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Thermomechanical criteria for overlay alignment in flexible thin-film electronic circuits

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A simple mechanical model for a deposited film/substrate couple is presented to describe how film deposition at an elevated temperature induces change in the substrate's in-plane dimensions at room temperature. The model provides a quantitative guideline for reducing, or completely eliminating, this elongation, by tailoring the tensile built-in stress in the deposited film. The dimensional stability so achieved is necessary for accurate overlay alignment of photomasks during the fabrication of thin-film electronic circuits. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2161391]

Flexible displays built on metallic or plastic foil substrates are slowly becoming a reality. Many flat panel display companies around the world have manufactured flexible display prototypes using a variety of thin-film technologies.[1] When the substrate's thickness d_s is reduced, its product with Young's modulus Y_s, Y_sd_s, may become comparable to that of the deposited device film, Y_fd_f. (A mechanical theory comparing rigid ($Y_fd_f \ll Y_sd_s$) and compliant substrates ($Y_fd_f \approx Y_sd_s$) has been published previously.)[2] If a film-on-substrate structure with $Y_fd_f \approx Y_sd_s$ is unconstrained, any mismatch strain between the deposited film and the substrate forces the structure to roll to a cylinder with the film facing outward (film under compression) or inward (film under tension). When flattened for circuit fabrication, the work piece now has different dimensions compared to the substrate before film deposition. Hence, in general, the curvature of the work piece and its dimensions change during the fabrication of amorphous silicon thin-film transistors (TFTs) on free-standing Kapton polyimide foils. This change affects the alignment between subsequent device layers with photolithographic masks. Experimental results show that the built-in stress in the TFT's silicon nitride film can be adjusted to improve the alignment accuracy between the gate and the source-drain contacts.[3] Here, we present a thermomechanical model of a single-film-on-substrate structure that provides a quantitative guide to improving this overlay alignment.

Amorphous silicon TFTs are patterned by photolithography at room temperature T_r, whereas the semiconductor stack is deposited at elevated temperature T_d. The substrate is held flat during both steps. Hence the strain ε in the plane of the foil is identical in all directions. Because the film is bonded to the substrate, the strains in the film and the substrate are equal. The stress in the film σ_f and the substrate σ_s is equal biaxial, with $\sigma_s \neq \sigma_f$. The substrate/film couple is allowed to slide freely in its plane. When stresses develop, the resultant force vanishes, namely,

$$\sigma_f d_f + \sigma_s d_s = 0. \tag{1}$$

The substrate is stress free at room temperature before film deposition. This state is set as the reference state, in which the strain is zero, $\varepsilon = 0$. Therefore, within this entire paper, the strains ε in the substrate and the film are identical and their reference is the bare, unstressed substrate at room temperature.

Now we determine the strain ε and the stresses σ_f and σ_s after the temperature has been raised to the deposition temperature T_d. The bare substrate is still stress free, but has expanded by a thermal strain $\varepsilon = \alpha_s(T_d - T_r)$, where α_s is the coefficient of thermal expansion (CTE) of the substrate.

The film grows at T_d with a built-in stress σ_{bi}. This built-in stress is caused by complex atomic processes, which have been under intense study in recent years.[4] We assume that σ_{bi} is constant and known, e.g., from the measurement of the curvature of the substrate.[3] When the only stress in the film is the built-in stress, then $\sigma_f = \sigma_{\mathrm{bi}}$, and according to Eq. (1), the stress in the substrate is $\sigma_s = -\sigma_{\mathrm{bi}} d_f / d_s$. This stress causes an elastic strain in the substrate, given by $-(\sigma_{\mathrm{bi}} d_f / d_s)/Y_s^*$. Here $Y_s^* = Y_s/(1-\nu_s)$ is the biaxial elastic modulus, where ν_s is Poisson's ratio of the substrate. Consequently, at T_d after the film is deposited, the strain in the substrate is the sum of the thermal and elastic strains, namely,

$$\varepsilon(T_d) = \alpha_s \cdot (T_d - T_r) - \frac{\sigma_{\mathrm{bi}} d_f}{Y_s^* d_s}. \tag{2}$$

After the film is deposited and the film/substrate stack has been cooled to room temperature, the stresses in the film σ_f and the substrate σ_s will assume new values. The strain in this state is denoted as $\varepsilon(T_r)$. In the substrate, this strain is entirely due to the stress:

$$\varepsilon(T_r) = \frac{\sigma_s}{Y_s^*}. \tag{3}$$

In the film, the strain deviates from $\varepsilon(T_d)$ due to the change in the temperature and the change in the stress:

$$\varepsilon(T_r) = \varepsilon(T_d) + \alpha_f \cdot (T_r - T_d) + \frac{\sigma_f - \sigma_{\mathrm{bi}}}{Y_f^*}. \tag{4}$$

Here $Y_f^* = Y_f/(1-\nu_f)$ is the biaxial elastic modulus, where Y_f is Young's modulus and ν_f Poisson's ratio of the film.

From Eqs. (1)–(4), one gets

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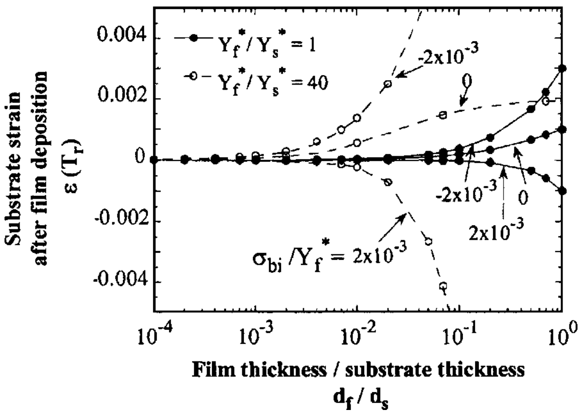

FIG. 1. Substrate strain at room temperature $\varepsilon(T_r)$ after film deposition as a function of film/substrate thickness ratio. The two substrates illustrated are steel with $Y_f^*/Y_s^* \cong 1$ and Kapton with $Y_f^*/Y_s^* \cong 40$, and $(\alpha_s - \alpha_f)(T_d - T_r) = 2 \times 10^{-3}$. The parameter σ_{bi}/Y_f^* represents the built-in stress measured in SiN_x films deposited by plasma enhanced chemical vapor deposition.

$$\varepsilon(T_r) = \frac{(\alpha_s - \alpha_f)\cdot(T_d - T_r)}{1 + \frac{Y_s^* d_s}{Y_f^* d_f}} - \frac{\sigma_{bi} d_f}{Y_s^* d_s}. \tag{5}$$

Equation (5) describes the strain of the substrate at room temperature, after film deposition at elevated temperature. It compares the in-plane dimensions of the substrate after and before film growth, which is a major source of alignment error in photolithography at those two stages. The first term on the right-hand side is the strain caused by the CTE mismatch between the film and the substrate, the second term is the strain resulting from the built-in stress in the film.

Figure 1 depicts the strain in the substrate $\varepsilon(T_r)$ at room temperature after film deposition, calculated from Eq. (5). See Fig. 2 for numerical values of Y, α, and ν. The three different values of σ_{bi}/Y_f^*, -2×10^{-3}, 0, and 2×10^{-3} were chosen to match typical values of built-in stress in silicon nitride films deposited by plasma-enhanced chemical vapor deposition.[3] The value of 2×10^{-3} taken for $(\alpha_s-\alpha_f)(T_d - T_r)$ is approximately the mismatch thermal strain between silicon nitride deposited at 150 °C and steel or Kapton E. For the values of σ_{bi}/Y_f^* used here, the steel substrate is seen to remain dimensionally stable ($\varepsilon=0$) up to $d_f/d_s \cong 0.05$, and for Kapton up to $d_f/d_s \cong 0.001$. It is clear that dimensionally stable flexible electronics can be achieved more easily on steel substrates.

The effect of film built-in stress σ_{bi} on substrate dimension $\varepsilon(T_r)$ is shown in Fig. 2 for 50-μm-thick foil substrates after 0.5-μm-thick silicon nitride film deposition at a temperature of 150 °C. Positive strain (tension) means that at room temperature the substrate is elongated after film growth, negative strain (compression) indicates shrinkage. [Note the opposite signs of σ_f and σ_s in Eq. (1)] $\varepsilon(T_r)$, given by Eq. (5), is plotted as a function of the built-in stress in the film for steel [Fig. 2(a)] and Kapton E [Fig. 2(b)] substrates. As mentioned above, the film/substrate couple is held flat, as required for the alignment procedure. Because the CTE of steel and Kapton are larger than that of silicon nitride, both substrates are elongated after deposition and cooling if no built-in stress is grown into the film. The steel substrate is elongated by ~20 ppm, Kapton by ~500 ppm. When the SiN_x film is grown with built-in *tensile* stress $\varepsilon(T_r)$ is reduced. For Kapton, a built-in stress of 0.37 GPa is seen to

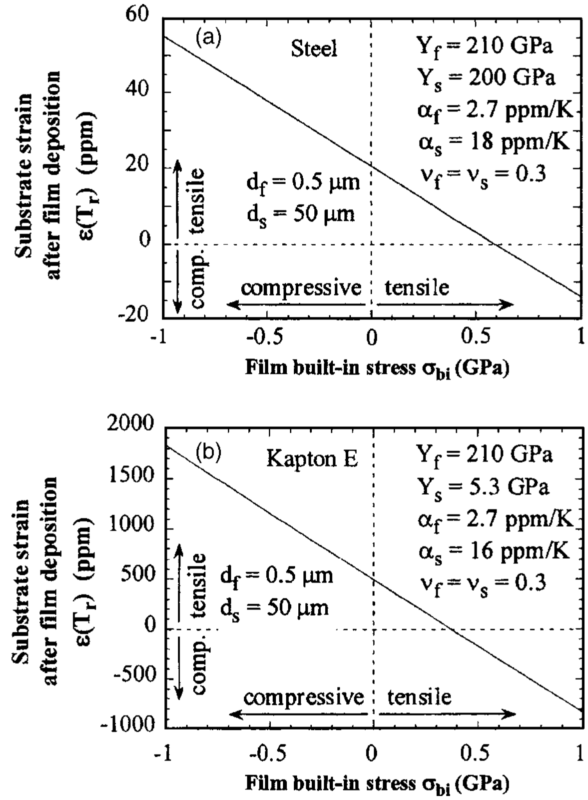

FIG. 2. Substrate strain $\varepsilon(T_r)$ after film deposition as a function of the built-in stress in a 0.5-μm-thick silicon nitride film deposited on 50-μm-thick (a) steel or (b) Kapton E foil substrates at 150 °C.

completely compensate for the CTE mismatch between the substrate and the film, leaving the dimensions of the work piece unchanged. Therefore, by tailoring the built-in stress in the TFT layers one can keep the film/substrate couple dimensionally stable for accurate photomask overlay alignment.

A simple mechanical model for a film-on-substrate structure describes how a film deposited at an elevated temperature induces a change in the in-plane substrate dimensions. The substrate/film couple is allowed to slide freely in its plane during the film growth. When stresses develop, for example due to the built-in stress in the growing film, the resultant force vanishes. The film/substrate couple is cooled after the deposition and kept flat as a necessary condition for alignment. The substrate strain $\varepsilon(T_r)$ is calculated with respect to the stress-free, bare, substrate before the deposition. When a 0.5-μm-thick silicon nitride film is deposited at a temperature of 150 °C on 50-μm-thick steel or Kapton foil, the film causes change in the in-plane dimensions of the substrate. If the silicon nitride film is grown without built-in stress, the elongation is ~20 ppm and ~500 ppm for steel and Kapton foil, respectively. The elongation becomes smaller when the film is grown with built-in tensile stress. By tailoring the built-in stress in the film, one can design the substrate to remain dimensionally stable, thereby eliminating alignment errors.

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