ELASTIC INSTABILITY OF MULITILAYER FILMS COATED ON SUBSTRATES*

Shu Guo, Martin Y.M. Chiang, Christopher M. Stafford
Polymers Division, National Institute of Standards and Technology Gaithersburg, Maryland 20899
Shu.guo@nist.gov

Introduction

Mechanical properties of ultra-thin (submicrometer) films coated on a substrate are paramount in many applications [1-4]. One question arises as to whether the physical and mechanical properties of supported thin films in applications can be significantly different from the properties of chemically identical bulk materials. There have been many methods developed to measure these properties of thin films for the purpose of understanding the relation between the microstructure and behavior of material in the bulk and material in thin films coated on a substrate. The basic concept among them is that these properties can be deduced from the response of a film/substrate system perturbed either mechanically, thermally, acoustically, or optically [5-17]. In some specialty or common applications, multilayer material system has been developed to meet the increasingly demanding cost and performance requirements. Therefore, we present here a theoretical analysis for the structural stability of a multilayer system on an elastic medium. Ultimately, rather than a single layer system reported in the literature [18-20], this stability analysis could facilitate the development of a measurement technique for deducing the mechanical properties of each constituent layer in a multilayer system. Also, the finite element analysis (FEA) has been performed on the multilayer system to clarify the assumptions used and validate the results in the theoretical analysis.

Method

We Adopt classic laminate theory [19] (CLT) to calculate the wavelength of a laminated multilayer. Figure 1 shows the schematic of a laminate. The constitutive relationship of a laminated multilayer can be written as

$$\begin{Bmatrix} N \\ M \end{Bmatrix} = \begin{bmatrix} A & B \\ B & D \end{bmatrix} \begin{Bmatrix} \varepsilon \\ \kappa \end{Bmatrix} \tag{1}$$

where N and M are the force and moment vectors acting on the laminate, ε and κ are the strain and curvature vectors. A, B and D are the extension stiffness, bending-extension coupling stiffness and bending stiffness matrices, respectively. They are related to the laminate stiffness matrix, Q, via

$$\begin{aligned} A_{ij} &= \sum_{k=1}^{n} \left(Q_{ij}\right)_k (z_k - z_{k-1}) \\ B_{ij} &= \frac{1}{2}\sum_{k=1}^{n} \left(Q_{ij}\right)_k (z_k^2 - z_{k-1}^2) \\ D_{ij} &= \frac{1}{3}\sum_{k=1}^{n} \left(Q_{ij}\right)_k (z_k^3 - z_{k-1}^3) \end{aligned} \tag{2}$$

where z_k denotes the axis coordinate perpendicular to the plate for each layer as shown in Figure 1. n is the number of layers, index i, j=1~6. The terms of Q for each isotropic layer are given by

$$\begin{aligned} &\left(Q_{11}\right)_k = \left(Q_{22}\right)_k = \frac{E_k}{1-\nu_k{}^2}, \qquad \left(Q_{12}\right)_i = \frac{\nu_k E_k}{1-\nu_k{}^2} \\ &\left(Q_{66}\right)_k = \frac{E_k}{2(1+\nu_k)}, \qquad \left(Q_{16}\right)_k = \left(Q_{26}\right)_k = 0 \end{aligned} \tag{3}$$

where E_k and ν_k denotes the modulus and Poisson's ratio of kth layer. The equilibrium equations for each layer can be expressed as follows

$$\begin{aligned} &\frac{\partial N_x}{dx} + \frac{\partial N_{xy}}{dy} = 0 \\ &\frac{\partial N_{xy}}{\partial x} + \frac{\partial N_y}{\partial y} = 0 \\ &\frac{\partial M_x}{\partial x^2} + 2\frac{\partial M_{xy}}{\partial x \partial y} + \frac{\partial M_y}{\partial x^2} + q = 0 \end{aligned} \tag{4}$$

and compatibility equation is:

$$\frac{\partial^2 \varepsilon_x}{\partial x^2} + \frac{\partial^2 \varepsilon_y}{\partial y^2} = \frac{\partial^2 \gamma_{xy}}{\partial x \partial y} \tag{6}$$

Eqn. 1 can be rewritten as

$$\begin{Bmatrix} \varepsilon \\ M \end{Bmatrix} = \begin{bmatrix} a & b \\ b & d \end{bmatrix} \begin{Bmatrix} N \\ \kappa \end{Bmatrix} \tag{7}$$

where matrices a, b, and d is given by

$$a = A^{-1},\ b = BA^{-1},\ d = D - BA^{-1}B$$

For cylindrical bending, $(\ )_{,y}=0$. If the elastic medium is assumed as an elastic foundation, the final governing equation for an isotropic multilayer with cylindrical bending can be obtained as follows

$$\left(d_{11}+\frac{b_{12}{}^{2}}{a_{22}}\right)\frac{\partial^4 w}{\partial x^4}+F\,\frac{\partial^2 w}{\partial x^2}+ky=0 \qquad (9)$$

where F is the compression force, k the foundation modulus of the substrate. If the substrate is treated as a Winkler foundation, the foundation modulus is given by [19]

$$k=\frac{E_s w}{1-\nu_s^2}\frac{\pi}{\lambda} \qquad (10)$$

where E_s and ν_s are the modulus and Poisson's ratio of the substrate respectively, w is the width of the film and λ wavelength. Assume a sinusoidal buckled shape:

$$w=A\sin\frac{2\pi}{\lambda}x \qquad (11)$$

where A is the magnitude of the buckled shape. The compressive force, F, can be found by substituting (11) and (10) into (9). F has a minimum value at some wavelength, which can be express as follows

$$\lambda=2\pi\left(b_{12}{}^{2}+a_{22}d_{11}\right)\sqrt[3]{\frac{1-\nu_s^2}{a_{22}E_s}} \qquad (12)$$

Discussion

Finite element analysis was conducted to verify the analytical calculation introduced in the proceeding section. Plane strain quadratic isoparametric elements were used to model the films and elastic medium. Eigen value buckling analysis was activated to obtain the buckled shape of the beam. Figure 2 illustrates the schematic of the model. A film consisting of two layers of same thickness was embedded on an elastic substrate. Figure 3 shows relationship between the wavelength and modulus ratio for the two layers. A perfect agreement between analytical solution (12) and FEA results is observed.

Conclusions

In this presentation, an analytical solution based on CLT was developed to describe the instability of multilayer thin film supported by an elastic media. A perfect agreement was observed between FEA simulation and this solution. This solution can be applied to the buckling-based metrology for measuring the modulus of an ultra thin film, in which a multilayer thin film structures is involved.

* Contribution of the National Institute of Standards and Technology, not subject to copyright in the United States.

References

1. A. A. Elshabini-Riad and E. D. Barlow, Thin Film Technology Handbook, 1997, McGraw-Hill, New York.
2. H. Namatsu, K. Kurihara, M. Nagase, K. Iwadate and K. Murase, *Applied Physics Letter*, 1995, 66, pp2655-2657.
3. H. B. Cao, P. F. Nealey and W.-D. Domke, *Journal of Vacuum Science and Technology*, B, 2000 18, pp3303-3307.
4. T. Tanaka, M. Morigami and N. Atoda, *Japanese Journal of Applied Physics*, 1995, 32, pp6059-6064.
5. T.F. Retajczyk, Jr., A.K. Sinha, *Thin Solid Films*, 1980, 70, pp241-247.
6. M. R. VanLandingham, *Journal of Research of the National Institute of Standards and Technology*, 1993, 108, 249-265.
7. A. G. Every, *Measurement Science and Technologies*, 2002, 13, ppR21-R39.
8. D. Du, O. K. C. Tsui, Q. Zhang and H. He, *Langmuir*, 2001, 17, pp3286-3291.
9. R. Hartschuh, Y. Ding, J. H. Roh, A. Kisliuk, A. P. Sokolov, C. L. Soles, R. L. Jones, T. J. Hu, W. L. Wu, and A. P. Mahorowala, *Journal of Polymer Science*, B, 2004, 42, pp1106-1113.
10. J. A. Forrest, K. Dalnoki-Veress and J. R. Dutcher, *Physical Review E*, 1998, 58, pp6109-6114.
11. D. Schneider, T. Witke, T. Schwarz, B. Schöneich and B. Schultrich, B., *Surface and Coatings Technology*, 2000, 126, pp136-141.
12. M. G. Allen, M. Mehregany, R. T. Howe, and S. D. Senturia, *Applied Physics Letter*, 1987, 51, pp241–243.
13. M. K. Small and W. D. Nix, *Journal of Materials Research*, 1992, 7, pp1553–1563.
14. J. J. Vlassak, and W. D. Nix, *Journal of Materials Research*, 1992, **7**, pp3242–3249.
15. D. Maier-Schneider, J. Maibach and E. Obermeier, *Journal of Microelectromechanical Systems*, 1995, 4, pp238–241.
16. M.Y.M. Chiang, C.K. Chiang, W.L. Wu, *J. of Engineering Materials and Technology, Trans. of ASME*, 2002, **124**, 274.
17. C.M. Stafford, C. Harrison, K. L. Beers, A. Karim, E. Amis, M. R. Vanlandingham, H.-C. Kim, W. Volksen, R. D. Miller, and E. Simonyi, *Nature Materials*, 2004, 3, pp545-550.
18. G. S.Gough, C. F. Elam, and G. H. De. Tipper, *The journal of Royal Aeronautical Society*, 1939, 13, pp12-45.

19. H. G. Allen, Analysis and Design of Structural Sandwich Panels, 1969, Pergamon, New York.
20. A. L. Volynskii, S. Bazhenov, O. V. Lebedeva. and N. F. Bakeev, *J. Mater. Sci*., 2000, 35, pp547–554.
21. R. M. Jones, Mechanics of Composite Materials, 1999, Taylor and Francis, Philadelphia, PA.

Figures

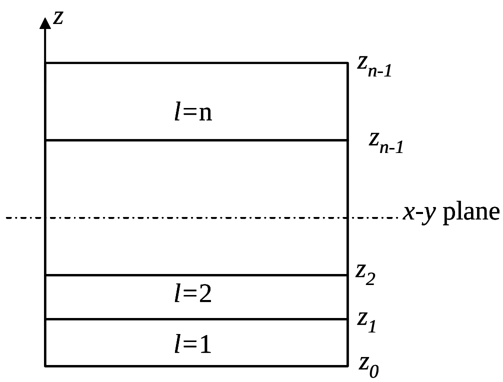

Figure 1. Cross-section of a laminate

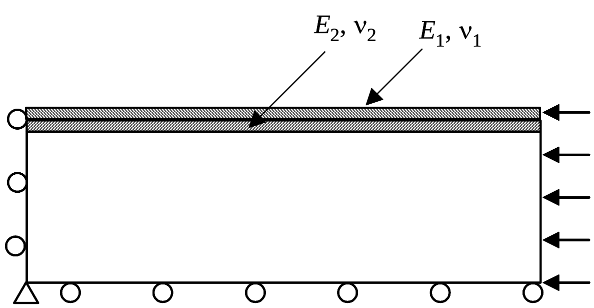

Figure 2. Schematic of the FEA model.

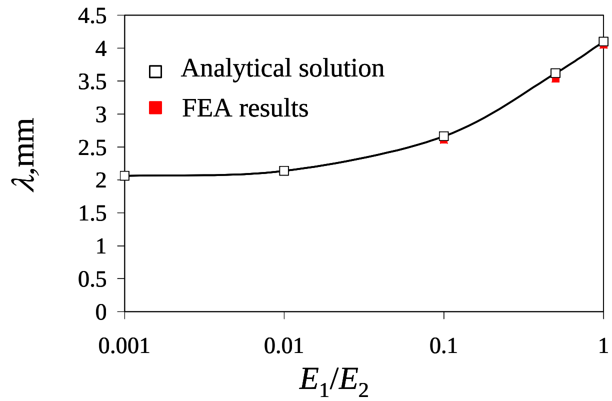

Figure 3. Wavelength as a function of the modulus ratio between two layers.