A Finite Element Analysis on the Residual Stresses in a Thin Film/Substrate System

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Summary

A finite element analysis (FEA) is performed to study the edge effects on the residual stress distribution in a thin film/substrate system. The results obtained by the present FEA are benchmarked with those obtained by the existing analytical and computational works.

Introduction

Epitaxy leads to a structurally perfect film and is critically important in the formation of modern device structures [1,2]. However, the film deposition process generates mismatch dislocations, residual stresses and strains leading to the formation of damage in the devices. Residual stresses due to coefficient of thermal expansion (CTE) mismatch in a film strip overlaid on a substrate is studied in the present model. Furthermore, the effects of film-edge and the material properties on the stress transfer in a film/substrate system are examined.

Finite Element Analysis

The model employed in the present work is shown in Figure 1. The dimensions of the film and the substrate in the z-direction are assumed to be infinite. Therefore, a plane strain condition is employed. The dimensions of the systems considered are $t_f = 1$, $l_f = 20$, $t_s = l_s = 50$ units unless stated otherwise. The Young modulus, Poisson's ratio and CTE of each of the material systems are listed in Table 1 [3,4]. The present FEAs are completed using the commercial code ANSYS. Because of symmetry, only half of the film/substrate system needs to be considered; see Figure 1. The boundary conditions employed in the present analysis are given by

$$u_x = 0 \qquad \text{for } -t_s \le y \le t_f, \quad x = 0 \tag{1}$$

$$u_x = u_y = 0 \qquad \text{for } 0 \le x \le l_s, \quad y = -l_s \tag{2}$$

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where u_x and u_y are the displacement in the x- and y-direction, respectively. During the film growth and cooling down process, the following temperature change occurs in the film:

$$\Delta T = T_g - T_r = 88.9^{\circ}K \quad (3)$$

where T_g is the growth temperature, and T_r is the room temperature.

Table 1: Properties of film/substrate system

Type of material	Young's modulus (GPa)	Poisson's ratio	CTE (10^{-6}/K)
Si	163.1	0.28	4.68
$Ge_{0.5}Si_{0.5}$	147.2	0.28	5.39
GaAs	85.5	0.31	5.35

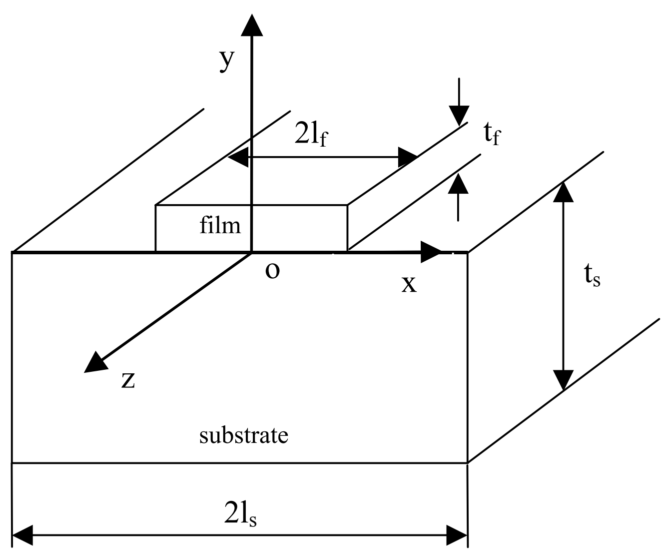

Figure 1: A thin film/substrate system

Results and Discussions

The normalized film stress σ_x/σ_o as a function of the normalized position x/t_f is shown in Figure 2.The biaxial stress σ_o is the stress $\sigma_x(=\sigma_z)$ in the film of a film/substrate system, which is infinitely long in both the x- and z- directions and is given by [5]

$$\sigma_o = \frac{E_f}{\nu_f - 1}\Delta\varepsilon = \frac{E_f}{\nu_f - 1}[\alpha_f \times (T_g - T_r)] \quad (3)$$

where α_f, E_f and ν_f are CTE, Young's modulus and Poisson's ratio of the thin film, respectively. It is shown that the results of the analytic model by Hsueh [5] are quite different from those of the present work for x = 8~18. The results are further compared with the existing analytic models [5~7] in Figure 3. All models predict the increase of σ_x/σ_o (at x = 0 and y = 0) with an increase in l_f. However, σ_x/σ_o approaches asymptotic values at l_f ~30. The results of the present work also agree well with the experimental data [8,9]; see Figure 4. The stress σ_x in the substrate as a function of y is shown in Figure 5. In the region that is close to film (y = -0.5 and -1) σ_x firstly increases, changes dramatically at the edge, and then decreases as x increases. On the other hand, in the regions away from the film (y = -10, -25, and -37.5) stresses gradually decrease as x increases. Figure 6 shows the effect of elastic properties of the film/substrate on σ_x/σ_o. It is concluded that Hsueh's analytical models agrees well with the present FEA when E_s/E_f is relatively high. The discrepancies between the two models are significant when E_s/E_f = 0.2.

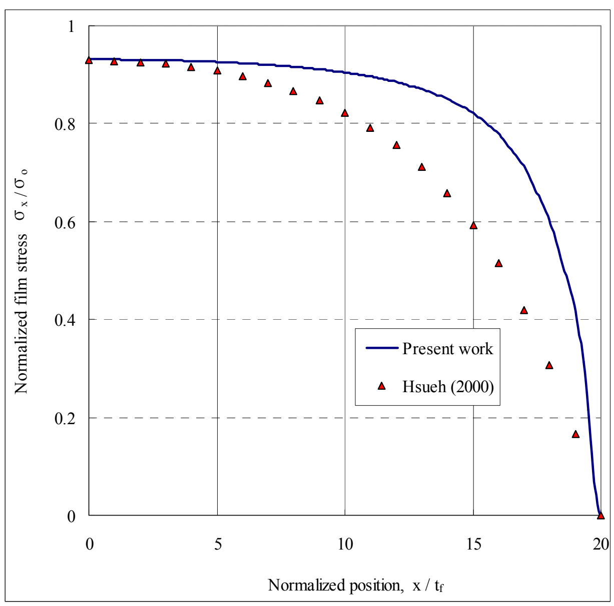

Figure 2: Normalized stress σ_x/σ_o at y = 0.5 as a function of normalized position, x/t_f

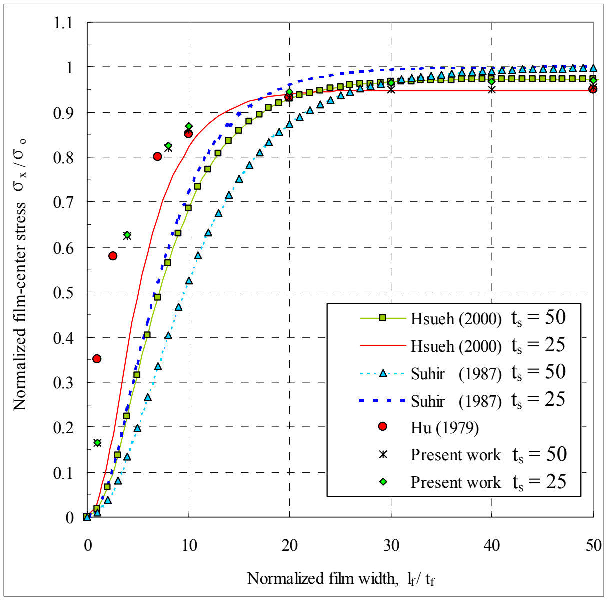

Figure 3: σ_x/σ_o at x = 0 and y = 0.5 as a function of l_f/t_f for t_s = 25 and 50

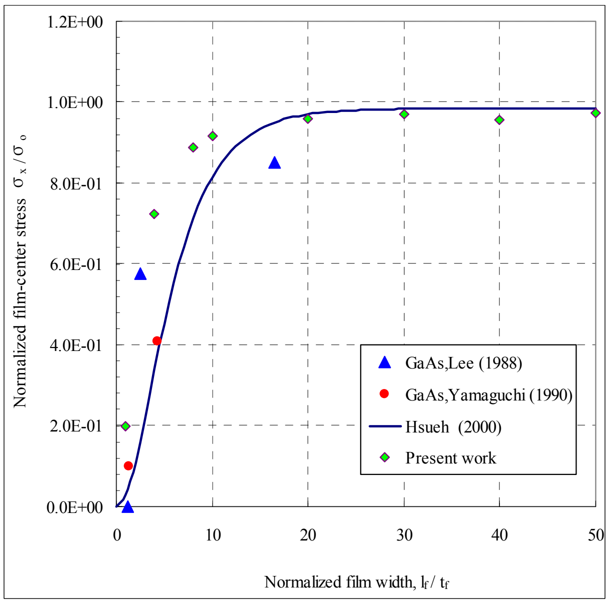

Figure 4: σ_x/σ_o at x = 0 and y = 0.5 as a function of l_f/t_f

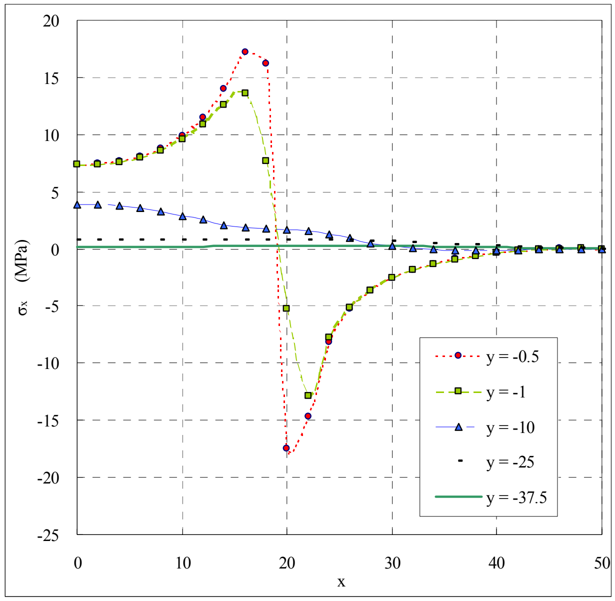

Figure 5: Stress σ_x as a function of x at y = -0.5, -1, -10, -25 and -37.5

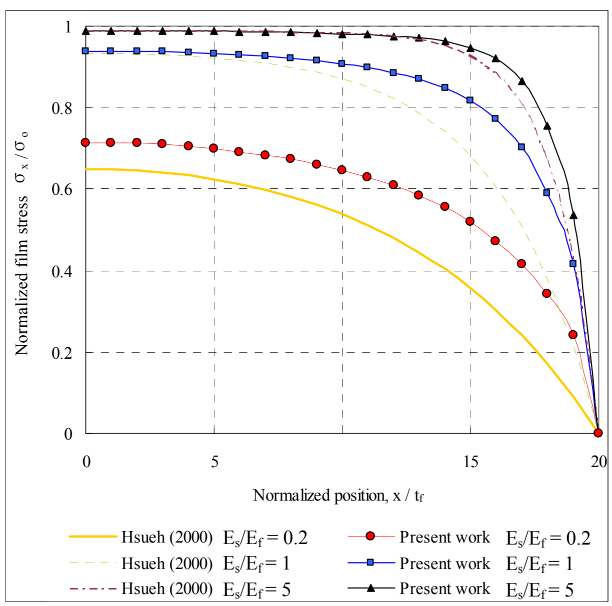

Figure 6: σ_x/σ_o (at y = 0.5) as a function of x/t_f for E_s/E_f = 0.2, 1 and 5 at t_s = 25

Conclusions

The present work investigates the stress distribution in a film/substrate system subjected to a temperature change in the film. It is concluded that (1) the variation of the stresses in the system near the film edges is significant no matter whether the film length and the film thickness are large or small; (2) the normalized stresses σ_x/σ_o of the film are related to film width l_f/t_f and approach asymptotic values as $l_f/t_f \geq 30$; (3) the stresses in the substrate have significant variation only within a certain distance close to the film edge; and (4) the film-edge residual stress distribution depend on both film and substrate properties.

Acknowledgments

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