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Predicting multilayer film's residual stress from its monolayers

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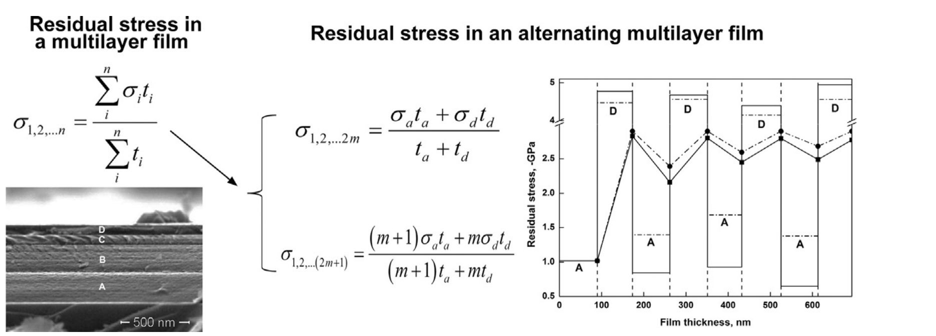
HIGHLIGHTS

- Residual stress in a multilayer film equals the weighted average of its monolayers' stresses.
- Relative errors in predicting multilayers' stresses are in the range of 0.2% to 10.7% in this paper.
- Alternating multilayers' stresses gradually approach a constant value as its monolayer number increases.
- Si-DLC interfaces can either rise or lower DLC films' residual stresses.

GRAPHICAL ABSTRACT



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ABSTRACT

Multilayer film's residual stress was deduced from Stoney formula. A simple stress formula, which means that multilayer residual stress can be given by the weighted average of each monolayer's residual stress, was proposed and verified through experiments on gradient diamond-like carbon (DLC) and CrN/DLC multilayers prepared by cathodic vacuum arc technology. Typical stress formulas for alternating multilayers were also investigated on corresponding DLC multilayers. Multilayer samples, together with monolayers existed in multilayers, were prepared and studied. Surface profilometry and film stress tester were used to measure films' thicknesses and residual stresses, respectively. Cross-sectional morphologies of multilayers were observed by scanning electron microscope. Results showed that the proposed stress formula was correct and could provide useful instructions on multilayer design. The formula's accuracy of predicting multilayer's residual stress through its monolayers was also investigated. In the present paper, relative errors of theoretical values were in the range of 0.2% to 10.7%, which had a strong relationship with the substrate–film interfaces. In addition, as to alternating multilayer film, its residual stress is a constant value as the number of monolayers is even; while this number is odd, multilayers' residual stress gets close to the constant value gradually and monotonously.

1. Introduction

Residual stresses in films have been of interest to scientists for a long time, especially for multilayers [1–6]. Proper residual stress is good to raise films' toughness and adhesion to substrates [7,8], while excessively high stress may lead to film failure [9–11]. Therefore, lots of researchers tried to take efforts to predict residual stress to design multilayers with high performance.

Numbers of methods for predicting residual stresses in multilayer films or structures have been proposed. In the research of Hsueh [12], an exact closed-form solution was formulated to predict thermal stress in elastic multilayer systems. Strain distribution in the system was decomposed into a uniform strain component and a bending strain

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component. Zhang et al. [13] proposed an analytical model based on force and moment balances to predict thermal residual stress distributions in multilayered coating systems. A closed-form solution of thermal stress was obtained which is independence of the number of coating layers. They also used a similar model to predict distribution and magnitude of thermal residual stress in multilayer coatings with graded properties and compositions [14]. Systematical analysis of effects of the gradient exponent, elastic modulus of ceramic component, number of coating layers and substrate's properties on thermal residual stress was conducted on $ZrO_2Y_2O_3$/NiCrAlY functionally and compositionally graded thermal barrier coatings. In another study, Zhang et al. [15] put forward a numerical model to predict the thermally induced residual stresses in the multilayer coating on a substrate with cylindrical geometry. This model is based on that the axial forces in the longitudinal direction and the interfacial pressures in the radial direction, which were derived from differential thermal contraction between the adjacent layers, could be determined by the continuity conditions at the interfaces using layer-by-layer procedure. In addition, finite element simulation has also been used to predict residual stresses in thermal barrier coatings [16–18]. Though all these methods can help people understand residual stress distribution or magnitude within multilayers, they either can't be applied to films with high intrinsic stresses or can't provide specific value when some parameters involved in the model are hard to obtain.

In the present study, a concise and practical method based on that Young's modulus and Poisson ratio of the multilayer-substrate system are approximately equal to that of substrate was put forward. A weighted average formula of multilayer's residual stress derived from Stoney formula was presented and then verified by gradient amorphous (DLC) as well as composite (CrN/DLC) multilayers. What's more, alternating multilayer's stress formulas derived from the former weighted average formula were also displayed and investigated through corresponding multilayer DLC films. By analyzing relative errors of theoretical values, the formulas' feasibility of predicting multilayer's residual stress was discussed in detail.

2. Theory and experimental details

2.1. Theory

When using Stoney formula to calculate residual stress in a film, it is considered that thickness of the film is much less than that of substrate [4]. The modified Stoney formula can be written as follows:

$$\sigma = \frac{Et_s^2}{6(1-\upsilon)}\frac{1}{t_f}\left(\frac{1}{R}-\frac{1}{R_0}\right), \quad (1)$$

where t_f is the thickness of film, R_0 and R correspond to radii of curvature of substrate measured before and after film deposition [19]. As for certain substrates, Young's modulus (E), Poisson's ratio (υ) and thickness (t_s) are all invariable values. So the part $Et_s^2/[6\,(1-\upsilon)]$ in Eq. (1) can be replaced by a constant: K. Hence, the modified Stoney formula could be rewritten as

$$\sigma = \frac{K}{t_f}\left(\frac{1}{R}-\frac{1}{R_0}\right). \quad (2)$$

Under harsh conditions, films made up by one single layer sometimes can't meet the needs any more. Fig. 1 illustrates a common design of a gradient multilayer film consisting of four kinds of monolayers: A, B, C and D. Here, t_i and σ_i represent thickness and residual stress of a certain monolayer, respectively. Several assumptions are made for later derivation.

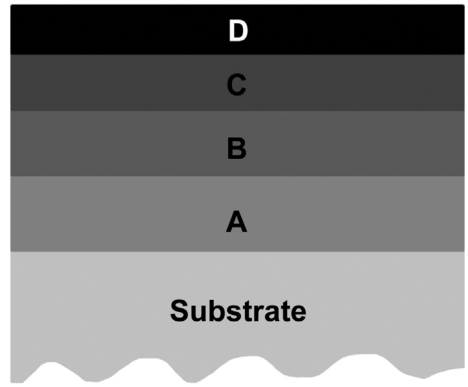

Fig. 1. Schematic diagram of a gradient multilayer film.

(1) $t_f = \sum_i ti \ll ts$.
(2) Young's modulus and Poisson's ratio of the system composed of film and substrate are approximately equal to that of substrate.
(3) No cracks or delamination occur in the film–substrate system.
(4) Deformation of substrate is in the range of elastic deformation.

Table 1 shows residual stresses of multilayers as well as substrate's radii of curvature with corresponding multilayers. Substrate's radius of curvature changes from R_0 to R_A after layer A is deposited.

Then, following equations can be obtained, according to Eq. (2).

$$\sigma_a = \frac{K}{t_a}\left(\frac{1}{R_A}-\frac{1}{R_0}\right) \quad (3)$$

$$\sigma_{ab} = \frac{K}{(t_a+t_b)}\left(\frac{1}{R_B}-\frac{1}{R_0}\right) \quad (4)$$

$$\sigma_{abc} = \frac{K}{(t_a+t_b+t_c)}\left(\frac{1}{R_C}-\frac{1}{R_0}\right) \quad (5)$$

$$\sigma_{abcd} = \frac{K}{(t_a+t_b+t_c+t_d)}\left(\frac{1}{R_D}-\frac{1}{R_0}\right) \quad (6)$$

The first and second assumptions suggest that when layer $(i+1)$ is deposited, the original substrate together with layers from 1 to i acts as new substrate for layer $(i+1)$. Therefore, residual stresses of monolayers B, C and D can be expressed as

$$\sigma_b = \frac{K}{t_b}\left(\frac{1}{R_B}-\frac{1}{R_A}\right), \quad (7)$$

$$\sigma_c = \frac{K}{t_c}\left(\frac{1}{R_C}-\frac{1}{R_B}\right) \quad (8)$$

and

$$\sigma_d = \frac{K}{t_d}\left(\frac{1}{R_D}-\frac{1}{R_C}\right). \quad (9)$$

Table 1
Residual stresses of multilayers and corresponding radii of curvature.

Multilayers	AB	ABC	ABCD
Residual stress	σ_{ab}	σ_{abc}	σ_{abcd}
Radius of curvature	R_B	R_C	R_D