Modeling of Substrate-Induced Anisotropy in Through-Plane Thermal Behavior of Polymeric Thin Films

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SYNOPSIS

Polymeric thin films are widely used in microelectronic applications for a variety of purposes. These films may possess completely isotropic material properties and yet still exhibit anisotropic effects due to the constraining influence of the substrate coupling into the film behavior via the film Poisson ratio. A theoretical model of this effect on the through-plane thermal properties of isotropic thin films for single layer (thin film rigidly clamped) and bilayer (thin film on substrate, e.g., silicon wafer) has been developed based on the assumption that the material follows Hooke's law in all directions. Finite element analyses using ANSYS 5.0A have also been performed to confirm theoretical results both for single-layer and bilayer models. In the case of Poisson ratio of 0.5, the effective coefficient of thermal expansion (CTE) in the thickness direction can be as high as three times that of the unconstrained film.

Keywords: anisotropy • polymeric thin film • coefficient of thermal expansion (CTE) • Poisson's ratio • through-plane direction • finite element modeling

INTRODUCTION

Various kinds of polymeric thin films are used in microelectronic applications. Examples include spin-coated polymeric thin films as interlayer dielectrics in multichip module-deposited (MCM-D) applications. Bulk material properties of polymers are relatively easy to measure and are usually well known. In contrast, thin film material properties are relatively hard to measure. Several investigations have been performed to characterize the thin film material properties because *in situ* material properties are vital for practical device design. The through-plane thermal properties of thin films are of great interest and have been investigated experimentally.[1,2] These investigations have been performed on polyimide films which have been deposited and subsequently removed totally[1] or partially[2] from a substrate, reducing or eliminating any substrate constraining effect. These investigations have yielded higher coefficient of thermal expansion (CTE) in the through-plane direction than that of the in-plane direction. One possible reason for these deviations is in-plane orientation of molecular chains in spin-coated polymeric thin films. Since most polymeric thin films used in MCM-D structures are deposited on substrates, the substrate constraining effect should also be considered in practical device design. For highly anisotropic polymeric thin films, however, such as BPDA//PPD (biphenyl dianhydride//para-phenylenediamine) polyimide which showed anisotropy of 49.3[1] (the ratio of the through-plane CTE to the in-plane CTE), the molecular orientation effect could be a dominating effect in the thermal behavior of the films. In contrast, for relatively less anisotropic polymeric thin films, such as PMDA//ODA (pyromellitic dianhydride//oxydianiline), BTDA//ODA//MPD (benzophenone-tetracarboxylic dianhydride//oxydianiline/meta-phenylenediamine), and Kapton which showed anisotropy of 3.8,[1] 1.2,[1] and 2.4,[2] respectively, the substrate constraining effect could

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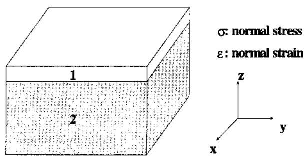

Figure 1. Deposited thin film on a substrate (bilayer).

contribute to the anisotropy in the thermal behavior of the film. The purpose of this article is to quantify through analytical models as well as finite element models the effect of this substrate-induced anisotropy alone based solely on the assumption that the thin film follows Hooke's law and possesses isotropic, bulk material properties. For isotropic films, this effect will dominate the effective anisotropy of the film/substrate system; any inherent material anisotropy will additionally affect the system anisotropy. It is shown that the effect of Poisson's ratio on the constrained thin polymeric films can explain how much the substrate-induced effects contribute to the anisotropy of thermal expansion behavior of films.

Since the anisotropy described here is due to the constraining influence of the substrate coupling into the film behavior via the film Poisson ratio, it should be noted that this anisotropy is separate and distinct from anisotropy due to crystalline morphology in crystallizable thermoplastics.[3] If a crystallizable thin film is deposited on a substrate resulting in subsequent anisotropy in thermal behavior, this anisotropy could result from two causes: the anisotropy due to the presence of a rigid substrate alone (the subject of this article) and the anisotropy caused by phase changes in the polymer.[3]

Theory

If a material follows Hooke's law, the three-dimensional normal strains can be expressed by eq. (1)

$$\varepsilon_x = \frac{\sigma_x}{E} - \frac{\nu}{E}(\sigma_y + \sigma_z)$$

$$\varepsilon_y = \frac{\sigma_y}{E} - \frac{\nu}{E}(\sigma_z + \sigma_x),$$

$$\varepsilon_z = \frac{\sigma_z}{E} - \frac{\nu}{E}(\sigma_x + \sigma_y) \qquad (1)$$

where ε_x, ε_y, ε_z and σ_x, σ_y, σ_z are normal strains and stresses in x, y, and z direction, respectively, E is the Young's modulus, and ν is the Poisson ratio. Equation (1) can be rearranged for normal stresses σ_x, σ_y, and σ_z yielding:

$$\sigma_x = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_x + \nu(\varepsilon_y + \varepsilon_z)]$$

$$\sigma_y = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_y + \nu(\varepsilon_z + \varepsilon_x)]$$

$$\sigma_z = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_z + \nu(\varepsilon_x + \varepsilon_y)]. \qquad (2)$$

Equations (1) and (2) are called the generalized Hooke's law.[4] The through-plane normal strain can be expressed by (Fig. 1):

$$\varepsilon_z = \varepsilon_z^z - \varepsilon_z^p, \qquad (3)$$

where ε_z^z is the through-plane strain induced by through-plane stress, ε_z^p is the through-plane strain induced by in-plane stress, and the minus sign indicates that if the in-plane stress is tensile, the film shrinks in the through-plane direction. The strain ε_z is the strain that is measured when the film thickness changes due to thermal expansion. The through-plane strain induced by in-plane stress ε_z^p can be calculated by setting the through-plane stress σ_z equal to zero (since the top of the film is a free surface) in eq. (2):

$$0 = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_z^p + \nu(\varepsilon_x + \varepsilon_y)]. \qquad (4)$$

If there is no applied stress in any direction other than thermally induced stresses, and if the material is completely isotropic, then:

$$\varepsilon_x = \varepsilon_y = \varepsilon_z^z = \alpha\Delta T, \qquad (5)$$

where α is the CTE, and the ΔT is the temperature change. Equation (4) can be rearranged by substitution of eq. (5) as follows:

$$\varepsilon_z^p = \frac{-\nu}{(1-\nu)}(\varepsilon_x + \varepsilon_y) = \frac{-2\nu}{(1-\nu)}\alpha\Delta T. \qquad (6)$$

Thus, the through-plane normal strain ε_z, can be represented by:

Table I. Parameters Used in Finite Element Modeling (FEM)

	Parameters Used in FEM			Literature Value	
	Free CTE (ppm/°C)	Poisson Ratio	Thickness (μm)		Free CTE (ppm/°C)
Thin film	60	0 ~ 0.49	1 ~ 50	BCB	about 60[5,6]
Substrate	2.3 ~ 60	0.33	500	Si	typical 2.3[7]

Ref. 5: BCB with antioxidant; ref. 6: BCB without antioxidant.

$$\varepsilon_z = \varepsilon_z^t - \varepsilon_z^p = \alpha\Delta T + \frac{2\nu}{(1-\nu)}\alpha\Delta T = \left(\frac{1+\nu}{1-\nu}\right)\alpha\Delta T. \quad (7)$$

Therefore, the effective through-plane CTE ($\alpha_{1z,\text{in situ}}$) of the deposited thin film on a rigid substrate (i.e., a substrate which does not warp out of the plane and has zero CTE) can be represented as a function of the free CTE and Poisson ratio of the film by:

$$\alpha_{1z,\text{in situ}} = \left(\frac{1+\nu}{1-\nu}\right)\alpha = \left(\frac{1+\nu}{1-\nu}\right)\alpha_{1\,\text{free}}, \quad (8)$$

where $\alpha_{1\,\text{free}}$ is the CTE of free standing film, and equal to α in eq. (7).

In the case of a bilayer structure, and neglecting the effect of substrate curvature and assuming that the substrate is isotropic, the thin film structure can also expand or shrink in the in-plane direction by the amount which the substrate expands or contracts in the in-plane direction due to the substrate CTE. The in-plane expansion of the substrate also affects the stress in the thin film. Thus, eq. (5) can be modified for a bilayer by:

$$\varepsilon_{1x} = \varepsilon_{1y} = \varepsilon_{1z}^t = \alpha_1\Delta T - \alpha_2\Delta T$$
$$\varepsilon_{2x} = \varepsilon_{2y} = \varepsilon_{2p} = \alpha_2\Delta T, \quad (9)$$

where 1 denotes the thin film and 2 denotes the substrate. This equation holds as long as the free CTE of the thin film ($\alpha_{1\,\text{free}}$) is greater than or equal to the CTE of substrate (α_2). Equation (6) can be modified for a bilayer by:

$$\varepsilon_{1z}^p = \frac{-\nu}{(1-\nu)}(\varepsilon_{1x} + \varepsilon_{1y}) = \frac{-2\nu}{(1-\nu)}(\alpha_1\Delta T - \alpha_2\Delta T). \quad (10)$$

Thus, the effective through-plane CTE of the thin film on a substrate, such as a Si wafer, can be represented as a function of the free CTE of the thin film, the CTE of the substrate, and the Poisson ratio of the thin film by:

$$\alpha_{1z,\text{in situ}} = \left(\frac{1+\nu}{1-\nu}\right)\alpha_{1\,\text{free}} - \left(\frac{2\nu}{1-\nu}\right)\alpha_2. \quad (11)$$

Equation (11) gives the measured CTE, $\alpha_{1z\text{in situ}}$, as a function of the free film and substrate parameters. It should be noted that the measured CTE can be as high as three times the free standing film value for the case of an incompressible film ($\nu = 0.5$) and low CTE substrate ($\alpha_2 = 0$).

FINITE ELEMENT MODELING

Finite element modeling (FEM) has been performed using three dimensional (3-D) tetrahedron and block elements in ANSYS 5.0A for single and bilayer structures in order to confirm the analytical derivation. The test case modeled using FEM was spin-coated benzocyclobutene (BCB) as the thin film and a Si wafer as the substrate. Parameters used in FEM are listed in Table I. Those parameters are based on previous literature values.[5-7] The free CTE of the thin film (BCB in this FEM) is about 60 ppm/°C based on the literature values for BCB with antioxidant[5] and without antioxidant.[6] The model values for the free CTE of the substrate range from the free CTE of Si (2.3 ppm/°C[7]) to the free CTE of the thin film (60 ppm/°C). Since the maximum Poisson ratio is 0.5, the Poisson ratio chosen for the thin film is ranging from 0 to 0.49. Since this FEM is a general model, it can be applicable to various materials with different material properties. The bottom of the thin film in the single layer and the bottom of the substrate in the bilayer were clamped as boundary conditions so that the bottom cannot be displaced in any direction. Both 3-D tetrahedron elements for cylindrical-shaped single and bilayer structures, as well as 3-D block elements for square-shaped single and bilayer structures, have been modeled. For the cylindrical shaped model, several different radii have been tested ranging from 100 to 5,000 μm, resulting in less than 1% discrepancy of effective through-plane CTE when the radius of the model was larger than 1000 μm. Several different angular sections of the model also have been tested ranging from 7.5° to 360° (i.e., the full circular substrate) resulting in less than 1% discrepancy when the angle of the model was larger than 15°. Figure 2 shows the generated meshed element diagrams for 3-D tetrahedron elements for the cylindrical shaped bilayer FEM. The angle of the model is 15°, the radius is 3000 μm, the thickness of the substrate is 500 μm, and the thickness of the thin film is 30 μm. The FEM results and the theoretical models are well matched to each other and also the FEM results for both 3-D tetrahedron and block elements are matched within 1%. The effective through-plane CTE of the thin film for both single layer and bilayer theoretical models and FEM as a function of the Poisson ratio of the thin film are shown in Figure 3. As seen in Figure 3, the effective through-plane CTE of the film is the same as that of the unconstrained film in the case of Poisson ratio of 0, doubles in the case of Poisson ratio of 0.33, and can be three times higher in the case of Poisson ratio of 0.5. In this figure, the thin film modeled is BCB (CTE of 60 ppm/°C) and the substrate modeled is Si (2.3 ppm/°C). Since the substrate modeled has relatively low value of CTE (2.3 ppm/°C), the effective through-plane CTE values for single and bilayer models are similar. In the case of a substrate having relatively larger values of CTE, the effective through-plane CTE values for the single-layer and

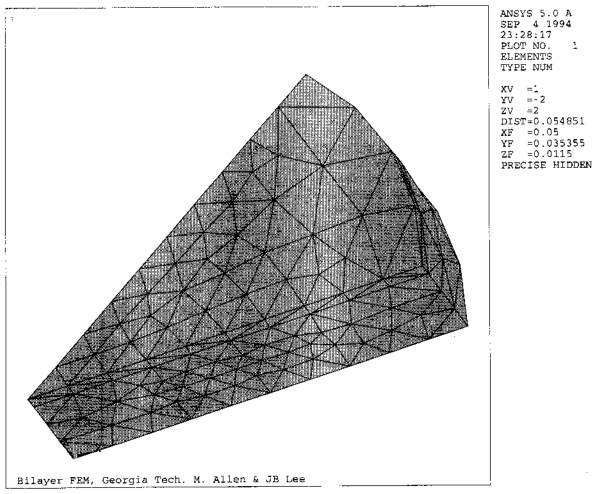

Figure 2. A meshed diagram for bilayer FEM using 3-D tetrahedron elements in ANSYS 5.0A. Fifteen degrees of a cylindrical shape bilayer structure is modeled.

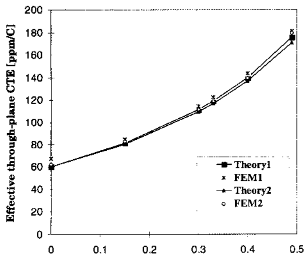

Figure 3. Effective through-plane CTE of the film as a function of the Poisson ratio of the film; 1 denotes the single layer and 2 denotes the bilayer modeling; in this case the thin film is BCB (CTE of 60 ppm/°C) and the substrate is Si (CTE of 2.3 ppm/°C).

bilayer models would no longer be similar, as predicted by eq. (11). The dependence of the effective through-plane CTE of the film as a function of the CTE of the substrate is shown in Figure 4. The thin film can expand or shrink in the in-plane direction by the amount which the substrate expands or contracts in the in-plane direction, resulting in the change of the effective through-plane CTE of the

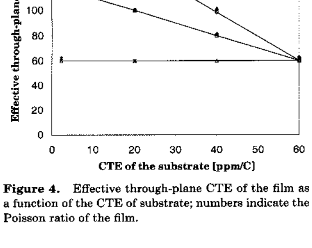

Figure 4. Effective through-plane CTE of the film as a function of the CTE of substrate; numbers indicate the Poisson ratio of the film.

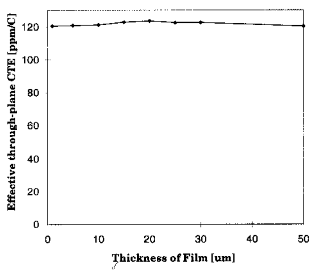

Figure 5. Effective through-plane CTE of the film as a function of the thickness of the film; in the case of thin film Poisson ratio of 0.33, thus the effective through-plane CTE is about double (120 ppm/°C) that of the free film.

film. When the CTE of the substrate is relatively low, the effective through-plane CTE of the film can be determined by the Poisson's ratio of the thin film. As the substrate CTE approaches the free film CTE, the effective through-plane film CTE approaches the free standing film CTE (60 ppm/°C). Figure 5 shows the effective through-plane CTE of the film which is independent of the thickness of the film (to within 1 ~ 2%, the precision of the finite element simulator) when the thickness of the film is very small compared to the length and width of the film (less than 1 : 500). As the thickness of the film increases, the effective through-plane CTE gets smaller and finally, if the thickness approaches the magnitude of the length and width of the film (i.e., no longer the thin film case), the effective through-plane film CTE approaches the free standing film CTE.

CONCLUSIONS

A theoretical model and a finite element model for a completely isotropic polymeric thin film which is deposited on a relatively rigid substrate has been developed and shows substrate-induced effective anisotropy in the thermal expansion behavior of the polymeric thin film, even when the intrinsic film properties are isotropic. Even though the film used in this study is isotropic, it is clear that when anisotropic polymeric thin films are deposited on a substrate, we can expect the effective anisotropy will be affected by intrinsic film anisotropy as well as this substrate-induced effect.

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