Effects of elastic anisotropy on the surface stability of thin

film/substrate system

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**Abstract:** The surface stability of thin film/substrate system is an important problem

both in the film synthesis and reliability of micro electrical and mechanical system

(MEMS). In this work, the elastic anisotropy effect on surface stability of thin

film/substrate system was considered. The theoretical analysis indicates that elastic

anisotropic influence could play an important role in the surface stability of thin

film/substrate system. And the anisotropy effect should be considered both in the thin

film synthesis process and its service reliability. In addition, there exists an

nondimensional parameter k for cubic crystalline thin film materials in evaluating the

anisotropic effect. When k is larger than one unit, the surface stability will be

weakened by anisotropic effect; vice versa. The method used in present work could be

easy extended to multi-layered thin film/substrate system and help us to consider the

elastic anisotropy effect.

**Key Words**: thin film; elastic anisotropy; surface stability; cubic crystalline;

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### 1. Introduction

More and more new characterizations are found extensively in the semiconductor, display and micro electrical and mechanical system (MEMS), such as portability, energy-saving and high-performance. The devices in these systems consist of many thin film/substrate systems, which play important role in these devices. Therefore, the reliability problem has attracted more and more attentions on film/substrate systems. Since there are many different failure mechanisms, as early as the year 1972, Asaro and Tiller [1] discovered the morphological instability of a free surface under tension. Similarly, the surface stability is indeed very important both in the synthesis and practical application of thin film/substrate system, especially when the scale of MEMS decrease in to nanoscale and become NEMS (nano electrical and mechanical system) [1, 2]. There are many works having been done on the surface stability of thin film/substrate system. Gao [3, 4] and Freund [5, 6] have studied the morphology instability of epitaxial thin films by considering the competition between elastic strain energy and surface energy of thin film. Suo and Zhang [7] have considered the effect of long-range force on surface stability of epitaxial thin films. Recently, Kim and Vlassak [8] have given perturbation analysis of an undulation free surface in a multi-layered system. However, these works mentioned above did not consider elastic anisotropy effect on surface stability of film/substrate system. Obayashi and Shintani [9] reported the direction dependence of surface morphological stability of heteroepitaxial layers. Liu et al. [10] carried out computer simulation on the Stranski-Krastanov growth of heteroepitaxial films with elastic anisotropy. And Pang

and Huang [11] theoretically predicted the bifurcation of epitaxial thin films induced by anisotropic mismatch stresses. However, these works also did not give a systematic analysis of elastic anisotropy effect on the surface stability of film/substrate system.

Therefore, the elastic anisotropy of cubic crystalline films, such as Au, Cu, Ni et al., which are extensively used in MEMS and NEMS, was systematically considered in this work. The Airy stress functions were used to derive the anisotropic effect on surface stability of thin film/substrate system for a linear perturbation analysis. In order to deal with this problem easily, the geometry of thin film/substrate system is taken to be two-dimensional, such as the length of the system is much greater than its thickness. The system is just considered as a single layered system; however, this method can be easily extended to multi-layered films system as given by Kim and Vlassak [8].

### 2. Linear perturbation analysis of thin film/substrate system

### 2.1 Elastic properties of cubic crystal

The stress/strain constitutive equation of cubic crystal is as follow:

$$\begin{bmatrix} \varepsilon_{x} \\ \varepsilon_{y} \\ \varepsilon_{z} \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{bmatrix} \begin{bmatrix} \sigma_{x} \\ \sigma_{y} \\ \sigma_{z} \\ \tau_{yz} \\ \tau_{xz} \\ \tau_{xy} \end{bmatrix}$$
(1)

where  $S_{11}$ ,  $S_{12}$ ,  $S_{44}$  are elastic constants of cubic crystal. Some elastic constants for cubic crystalline materials used in thin film/substrate system are listed in Table 1. The

degree of departure from isotropy in response of a cubic material can be characterized by anisotropy ratio AR defined as follow:

$$AR = \frac{2(S_{11} - S_{12})}{S_{44}} \tag{2}$$

Note that AR=1 for an isotropic crystal. In this paper, another parameter is defined to characterize the elastic anisotropy of cubic crystal as

$$k = \frac{S_{11}S_{12} + \frac{1}{2}S_{11}S_{44} - S_{12}^2}{S_{11}^2 - S_{12}^2}$$
(3)

Also note that k=1 for an isotropic crystal and k is always larger than -1 for all of the cubic crystals. According to parameter k, different Airy stress functions will be used for different cubic crystalline films shown in part 2.3. The values of AR and k for cubic crystalline materials, which is widely used in MEMS, can be found in the Fig. 1.

### 2.2 Stress distributive state in thin film/substrate system

Considering the stress distribution in thin film/substrate system can be written as follow [1]:

$$\tilde{\sigma} = \tilde{\sigma}_0 + \tilde{\sigma}_n \tag{4}$$

where  $\tilde{\sigma}$ ,  $\tilde{\sigma}_0$  and  $\tilde{\sigma}_p$  are defined as total stress tensor, unperturbed stress tensor and perturbed stress tensor for thin film/substrate system, respectively. For simplified representation, it is assumed that the unperturbed film is in a state of uniform uniaxial stress of magnitude  $\sigma_0$  and the substrate is stress free. The  $\sigma_0$  may be generated by the strain or deformation mismatch between the film and substrate or the loading misfit of thin film/substrate system. Therefore,  $\tilde{\sigma}_0$  for thin film is as follow:

$$\tilde{\sigma}_0 = \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{5}$$

Due to the amplitude of perturbation is much smaller than the wavelength of thin film free surface, the perturbed stress tensor  $\tilde{\sigma}_p$  can be written as follow [8, 12]:

$$\widetilde{\sigma}_p = \frac{a}{\lambda} \widetilde{\sigma}_f + O(\frac{a^2}{\lambda^2}) \tag{6}$$

where a and  $\lambda$  are perturbation amplitude and wavelength, respectively. Obviously, this is a linear perturbation analysis of thin film systems and only considers the first order of perturbation. Due to the wavelength  $\lambda$  is much larger than amplitude a, the high order items of  $\lambda$  were ignored.  $\tilde{\sigma}_f$  represents the first order perturbed stress tensor for thin film/substrate system. The free surface perturbation of cubic crystalline thin film always toward the <100> directions if AR>1 [9, 10]. Therefore, the coordinate system and crystal orientation are as shown in Fig.2.

# 2.3 Airy stress function for perturbed stress tensor $\tilde{\sigma}_{\scriptscriptstyle f}$

Assuming the stress status in thin film is plane strain ( $\varepsilon_{zz} = 0$ ), the strain coordinative equation is as follow:

$$\frac{\partial^2 \varepsilon_x}{\partial y^2} + \frac{\partial^2 \varepsilon_y}{\partial x^2} = \frac{\partial^2 \gamma_{xy}}{\partial x \partial y} \tag{7}$$

The stress components can be written in terms of Airy stress function:

$$\sigma_{x} = \frac{\partial^{2} F}{\partial y^{2}}, \sigma_{y} = \frac{\partial^{2} F}{\partial x^{2}}, \quad \tau_{xy} = -\frac{\partial^{2} F}{\partial x \partial y}$$
 (8)

The compatible function for Airy stress function can be obtained by substitute Eq. (1) and Eq. (8) into Eq. (7) as follow

$$\frac{\partial^4 F}{\partial y^4} + 2k \frac{\partial^4 F}{\partial x^2 \partial y^2} + \frac{\partial^4 F}{\partial x^4} = 0 \tag{9}$$

By assuming  $F = \cos(\omega x) f(y)$  where  $\omega$  is the frequency of perturbation as  $\omega = 2\pi/\lambda$ , Eq. (9) could be rewritten as

$$\frac{d^4 f(y)}{dy^4} - 2k\omega^2 \frac{d^2 f(y)}{dy^2} + \omega^4 f(y) = 0$$
 (10)

Solving the ordinary differential equation (10), the Airy stress function for perturbed film is as follow

$$F = \cos(\omega x)(C_1 e^{\omega y \sqrt{k + \sqrt{k^2 - 1}}} + C_2 e^{-\omega y \sqrt{k + \sqrt{k^2 - 1}}} + C_3 e^{\omega y \sqrt{k + \sqrt{k^2 + 1}}} + C_4 e^{-\omega y \sqrt{k + \sqrt{k^2 + 1}}})$$
 if k>1

$$F = \cos(\omega x)[e^{\omega y}(C_1 + C_2 y) + e^{-\omega y}(C_3 + C_4 y)]$$
 if k=1 (11)

$$F = \cos(\omega x) \{e^{\omega y \sqrt{(1+k)/2}} [C_1 \cos(\omega y \sqrt{\frac{1+k}{2}}) + C_2 \sin(\omega y \sqrt{\frac{1+k}{2}})] + e^{-\omega y \sqrt{(1+k)/2}} [C_3 \cos(\omega y \sqrt{\frac{1-k}{2}}) + C_4 \sin(\omega y \sqrt{\frac{1-k}{2}})] \}$$
 if  $|k| < 1$ 

where C<sub>1</sub>, C<sub>2</sub>, C<sub>3</sub> and C<sub>4</sub> are constants and can be solved by the boundary conditions of thin film/substrate system. The Airy stress function for thin film could be chosen according to parameter k of thin film material. In this work, the substrate is considered as elastic isotropic material because the thickness of substrate is assumed much larger than that of thin film so its k equals 1. Therefore, the Airy stress function for substrate is the middle one of Eq. (11). Of course, if the substrate is elastic anisotropy, the corresponding Airy stress function could be used to solve the perturbed stress field. However, this situation is not considered in present work.

### 2.4 Perturbed stress distribution in thin film

The conditions for traction-free surface of thin film can be expressed as follow [8]:

$$\sigma_{yy} = 0$$
 for y=0 (12)

$$\sigma_{xy} = -2\pi\sigma_0 \sin(\omega x) \qquad \text{for y=0}$$

Similarly, the conditions for traction-free surface of substrate can be expressed as follow:

$$\sigma_{yy} = 0 \qquad \text{for } y = -h_f - h_s \tag{14}$$

$$\sigma_{xy} = 0 \qquad \text{for } y = -h_f - h_s \tag{15}$$

where  $h_f$  and  $h_s$  denote the thickness of thin film and substrate, respectively. The traction and displacement at the interface ( $y = -h_f$ ) between thin film and substrate should be continuity as follow

$$\sigma_{yy}^f = \sigma_{yy}^s \qquad \text{for } y = -h_f$$
 (16)

$$\sigma_{xy}^f = \sigma_{xy}^s \qquad \text{for } y = -h_f$$
 (17)

$$\frac{\partial u^f}{\partial x} = \frac{\partial u^s}{\partial x} \qquad \text{for } y = -h_f$$
 (18)

$$\frac{\partial v^f}{\partial x} = \frac{\partial v^s}{\partial x} \qquad \text{for } y = -h_f$$
 (19)

where u and v are the displacement in the x and y direction, respectively. The superscript f and s represent film and substrate, respectively. The equivalent elastic

constants of cubic crystalline film in plane strain state are defined as follow

$$\overline{E}_f = \frac{S_{11}}{S_{11}^2 - S_{12}^2}, \overline{\mu}_f = -\frac{S_{12}}{S_{11} + S_{12}}, \quad G_f = \frac{\overline{E}_f}{2(k + \overline{\mu}_f)}$$
 (20)

where  $\overline{E}_f$ ,  $\overline{\mu}_f$  and  $G_f$  are the equivalent Young's modulus, Poisson's ratio and shear modulus of thin film in plane strain state, respectively. Using the same definition of Dundur's parameters for two materials at interface, it could be known

$$\alpha = \frac{\overline{E}_f - \overline{E}_s}{\overline{E}_f + \overline{E}_s} , \beta = \frac{1}{2} \frac{G_f (1 - 2\overline{\mu}_s) - G_s (1 - 2\overline{\mu}_f)}{G_f (1 - \overline{\mu}_s) + G_s (1 - \overline{\mu}_f)}$$

$$(21)$$

where  $\overline{E}_s$ ,  $\overline{\mu}_s$  and  $G_s$  are the equivalent Young's modulus, Poisson's ratio and shear modulus of substrate in plane strain state, respectively. The Eqs (12)-(19) could be rewritten in terms of Airy stress function as the same form given by Kim and Vlassak [8]

$$\frac{\partial^2 F_f}{\partial x^2} = 0 \qquad \text{for y=0}$$

$$\frac{\partial^2 F_f}{\partial x \partial y} = -2\pi \sigma_0 \sin(\omega x) \qquad \text{for y=0}$$
 (23)

$$\frac{\partial^2 F_f}{\partial x^2} = \frac{\partial^2 F_s}{\partial x^2} \qquad \text{for } y = -h_f$$
 (24)

$$\frac{\partial^2 F_f}{\partial x \partial y} = \frac{\partial^2 F_s}{\partial x \partial y} \qquad \text{for } y = -h_f$$
 (25)

$$\frac{1-\alpha}{2}\frac{\partial^2 F_f}{\partial y^2} + (\alpha - \beta)\frac{\partial^2 F_f}{\partial x^2} = \frac{1+\alpha}{2}\frac{\partial^2 F_s}{\partial y^2} + \beta\frac{\partial^2 F_s}{\partial x^2} \quad \text{for } y = -h_f - h_s$$
 (26)

$$\frac{1-\alpha}{2}\frac{\partial^{3}(\int F_{f}dy)}{\partial x^{3}} + (\alpha - \beta)\frac{\partial^{2}F_{f}}{\partial x\partial y} = \frac{1+\alpha}{2}\frac{\partial^{3}(\int F_{s}dy)}{\partial x^{3}} + \beta\frac{\partial^{2}F_{s}}{\partial x\partial y} \quad \text{for } y = -h_{f} - h_{s} \quad (27)$$

$$\frac{\partial^2 F_s}{\partial x^2} = 0 \qquad \text{for } y = -h_f - h_s \tag{28}$$

$$\frac{\partial^2 F_s}{\partial x \partial y} = 0 \qquad \text{for } y = -h_f - h_s \tag{29}$$

According to the k of cubic crystalline film, the corresponding Airy stress function  $F_f$  could be chosen and the middle Airy stress function of Eq. (11) is used for substrate as  $F_s$ . Solving Eqs. (22)-(29), the constants in  $F_f$  and  $F_s$  can be obtained, so dose the perturbed stress field  $\tilde{\sigma}_f$  of thin film. As the exact expressions of  $C_1$ ,  $C_2$ ,  $C_3$  and  $C_4$  are very complicated, we do not give them here. According to the Eq. (4), the whole stress field of thin film will be known.

### 3. Energy of thin film/substrate system

In this work, the potential energy,  $\Delta U$ , consists of surface energy,  $\Delta U_s$ , and strain energy at the free surface of thin film,  $\Delta U_e$  [2, 8]. Although the effects of long-range force [7], van der Waals interactions [13] or anisotropic interfacial energy [14] may influence the surface stability of thin film. A more accurate result could be obtained for the surface stability by considering these factors, but this is not our purpose in this work. The variation of potential energy

$$\Delta U = \Delta U_s + \Delta U_e \tag{30}$$

is considered to show the elastic anisotropy effect on surface stability of thin film/substrate system.

### 3.1 Calculation the potential energy of thin film/substrate system

According to Gao [3], the change of surface energy between an unperturbed surface and a flat surface for one period of undulating is as

$$\Delta U_s = \int_0^{\lambda} \gamma (\sqrt{1 + (\partial A/\partial x)^2} - 1) dx = \frac{\gamma \pi^2 a^2}{\lambda} + O(\frac{a^2}{\lambda^2})$$
 (31)

A is the perturbing function as

$$A = a \times \cos(\omega x) \tag{32}$$

 $\gamma$  is the surface energy density and for simplicity, it is assumed as a constant number.

The strain energy density w can be given as follow

$$w = \frac{1}{2} (\sigma_x \varepsilon_x + \sigma_y \varepsilon_y + \tau_{xy} \gamma_{xy})$$
 (33)

The strain energy density w at the film surface(y=0) is as follow

$$w = \frac{4\sigma_0^2}{\overline{E}_f} \left[ 8 - \frac{a}{\lambda} \cos(\omega x) g \right] + O(\frac{a^2}{\lambda^2})$$
(34)

where g is a function of the constants in Airy stress function and other parameters as follow:

$$g = \frac{\omega^2}{2\sigma_0} \sqrt{k^2 - 1} (C_3 + C_4)$$
 for k>1

$$g = -\frac{\omega}{2\sigma_0}(C_2 - C_4) \qquad \text{for k=1}$$

$$g = -\frac{\omega^2}{8\sigma_0} \sqrt{2} \sqrt{1 - k^2} (C_2 - C_4)$$
 for  $|k| < 1$ 

If thin film is elastic isotropy and  $\alpha = \beta = 0$ , it could get  $g = \pi$ , which is in good agreement with the previous works [3, 8]. Using the method given by Gao [3], the change of strain energy at free surface of thin film is as follow:

$$\frac{\partial U_e}{\partial a} = \int_0^{\lambda} w \cos(\omega x) dx = -\frac{a\sigma_0^2}{4\overline{E}_f} g$$
 (36)

$$\Delta U_e = \int_0^a \frac{\partial U_e}{\partial a} da = -\frac{a^2 \sigma_0^2}{8\overline{E}_f} g \tag{37}$$

Therefore, the variation of potential energy is given as

$$\Delta U = \frac{\gamma \pi^2 a^2}{\lambda} - \frac{a^2 \sigma_0^2}{8\overline{E}_f} g \tag{38}$$

### 3.2 The critical wavelength and preferred wavelength of perturbation

From the previous analysis, when the surface of thin film begin to perturb, there exists a competition between surface energy,  $\Delta U_s$ , and strain energy  $\Delta U_e$ . The undulation always leads to the increment of surface energy, but, decrement of strain energy. When the variation of potential energy equals to zero, the wavelength of undulation reaches a critical point  $\lambda_c$ . For the perturbed wavelength  $\lambda$ , if  $\lambda > \lambda_c$ , the strain

energy relaxation will dominate the process, and therefore, the surface roughening and island formation will energetically favorable. However, if  $\lambda < \lambda_c$ , the surface energy increment will dominate the process, and therefore, the surface of thin film will remain flat. Therefore, if the critical wavelength is upgraded, thin film surface stability will be enhanced; vice verse. From Eq. (38), the critical wavelength of thin film perturbation can be obtained as

$$\Delta U = 0 \tag{39}$$

The critical wavelength can be solved from following equation

$$\lambda g = \frac{8\gamma \pi^2 \overline{E}_f}{\sigma_0^2} \tag{40}$$

The Eq. (40) could be rewritten as

$$\frac{\lambda}{\lambda_0} = \frac{\pi}{g} \tag{41}$$

by defining

$$\lambda_0 = \frac{8\gamma\pi\overline{E}_f}{\sigma_0^2} \tag{42}$$

The Eq. (41) also has the same form as given by Kim and Vlassak for the surface stability of elastic isotropy thin film [8]. The critical wavelengths for some cubic crystalline films, such as Au, Ni, Mo, are shown in Fig. 3. The film and substrate are assumed as the same materials and substrate is elastic isotropy and semi-infinity. Gao [3] has justified that the most unstable perturbation mode of thin film undulation

corresponded to maximizing the quantity –  $\Delta U/\lambda^3$  , so the preferred wavelength of undulation is

$$\frac{\partial}{\partial \lambda} \left( -\frac{\Delta U}{\lambda^3} \right) = 0 \tag{43}$$

Using Eqs. (38) and (42), Eq. (43) can be rewritten as

$$4\pi \frac{\lambda_0}{\lambda^5} + \frac{\partial}{\partial \lambda} (\frac{g}{\lambda^3}) = 0 \tag{44}$$

The Eq. (44) also has the same form give by Kim and Vlassak [8]. The preferred wavelength of thin film perturbation is shown in Fig. 4.

### 3.3 Elastic anisotropy effect on surface stability

If assuming both the film and substrate are elastic isotropy and have same elastic properties (k=1), the critical or preferred wavelength of perturbation will not change as film thickness changing as shown in Fig.3 and Fig.4. It is interesting to find that the relationship between the film thickness and wavelength is not longer linear for k<1, while the relationship for k>1 is almost as linear as k=1. There exists a critical point  $h_c = 0.1\lambda_0$  for k<1 as the wavelength reaches its minimum value. When the film thickness is beyond this point, the relationship between wavelength and film thickness is like a waviness curve. Therefore, a thickness window may exist between the critical point  $h_c = 0.1\lambda_0$  and point  $h_f = 1\lambda_0$  (as we know that the larger the wavelength, the more difficult the film roughing occurred). The smooth films could be formed in the

thickness window. The thickness window is also found by Suo and Zhang [7] when they considered the effect of dispersion force. Although the thickness window in this work is induced by elastic anisotropy effect, it also indicates that such an anisotropic effect can not be ignored.

If k is less than one unit, the wavelength for anisotropic thin film is larger than that for isotropic film (k=1) about 40~80%. Therefore, elastic anisotropy effect could enhance thin film surface stability. On the other hand, the anisotropic effect could also weaken the surface stability if k>1 because the wavelength is less than that for k=1 about 40~60%. Such anisotropic effect also appeared in Liu et al.'s work [10]. When AR>1 (k<1), thin film is stable at the first and ripples at a critical thickness. However, when AR<1(k>1), the film is almost unstable and ripples immediately at begin of the film growth [10]. Therefore, the elastic anisotropy effect in this work is in good agreement with the previous work [10] and should be considered. However, if k is large than one unit, AR will less than one unit, such as Nb, Mo, then the undulation direction will not along <100> and change to other directions. Such effect is not considered in present work and the wavelength along <100> here is as a reference to compare it with other results for different k values. All of the differences mentioned above may greatly influence the surface stability of thin film/substrate system, especially, when the film is ultra-thin or k deviates one unit too much. Therefore, the elastic anisotropic effect should be considered both in the film synthesis and its application. From the calculation, the perturbed wavelength for anisotropic aluminum film is almost coincidence with that for isotropic film. Therefore, it is also proper to ignore the

elastic anisotropic effect when the k is closed to one unit.

Gao [3] has obtained the relationship between critical wavelength and preferred wavelength for isotropic film on the same semi-infinite homogeneous solid as

$$\lambda_p = \frac{4}{3}\lambda_c \tag{45}$$

Eq. (45) is also theoretical validated by Obayashi and Shintani [9] when both the film and substrate are the same elastic anisotropy materials. From Fig.3 and Fig.4, the relationship between  $\lambda_p$  and  $\lambda_c$  shown in Eq. (45) still exists when the film is elastic anisotropy and substrate is isotropy but the same material as film.

By considering the preferred wavelength at critical film thickness  $h_c=0.1\lambda_0$ , the relationship between k and normalized preferred wavelength is shown in Fig. 5. The normalized preferred wavelength is parabolic decreasing as increasing k. Such phenomenon is also observed by Liu et al. [10] through finite element simulation. In Liu et al.'s work [10], they use AR as the material parameter for simulation and found that the larger the value of AR, the larger the preferred wavelength. Considering k has the following relationship with AR in cubic crystal

$$k = \frac{S_{12}}{S_{11} + S_{12}} \left( 1 + \frac{S_{11}}{S_{12}} \frac{1}{AR} \right) \tag{46}$$

the relationship shown in Fig. 5 is also proved the simulation results given by Liu et al.[10].

When multi-layered thin film/substrate system is considered, i.e. Cu/Ni, the

corresponding Airy stress function for Cu film and Ni film could be chosen from Eq.(11). Incorporated with the corresponding boundary conditions, the stress field for Cu film and Ni film could be easily obtained. By following the procedures given above, the surface stability of Cu/Ni multi-layered film could be known. Therefore, the method given here is easily extended to the multi-layered film/substrate system and used for considering elastic anisotropy effect.

### 4. Summary

In this work, the elastic anisotropy effect on surface stability of thin film/substrate system was considered. The method used in present work can be easily extended to the multi-layered system, which could have different cubic crystalline materials such as Au, Ni, Cu, et al.. From systematic analysis, the effect of elastic anisotropy could not be ignored, especially, when the film is ultra-thin or k deviates one unit very much.

The anisotropic effect could enhance the surface stability of thin film/substrate system if k<1; it also can weaken the surface stability if k>1. There exists a critical thickness  $h_c = 0.1\lambda_0$  for cubic crystalline film on the semi-infinity substrate with same material if k is less than one unit. When k is closed to one unit, it is proper to ignore the elastic anisotropy effect.

Although the direction effect of cubic crystal is not considered here, the ripples and

islands of film are always toward to <100> direction during the epitaxial growth when AR is larger than one unit. In general, an effective method was given here to evaluate elastic anisotropy effect on the surface stability of thin film/substrate system. This work may improve our understanding in the stability problems of thin film/substrate system and help us to utilize the anisotropic effect both in thin film synthesis and its application.

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### References

- [1] R.J Asaro, W.A. Tiller, Metall. Trans. 3(1972) 1789-1796.
- [2] Y. Li, X.S. Wang, X.K Meng, Appl. Phys. Lett. 92(2008) 131902.
- [3] H. Gao, Int. J. Solids Structures 28(1991) 703-725.
- [4] H. Gao, J. Mech. Phys. Solids 42(1994), 741-772.
- [5] L.B, Freund, F. Jonsdottir, J. Mech. Phys. Solids 41(1993) 1245-1264.
- [6] L.B. Freund, Int. J. Solids Structures 32(1995) 911-923.

- [7] Z. Suo, Z. Zhang, Phys. Rev. B 58(1998) 5116-5120.
- [8] J.H. Kim, J.J. Vlassak,. Int. J. Solids Structures. 44(2007) 7924-7937.
- [9] Y. Obayashi, K. Shintani, J. Appl. Phys. 84(1998) 3141-3146.
- [10] P. Liu, Y.W. Zhang, C. Lu, Surf. Sci. 526(2003) 375-382.
- [11] Y. Pang, R. Huang, J. Appl. Phys. 101(2007) 023519.
- [12] K.U. Urazgil'dyaev, A.G. Cheberyak, V.A Chubok., P.G. Shishkin, Int. Appl. Mech. (1975) 1283-1287.
- [13] Y. P. Zhao, Arch. Appl. Mech. 72 (2002) 77-84.
- [14] B.J. Spencer, Phys. Rev. B. 59(1999) 2011.

## Figures and Table captions

Figure 1. The k and AR for some cubic crystals

Figure 2. Schematic of thin film/substrate system with perturbed free surface

Figure 3. Normalized critical wavelength vs. normalized film thickness

Figure 4. Normalized preferred wavelength vs. normalized film thickness

Figure 5. k vs. the normalized preferred wavelength

Table 1. Some elastic properties of cubic crystals

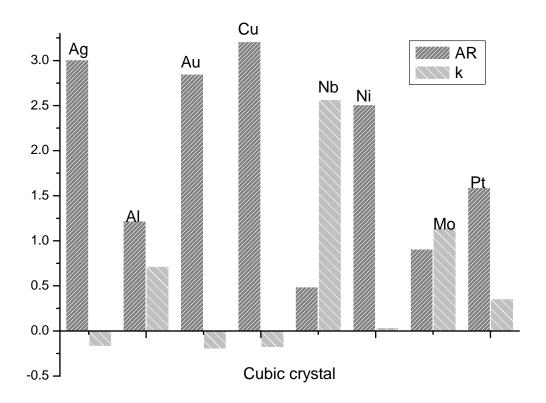


Figure 1. The k and AR for some cubic crystals

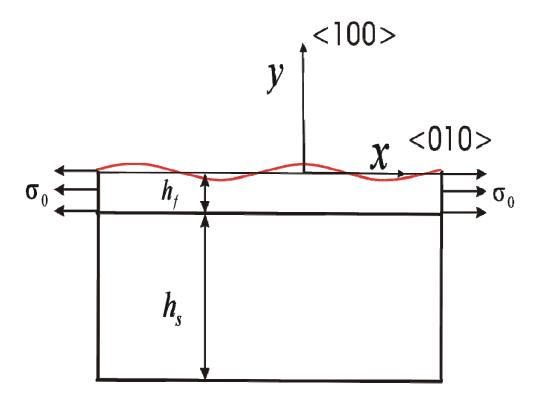


Figure 2. Schematic of thin film/substrate system with perturbed free surface

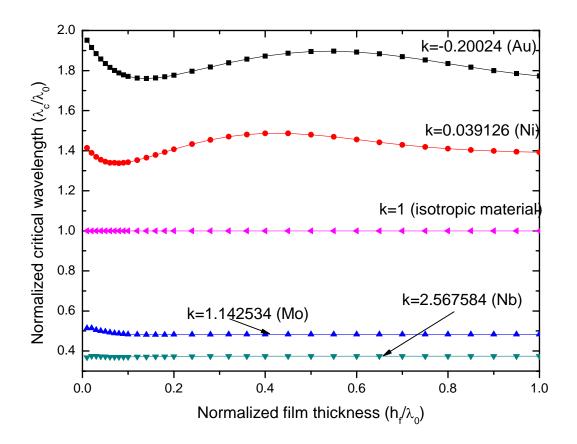


Figure 3. Normalized critical wavelength vs. normalized film thickness

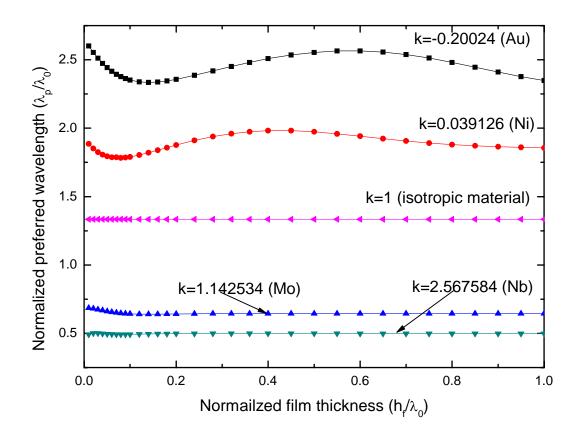


Figure 4. Normalized preferred wavelength vs. normalized film thickness

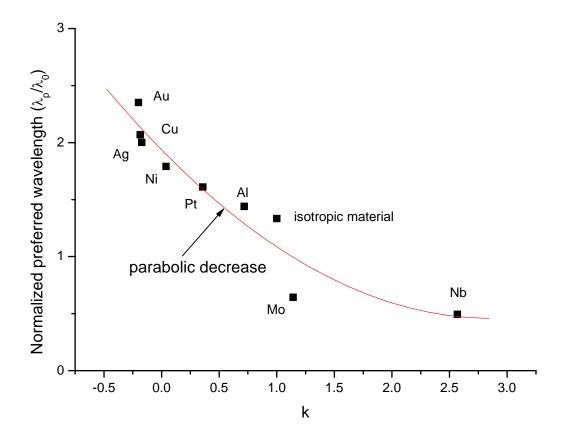


Figure 5. k vs. the normalized preferred wavelength

Table 1. Some elastic properties of cubic crystals

Material	$S_{11}$	$S_{12}$	$S_{44}$	E	G	μ
	$(GPa^{-1} \times 10^3)$	$(GPa^{-1} \times 10^3)$	$(GPa^{-1} \times 10^3)$	(GPa)	(GPa)	
Au	23.55	-10.81	24.10	77.2	27.2	0.42
Nb(Cb)	6.5	-2.23	35.44	103	37.5	0.38
Ni	7.34	-2.74	8.02	207	76	0.31
Mo	2.91	-0.818	8.22	330	120	0.375