):

$$\alpha=\alpha_1+\frac{f_2(\alpha_2-\alpha_1)}{\dfrac{12K_1G_1}{3K_1+4G_1}\cdot\left(\dfrac{f_2}{3K_1}+\dfrac{1}{4G_1}+\dfrac{1-f_2}{3K_2}\right)}, \quad (2)$$

where α, α_1 and α_2 are the thermal expansion coefficient of graded layer, substrate and PCD, respectively. f_2 is the volume faction of PCD. K_1 and K_2 are the bulk modulus of substrate and PCD, respectively, and G_1 is the shear modulus of substrate. They are calculated by the following functions:

$$G_1=\frac{E_1}{2(1+\mu_1)}, \quad K_1=\frac{E_1}{3(1-2\mu_1)},$$

E_1 is Young's modulus and μ_1 is Poisson's ratio of substrate.

Density, Young's modulus and Poisson's ratio of graded layer are computed by the following equation (Huang *et al.*, 2001):

$$p=f_2p_2+(1-f_2)p_1,$$

in which p, p_1 and p_2 represent corresponding properties (i.e. density, Young's modulus and Poisson's ratio) of graded layer, substrate and PCD, respectively. f_2 is the volume faction of PCD.

The residual stress of FGM PDC is analyzed by the FEM (ANSYS9.0). An axial symmetric model is again used. A fine mesh is introduced to model both the coating and the substrate, and in graded region the element mesh is refined in order to gain accurate results. An analytical model and element mesh model are given in Fig.5.

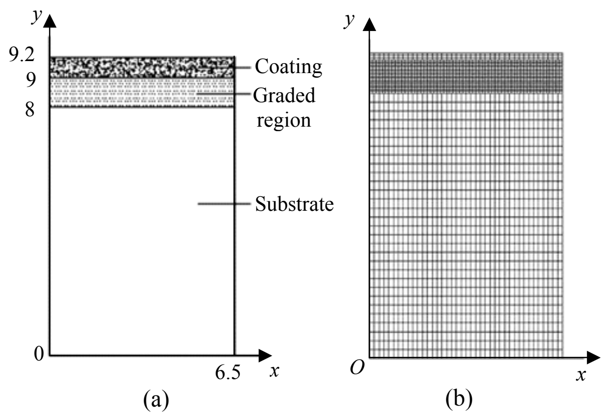

Fig.5 Analytical model (a) and the element mesh model (b) of FGM PDC

Relations between residual stresses and compositional distribution factor *n*

Keeping the number of the graded layer L=6 and the thickness of the graded region H=1 mm, different n values have been investigated in order to study the effect of compositional distribution factor on the level of residual stresses, including n=0.2, 0.4, 0.6, 0.8, 1.2, 1.4, 1.6, 1.8, 2.0, 2.4 (Li *et al.*, 2003; Wang and Sun, 1999). The calculation results are given in Fig.6.

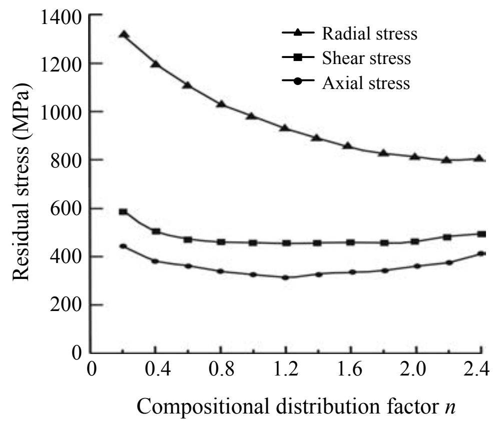

Fig.6 Relations between residual stresses and compositional distribution factor *n*

From Fig.6, we can see that the maximum axial tensile stress and the shear stress decrease with an increase of the value n until n=1.2, and after that they increase with increasing n value. The maximum radial tensile stress continuously decreases with increase of the value n. Generally, the large axial tensile stress at the PCD surface may result in micro-cracks that can propagate vertically toward the interface and cause macroscopic cracks in the PCD coating. And large shear stress can contribute either shear or mixed modes of failure of coating. Therefore, the optimum n is 1.2.

Relations between the residual stresses and the number of graded layers

Fig.7 shows the calculation results when n=1.2, H=1 mm, and taking the number of the graded layers as 2, 4, 6, 8, 10, respectively.

It can be seen from Fig.7 that both the maximum axial tensile stress and the shear stress decrease rapidly before L=6, but after that the stresses change little. The fabrication cost considered, the optimum number of graded layers is 6.

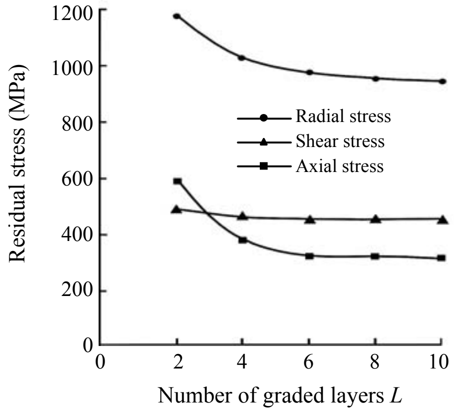

Fig.7 Relations between residual stress and number of graded layers

Contour plot of residual stress distribution of FGM PDC

The residual stress of FGM PDC were studied by the finite element method when n=1.2 and L=6. The results are given in Fig.8.

FEM results showed that there is a large stress concentration near the interface of the specimen. The radial stress distribution is similar to that of the single coating, but the maximum tensile stress is reduced from 1290 MPa to 813 MPa. The maximum shear stress is reduced from 671 MPa to 417 MPa compared with single coating. Fig.8b shows that the axial stress distribution differs from that of the single coating. The maximum axial tensile stress is not generated at the interface but in the substrate interior, and the stress value is reduced from 840 MPa to 229 MPa.

STRESSES COMPARISION OF SINGLE LAYER PDC AND FGM PDC

Fig.9 shows the distributions of radial stress, shear stress and axial stress along the radius at the interface between substrate and coating. It can be seen that there is a remarkable stress concentration at the edge of the interface and that it may cause the spallation of the coating. It also can be seen that the compressive radial stress decreases with an increase of radius. The maximum compressive stress occurred near the center of the interface.

Like the axial stress, the tensile stress occurred near the edge of the specimen and decreased abruptly and changed to compressive stress with the decrease of specimen radius, and then changed to tensile stress gradually. Fig.9b shows that the tensile stress in single layer PDC is larger than the stress in the FGM coating. The maximum tensile stress at the interface of the single coating is 943.4 MPa, while it is 323 MPa in the FGM coating. Generally, this large tensile stress may cause the spallation and buckling of PCD coatings. So the single coating is more prone to spallation and cracking than the FGM coating.

The shear stress is always tensile for the single coating, and the maximum stress that occurred near the edge of the interface is 615.3 MPa, which is three times that of the single coating's 205 MPa. Because these shear stresses can contribute either shear or mixed modes of failure of coatings, the single coating is more prone to shear failure.

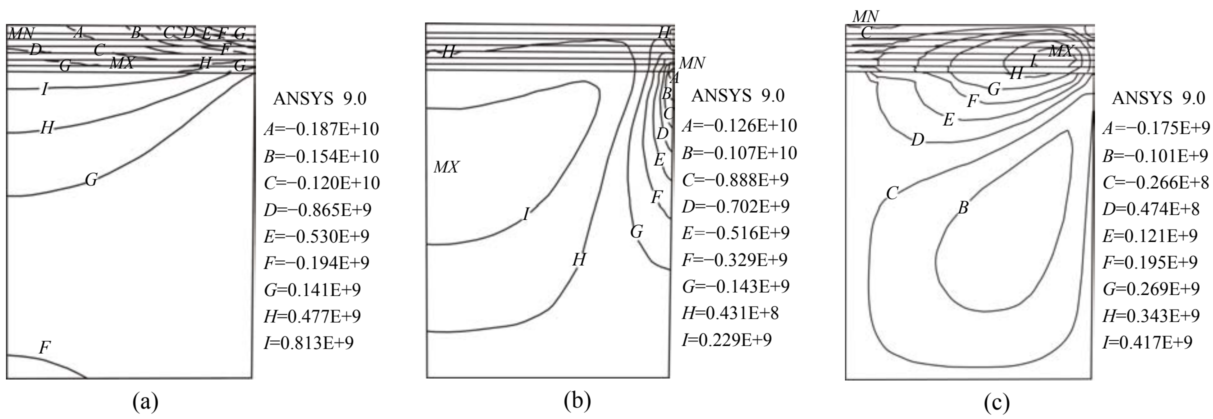

Fig.8 Contour plot of residual stresses distribution of FGM coating. (a) Radial stress; (b) Axial stress; (c) Shear stress

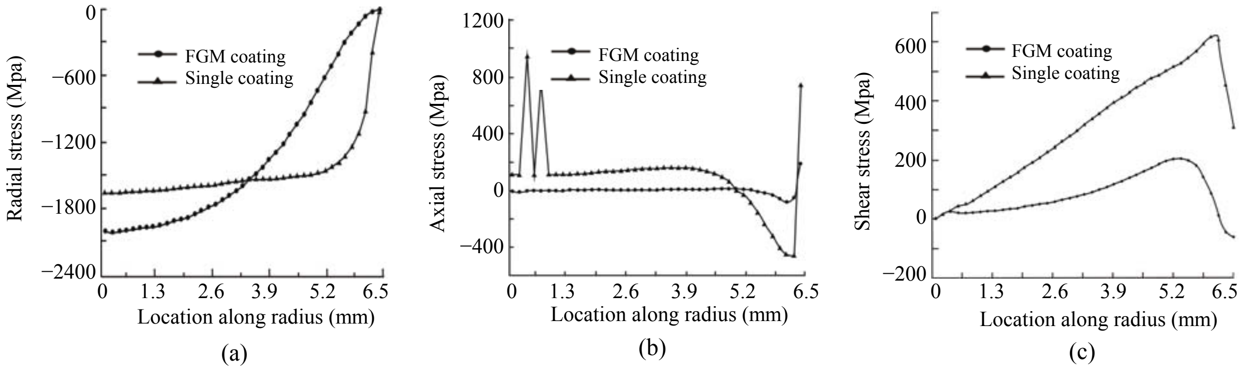

Fig.9 Comparison of residual stress distribution at interface along radius. (a) Radial stress; (b) Axial stress; (c) Shear stress

DISCUSSION AND CONCLUSION

Based on the results obtained in the present work, the following conclusions can be drawn:

The residual stress of the FGM coating is smaller than that of the single coating, which indicates that the single coating is more prone to surface cracking than FGM coating during facture. The maximum axial stress of FGM coating is reduced from 986 MPa of single coating to 323 MPa, and the maximum shear stress is reduced from 722 MPa to 454 MPa.

The axial stress and the shear stress are smallest when the number of FGM layer L=6 and the composition distribution factor n=1.2. They are the optimum parameters for FGM PDC discussed in this paper.

The stress distribution is improved in the interface of FGM PDC, and bond strength is greatly increased. It is indicated that the FGM has great influence on the thermal stress distribution.

For simplicity, FEM analysis in this paper is on the basis of elastic model, so that the results may be somewhat different from the real status. The real stresses and stress distribution of FGM PDC can be analyzed by synchrotron x-rays and neutrons diffraction analysis, which will be used in future work.

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