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Deformation of thin solid film/liquid layer/substrate structures with rough liquid layer/substrate interface

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Abstract

This paper investigates the consequence on deformation of the compressive solid film in a laminate structure with thin solid film, liquid layer and rigid substrate from top to bottom, by taking consideration of the roughness in the liquid layer/substrate interface. Two roughness morphologies, self-affine and mound roughness, are studied. The solid film corrugates when subjected to internal compressive stresses. Deformation of the solid film is determined by calculation of energies in this structure. Our analogy indicates that rough morphologies may affect the deformation of the structure. Interestingly, further investigation shows that the solid film with nonplanar liquid/substrate interface can be stable under certain wrinkling wave numbers, while that with a planar liquid/substrate interface under the same wave numbers can be unstable. Our findings supplement rather than overthrow the previous theory obtained without considering the roughness in interfaces. Self-affine interface is characterized by an roughness amplitude A, and the fractal dimension s. As for mound roughness, the characteristic parameters are interface width ω, and average mound separation λ. With increasing amplitude or interface width of a rough interface, the roughness in interface exhibits more influence on the stability of the structure. Variation of critical wave numbers increases in parallel to the increase of fractal dimension s in the structure with a self-affine roughness interface, or decrease of the average mound separation λ in the structure with a mound rough interface. The influence of the rough interface on the stability of the structure reach to a plateau when s or λ is large enough or when λ is little enough. As sequences, the stable state when the vicious/substrate interface is supposed to be planar is very different from that when the interface is nonplanar for both rough morphologies.

Keywords: Surface energy; Surface roughness; Multilayers internal stress

1. Introduction

In thin film systems, the film suffers biaxial stresses, an inevitable consequence of the manufacturing process. Complaint or liquid substrates have been used to release such stresses in those thin films with low dislocation density. Structures with thin solid film bonded to a liquid layer, which lies on a rigid substrate (Fig. 1), is widely used in microelectromechanical systems, biological engineering, and optoelectronical equipments (Fig. 1) [1–5]. We use solid film/liquid layer/substrate structure to refer to such structure. When subjected to a compressive membrane force, the solid film in the structure wrinkles, resulting in flowing of the underneath liquid layer. More than one wrinkling pattern may simultaneously occur in the solid film under non-uniform stresses. Mechanism of this patterning process is utilized in optical devices such as diffraction gratings and optical sensors, and in measurement of strain in materials. Huang and several other researchers investigated the stability of this structure with compressive solid film, and proposed a critical wave number in calculation of wrinkle deformation of the solid film [6–10].

The above studies ignored the roughness of the interface between liquid film and substrate. In another word, these studies assumed the liquid/substrate interface being planar, which did not represent the actual situation. In this paper, we study on random self-affine and mound rough interfaces, which are widely accepted in models of rough interfaces and surfaces [11–14]. We considered the consequences of the alteration of parameters, such as amplitude of the roughness, fractal dimension of the self-affine interface, and average mound separation in mound rough interface, on stability of the solid

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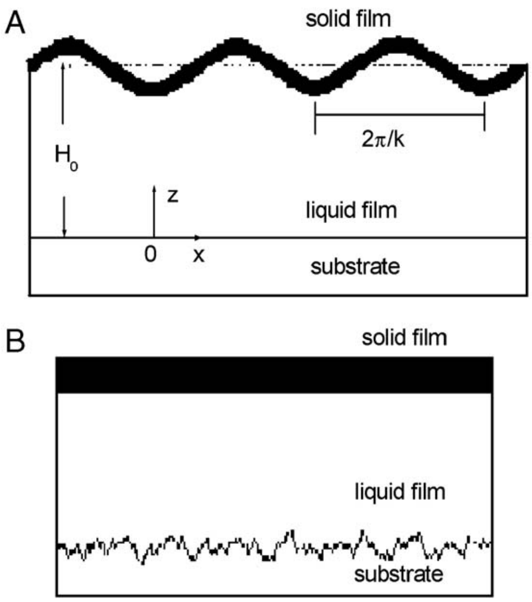

Fig. 1. The solid film/liquid layer/substrate structure. (A): The solid film suffers internal compressive stresses and wrinkles. (B): The nonplanar liquid layer/substrate interface.

film. Our result shows that rough morphologies of the liquid/substrate interface affect the deformation of the solid film in thin solid film/liquid layer/substrate structures.

2. Self-affine rough interface

The interface height profile is denoted by $h(x)$, which exhibits a single-valued function of x. $h=0$ represents the planar interface (Fig. 2). The deflection of the solid film under internal compressive stress is $w=q_1 \sin(kx)$, in which q_1 is the amplitude and k is the wave number [6–10]. $\Delta\bar{U}$ represents the average change of the free energy of the structure per unit area. For nonplanar interface:

$$\Delta\bar{U} = \frac{q_1^2 D}{4l^4}\left[(kl)^4 + \mathrm{sign}(N)(kl)^2 + (1+u)\xi\right] \tag{1}$$

where $D=\frac{Eh^3}{12(1-v^2)}$, D is the flexural rigidity. $N=\sigma h+f$, $l=\left(\frac{D}{|N|}\right)^{1/2}$, and $\xi=\frac{DU_L''}{N^2}$. σ is the residual stress in the solid film at the reference state. f is the sum of surface stresses on the top and bottom of the solid film. $U_L''=\partial^2 U_L/\partial H^2$, where U_L is the interaction energy and H is the thickness of the liquid layer. For example, the interaction energy caused by van der Waals force [6] turns out to be $U_L(H)=-\frac{B}{12\pi H^2}$, where B is the Hamaker constant. Roughness of the liquid layer/substrate interface affects the free energy of the structure, and such influence is denoted as u, where $u=\frac{2k}{q_1\pi}\int_0^{\frac{2\pi}{k}} h(x)\sin(kx)\mathrm{d}x$. Apparently, the influence of a rough surface can be neglected if H is significant.

The self-affine function, $h(x)$, can be presented in the following form of Weierstrass–Mandelbrot (W–M) function [11–14].

$$h(x) = \sum_{n=1}^{\infty} A\lambda^{(s-2)n}\sin(2\pi\lambda^n x) \tag{2}$$

where A is a constant, s is the fractal dimension ($1<s<2$), and λ has been assigned to be 1.5 in literatures [13,14]. Eq. (2) is similar to Fourier series, except that the frequencies increase in an arithmetic progression in Fourier series but in a geometric progression in Eq. (2). We choose $n=1000$, large enough to obtain a stable curve as shown in Fig. 2. The profile of the function with fractal dimensions varies between 1.1 and 1.9. It appears that the larger the value of s, the more uneven the interface.

By substituting Eq. (2) into Eq. (1), we acquire Eq. (3) which determines the free energy of the structure with a self-affine rough interface between the liquid layer and the substrate.

$$\Delta\bar{U} = \frac{q_1^2 D}{4l^4}\left[(kl)^4 + \mathrm{sign}(N)(kl)^2 + \left(1+\sum_{n=1}^{\infty}\left(-\frac{Ak^2 q_1\lambda^{n(-2+s)}\sin\left(\frac{4\pi^2\lambda^n}{k}\right)}{2\pi(k-2\pi\lambda^n)(k+2\pi\lambda^n)}\frac{4}{q_1^2}\right)\right)\xi\right] \tag{3}$$

Eq. (3) indicates that the influence of nonplanar interface on free energy will be more distinguished with large

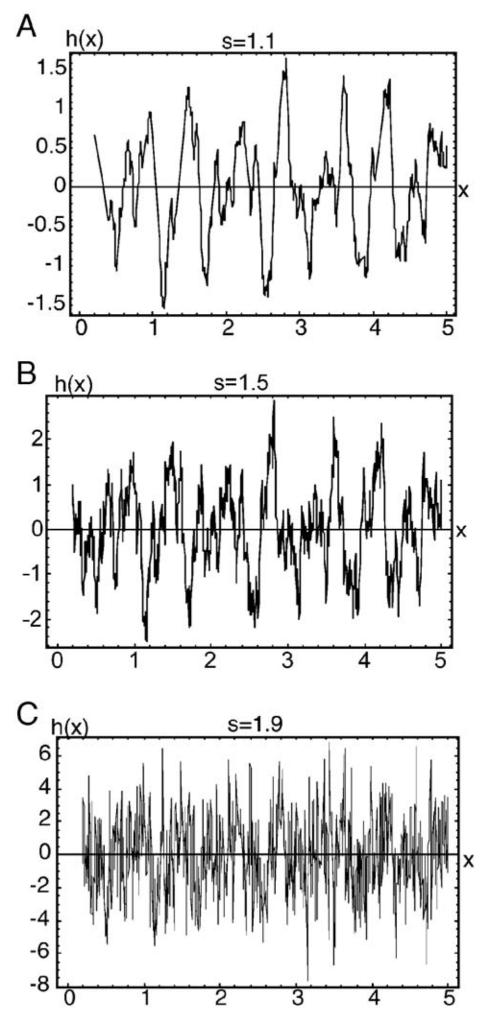

Fig. 2. Self-affine fractal profiles in W–M function with different fractal dimensions.

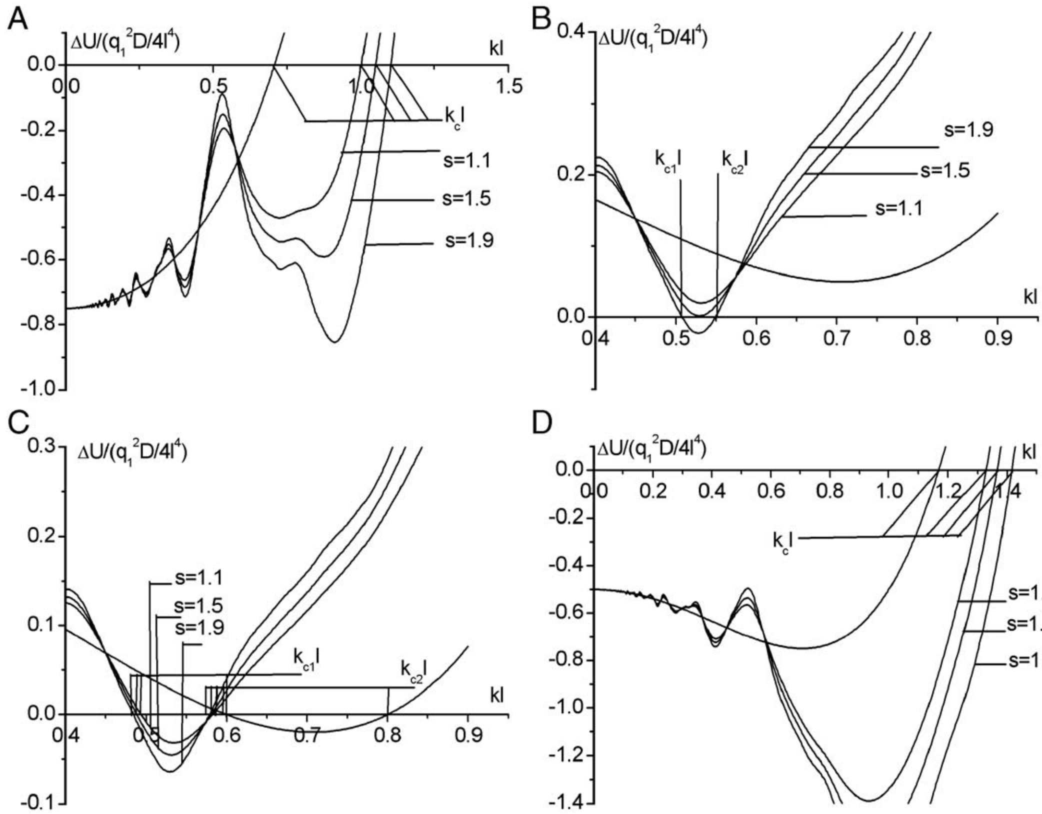

Fig. 3. Diagram of $\Delta U/\left(\frac{q_1^2 D}{4l^4}\right)-kl$ in the solid film/liquid layer/substrate with self-affine rough interface (the material and dimensional parameters of the solid film are: $E=100\,\text{GPa}$, $v=0.3$, $h=10\,\text{nm}$, $A=5\,\text{nm}$, $q_1=5\,\text{nm}$, $\sigma=\pm 100\,\text{MPa}$). (A): $N>0$, $\xi=-0.75$, (B): $N<0$, $\xi=0.3$, (C): $N<0$, $\xi=0.23$, (D): $N<0$, $\xi=-0.5$.

amplitude A. The solid film is stable when $\Delta\bar{U}>0$. The critical wave number k_c can be calculated (Fig. 3). Fig. 3 shows a critical wave number k_c in a situation that $N>0$ and $(1+u)\ \xi<0$. When $k>k_c$, the solid film is stable, and the value of the wave number increases along with the fractal dimension s. On the other hand, if $N<0$, there will be two possibilities (Fig. 3). When $(1+u)\ \xi>0.25$, the solid film is stable with wrinkles of all wave numbers. When $0<(1+u)\ \xi<0.25$, two critical wave numbers k_{c1} and k_{c2} co-exist and the solid film is unstable with an intermediate wave number k, where $k_{c1}<k<k_{c2}$. The two critical values in unstable region differ more if s increases. Furthermore, when s becomes large enough, an unstable wave number region will appear, however the structure would be always stable with wrinkles of these wave numbers if the interface were planar. Further, as shown in Fig. 4, the influence of the self-affine rough interface on the free energy will reach to a plateau when s is large enough.

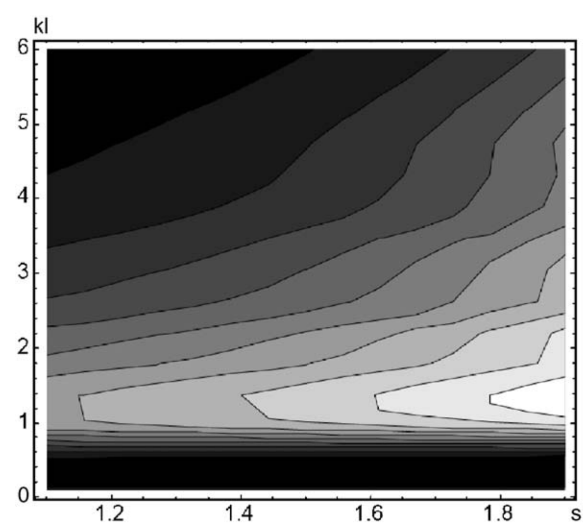

Fig. 4. Contour Diagram of u with different kl and s for self-affine rough interface (the material properties and dimensions are the same as Fig. 3).

3. Mound rough interface

Besides self-affine fractal morphologies, mound roughness is another important rough morphology in surfaces and interfaces. Mound roughness morphologies are determined by four parameters: the interface width ω, the system correlation length ς, the roughness exponent α, and average mound separation λ. To mound roughness surfaces, $\alpha=1$ [11,15]. Thus, the mound roughness morphology can be described as Eq. (4) [15].

$$<h(0)h(x)> = \omega^2 e^{-(x/\varsigma)^{2\alpha}} \cos\left(\frac{2\pi x}{\lambda}\right) \tag{4}$$

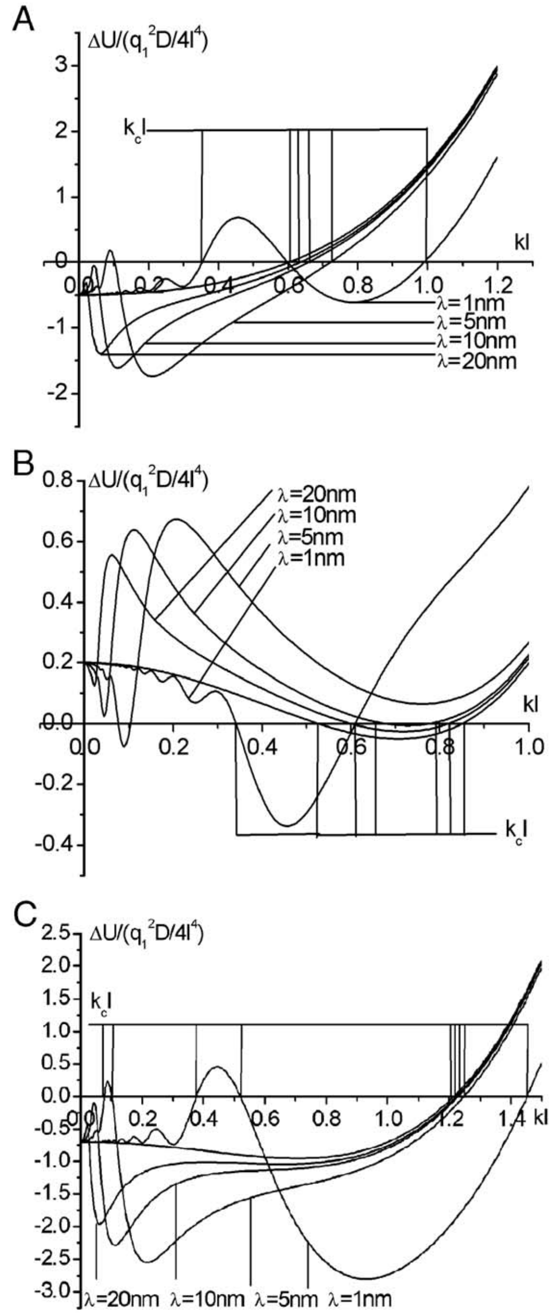

Fig. 5. Diagram of $\Delta U/\left(\frac{q_1^2 D}{4l^4}\right)-kl$ in the solid film/liquid layer/substrate with mound rough interface (the material properties and dimensions are: $E=100\,\mathrm{GPa}$, $\nu=0.3$, $h=10\,\mathrm{nm}$, $\omega=5\,\mathrm{nm}$, $\varsigma=10\,\mathrm{nm}$, $<h(0)>=3\,\mathrm{nm}$, $q_1=5\,\mathrm{nm}$, $\sigma=\pm 100\,\mathrm{MPa}$). (A): $N>0$, $\xi=-0.5$, (B): $N<0$, $\xi=0.2$, (C): $N<0$, $\xi=-0.7$.

We use $\frac{<h(0)h(x)>}{<h(0)>}$ to replace the value of $h(x)$. $<>$ means the assemble average of all possible configurations of roughness. Hence, change of free energy caused by application of mound roughness in the solid/liquid interface can be calculated with Eq. (5).

$$\Delta\bar{U}=\frac{q_1^2 D}{4l^4}\Bigg[(kl)^4+\mathrm{sign}(N)(kl)^2 + \left(1+\left(-\frac{\mathrm{e}^{-\frac{2\pi}{k\varsigma}}k\lambda^2\varsigma^2\left(\mathrm{e}^{\frac{2\pi}{k\varsigma}}(\lambda^2-4\pi^2\varsigma^2+k^2\lambda^2\varsigma^2)-(-4\pi^2\varsigma^2+\lambda^2(1+k^2\varsigma^2))\cos\left(\frac{4\pi^2}{k\lambda}\right)+4\pi\lambda\varsigma\sin\left(\frac{4\pi^2}{k\lambda}\right)\right)}{\lambda^4+8\pi^2\lambda^2\varsigma^2+2k^2\lambda^4\varsigma^2+16\pi^4\varsigma^4-8k^2\pi^2\lambda^2\varsigma^4+k^4\lambda^4\varsigma^4}\frac{4k\omega^2 q_1}{2\pi<h(0)>q_1^2}\right)\right)\xi\Bigg] \tag{5}$$

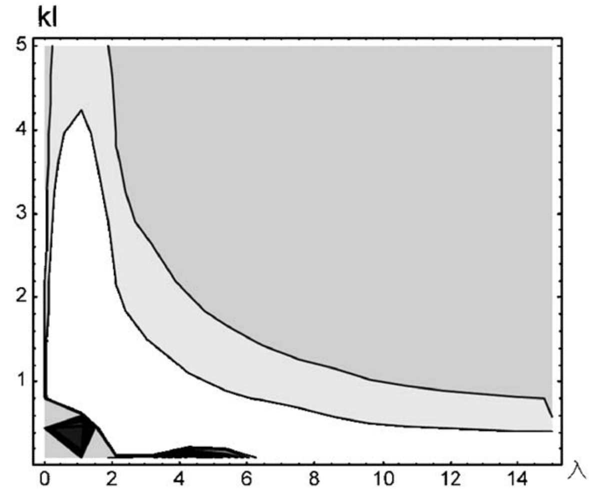

Fig. 6. Contour Diagram of u with different kl and λ for mound rough interface (the material properties and dimensions are the same as Fig. 4).

From Eq. (5), it is obvious that the influence of nonplanar interface is more distinguished with large interface width ω. Fig. 5 shows the critical wave number k_c. If one critical wave number is given, the critical value increases in parallel to the average mound separation λ. If two critical wave numbers are given, the unstable region becomes smaller when λ increases. Eq. (5) also illustrates a situation that the structure is always stable in regardless of the values of wave numbers. Finally, if λ is large enough, three critical wave numbers may occur at once. All above observations indicate that roughness of the interfaces shall not be ignored in analysis of the stability of the structure. The critical wave numbers and the stable state of the structure are very different between the structure with or without the consideration of the roughness of the interfaces. What's more, as shown in Fig. 6, the influence of the mound rough interface on the free energy will reach to a plateau when λ is large enough or little enough. The number of wounds on the surface is anti-correlated with mound separation λ. Therefore, the larger the λ, the fewer the wounds, and vice versa. Besides, if there are no enough mounds on the surface, the influence of the mounds or the roughness can be neglected.

4. Conclusions

In order to investigate the effect of roughness morphologies in liquid/substrate interface on stability of the solid film/viscous layer/substrate structure, we combine the knowledge of stability of the structure with the description of self-affine and mound rough morphologies. In this investigation, the liquid film is not so thick compared to the solid film. The results indicate that the roughness morphology may affect the stability of the structure. A stable structure with nonplanar liquid/substrate interface is very different from that with a planar interface. Taking rough interface into consideration may set a new angle in mechanical research of such structures. More interesting findings are anticipated.

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