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Thermomechanical Analysis of Film-on-Substrate System With Temperature-Dependent Properties

Thermomechanical analysis of global and local buckling is presented to show temperature effects on the stress/strain and shape of a film-on-substrate system. First, the strain is expressed as a function of three key temperatures (room, working, and deposit temperatures). Through sensitivity analysis on temperature, polydimethylsiloxane (PDMS) selection is determined to theoretically design film-on-substrate systems with the minimum variation in stress caused by temperatures. Then, the wrinkling behaviors are studied to establish the relationships of critical strain, wavelength, and amplitude with temperature. In addition, the critical working temperature is determined for local buckling. The approximate semi-analytical solution and the finite element simulation are compared by the use of a two-dimensional case of film on a half-space substrate.

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1 Introduction

With the development of microelectronics technology, there are functions that are not well addressed by the established rigid semiconductor technology. Realization of flexible electronics with performance equal to conventional microelectronics built on brittle wafers, but in high mobility, optical transparency, light-weight and bendable/stretchable formats would enable many new applications, such as solar cell, flexible display, smart skin, and radio frequency identification (RFID) [1–3].The film-on-substrate system is a typical structure in flexible electronics. A main challenge is how to design a structure free from the temperature's variation and meeting the requirement of bendability and stretchability [4].

Reported studies on film-on-substrate system made large progress in duality, crack, and bendability/stretchability [5–10]. Freestanding Si/metal thin film ruptures when stretched beyond 1–2% [11]. However, when bonded onto an organic substrate, it can sustain plastic deformation ten times larger than its fracture strain, yet still remains electrically conductive [12,13]. Park et al. [5] carried out theoretical and experimental studies on bending in structure relevant to inorganic flexible electronics, and the effects of edges and finite device sizes were also considered. Wrinkles are usually nuisance in many applications, but may be used as stretchable interconnects, templates for device fabrication, or means to evaluate mechanical properties of materials [4]. A compressively strained elastic film bonded onto the compliant substrate will form wrinkles, which is a simple approach for flexible integrated circuits to circumvent the limitations of stretchability and their low flexural rigidity. Khang et al. [7], Kim et al. [8], Jiang et al. [14], and Sun et al. [15] studied the buckling behavior of the film-on-substrate system and the controllability of the structure formation, and developed a stretchable and foldable silicon integrated circuits with high-performance. Huang et al. [6], Huang et al. [4], and Lacour et al. [13] studied buckling behavior with nonlinearity and a viscous layer, and discussed the mechanisms of reversible stretchability of thin metal films on elastomeric substrates. Circuits in wavy patterns offer fully reversible stretchability/compressibility without substantial strains in circuit materials themselves. The resulting mechanical advantages are critically important for achieving stretchability. In these systems, strains at the circuit level can exceed the fracture limits of almost all known electronic materials [7].

However, temperature effects are highlighted in flexible electronics because of the existence of stiff inorganic film and flexible organic substrate. Few papers reported on thermal analysis of film-on-substrate structure, where the temperature is uniform or nonuniform [16,17], the structure has only one film or multilayer film [18], the deposit and room temperatures are discussed [19], and the film may be stiff and soft [20]. So far, there are still many temperature effects unaddressed such as the temperature-dependent properties of a polymeric material. Elastomer has wide ranges of mechanical properties such as coefficient of thermal expansion (CTE) from 16 ppm/K to 310 ppm/K [16,19], and Young's modulus from 50 KPa to 50 MPa [21]. A thin film with thickness measured in tens of nanometers is vapor deposited onto a thick elastomeric substrate at an elevated temperature. When the film-on-substrate structure is cooled, the large mismatch of CTEs and Young's modulus between film and substrate produces a state of compression, even buckling in film [19]. The temperature-dependent properties are often considered as nuisance in structural design. It will be addressed in this work how to use these temperature-dependent properties to increase the reliability, and what the temperature effects are in buckling format. The film will buckle into modes with wavelengths, typically measured in microns at a critical temperature. As the temperature is further lowered, the amplitude of the buckles grows and distinctive patterns emerge [22]. The temperature plays an important role in manufacturing and running, however, there is still a large blank space not investigated.

In this work, the model of the strain of the film-on-substrate structure is established based on interface continuity and is considered as a function of room, working, and deposit temperatures. In the wrinkle state, the amplitude and the wavelength are func-

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tions of the ratio of Young's modulus and thicknesses of the film and the substrate. The Young's modulus of the substrate is affected severely by temperature. In other words, the temperature may directly determine the structural format, including wavelength, amplitude, and critical strain. In order to keep the stability of the flexible electronics system, the critical working temperature needs to be studied. Analytical solution and finite element analysis reveal the physics in temperature change. Deep studies on temperature effects are useful for structural optimization design of flexible electronics.

2 Formation of Film-on-Substrate Structure

The film-on-substrate structure in flexible electronics is mostly realized through the thin film deposited, typically by vapor phase or physical transfer processes, onto a prestrained elastomeric substrate. The prestrain is usually generated in two ways: thermally expanded elastomeric substrate and mechanically stretched elastomeric substrate [14]. In the former, depositing film onto a heated substrate and cooling this system led to compressive strains in film due to the mismatch of the CTEs of the film and substrate. Sufficiently large compression will lead to buckling instabilities in the film. The mechanically stretched elastomeric substrate may be found in many references [7,8]. In our work, a hybrid method by combining the above two ways is adopted to create a prestrained elastomeric substrate. We wondrously observe that there are nonlinear phenomena when the substrate is elongated by the thermal and mechanical loads collectively. The thin film and the substrate are supposed to be coupled at the interface where the strain is continuous. If structures with $E_f h_f \approx E_s h_s$ are unconstrained, any mismatch strain between the deposited film and the substrate forces them to form a wavy format (local buckling) [16], or to roll to an arch geometry (global buckling) with the film facing outward or inward [19], where h_f and h_s, and E_f and E_s are the thickness and the Young's modulus of the film and the substrate, respectively. Usually, the thickness effect of the substrate is not considered because the substrate is much thicker than the film. The film-on-substrate system is always considered as a semi-infinite solid. In this case, it appears as local buckling. However, when the substrate becomes thinner, global buckling will be observed. Wang et al. [23] definitely gave the critical condition separating the local and global buckling modes. The critical condition of the local buckling is $\varepsilon_{\text{critical}}^{\text{local}} = (3\bar{E}_s / 8\bar{E}_f)^{2/3}$ and that of global buckling is $\varepsilon_{\text{critical}}^{\text{global}} = \bar{G}(h_s+h_f)F_{\text{cr}}^0 / (\overline{EA}(\bar{G}(h_s+h_f)+1.2F_{\text{cr}}^0))$, where $\overline{EA}$, $\bar{G}$, and F_{cr}^0 can be referred to in the literature [23]. When $\varepsilon_{\text{critical}}^{\text{local}} < \varepsilon_{\text{critical}}^{\text{global}}$, local buckling occurs. When $\varepsilon_{\text{critical}}^{\text{local}} > \varepsilon_{\text{critical}}^{\text{global}}$, global buckling occurs. Because $\varepsilon_{\text{critical}}^{\text{global}}$ is related with the thickness of the substrate and the length of the film-on-substrate structure, whether the film-on-substrate structure generates local or global buckling is not determined only by the ratio of the Young's modulus of the film and substrate, but also by the length of the film-on-substrate structure and the thickness of the film and substrate.

Figure 1 schematically illustrates the hybrid method to integrate thin films (e.g., silicon) with elastomeric substrates (e.g., polydimethylsiloxane (PDMS)). The length of the substrate is L_0 when relaxed (Fig. 1(*a*)), and L_1 when stretched by external force (mechanically stretched elastomeric substrate), as shown in Fig. 1(*b*). Then the length becomes L_2 when the temperature is up to the deposit temperature (thermally expanded elastomeric substrate) shown in Fig. 1(*c*). The thin film is deposited onto the stretched substrate (Fig. 1(*d*)). When the elastomeric substrate is released, the thin film will form a pattern of wrinkles or roll to an arch geometry (Fig. 1(*e*)). When this wrinkling structure is stretched, the deformation of the thin film matching the elongation of the substrate is compensated by the shape change in the thin film from a sharp shape to a flat shape, namely, the amplitude becomes small. It is known that large elongation of substrates induce only small strains in thin films.

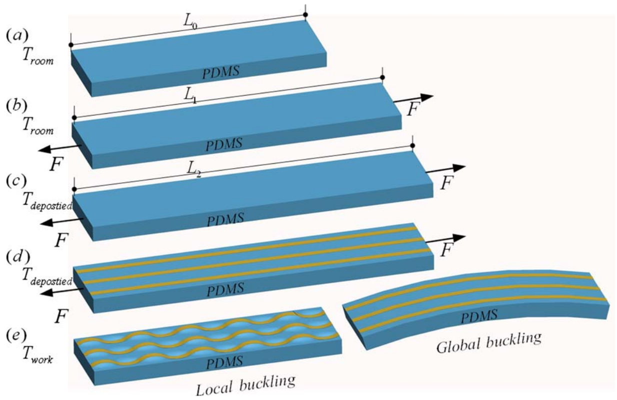

Fig. 1 Wrinkling steps for thin films onto a prestretched and thermally expanded PDMS substrate. (*a*) PDMS substrate with L_0 when relaxed; (*b*) prestretched PDMS with L_1 when stretched in T_{room} by external mechanical load F; (*c*) prestretched PDMS with L_2 when stretched in $T_{\text{deposited}}$ by external mechanical load F and thermal load $T_{\text{deposited}} - T_{\text{room}}$; (*d*) thin films evaporated on the stretched substrate; (*e*) release from prestretch in T_{work} environment, and thin films wrinkle or bend. When the structure is stretched, thin films deflect out of plane so that large elongation of substrate induces only small elastic strains in thin films.

Mismatch strain ε composes of three dominant components: (1) thermal mismatch of CTEs between substrate α_s and thin film α_f; (2) built-in strain in a deposited film [19]; and (3) mechanical load acting on a substrate. The substrate does not have temperature-induced stress at the room temperature T_{room} before the thin film deposited (Fig. 1(*a*)). When the substrate is elongated from L_0 to L_2 (see Fig. 1(*c*)), one can get $\varepsilon_{s0}(T_r) = (L_1 - L_0)/L_0$ and $\sigma_{s0}(T_r) = \bar{E}_s \cdot \varepsilon_{s0}$, where $\bar{E}_s = E_s/(1-\nu_s^2)$, and E_s is the Young's modulus of the substrate. Now, one determines the strain ε_s and the stress σ_s after the temperature raised to the deposit temperature $T_{\text{deposited}}$. The elongation from L_0 to L_2 results from two parts: one is the strain induced by force, and another is induced by temperature. Supposing the external load σ_{s0} keeps constant before and after temperature changes. Consequently, at $T_{\text{deposited}}$ after thin film deposited, the strain in the substrate is the sum of the thermal strain and the mechanical strain (see Fig. 1(*c*)), namely

$$\varepsilon_s(T_{\text{deposited}}) = \alpha_s(T_{\text{deposited}} - T_{\text{room}}) + \frac{\sigma_{s0}}{\bar{E}_s(T_{\text{deposited}})} \qquad (1)$$

3 Temperature-Dependent Global Buckling Analysis and Structural Design

3.1 Geometrical Model and Governing Equations. It is important to address that properties of the thin film can be significantly different from those of bulk materials. Inorganic materials can be made flexible by taking advantage of two facts: making them thinner and softer. According to the elementary beam theory, when a film with thickness h_f is bent to a curvature with radius r, the strain is $\varepsilon = h_f/2R$. One gets $\varepsilon \leq 2\%$ when $h_f = 1$ μm and $R \geq 25$ μm. If a structure of two layers with similar modulus such as silicon and steel, the neutral surface is the midsurface of the structure, and the strain in the top surface is given by $\varepsilon = (h_f + h_s)/2R$ [24]. Now let us consider a stiff film deposited onto a compliant substrate such as PDMS. The film and the substrate have different elastic moduli, and $E_f \gg E_s$, so that the neutral surface shifts from the midsurface toward the film. Then one can get the strain on the top [25],

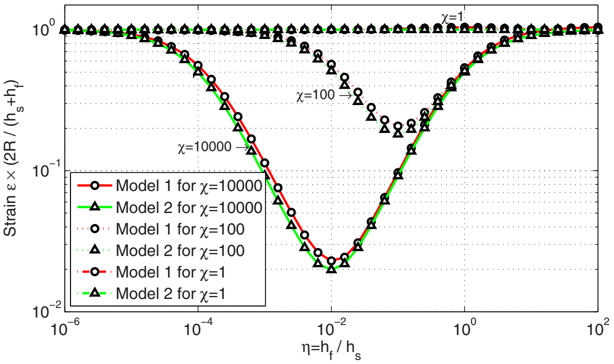

Fig. 2 Normalized strain in the film as a function of film/substrate thickness ratio

$$\varepsilon_{\mathrm{Model\ 1}} = \frac{(h_s + h_f)}{2R} \frac{(1 + 2\eta + \chi\eta^2)}{(1 + \chi)((1 + \chi\eta) - h_s\eta(1 - \chi)/2R)} \times 100\% \tag{2}$$

where, $\eta = h_f/h_s$, $\chi = \bar{E}_f/\bar{E}_s$, $\bar{E}_s = E_s/(1-\nu_s^2)$, and $\bar{E}_f = E_f/(1-\nu_f^2)$. In a biaxial tensile condition, the strain of the film can be written as [24]

$$\varepsilon_{\mathrm{Model\ 2}} = \frac{(h_s + h_f)}{2R} \frac{(1 + 2\eta + \chi\eta^2)}{(1 + \eta)(1 + \chi\eta)} \times 100\%$$

Strains in thin films calculated by the two models are shown in detail in Fig. 2, which plots the normalized strain in the film versus η. Three kinds of substrates are compared: steel ($E_f/E_s \approx 1$), plastic ($E_f/E_s \approx 100$), and rubber ($E_f/E_s \approx 10000$) when the thin film is Si. One can observe that the more compliant the substrate is, the less the strain is.

In the fabrication process, the room temperature T_{room} may act as a reference temperature for thermal expansion of the substrate. The thin film, however, is stress-free at the deposit temperature $T_{\mathrm{deposited}}$ when it is deposited onto the substrate. $T_{\mathrm{deposited}}$ is set as a reference temperature for thermal expansion of the thin film. In the initial state, the thin film's strain is zero, namely, $\varepsilon_f(T_{\mathrm{deposited}}) = 0$. If the temperature decreased from $T_{\mathrm{deposited}}$ to T_{room} and the thin film is subjected to mechanical force, one gets $\varepsilon_f(T_{\mathrm{room}}) = \alpha_f \cdot (T_{\mathrm{room}} - T_{\mathrm{deposited}}) + \sigma_{f0}/\bar{E}_f$. Figure 3(*a*) shows the strain as a function of the Young's modulus ratio of film/substrate, where the thickness of the thin film is kept constant, but that of the substrate is varied. It is well known that the polymeric materials are temperature dependent. Several models for the temperature-dependent Young's modulus of polymeric materials have been presented such as a nonlinear model $E_s = E_{s0}^2/(E_{s0} + k(T - T_{\mathrm{ref}}))$ and a linear model $E_s = E_{s0} + k(T - T_{\mathrm{ref}})$. If the linear model is adopted, one can get the strain as a function of temperature plotted as Fig. 3(*b*), where the parameters of the substrate are $h_s \sim 1$ mm, $v_s \sim 0.48$, and $E_s \sim 2$ MPa, and those of the thin film are $h_f \sim 200$ nm, $v_f \sim 0.27$, and $E_f \sim 20$ GPa. It can be noted that the temperature plays an important role in the variation in strain. The thin film adhering to the substrate (see Fig. 1(*d*)) is coupled with the strain of the substrate. When the external force σ_{s0} is released (see Fig. 1(*e*)), the resultant force vanished, namely

$$\sigma_f h_f + \sigma_s h_s = 0 \tag{3}$$

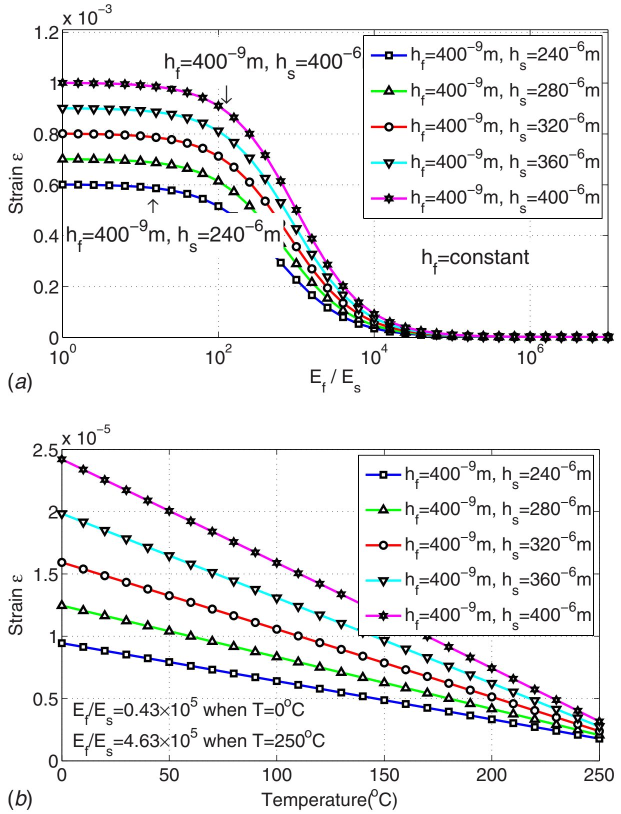

Fig. 3 Normalized strain as a function of Young's modulus of substrate. (*a*) Normalized strain as a function of film/substrate Young's modulus ratio. (*b*) Normalized strain as a function of temperature.

This equation is derived by considering the thin film and substrate as two strips in order to simplify the process of description. The bending effect is not considered here, more about which can refer to literatures in Refs. [17,18]. After the thin film is deposited and the film/substrate stack has been cooled down to room temperature or heated up to higher temperature, they will be evaluated to new values. During the running of the device, the resistive layer dissipates the heat that it generates in two ways: on its up-side to the surrounding air, and on its down-side to the elastomeric substrate, so there is the third temperature named work temperature T_{work} for flexible electronics, in addition to the room and deposit temperatures (T_{room} and $T_{\mathrm{deposited}}$). The strain will change with the variation in temperature and external stress. One gets

$$\begin{aligned}\bar{E}_f \cdot \left(\varepsilon_f(T_{\mathrm{work}}) + \alpha_f \cdot (T_{\mathrm{deposited}} - T_{\mathrm{work}}) + \frac{\sigma_{f_0}}{\bar{E}_f} \right) \cdot h_f \\ = \bar{E}_s(T_{\mathrm{work}}) \cdot \Bigg(\alpha_s \cdot (T_{\mathrm{deposited}} - T_{\mathrm{room}}) + \frac{\sigma_{s0}}{\bar{E}_s(T_{\mathrm{deposited}})} \\ - \alpha_s \cdot (T_{\mathrm{deposited}} - T_{\mathrm{work}}) - \varepsilon_f(T_{\mathrm{work}}) \Bigg) \cdot h_s\end{aligned} \tag{4}$$

where $E_s(T)$ is a temperature-dependent Young's modulus, E_f is usually considered as a constant, and σ_{f_0} is a built-in stress. Then one can get the strain of the thin film as

$$\varepsilon_f(T_{\mathrm{work}}, T_{\mathrm{deposited}}, T_{\mathrm{room}}) = \frac{\bar{E}_s(T_{\mathrm{work}}) \cdot h_s \cdot \alpha_s(T_{\mathrm{work}} - T_{\mathrm{room}}) - \bar{E}_f \cdot h_f \cdot \alpha_f(T_{\mathrm{deposited}} - T_{\mathrm{work}})}{\bar{E}_s(T_{\mathrm{work}}) \cdot h_s + \bar{E}_f \cdot h_f} + \frac{\bar{E}_s(T_{\mathrm{work}}) \cdot h_s \cdot \sigma_{s0}/\bar{E}_s(T_{\mathrm{deposited}}) - h_f \cdot \sigma_{f_0}}{\bar{E}_s(T_{\mathrm{work}}) \cdot h_s + \bar{E}_f \cdot h_f} \tag{5}$$

Here, a thermomechanical model of a film-on-substrate structure is presented to provide a quantitative guide for improving overlay alignment. Equation (5) describes the strain of the film at the working temperature T_{work} after being deposited at $T_{\text{deposited}}$. The first term on the right-hand side is the strain caused by CTEs' mismatch, and the second term is caused by the initial stress and the built-in stress in the substrate and the thin film. They are the major sources of alignment errors.

3.2 Structure Design Based on Temperature-Dependent Properties. The linear model $E_s = E_{s0} + k(T - T_{\text{ref}})$ is adopted here and submitted into Eq. (5). Then one can observe that there exists a nonlinear behavior, even by the use of this linear model. Figure 4(*a*) indicates that the Young's modulus models with and without temperature-dependent effects show two different laws of change with temperature. Figure 4(*b*) shows different nonlinear relationships between the strain and the temperature with different initial values of strain. It also can be observed from Fig. 4 that the degree of nonlinearity lies heavily on the thermal and mechanical load together. However, we discover an interesting phenomenon that nonlinearity disappears when thermal or mechanical load acts on structures separately. The nonlinearity gives us a chance to design a structure with high stability. It is important that there exists an extreme point so that one can get a working temperature for flexible electronics with minimum strain variation corresponding to the room temperature. In other words, a key parameter k can be found to design a structure with minimum strain variation for special working temperature. If a nonlinear temperature-dependent model is adopted, there are more fruitful nonlinear behaviors. For example, there are more than one extreme points, so several working temperature without strain variation can be acquired.

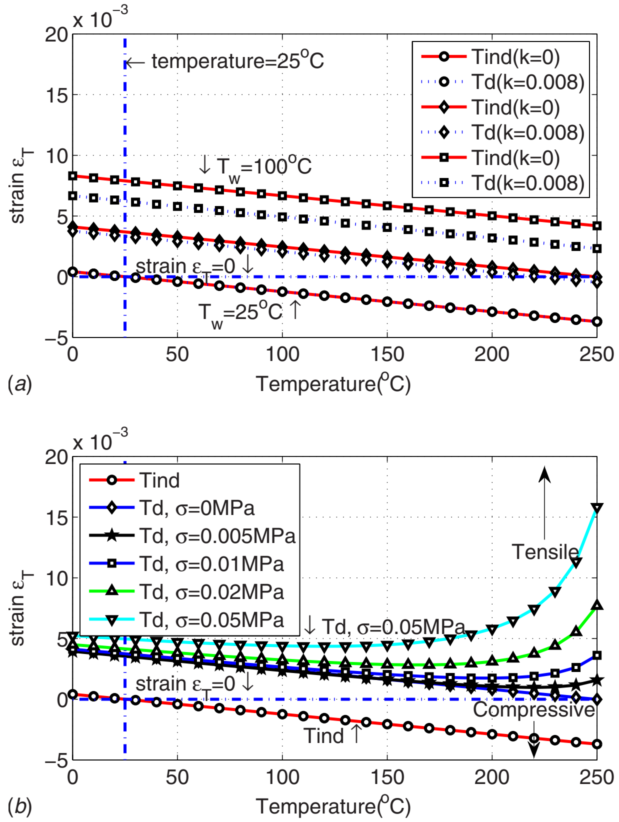

Fig. 4 Substrate strain $\varepsilon_f(T_{\text{ref}})$ as a function of the temperature and the initial stress. (*a*) Without external stress, temperature independent or dependent moduli are considered. (*b*) The degree of nonlinearity is dependent on the external stress. *T*-independent and *T*-dep mean temperature independent and dependent, respectively.

Through the critical parameter k, a temperature-free structure can be designed to keep the strain constant. The sensitivity analysis of the three different temperatures, T_{room}, T_{work} and $T_{\text{deposited}}$, can be given as

$$a{:}\,\partial\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})/\partial T_{\text{work}} = 0$$

$$b{:}\,\partial\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})/\partial T_{\text{deposited}} = 0$$

$$c{:}\,\partial\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})/\partial T_{\text{room}} = 0 \tag{6}$$

It is noted from Fig. 4 that there exits k that can meet $\partial\varepsilon_f/\partial T_i = 0, (i = \text{room},\ \text{deposited},\ \text{work})$. It means that there exists some value for parameter k to keep the strain invariable, according to the three different temperatures, respectively. The second equation of Eq. (6) is adopted to show how to calculate the parameter k

$$\frac{\partial\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})}{\partial T_{\text{deposited}}} = \frac{k\cdot h_s\cdot\alpha_s\Delta T_{dr} + \bar{E}_f\cdot h_f\cdot\alpha_f + \dfrac{k\cdot h_s\cdot\sigma_{s0}}{(\bar{E}_{s0}+k\cdot\Delta T_{dr})}}{(\bar{E}_{s0}+k\Delta T_{wr})\cdot h_s+\bar{E}_f\cdot h_f} - \frac{k\cdot h_s\cdot\left[(\bar{E}_{s0}+k\cdot\Delta T_{wr})\cdot\left(h_s\cdot\alpha_s\cdot\Delta T_{dr}+\dfrac{h_s\cdot\sigma_{s0}}{(\bar{E}_{s0}+k\cdot\Delta T_{dr})}\right)-\bar{E}_f\cdot h_f\cdot\alpha_f\cdot\Delta T_{dw}-h_f\cdot\sigma_{fbi}\right]}{((\bar{E}_{s0}+k\cdot\Delta T_{wr})\cdot h_s+\bar{E}_f\cdot h_f)^2} \tag{7}$$

where $\Delta T_{dr} = (T_{\text{deposited}} - T_{\text{room}})$, $\Delta T_{wr} = (T_{\text{work}} - T_{\text{room}})$, $\Delta T_{dw} = (T_{\text{deposited}} - T_{\text{work}})$.

The material properties for calculation are listed as follows: $E_{si} = 130$ GPa, $\upsilon_{si} = 0.27$, $\alpha_{si} = 2.7$ ppm/K, $E_{\text{PDMS}} = 2$ MPa, $\upsilon_{\text{PDMS}} = 0.48$, and $\alpha_{\text{PDMS}} = 16$ ppm/K [7,14], from which one can note that the Young's modulus of PDMS is nearly five orders of magnitude more compliant than the thin film. The temperature effects have been shown in Fig. 4 for a 1-mm-thick PDMS substrate after a 100-nm-thick film was deposited at different temperatures. If $T_{\text{room}} = 25°\text{C}$, $T_{\text{work}} = 75°\text{C}$, $T_{\text{deposited}} = 200°\text{C}$, and

$\sigma_{f_0}=0.5$ MPa, by combining Eqs. (5) and (6), one gets three values that have one complex number and two real numbers, $k=-0.000207$ and $k=-0.900640$, and $k=-0.000207$ is reasonable and feasible for practical PDMS. That is to say, a structure with strain free from temperature can be designed to meet special needs such as reducing the response of the dynamic temperature load in solar cell, because the Young's modulus of the same material can be tuned over two orders of magnitude by controlling the amount of cross linking between polymer chains [14].

4 Temperature-Dependent Local Buckling Analysis and Critical Condition

4.1 Sinusoidal Wrinkles for Thermomechanical Buckling Behavior. When wrinkles appear, the shear stresses between the thin film and substrate may be neglected. To analyze the buckling behavior of a film-on-substrate structure, the following bending equation for a thin film can be written as [26,27]:

$$\bar{E}_f I \frac{\partial^4 z}{\partial x^4} + F \frac{\partial^2 z}{\partial x^2} + Kz = 0 \tag{8}$$

where $I=h_f^3/12$ is the area moment of inertia of film per unit length. According to Biot (Winkler's modulus of half-space), the response of an elastic half-space to sinusoidal load is a function of wavelength, and the substrate stiffness is given by

$$K = \frac{\bar{E}_s \pi}{\lambda} \tag{9}$$

where λ is the buckling wavelength.

Theories have proven that wavy structures are highly sinusoidal, and experiments have shown that they have excellent uniformity in wave amplitudes (less than ±5%) and wavelengths (less than ±3%) over large areas (up to 15×15 mm^2) [14]. Chen and Hutchinson [22] analyzed sinusoidal wrinkles of the deflection field $w=A\cos((2\pi/\lambda)\cdot x)$, in a film on a substrate with infinite thickness, where A is the amplitude. When temperature effects are considered, the deflection field becomes $w=A(T)\cdot\sin((2\pi/\lambda(T))\cdot x)$. From Eqs. (8) and (9), one can observe that K is affected directly by the Young's modulus of the substrate, which, however, is temperature dependent. When it is substituted into Eq. (8), the uniformity of strains requires the in-plane displacement field be

$$u = \frac{1}{2}\frac{\pi}{\lambda(T)} \cdot A^2(T) \cdot \sin\left(\frac{4\pi}{\lambda(T)} \cdot x\right)$$

The compressive force in the thin film can be written as

$$F = \frac{\bar{E}_f h_f^3}{12}\left(\frac{2\pi}{\lambda}\right)^2 + \frac{\bar{E}_s \lambda}{4\pi} \tag{10}$$

if the linear temperature model $\bar{E}_s=(E_{s0}+k(T-T_{\text{room}}))/(1-\upsilon^2)$ is submitted into Eq. (8). The minimum of the function is found from the condition $dF/d\lambda$ leading to buckling wavelength

$$\lambda = \frac{\pi h_f}{\sqrt{\varepsilon_c}} = \frac{2\pi}{k_{\text{wave}}} = 2\pi h_f \left(\frac{\bar{E}_f(1-\upsilon_s^2)}{3(E_{s0}+k(T-T_{\text{room}}))}\right)^{1/3} \tag{11}$$

where

$$k_{\text{wave}} = \frac{1}{h}\left[\frac{12\bar{E}_s(T)}{\bar{E}_f}\right]^{1/3}$$

depends on mechanical parameters and geometry. Then one can get the stiffness of the substrate

$$K = \frac{\bar{E}_s \pi}{2\pi h}\left(\frac{3(E_{s0}+k(T-T_{\text{room}}))}{\bar{E}_f(1-\upsilon_s^2)}\right)^{1/3} \tag{12}$$

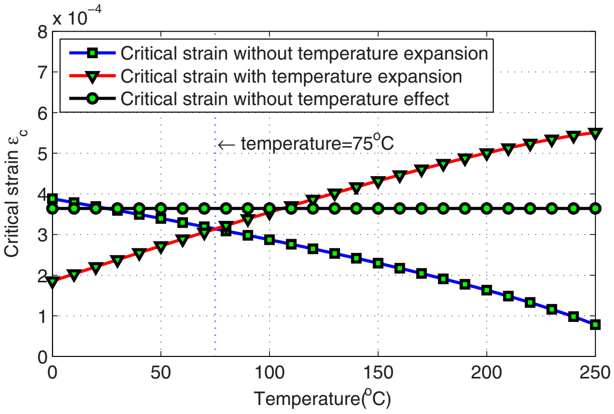

Fig. 5 The relationship of critical strain with temperature

The behavior in wavy configuration is consistent with the linear analysis of initial buckled geometry in a uniform, thin, high-modulus layer on half-space low-modulus support; one can get the critical strain $\varepsilon_c=(3\bar{E}_s/8\bar{E}_f)^{2/3}$ [4,22]. For $\varepsilon_c=\sigma_c/\bar{E}_f$ and $E_s=E_{s0}+k(T_{\text{work}}-T_{\text{room}})$, one can get the stress as a function of temperature as follows:

$$\frac{\sigma_c}{\bar{E}_f} = \left[\frac{3}{8}\frac{(E_{s0}+k(T-T_{\text{room}}))}{\bar{E}_f(1-\upsilon_s^2)}\right]^{2/3} \tag{13}$$

Then one can get the critical strain of the thin film in view of temperature-dependent properties of the substrate and thermal expansion of thin film as follows:

$$\varepsilon_{f_c}(T_{\text{work}},T_{\text{deposited}},T_{\text{room}}) = \left[\frac{3}{8}\frac{(E_{s0}+k(T_{\text{work}}-T_{\text{room}}))}{\bar{E}_f(1-\upsilon_s^2)}\right]^{2/3} - \alpha_f(T_{\text{work}}-T_{\text{deposited}}) \tag{14}$$

The strain of the thin film $\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})$, given by Eq. (5), acts as the prestrain here. When $|\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})| < |\varepsilon_{f_c}(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})|$, the thin film remains flat. When $|\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})| > |\varepsilon_{f_c}(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})|$, the thin film will wrinkle. Due to temperature effects, the critical strain of wrinkling usually cannot be determined directly as usual, and it is more convenient by the critical stress than the critical strain. Temperature will affect the critical strain and the amplitude. Combining Eq. (5) with $A=h_f\sqrt{\varepsilon_{\text{pre}}/\varepsilon_c-1}$ [4,22], one can get

$$A(T_{\text{work}},T_{\text{deposited}},T_{\text{room}}) = h_f\sqrt{\frac{\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})}{\varepsilon_{f_c}(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})} - 1} \tag{15}$$

Figure 5 shows the relation between the critical strain and the temperature. There are three different trends in this figure. When thermal expansion and the temperature-dependent Young's modulus are not considered, the results (the horizontal line in Fig. 5) are free from temperature. When the temperature-dependent Young's modulus is considered, two different trends with temperature can be observed, which mainly depends on the thermal expansion considered or not. Figure 6 shows the relation of the wavelength with temperature. If the temperature-dependent Young's modulus is not considered, the wavelength is not varied with temperature (horizontal line in Fig. 6). The other curve shows that the wavelength is heavily influenced by temperature. The wavelength is a monotone increasing function of temperature. Figure 7 shows the relation of amplitude with temperature. Among these results, the two critical strain models (the critical strain without thermal expan-

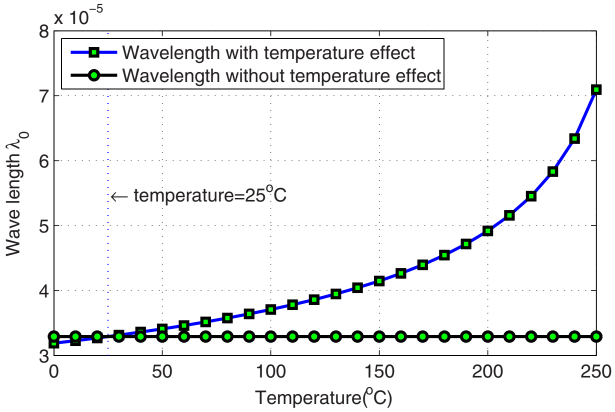

Fig. 6 The relationship of wavelength with temperature

sion, and the critical strain without thermal expansion and temperature-dependent Young's modulus) have the similar trends with the results in Fig. 6. However, the other two results monotonously decrease with temperature.

4.2 Critical Working Temperature for Thermomechanical Buckling. The temperature changes from room temperature to working temperature when flexible electronics are running. Flexible electronics may create wrinkling when the working temperature changes heavily. So the critical working temperature is very important for systemic stability. According to Eqs. (5) and (14), the critical working temperature can be calculated from the following equation:

$$\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})=\varepsilon_{f_c}(T_{\text{work}},T_{\text{deposited}},T_{\text{room}}) \tag{16}$$

When the built-in stress and the external stress acting on the substrate are not considered in the process of deposition, one can get the following equivalent equation:

$$\frac{\bar{E}_s(T_{\text{work}})\cdot h_s\cdot\alpha_s\cdot\Delta T_{wr}-\bar{E}_f\cdot h_f\cdot\alpha_f\cdot\Delta T_{dw}}{\bar{E}_s(T_{\text{work}})\cdot h_s+\bar{E}_f\cdot h_f}=\left[\frac{3}{8}\frac{\bar{E}_s(T_{\text{work}})}{\bar{E}_f}\right]^{2/3}+\alpha_f\cdot\Delta T_{dw} \tag{17}$$

Suppose

$$\text{function}(T_{\text{work}})=\frac{\bar{E}_s(T_{\text{work}})\cdot h_s\cdot\alpha_s\cdot\Delta T_{wr}-\bar{E}_f\cdot h_f\cdot\alpha_f\cdot\Delta T_{dw}}{\bar{E}_s(T_{\text{work}})\cdot h_s+\bar{E}_f\cdot h_f}-\left[\frac{3}{8}\frac{\bar{E}_s(T_{\text{work}})}{\bar{E}_f}\right]^{2/3}-\alpha_f\cdot\Delta T_{dw} \tag{18}$$

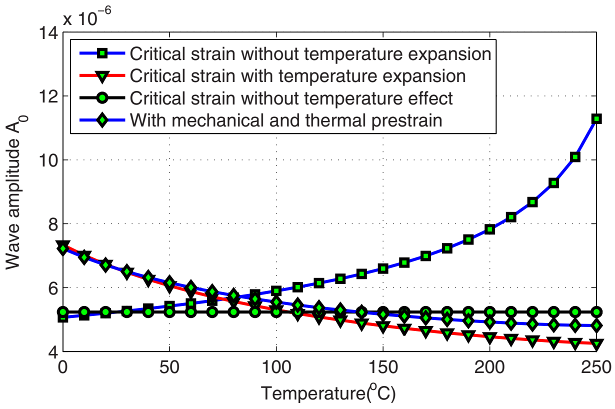

Fig. 7 The relationship of wave amplitude with temperature

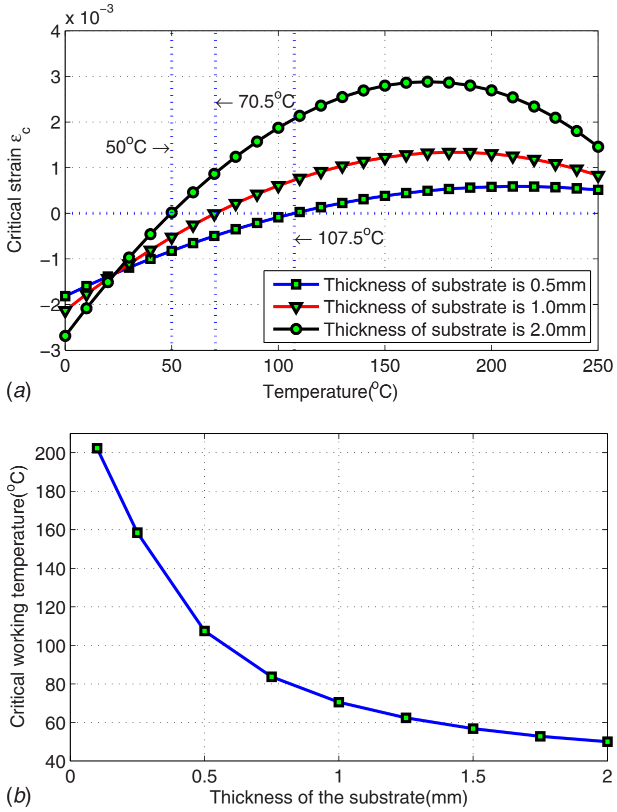

Fig. 8 The critical working temperature with deposit temperature 200°C. (*a*) Calculation of critical strain for three kinds of thickness of substrate. (*b*) The law of the critical working temperature relative to the thickness of the substrate.

When function(T_{work}) > 0, the thin film buckles. If $E_s=E_{s0}+k\cdot\Delta T_{wr}$ is submitted into Eq. (18), where $k=0.008$, one can get the critical temperatures (the critical working temperature for certain deposit temperature) for thermomechanical buckling as follows:

$$T_{\text{work-critical 1}}\approx\begin{cases}50\,^\circ\text{C} & \text{for 2.0 mm: thickness substrate}\\ 70.5\,^\circ\text{C} & \text{for 1.0 mm: thickness substrate}\\ 107.5\,^\circ\text{C} & \text{for 0.5 mm: thickness substrate}\end{cases},\quad \text{for}\quad T_{\text{deposited}}=200\,^\circ\text{C} \tag{19}$$

It can be noted from Eqs. (18) and (19) that the critical working temperature is related with the other two temperatures (room temperature and deposit temperature). The results of Eq. (18) for three special cases of Eq. (19) are shown in Fig. 8(*a*), where the three results hold a similar trend. However, function(T_{work}) are not monotonic. Figure 8(*b*) is the law of the critical working temperature relative to the thickness of the substrate. It can be noted that the critical working temperature is a monotonic function of the thickness of the substrate. The thicker the substrate is, the lower the critical temperature is. When the thickness of the substrate is 2 mm, the critical temperature is 50°C. 50°C usually appears in computers and other electronic devices, so the analysis of the critical working temperature is very important in practical applications. In order to design a structure influenced less from temperature, a feasible method is to optimize the thickness of the substrate.

When the Young's modulus of the substrate is invariable with temperature, one can get the critical working temperature and the critical deposit temperature as follows:

$$T_{\text{work-critical }2}=\frac{(\bar{E}_sh_s+\bar{E}_fh_f)\left(\frac{3}{8}\frac{\bar{E}_s}{\bar{E}_f}\right)^{2/3}+\bar{E}_sh_s\alpha_sT_{\text{room}}+\bar{E}_sh_s\alpha_fT_{\text{deposited}}+2\bar{E}_fh_f\alpha_fT_{\text{deposited}}}{\bar{E}_sh_s\alpha_s+\bar{E}_sh_s\alpha_f+2\bar{E}_fh_f\alpha_f} \qquad (20)$$

$$T_{\text{deposited-critical}}=\left(\frac{3}{8}\frac{\bar{E}_s}{\bar{E}_f}\right)^{2/3}\frac{(h_f\bar{E}_f+h_s\bar{E}_s)}{h_s\bar{E}_s(\alpha_s-\alpha_f)}+T_{\text{room}} \qquad (21)$$

The following can be acquired:

$$T_{\text{work-critical }2}\approx 77.1\,^\circ\text{C for 1.0 mm:}$$

$$\text{thickness substrate and}\quad T_{\text{deposited}}=200\,^\circ\text{C} \qquad (22)$$

From the above, the critical working temperature is related with the deposit temperature, the room temperature, and even the thickness ratio of the film and the substrate. Due to the temperature-dependent Young's modulus, $T_{\text{work-critical }2}$ is 6.6°C larger than $T_{\text{work-critical }1}$.

4.3 Peak Strain in Thin Film. Peak strain $\varepsilon_{\text{peak}}$ is the maximum strains in thin films during deformation. In manufacturing and running, $\varepsilon_{\text{peak}}$ is forbidden to exceed the ultimate strain. In the flat case, $\varepsilon_{\text{peak}}$ is equal to: (1) the strain of the substrate without prestrain; and (2) the applied strain $\varepsilon_{\text{applied}}$ minus $\varepsilon_f(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})$. However, in the wrinkling case, $\varepsilon_{\text{peak}}$ is much less than $\varepsilon_{\text{applied}}$. The peak strain is equal to the sum of the membrane strain ε_{mem} and the strain induced by the buckling geometry, and can be written as [14]

$$\varepsilon_{\text{peak}}=2\sqrt{\varepsilon_{\text{pre}}\varepsilon_c(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})}\frac{(1+\xi)^{1/3}}{\sqrt{1+\varepsilon_{\text{pre}}}} \qquad (23)$$

where $\xi=5\varepsilon_{\text{pre}}\cdot(1+\varepsilon_{\text{pre}})/32$. Figure 9 shows the peak strain, from which one can observe that there are two completely different trends when the temperature effects are considered or not. The main reason lies on the temperature-dependent Young's modulus. The peak strain is a monotone decreasing function with temperature.

If the fracture strain is in the range of $\varepsilon_{\text{fracture}}$, the maximum allowable prestrain is approximately

$$\frac{\varepsilon^2_{\text{fracture}}}{4\varepsilon_c(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})}\left(1+\frac{43}{48}\frac{\varepsilon^2_{\text{fracture}}}{4\varepsilon_c(T_{\text{work}},T_{\text{deposited}},T_{\text{room}})}\right) \qquad (24)$$

which, for the system examined in [14], is ≈37% or almost 20 times larger than $\varepsilon_{\text{fracture}}$. A recent experiment shows that a 7 nm-thick silica film can sustain strains beyond 5%; theoretically, the maximum allowable prestrain is ≈487% or over 97 times larger than $\varepsilon_{\text{fracture}}$. Figure 10 indicates the maximum allowable prestrain, which is a monotone increasing function with temperature.

4.4 Comparison and Discussion. The finite element simulation based is employed to verify the approximate analytical derivation presented in Sec. 4.1. A solution for the wrinkling of a stiff film bounded to a compliant elastic half-space and subjected to uniform axial compression is studied in this section. The mechanical properties of Si and PDMS that use literature value [7,14] are listed as follows: $E_{\text{Si}}=130$ GPa, $E_{\text{PDMS}}=2$ MPa, $\upsilon_{\text{Si}}=0.27$, $\upsilon_{\text{PDMS}}=0.48$, $\alpha_{\text{Si}}=2.7$ ppm/K, and $\alpha_{\text{PDMS}}=16$ ppm/K. A 200-nm-thick gold film is evaporated on a 1-mm-thick prestretched (20%) PDMS membrane. And $T_{\text{room}}=25\,^\circ\text{C}$ and $T_{\text{deposited}}=200\,^\circ\text{C}$ are adopted as room temperature and deposit temperature, respectively.

The aim is to analyze the temperature effects of the film-on-substrate structure such as the wavelength and amplitude. An FEM software, COMSOL, is adopted in our work. Due to the severe mismatch between the thin film and the substrate, there appears to have severe edge effects leading to unconvergence. So the periodic boundary is employed to avoid problems resulting from the edge effect. In order to achieve reasonable accuracy, the size of the FE model is chosen to be big enough to accommodate about ten buckling waves. Even so many wavelengths have been adopted, there may still be comparable errors. The main reason is that the number of the wave is not an integer but a decimal, which result in jumping in the number of the wave. The second difficulty

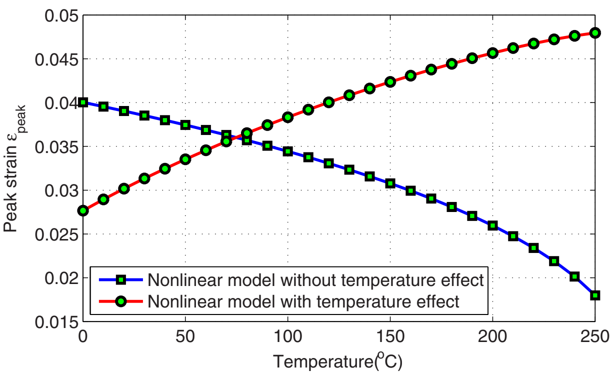

Fig. 9 The peak strains of thin film

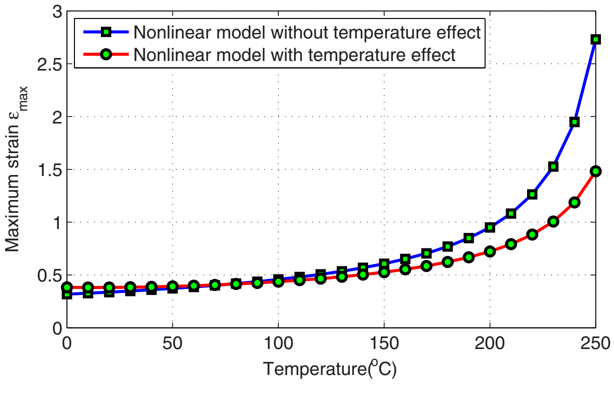

Fig. 10 The maximum allowable prestrain

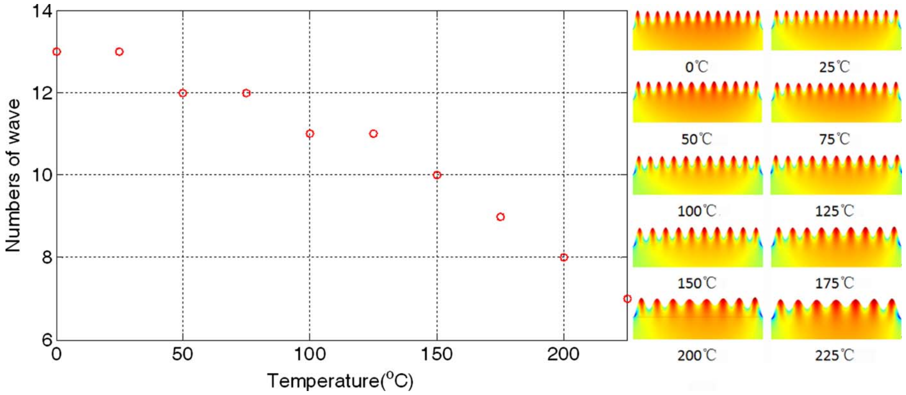

Fig. 11 Different number of waves at different temperatures

is how to model the interface. In order to improve the continuity of the interface, an interface element is adopted between the thin film and the substrate. The corresponding faces of the film and the substrate are adhered onto the interface element. Before simulation, a small disturbance, a sinusoidal force adopted here, is added onto the surface of the film. The force is so small that it cannot influence the final results of the simulation. The different simulations are shown in Fig. 11. The number of waves is from 7 to 13, distributed from 0°C to 250°C. The comparisons of the wavelength with the temperature between the analytical solution and the FE simulation are shown in Fig. 12. There exists a certain degree of difference in the analytical solution and the FE simulation. It partly roots in the imposed periodic boundary so that the number of waves has to be an integer. For example, if the number of waves changes from 10 to 9 suddenly, according to 150°C and 175°C, respectively, there may be a 10% error. Even when the temperature is increased or decreased, the wavelength does not vary, such as 50°C to 75°C, and 100°C to 125°C. However, it can be observed from the contour of Fig. 11 that the internal stress is different from each other. On the other hand, the analytical solution is also an approximate linear model, which may lead to a 5% error [14]. If the extension of Stoney's formula is adopted, the analytical solution should be more accurate by the bending effect of the thin film [17,18]. The trend of the analytical solution tallies closely with that of the FE simulation. The comparison shows that temperature plays a key role in buckling.

5 Conclusion

This work has represented routes to analyze temperature effects of a stiff thin film on a compliant substrate to meet the requirement of extreme mechanical deformations. First, three key temperatures are highlighted in calculating the strain of the thin film, based on which, the temperature effects have been identified. Meanwhile, we studied the nonlinearity induced jointly by the temperature and external load. By tailoring the parameter k, the CTEs mismatch between thin film and substrate is able to be compensated, so that a multilayer structure can be designed to decrease the strain variation with the working temperature. In other words, the temperature effects play important roles in increasing the reliability in circumstances with temperature varying severely. Second, the trends of wavy varying with temperature have been studied. The critical working temperature for buckling has been formulated for several structures with different thicknesses of film. The approximate semi-analytical solution and FE simulation are obtained and compared. The comparison demonstrates that the two-dimensional solution can be applied to predict the buckling wavelength, critical compressive strain.

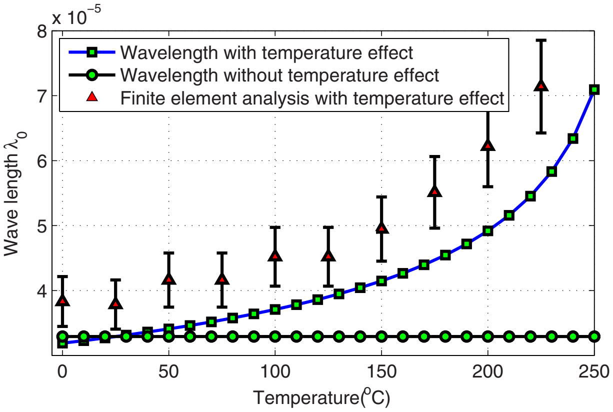

Fig. 12 The analytical solution and the finite element simulation of wavelength with temperature

This work is useful for making flexible and stretchable electronic circuits, including: (1) structural design and thermal management such as selection of substrate; (2) the temperature effect on wrinkling (critical strain, wavelength and wave amplitude); (3) the peak strain considering thermal load; and (4) the critical working temperature for wrinkling.

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