Chapter 31 Film Residual Stress Assessment Method via Temporarily Thermal Relaxation

Xin-Xin Cheng and Chen-Wu Wu

Abstract The concept of temporarily thermal relaxation is extended theoretically to assess the film residual stress. First, the contribution of the initial stress to the observable displacement field is separated with eliminating the thermal expansion effect of the material. Then, the residual stress is inversely derived through the displacement increment. Finally, finite element analysis was carried out to provide numerical description of the partial relieve of the residual stress.

Keywords Film • Residual stress • Assessment • Temporarily thermal relaxation

31.1 Introduction

Almost all of the films used in many products are formed with large residual stress. To describe accurately the film residual stress is of importance for designing a product or evaluating its reliability [1, 2]. A great many of research have been attracted to focus on the measurement and assessment of the film residual stress [3, 4].

The method of temporarily thermal relaxation [5] is theoretically extended herein to assess film residual stress. The basic mechanism on such concept can be reviewed briefly herein. It is well known that non-uniform temperature elevation will lead to non-uniform distribution of elastic modulus in an initial homogeneous solid of material with temperature-dependent elasticity [6]. The non-uniform change of modulus should result in the redistribution of the initial stress (herein identical to the term residual stress), which will contribute to the observable displacement field upon thermal loading experiment. Furthermore, the contribution is determined by the initial stress, the initial and present elastic properties of the material, among which the analytical relationship could be established. Therefore, the initial (residual) stress could be inversely derived after extracting the contribution of the initial stress from the observable displacement field. Theoretically speaking, such separation can be achieved by solving the heat conduction partial difference equations and thermo-elastic partial difference equations for an actual experiment.

In this article, the displacement increment accompanied with the thermal softening of modulus in an initially stressed film subjected to non-uniform heating is calculated based on an axis-symmetry model. For the sake of simplicity, the preliminary analytical solution is derived for a freestanding film and numerical modeling is utilized to investigate the influences of the substrate on the film deformation. First, the contribution of the redistribution of the initial (residual) stress to the observable displacement field is separated by eliminating the thermal expansion effect of the material. Then, the residual stress is derived inversely from such contribution of the initial stress. Finally, finite element analysis was carried through to provide numerical description of the partial relief of the initially stressed film.

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31.2 Theoretical Analysis

31.2.1 Formularization

Consider a double layer structure of homogeneous film and homogeneous substrate as shown in Fig. 31.1, in which the film is initially equiaxial tensioned in plane, i.e., the residual stress can be described via

$$\sigma_{\rho} = T_{rs}, \sigma_{\varphi} = T_{rs}, \tau_{\rho\varphi} = 0, \tag{31.1}$$

where σ refers to the normal stress component, τ is the shear stress component, ρ and φ represents the radial and tangent direction, respectively. Of course, such stress state shall develop a displacement vector field relative to the stress free state and can be expressed with the radial component as

$$u_{\rho[rs]} = \frac{1 - v}{E} T_{rs} \rho, \tag{31.2}$$

where E and v is the Yang's modulus and Poisson's ratio, respectively.

Now, assume the film is subjected to non-uniform temperature elevation, i.e., the temperature of the material within a circular region of radius r is increased via some heating technique, as shown in Fig. 31.2a, b. One can easily understand that the initial equilibrium state will be disturbed due to the non-uniform thermal softening of the material. A new equilibrium state will be developed, which, generally speaking, should be accompanied with the redistribution of the displacement.

Divide the temperature elevated circular region into the center circle and a series of annuluses, therefore the elastic properties can be assumed to be identical in every annulus as shown in Fig. 31.2c.

The interface traction and displacement should be continuous, that is,

$$\sigma_{\rho[k]} = \sigma_{\rho[k]}' = \sigma_{[k]}, \qquad (31.3)$$

And

$$u_{\rho[k]} = u_{\rho[k]}' = u_{[k]}.$$
(31.4)

Moreover, the radial displacement can be related to interface traction [7] as:

$$u_{\rho[1]} = \frac{1 - v_{[0]}}{E_{[0]}} \sigma_{[1]} r_1, \tag{31.5}$$



Fig. 31.1 Sketch of the initially equiaxially stressed film and substrate



Fig. 31.2 Sketch of the non-uniform temperature elevated film

$$u_{\rho[1]}' = \frac{1}{E_{[1]}} \left[\left(1 - v_{[1]} \right) \frac{\sigma_{[2]} r_2^2 - \sigma_{[1]} r_1^2}{r_2^2 - r_1^2} r_1 - \left(1 + v_{[1]} \right) \frac{r_2^2 r_1 \left(\sigma_{[1]} - \sigma_{[2]} \right)}{r_2^2 - r_1^2} \right], \tag{31.6}$$

across the interface between annulus denoted by k = 1 and that by k = 2.

$$u_{\rho[k]} = \frac{1}{E_{[k-1]}} \left[\left(1 - v_{[k-1]} \right) \frac{\sigma_{[k]} r_k^2 - \sigma_{[k-1]} r_{k-1}^2}{r_k^2 - r_{k-1}^2} r_k - \left(1 + v_{[k-1]} \right) \frac{r_{k-1}^2 r_k \left(\sigma_{[k-1]} - \sigma_{[k]} \right)}{r_k^2 - r_{k-1}^2} \right], \tag{31.7}$$

$$u_{\rho[k]}' = \frac{1}{E_{[k]}} \left[\left(1 - v_{[k]} \right) \frac{\sigma_{[k+1]} r_{k+1}^2 - \sigma_{[k]} r_k^2}{r_{k+1}^2 - r_k^2} r_k - \left(1 + v_{[k]} \right) \frac{r_{k+1}^2 r_k \left(\sigma_{[k]} - \sigma_{[k+1]} \right)}{r_{k+1}^2 - r_k^2} \right], \tag{31.8}$$

across the interface between No. k annulus and No. (k + 1) annulus.

$$u_{\rho[n]} = \frac{1}{E_{[n-1]}} \left[\left(1 - v_{[n-1]} \right) \frac{\sigma_{[n]} r_n^2 - \sigma_{[n-1]} r_{n-1}^2}{r_n^2 - r_{n-1}^2} r_n - \left(1 + v_{[n-1]} \right) \frac{r_{n-1}^2 r_n \left(\sigma_{[n-1]} - \sigma_{[n]} \right)}{r_n^2 - r_{n-1}^2} \right], \tag{31.9}$$

$$u_{\rho[n]}' = \frac{1}{E} \left[2r_n T_{rs} - (1+v)r_n \sigma_{[n]} \right], \tag{31.10}$$

across the interface between the annulus denoted by k = n and the annulus beyond the thermal softening region, in which it is also implied that $E_{[n]} = E$ and $v_{[n]} = v$ with E and v being the initial elastic constants of the material.

By utilizing the displacement continuous condition at the interface as indicated in Eq. 31.4 and dividing the radius evenly, which means that the width of every annulus is d = r/n, one can get the series of equations:

$$[A]\{\sigma\} = \{F_{rs}\},\tag{31.11}$$

where the elements of the coefficient matrix are

$$A_{11} = 3E_{[1]}(1 - v_{[0]}) + E_{[0]}(5 + 3v_{[1]})$$

$$A_{12} = -8E_{[0]}$$

$$A_{k,k-1} = -2E_{[k]}(2k + 1)(k - 1)^{2}$$

$$A_{k,k} = \begin{cases} E_{[k]}(2k + 1)\left[(1 - v_{[k-1]})k^{2} + (1 + v_{[k-1]})(k - 1)^{2}\right] \\ +E_{[k-1]}(2k - 1)\left[(1 - v_{[k]})k^{2} + (1 + v_{[k]})(k + 1)^{2}\right] \end{cases} k = 2, 3 \dots n - 1,$$

$$A_{k,k+1} = -2E_{[k-1]}(2k - 1)(k + 1)^{2}$$

$$A_{n,n-1} = -2E(n - 1)^{2}$$

$$A_{n,n} = E(1 - v_{[n-1]})n^{2} + E(1 + v_{[n-1]})(n - 1)^{2} + E_{[n-1]}(2n - 1)(1 + v)$$
(31.12)

and the elements of the force vector are

$$F_{rs[i]} = 0 \quad i = 1, 2, 3 \dots n - 1$$

$$F_{rs[n]} = 2E_{[n-1]}(2n-1)T_{rs}.$$
(31.13)

Solving the equation, the interface traction can be obtained as

$$\{\sigma\} = [A]^{-1}\{F_{rs}\}.$$
(31.14)

Thus, the displacement can be obtained at every interface as

$$u_{[1]} = \frac{1 - v_{[0]}}{E_{[0]}} \sigma_{[1]} d$$

$$u_{[k]} = \frac{d}{E_{[k-1]}} \left[\left(1 - v_{[k-1]} \right) \frac{\sigma_{[k]} k^2 - \sigma_{[k-1]} (k-1)^2}{(2k-1)} k - \left(1 + v_{[k-1]} \right) \frac{(k-1)^2 k \left(\sigma_{[k-1]} - \sigma_{[k]} \right)}{(2k-1)} \right] \quad k = 2, 3 \dots n - 1.$$

$$u_{[n]} = \frac{d}{E} \left[2nT_{rs} - (1+v) n\sigma_{[n]} \right]$$
(31.15)

Again, if the specimen dimension is large enough that boundary effect can be neglected, the displacement outside the thermal softening disc region is

$$u_{\rho} = \frac{1}{E} \left[(1 - v)T_{rs}\rho - (1 + v)\frac{r^2 (\sigma_{[n]} - T_{rs})}{\rho} \right].$$
(31.16)

Therefore, the radial displacement increment due to the material thermal softening is

$$\{u_{\rho}\} = \{u_{\rho}\} - \{u_{\rho[rs]}\}$$
(31.17)

Let $[B] = [A]^{-1} = \begin{pmatrix} B_{11} & \dots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \dots & B_{nn} \end{pmatrix}$, then Eq. 31.14 can be rewritten as

$$\{\sigma\} = T_{rs} \cdot 2E_{[n-1]}(2n-1)\{B_{1n}\cdots B_{nn}\}^T.$$
(31.18)

Thus the radial displacement at the location $\rho = r$ can be obtained as following

$$u_{[n]} = \frac{2r}{E} \left[1 - (2n-1)(1+\nu)E_{[n-1]}B_{nn} \right] T_{rs}.$$
(31.19)

From Eq. 31.2, the initial radial displacement at the same location can be expressed directly as

$$u_{[n][rs]} = \frac{1-v}{E} r T_{rs}.$$
(31.20)

Substitute the relevant components in Eq. 31.17 by Eqs. 31.18 and 31.19, one can get the equation relating the residual stress and the displacement increment as

$$U_{IN[n]} = \left[2 - 2(2n-1)(1+\nu)E_{[n-1]}B_{nn} - (1-\nu)\right]\frac{r}{E} \times T_{rs}.$$
(31.21)

Therefore, the residual stress can be derived through Eq. 31.21 as

$$T_{rs} = U_{IN[n]} \frac{E}{r \left[2 - 2(2n-1)(1+\nu)E_{[n-1]}B_{nn} - (1-\nu)\right]}.$$
(31.22)

As a simple illustration, assuming the film is partially subjected to even temperature elevation, which indicates that the elastic modulus *E* and the Poisson's ratiovchange into $E_{[0]}$ and $v_{[0]}$ throughout the whole thermal softening region, respectively. Then one can describe the residual stress as

$$T_{rs} = \Delta U_{IN} \frac{E[E(1-v_{[0]}) + E_{[0]}(1+v)]}{r(1+v)[E(1-v_{[0]}) - E_{[0]}(1-v)]}.$$
(31.23)

To sum up, the radial displacement increment is dependent on the initial residual stress T_{rs} and elastic parameters of the material. Therefore, the initial stress T_{rs} can be calculated inversely once the displacement increment $\{u_{\rho}\}$ and temperature profile of the specimen are obtained by measurement and analysis. To this end, heat transfer analysis and direct thermoelastic analysis [5] should also be carried out, of which the former is used to determine the softened elastic properties while the latter is used to eliminate the thermal expansion effect, which is always inevitably included in the real experimental process.

31.2.2 Analytical Results

Suppose the radius of the circular film specimen to be R = 0.1 m and the radius of the thermal softening region r = 0.01 m. Assume the lowest value of the modulus at the center of the thermal softening region is 100, 125 and 150 GPa for three cases and increase linearly up to the initial value of 200 GPa at the location of r = 0.01 m. Moreover, the Poisson's ratio v = 0.3 is assumed to be temperature-independent for simplicity.

The results are shown in Figs. 31.3 and 31.4 with the numerical deviation being lower than 0.1%, which is maintained after the division number n is larger than 400.

Figure 31.3a shows the radial displacement increment $\{u_{IN}\}$ induced by the thermal softening of the film stiffness, of which the lowest elastic modulus is 100, 125 and 150 GPa corresponding to the three cases. It is indicated that the displacement increment increases with decreasing the lowest elastic modulus. Moreover, the influences of the thermal softening of the material are neglectable when away from the temperature elevated region, which is seemed to be in accordance with the Saint-Venant's Principle.

The radial strain increment $\varepsilon_{\rho} = \partial U_{IN}/\partial \rho$ is diagramed in Fig. 31.3b, which also shows that the radial strain increment increases with decreasing the lowest elastic modulus. This is easy to understand because, in the extreme, the initial strain should be totally released if the material within the heated region were removed just like that appears in hole-drilling process, for which the lowest elastic modulus is certainly reduced to zero. Generally speaking, the higher the elevated temperature is the lower the minimum modulus will be maintained. Therefore, it can be expected that the displacement/ strain increments will increase with increasing the elevated temperature.

Moreover, the radial displacement increment and strain increment also increase with increasing the magnitude of the initial residual stress, as shown in Fig. 31.4a, b. Again, in the extreme, one can understand that if there is no initial residual stress, there'll still be no displacement even though the material stiffness is unevenly reduced due to non-uniform thermal softening. Of course, it should be noted again that no thermal expansion effect need to be taken into account in discussing this phenomenon.



Fig. 31.3 Radial (a) displacement and (b) strain increment for three cases of different thermal softening conditions

31.3 Numerical Computations

31.3.1 FEA Model

Considering the fact that the substrate has not been involved in the analytical analysis model, the Finite Element Analysis (FEA) model as shown in Fig. 31.5a is utilized to investigate the influence of the substrate on the deformation of the film. The dimension of the axis-symmetrical model is 100 mm × 100 mm and the thickness of the film is $t_f = 100 \mu m$, the initial residual stress is realized by stretching the rightmost side of the geometry by 0.15 mm along the radial direction.

As an example, the elastic modulus of the film is linearly correlated to the temperature and that of the substrate is fixed to be 200 GPa. The film elastic modulus is 200 GPa at room temperature and 100 GPa when temperature reaches 300°C and the its Poisson's ratio is always 0.3. The applied temperature profile is shown in Fig. 31.5b, in which the film temperature is 300° C at the center (x = 0) and ascends linearly to 25° C at the location x = 5 mm. In computation, the continuous conditions of both displacement and traction are adopted across the interface between the substrate and film.



Fig. 31.4 Radial (a) displacement and (b) strain increment for three cases of different initial residual stress levels



Fig. 31.5 FEA model of the film-substrate and temperature elevation profile

Fig. 31.6 Radial stress (a) contour and (b) mapped onto film surface path



31.3.2 Numerical Results

The redistributions of the residual stress are shown in Fig. 31.6a, b, and the radial displacement/strain increments are shown in Fig. 31.7a, b.

In Fig. 31.6a, one can see that the radial stress is partially relaxed around the region of elevated temperature. In comparison, the initial residual stress is uniform within the film as indicated in the curve portion away from the center graphed in Fig. 31.6b.

The radial displacement/strain increments as shown in Fig. 31.7a, b indicate that the magnitude of the displacement increment is nearly one order lower than that of the freestanding film although the tendency of the displacement/strain increments are similar to that of the freestanding film.





31.4 Conclusions

The analytical results show that displacement/strain increments will be developed by non-uniform temperature elevation in the initially stressed freestanding film. Such displacement/strain increments increase with increasing the magnitude of initial (residual) stress or elevated temperature. The initial (residual) stress can be derived inversely by the displacement increment and relevant temperature profile. The numerical results reveal that the constraint effect of the substrate will influence the magnitude of the displacement/strain increment while not alter the basic characteristics of them.

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References

- 1. Tonshoff HK, Seegers H (2000) Influence of residual stress gradients on the adhesion strength of sputtered hard coatings. Thin Solid Film 377-378:340-345
- 2. Teixeira V (2002) Residual stress and cracking in thin PVD coatings. Vacuum 64:393-399
- 3. Zhang T-Y, Chen L-Q, Fu R (1999) Measurements of residual stresses in thin films deposited on silicon wafers by indentation fracture. Acta Mater 47:389–3878
- 4. Chandra T, Ionescu M, Mantovani D (1999) Residual stress analysis of textured materials by X-ray diffraction method. Mater Sci Forum 706–709:1673–1678
- 5. Chen-Wu Wu (2012) Temporarily thermal relaxation of residual stress. In: Silva Gomes JF, Mário Vaz AP (eds) Proceedings for 15th international conference on experimental mechanics, Porto/Portugal, 22–27 July 2012
- 6. Fukuhara M, Sanpei A (1993) Elastic moduli and internal frictions of Inconel 718 and Ti-6Al-4V as a function of temperature. J Mater Sci Lett 12:1122–1124
- 7. Timoshenko SP, Goodier JN (2004) Theory of elasticity, 3rd edn. McGraw-Hill Companies, Inc., New York, pp 65-71