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Edge and size effects in micro composite structure

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Abstract—Because of the load transfer effect of interface layer, the stress distribution inside the composite structure of film/substrate can be very different from the Timoshenko's model. In this paper, we give the derivation and analysis of such load transfer effect of shear-lag (S-L) model. The micro-structure size (boundary conditions) effect together with interface load transfer effect becomes more and more important as the micro-structure size including the three dimensions of thickness, width and length shrinks. The microstructure size is also responsible for the so-called edge-induced stress. The edge effect and difference of S-L model and Timoshenko model are also demonstrated.

Keywords- Edge/size effects, interface layer, shear-lag model

I. INTRIDUCTION

Edge-induced stress problem has been intensively studied for its importance in the film/substrate composite structure of the micro-electronic components. For this topic, reader should refer to the excellent review article [1] and book by Freund and Suresh[2] for comprehensive reading. Hu [3] derived the stress distribution in a semi-infinite film on an infinite substrate. His derivation uses Flamant solution, which models the substrate as half-space. Therefore, the size effect of composite structure is not incorporated in the model. In Hu's model [3], the interface effect is incorporated in the compatibility condition as a constraint condition between the film and substrate at the interface. Unlike Hu's approach of using the interface effect as constraint condition, Chen and Nelson's shear-lag (S-L) model [4] assumes that there is an interface layer, in which the interfacial shear and normal stresses account for the load/stress transfer between the two material layers. Such interface layer, as for Cu/Si composite is about 1 nm, has been experimentally observed by Murray and Noyan et al [5, 6]. The interface layer itself demonstrates the quite different properties with those in the material layer, for example, in the bending case of the composite structure(which is thin enough to be modeled as Euler-Bernoulli beam) consisting of two layers, the interfacial shear stress is the same magnitude of the normal stress inside material layer. While, the shear stress inside the material layer is so small to be ignored. The interfacial shear stress plays an essential role in load/stress transfer between the material layers. Compared with Hu's model [3], S-L model, which is capable of describing size effect of the composite structure, has been successfully applied to explain the enlarging difference between the experimental data and Timoshenko's model as the micro-structure size reduces. Timoshenko's model [7] does not consider the interfacial effect and geometrically his structure is infinitely long (but finite in width and thickness). In this paper, both interfacial and size effects on the film stress distribution are presented. The stress distribution of S-L model is also compared with that of Timoshenko's model to demonstrate these effects. The significant results difference can be shown between those of S-L model considering both interfacial and size effects and those of Timoshenko's model. So for the recently developed ultra-thin micro-structures, for example, the one used for DNA sequencing (Au/SiNx composite structure) [8], the interfacial and size effects will be the significant and important factors influencing the measurement and performance of those micro-structures.

II. MODEL DEVELOPMENT AND RESULTS DISCUSSION

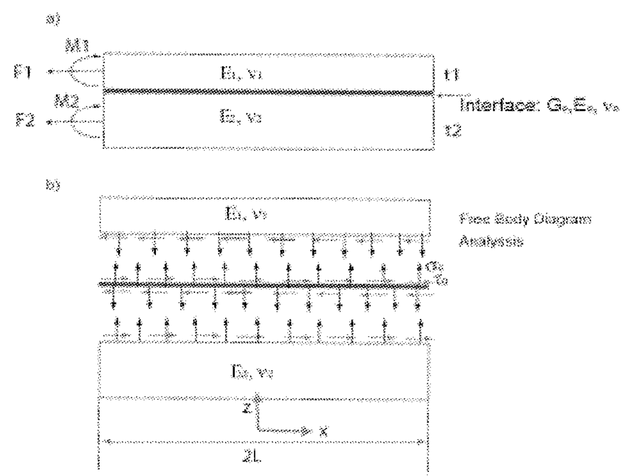

Figure 1. (a): The schematic diagram of bilayered composite structure with an interface under an unknown force couple and moments acting on the two material layers. (b) free body diagram analysis in S-L model on the both material layers and interface layer

We first derive the Timoshenko's model for the bilayer bending case. The equilibrium requires the balance of both force and moment as follows

$$F_1 + F_2 = 0, \tag{1}$$

and

$$M_1 + M_2 = 0. \tag{2}$$

As illustrated in figure 1(a), F_i and M_i (i = 1, 2) are the axial force per unit width and bending moment acting on the different layer. From (1), we have

$$F_1 = P = -F_2. \tag{3}$$

Substitute equation (3) into (2), it shows

$$\frac{P(t_1 + t_2)}{2} = M_1 + M_2. \tag{4}$$

For the longitudinal normal strains of the two layers, they have the following forms

$$\begin{aligned} \frac{du_1(x)}{dx} &= \varepsilon^1 + \frac{P}{E_1 t_1} + \frac{t_1}{2\rho} \\ \frac{du_2(x)}{dx} &= \varepsilon^2 + \frac{P}{E_2 t_2} + \frac{t_2}{2\rho}. \end{aligned} \tag{5}$$

ε^1 and ε^2 are the 'free" strains in the two layers, which can be induced by thermal expansion [5, 7] , dislocation [9] or other sources. Generally speaking, they are the functions of x and z [9]. For simplicity reason, here we treat them as constants as those in thermal expansion case [5, 7]. ρ is the radius of curvature at interface. The relation between the bending moment and curvature is the following

$$M_i = \frac{E_i t_i^3}{12\rho}. \tag{6}$$

Substitute (6) into (4), we have

$$M_i = \frac{6P(t_1 + t_2)}{E_1 t_1^3 + E_2 t_2^3}. \tag{7}$$

The compatibility requires that

$$\varepsilon^1 + \frac{P}{E_1 t_1} + \frac{t_1}{2\rho} = \varepsilon^2 + \frac{P}{E_2 t_2} + \frac{t_2}{2\rho}. \tag{8}$$

In Timoshenko's model, the middle-surface displacements are the only variables of describing the deflection of the composite beam, the equation above physically indicates that there is no relative slip between the two layers. From the equation above, we also derive the expression for P as

$$P = \frac{\varepsilon^2 - \varepsilon^1}{1/E_1 t_1 + 1/E_2 t_2 + 3(t_1 + t_2)^2/(E_1 t_1^3 + E_2 t_2^3)}. \tag{9}$$

The stress inside layer 1 is

$$\sigma_t(x) = \frac{F_1}{t_1} = \frac{P}{t_1}. \tag{10}$$

For the derivation of S-L model, it is extremely lengthy and omitted here. The reader can refer to the papers [4, 5] for the detailed derivation. Here we just give such governing equation for interfacial normal stress, $\sigma_0(x)$, illustrated in figure 1(b), as follows [5]

$$\frac{d^6\sigma_o(x)}{dx^6} - \frac{G_o c}{\eta}\frac{d^4\sigma_o(x)}{dx^4} + \frac{E_o b}{\eta}\frac{d^2\sigma_o(x)}{dx^2} - \frac{E_o G_o(bc - a^2)}{\eta}\sigma_o(x) = 0. \tag{11}$$

And for interfacial shear stress $\tau_0(x)$, the following equation sustains

$$\frac{d^6\tau_o(x)}{dx^6} - \frac{G_o c}{\eta}\frac{d^4\tau_o(x)}{dx^4} + \frac{E_o b}{\eta}\frac{d^2\tau_o(x)}{dx^2} - \frac{E_o G_o(bc - a^2)}{\eta}\tau_o(x) = 0. \tag{12}$$

Here E_0, G_0 and η are the interfacial Young's modulus, shear modulus and thickness, respectively. a, b and c are the followings:

$$\begin{aligned} a &= \frac{1}{2}\left(\frac{t_1}{D_1} - \frac{t_2}{D_2}\right), \\ b &= \frac{1}{D_1} + \frac{1}{D_2}, \\ c &= \frac{1}{3}\left(\frac{t_1^2}{D_1} - \frac{t_2^2}{D_2}\right). \end{aligned} \tag{13}$$

Here t_1 and t_2 are the thicknesses of the two material layers. D_1 and D_2 are bending stiffness of the structure.

Equation (11) is a sixth order ordinary differential equation (ODE) and its solution has the following forms

$$\begin{aligned} \sigma_o(x) = {} & A_1\cosh(\beta_1 x) + A_2\sinh(\beta_1 x) + A_3\cosh(\beta_h x)\cos(\beta_v x) \\ & + A_4\sinh(\beta_h x)\cos(\beta_v x) + A_5\sinh(\beta_h x)\sin(\beta_v x) + A_6\sinh(\beta_h x)\cos(\beta_v x). \end{aligned} \tag{14}$$

Here A_is (i = 1 to 6) are the unknown constants to be determined. B_1, β_h and β_v are the eigenvalues solved from characteristic equation of (11). The symmetry requires $\sigma_0(x)$ to be an even function, therefore (14) changes as

$$\sigma_o(x) = A_1\cosh(\beta_1 x) + A_3\cosh(\beta_h x)\cos(\beta_v x) + A_5\sinh(\beta_h x)\sin(\beta_v x). \tag{15}$$

The three boundary conditions are [5]

$$\begin{aligned} & \int_{-L}^{L} \sigma_o(x)dx = 0, \\ & \frac{d^2\sigma_o(L)}{dx^2} = 0, \\ & \frac{d^4\sigma_o(L)}{dx^4} - \frac{E_o b}{\eta}\sigma_o(L) = 0. \end{aligned} \tag{16}$$

With these three boundary conditions, A_1, A_3 and A_5 can be solved. In practice, for $\tau_0(x)$, it is unnecessary to solve the sixth order ODE of (12). The following equation is more convenient to be used to solve $\tau_0(x)$ once $\sigma_0(x)$ is solved [4, 5]

$$\frac{d^4\sigma_o(x)}{dx^4} - \frac{E_o b}{\eta}\sigma_o(x) = \frac{E_o a}{\eta}\frac{d\ \tau_o(x)}{dx}. \quad (17)$$

The longitudinal normal stress inside layer 1 is as follows

$$\sigma_1(x) = \frac{\int_{-L}^{x}\tau_o(x)dx}{t_1}. \quad (18)$$

The complex sixth order ODEs of S-L model make it hard for us to properly understand the physical nature of interfacial load/stress transfer mechanism as acknowledged by Murray and Noyan [5, 6]. The lap-shear (L-S) model developed by Suhir [10] has the similar sixth order ODEs for interfacial normal and shear stresses and such complex forms of governing equations might be the reasons why those models are not widely accepted and applied to multilayered structures [11]. Mathematically, the complex forms of governing equations are the concomitant results due to the self-equilibrium requirement for interface layer [11]. Physically, the nature of those interface layer models (both S-L and L-S) are a direct and convenient way of modeling the interface as non-ideal or say, damaged interface (DI), which allows the relative slip between the two material layers. As mentioned above, (8) does not allow such slip. In S-L model, the slip is related to parameter Go/η and the middle-surface longitudinal displacements of the two layers [4, 5]. In damaged interface model [12], similar relation also holds and the equivalence of DI and S-L models is proved by Tullini et al [13]. While, such complex and difficult mathematics still troubles us for better understanding of the interfacial influence on the stress transfer between the layers. Based on the previous works [4, 6], the following approximate solution for the longitudinal stress inside layer 1 is derived

$$\sigma_1(x) \approx E_1(\varepsilon^1 - \varepsilon^2)[\frac{\cosh(\beta x)}{\cosh(\beta L)} - 1],$$
$$\beta \approx \sqrt{\frac{G_o}{\eta}(\frac{1}{E_1 t_1} + \frac{1}{E_2 t_2})}. \quad (19)$$

We present our results derived from the equation above in the form of $\sigma_1(x)/\sigma_t(x)$ in order to make the comparison $\sigma_t(x)$ is the longitudinal stress derived by Timoshenko's model in (10). As shown in the derivation, there are no boundary conditions applied in Timoshenko's model as it assumes the beam is infinitely long. Another assumption in Timoshenko's model is worthy to be pointed out that the radius of curvature, ρ, is assumed constant. The two assumptions combined result in that $\sigma_t(x)$ is a constant as far as $\varepsilon^1 - \varepsilon^2$ is a constant..

Figure 2 shows the longitudinal stress distribution inside the layer 1 as the micro-structure length is fixed as 2μm and β varies as $2\times10^6\mathrm{m}^{-1}$, $1\times10^7\mathrm{m}^{-1}$ and $3\times10^7\mathrm{m}^{-1}$. In this case, when β increases, more and more areas inside the micro-structure except the edge parts approach to Timoshenko's value. The physical reason is that as β becomes larger, the interface becomes stronger and allows less slip between the two material layers, which approaches the case of no slip in Timoshenko's model. Figure 3 is the case when β is fixed as 3 × 106m^{-1} and length varies as 2 μm, 4 μm and 6 μm. The size effect is clearly shown. As β, which is directly related to interfacial properties indicated in (19), is fixed, the length variation is solely responsible for the stress distribution. When micro-structure size increases, more and more $\sigma_1(x)$ inside layer 1 approaches to or equals σ_t. In reality, for the two materials bonded to form interface, the properties like elastic constants, roughness and work of adhesion should keep constant if no further processing is applied after the formation of interface. Thus, the interfacial parameters should also keep constant and the size effect will be the dominant factor determining the micro-structure stress distribution. So the application, performance and reliability etc related to the micro-structure stress distribution will be greatly influenced, too.

III. CONCLUSION

Micro-structure size and interfacial properties are the two factors influencing the layers' stress distribution.

Mathematically, the size effect is embodied via boundary conditions and interfacial influence is incorporated in the governing equations. Fundamentally and physically, such size effect is a reflection of the micro-structure increasing interface effect due to the increasing ratio of surface to volume when its size decreases.

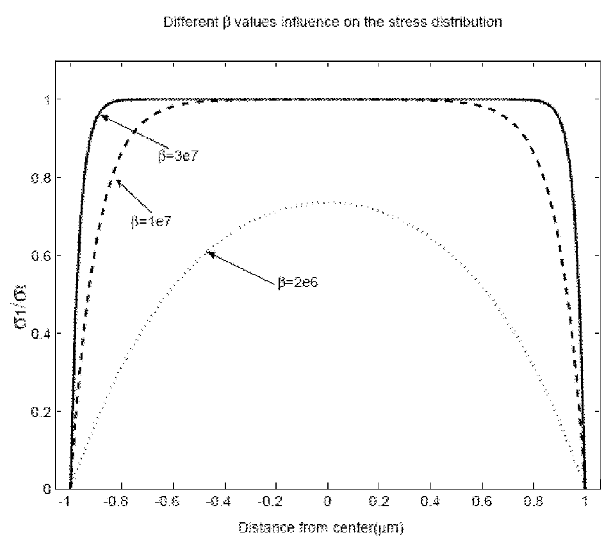

Figure 2. Interfacial effects on the longitudinal stress distribution of layer 1 when the structure length $2L$ is fixed as 2 μm. β varies as $2\times10^6 m^{-1}$, $1\times10^7 m^{-1}$ and $3\times10^7 m^{-1}$.

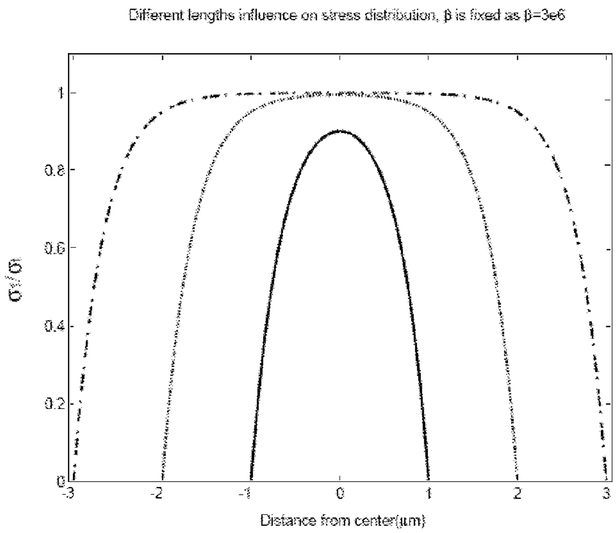

Figure 3. Size effect when the interfacial parameter β is fixed as 3×10^7 m $^{-1}$. The length varies as 2 μm, 4 μm and 6 μm.

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