Surface Effect on the Buckling of a Stretchable Electronic Structure

Abstract. The structure of a stiff thin film on a compliant substrate has important applications in stretchable electronics. However, such structures are micro-nano-order of magnitude, where surface effects cannot be ignored. Gurtin-Murdoch theory is applied to model the thin film including surface effects. Through energy method, the size-dependent relations between the buckling features, material properties and geometric parameters are deduced. At last the influence of surface effects is illustrated by the case of silicon film and PDMS substrate.

Streszczenie. Badano strukturę cienkiej warstwy nałożonej na podłoże. Taka struktura może mieć rzędu nanometrów kiedy efekt podłoża nie może być ignorowany. Zaproponowano model matematyczny struktury bazując na teorii Gurtin-Murdoch. (Wpływ podłoża na odkształcenie elastycznej struktury elektronicznej)

Keywords: Surface effects, compliant substrate, thin film, buckling

1. Introduction

The structure of a stiff thin film on a compliant substrate has important applications in microelectronics, biology, medicine, etc. Specially, the buckling of such structure is applied in international advanced stretchable electronics, making controlled deformation of electronic be realized [1]. Currently, the researches about the buckling of such structure are based on the classical plate theory [2] and do not consider surface effects. However, in microelectronics, such structures are micro-nano-order of magnitude. With the reduction of dimension, the proportion of surface region increase and surface effects cannot be ignored, which have essential influence on the mechanical behaviors for the whole structure.

To incorporate surface effects, Gurtin and Murdoch proposed surface constitutive equations [3, 4], defined surface elasticity constants and elaborated a generic continuum model of surface elasticity. In this model, the surface of a solid is regarded as a negligibly thin layer adhering to the underlying material without slipping, and the material constants for both are different. They also supposed that the deformation of surface and bulk is continuous. Based on the Gurtin-Murdoch theory, Miller and Shenoy studied the scale effect of nano-rods and nano-plate under stretching and bending, and their size-dependent elastic properties [5]. C.W.Lima and L.H.He studied size-dependent nonlinear response of thin elastic films by Hamilton’s principle [6]. P.Lu etc. proposed a general thin plate theory including surface effects, which can be used for size-dependent static and dynamic analysis of plate-like thin film structures [7].

In this paper, based on the Kirchhoff plate theory, the constitutive equations built by Gurtin and Murdoch are applied to model a stiff thin film on a compliant substrate which includes surface effects of the film. Through energy method, size-dependent governing equations for buckling are deduced. And the buckling features about material properties and geometric parameters are solved. At last the influence of surface effects is illustrated by the case of silicon film and PDMS substrate. In section 2, the theoretical analysis considering surface effects are made to deduce the equilibrium wave number, amplitude and critical condition. In section 3, the influence of surface effects on buckling is discussed quantitatively. In section 4, the summary is made.

2. Theoretical analysis considering surface effects

2.1 Model of a stiff thin film on a compliant substrate

An elastic stiff film is bonded to a compliant elastic substrate without slipping, which in turn is bonded to a rigid support. The substrate is imposed a uniaxial prestrain, but the film is free. After releasing the prestrain in the substrate, the film buckles. The thickness of the film and substrate are $h$ and $H$, respectively. A coordinate system is established, by setting the origin at the center in mid-plane of the film, as Fig 1. The substrate is described by the small deformation theory, while the film is described by the large deformation plate theory. Since the length of the system ($x_2$) is much larger than the amplitude of buckling, this problem can be simplified as a plane plain problem.

In the model proposed by Gurtin and Murdoch [3, 4], the surface of a solid is regarded as a negligibly thin layer adhering to the underlying material without slipping, and the material constants for both are different. The non-classical boundary conditions, the surface stress-strain relations, and the equations of classical elasticity for bulk material together form a coupled system of field equations. Here we neglect surfaces thickness, as Fig. 2. The upper and lower surfaces are $S'$ and $S$ ($x_3=\pm h/2$), respectively. The mid-plane is $S^0$ ($x_3=0$). The upper surface $S'$ is free, but the lower surface $S^0$ sustains a normal pressure $P_3$ caused by the interaction stress of the substrate.

![Fig.1 Model of a stiff thin film on a compliant substrate](image)

![Fig.2 Thin film and its surfaces](image)

2.2 Equilibrium equation and constitutive relation

The equilibrium equations without body force for the bulk and surfaces [3, 4] of the film are given by

\begin{align}
\sigma_{1,1} &= 0 \\
S^+ : \tau_{1,1}^+ - \sigma_{1,1}^+ &= 0, \quad S^- : \tau_{1,1}^- + \sigma_{1,1}^- = P_3 \delta_{13}
\end{align}

...
where $\sigma_{ij}$ and $\tau_{i\alpha}$ are bulk and surface stresses at $S'$ and $S'$. Integrating (1) through the thickness and then substituting (2), the equilibrium equations include surface stresses

$$N_{i\beta,\beta} + \tau_{i\alpha,\beta} + \tau_{i\beta,\beta} - P_i \delta_{ij} = 0$$

where the membrane forces $N_{i\beta}$ are the integral of the stresses $\sigma_{i\beta}$. The generalized membrane forces containing surface stresses are defined as $N'_{i\beta} = N_{i\beta} + \tau_{i\alpha,\beta} + \tau_{i\beta,\beta}$. Then the equilibrium equations (3) can be further written as

$$N'_{i\beta,\beta} - P_i \delta_{ij} = 0$$

Assuming that both the bulk and surfaces of the film are homogeneous and isotropic, the constitutive relation of the bulk is expressed by

$$\sigma_{ij} = \frac{E_i}{1-\nu_i} \left( \epsilon_{ij} + \frac{\nu_i}{1-2\nu_i} \epsilon_{kk} \delta_{ij} \right) + \frac{1}{1-\nu_i} \nu_i \epsilon_{kk} \delta_{ij}$$

The stress component $\sigma_{ij}$ is usually assumed to be zero in the classical plate theories. However, the surface balance conditions (2) cannot be satisfied. To consider the weakness, it is assumed that the stress component $\sigma_{ij}$ varies linearly through the thickness and satisfies the balance conditions on the surfaces,

$$\sigma_{ij} = \frac{1}{2} \left( \sigma_{ij}^{\text{bulk}} + \sigma_{ij}^{\text{surf}} \right) / \left( 1 + \nu_i \right)$$

It is noted that the relation (6) is also suitable for the materials with isotropic properties. The stress-strain relations (5) can be simplified as

$$\sigma_{ij} = \frac{E_i}{1-\nu_i} \left( \epsilon_{ij} + \frac{\nu_i}{1-2\nu_i} \epsilon_{kk} \delta_{ij} \right) + \frac{1}{1-\nu_i} \nu_i \epsilon_{kk} \delta_{ij}$$

If the upper and lower surfaces have same material properties, the stress-strain relations are described as [3,4,8]

$$\tau_{i\alpha} = \tau_0 \delta_{i\alpha} + \mu_\alpha \epsilon_{i\alpha} \delta_{i\alpha} + \left( \mu_\beta + \lambda_\alpha \right) \epsilon_{i\alpha} \delta_{i\alpha}$$

where $\tau_0$ is residual surface stress under unconstrained conditions, $\lambda_\alpha$ and $\mu_\alpha$ are the surface Lamé constants.

In Kirchhoff plate theory, the displacement components are assumed to have the form

$$u_i = u_i^0 - x_i u_i^0, \quad u_i^0 = x_i$$

where $u_i^0$ is the displacement components of the mid-plane. The nonlinear strains are

$$\epsilon_{i\alpha} = \epsilon_{i\alpha}^0 + \left( u_{i\beta} + u_{\beta i} + u_{i\beta} u_{\beta i} \right) / 2$$

where $\epsilon_{i\alpha}^0$ are prestrains.

2.3 The interaction stress

Now we deduce the interaction stress of the substrate. According to the stress compatibility equations $V^2 \sigma_{\alpha i} = 0$, a stress function $\phi(x_i, x_j)$ is introduced, $\sigma_{ij} = \phi_{ij}$, $\phi_{ij} = \phi_{ij}$, with the general solutions

$$\phi(x_i, x_j) = \left( C_j \cos(k_j x_j) + C_j \sin(k_j x_j) + C_j x_i \cos(k_j x_j) + C_j x_i \sin(k_j x_j) \right) \cos(k_j x_j)$$

By the small deformation theory, the strains are

$$\epsilon_{i\alpha} = \left( \epsilon_{i\alpha}^0 + \tau_{i\alpha} \right) / 2$$

The physical equations of plane strain are

$$\left\{ \epsilon_{i\alpha}^0, \epsilon_{i\alpha}^0 \right\} = 2 \left( \epsilon_{i\alpha}^0 - \epsilon_{i\alpha}^0 \right) / E_i, \quad \tau_{i\alpha} = \epsilon_{i\alpha}^0 / \left( 1 - \nu_i \right) \text{ and } \tau_{i\alpha} = \epsilon_{i\alpha}^0 / \left( 1 - \nu_i \right).$$

From the stress function, the stresses are

$$\sigma_{ij} = k \cos(k_j x_j) \left( C_j \cos(k_j x_j) + C_j \sin(k_j x_j) + C_j \left( 2 \sinh(k_j x_j) + \sinh(2k_j x_j) / \left( \tau_i + 1 \right) \right) \right)$$

By substituting (14) into (13) the strains are

$$\epsilon_{i\alpha}^0 = k \cos(k_j x_j) \left( C_j \cos(k_j x_j) + C_j \sin(k_j x_j) + C_j \left( 2 \sinh(k_j x_j) + \sinh(2k_j x_j) / \left( \tau_i + 1 \right) \right) \right)$$

By substituting (14) into (13) the stresses are

$$\sigma_{ij} = -k \cos(k_j x_j) \left( C_j \cos(k_j x_j) + C_j \sin(k_j x_j) + C_j \left( 2 \sinh(k_j x_j) + \sinh(2k_j x_j) / \left( \tau_i + 1 \right) \right) \right)$$

Because the buckling mode is similar to cosine curve, the deflection in the mid-plane of the film is assumed as

$$u_i = C \cos(k_j x_j)$$

The normal displacement is continuous and the shear stress is ignored at the interface [2]. The lower surface of the substrate is fixed, so the boundary conditions are

$$\sigma_{ij} (x_i, 0) = 0, \quad u_i (x_i, 0) = u_i^0 = A \cos(k_j x_j)$$

According to (14) and (16), the constants $C$ can be solved

$$C_i = -AE_i / 2k_i, \quad C_i = AE_i / 2k_i$$

By substituting (19) into (14) the interaction stress is

$$P_i = \delta_i (x_i, 0) = -g(t_i, H) A k_i E_i \cos(k_j x_j) \times \frac{4k_i H - 6 \cos(2k_i H) + 2 \sin(2k_i H)}{4k_i H - 6 \cos(2k_i H) + 2 \sin(2k_i H)}$$

For the thick substrate, $k_i H$ is so large that the interaction stress can be simplified as

$$P_i = \frac{1}{2} 4k_i E_i \cos(k_j x_j) = \frac{1}{2} k_i E_i u_i^0$$

2.4 Displacement of the film

Since the system only sustains uniaxial prestrain, it is believed that prestrains $\epsilon_{i\alpha}^0 = \epsilon_{i\alpha}^0 = 0$. For the plane plain problem, load, stress and displacement are independent of $x_2$ and $x_3$. Assuming that there is no residual surface...
To analyze the critical state, the energy density is minimized by setting \( \partial E_{\text{eq}} / \partial \varepsilon = \partial U_{\text{eq}} / \partial \varepsilon = 0 \). The equations about \( A \) and \( k \) are

\[ 4k' \left( E_E + 6\lambda_f + 12\mu_f \right) h^3 - h^2 \left( E_E + 2k + 2\lambda_f \right) - 12E_E = 0 \]

\[ 2A' k' \left( E_E + 2\lambda_f + 2\mu_f + 2k \right) (3h^2 k'^2 + 8\varepsilon_{11}^0 + 8\varepsilon_{11}^f) + E_E h \left( 2k + 8\varepsilon_{11}^f + 8\varepsilon_{11}^f \right) + E_E (3 - 5h^2 k' \gamma / 12 + 2hk \varepsilon_{22}^f) = 0 \]

From the first equation in (34), the equilibrium wave number \( k_{\text{eq}} \) can be solved, which is independent of prestrain. From the second equation in (34), the equilibrium amplitude \( A_{\text{eq}} \) is also solved, which is related to prestrain. By setting \( A_{\text{eq}} = 0 \), the critical prestrain \( \varepsilon_{\text{cr}} \) is obtained. From (25) and (26), the critical general membrane force is

\[ \varepsilon_{\text{cr}} = \frac{1}{4} \left( 3E_E / E_E \right)^{\frac{1}{3}} \]

They are the same as the result in the traditional analysis [2]. That is to say, the equilibrium equations (34) considering surface effects can degenerate to the traditional ones.

3. Discussion

3.1 Material parameters

In this section an example of silicon film and PDMS (Polydimethylsiloxane) substrate is applied to analyze quantitatively the influence of surface effects on buckling. Tab.1 shows the Young's modulus, Poisson's ratio [9,10] and their plane strain effective values. Tab.2 shows the silicon surface elastic constants [5] and Lamé' constants where \( \mu_0 = 0.28 \) and \( \lambda_0 = 0.48 \). Obviously, if the surface stresses are neglected, then \( \mu_0 = \lambda_0 = 0 \).

3.2 Influence of surface effects

Now two models are discussed. One is the classical model with the buckling features (36); the other is the model considering surface stress and surface balance where the buckling features can be solved by substituting the material parameters into (34). In the following text, the superscript I and II present these two models respectively.

Fig.3 shows the relation between the ratio of the equilibrium wave number \( k_{\text{eq}} / k_{\text{cr}} \) in two models and film thickness \( h \). Under the influence of surface effects, equilibrium wave number increase. When the film thickness is less than 5nm, such influence becomes significant. With the reduction of film thickness, this influence still increase.

Fig.4 shows the relation between the ratio of the critical prestrain \( \varepsilon_{\text{cr}} / \varepsilon_{\text{cr}}^0 \) and film thickness \( h \). Under the influence of surface effects, critical prestrain decrease, but the influence
is slight. Fig.5 shows the relation between the ratio of critical general membrane force $N_{cr}^{II}/N_{cr}^{I}$ and film thickness $h$. Because of surface effects, critical general membrane force decrease. When the film thickness is less than 5nm, such influence becomes significant. With the reduction of film thickness, this influence still increase.

Fig.5 shows the relation between the ratio of critical general membrane force $N_{cr}^{II}/N_{cr}^{I}$ and film thickness $h$.

Because of surface effects, critical general membrane force decrease. When the film thickness is less than 5nm, such influence becomes significant. With the reduction of film thickness, this influence still increase.

4. Conclusion

The governing equations about the buckling of a stiff thin film on a compliant substrate including surface effects are (37) and (38), whose real roots are equilibrium wave number $k_{eq}$ and equilibrium amplitude $A_{eq}$. For the silicon film and PDMS substrate, when the film thickness is less than 5nm, surface effects have significant influence on the equilibrium wave number, amplitude and critical membrane force. With the reduction of film thickness, this influence still increase. In other words, surface effects cannot be neglected for such nano system.

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REFERENCES


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