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The multilayer-modified Stoney's formula for laminated polymer composites on a silicon substrate

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The thermomechanical behavior of multilayer structures is a subject of perennial interest. Stoney's formula has long been one of the most important tools for understanding thermomechanical stress for single-layered structures like spin-coated polyimides or deposited metal thin film on substrates. In today's microelectronics, however, as multilayer substrates have become widely available, the ''modified version'' of Stoney's formula for multilayer applications is not only useful but necessary. While the majority of reports in the literature have focused on single-layer analysis, in this study, we examined an extended usage of Stoney's formula for multilayer analysis. A simple model, the multilayer-modified Stoney's formula, which predicts the stress contribution of each individual layer is proposed and verified through experiments and numerical analysis. Using various kinds of materials employed in a typical lamination-based multichip module technology, the thermomechanical behavior of the lamination-based multilayer substrates was measured by a laser profilometry during thermal cycling. The measured values were compared with calculated values using the multilayer-modified Stoney's formula. *© 1999 American Institute of Physics.* [S0021-8979(99)05822-3]

I. INTRODUCTION

The thermomechanical behavior of multilayer substrates is a subject of perennial interest. The difference in the coefficient of thermal expansion (CTE) between substrate, polymer, and metal leads to complicated stress fields in multilevel interconnect structures. A vast amount of literature exists on this topic for mechanical structures.[1–5] It is an important reliability and fabrication issue to realize cost-effective and high-reliability electronic devices.

One of the most well-known formulas for thermomechanical stress analysis of thin film on much thicker substrates is Stoney's formula.[6] The formula has long been one of the most important tools for understanding the thermomechanical phenomena in thin films in electronic devices.[7–11] However, while the formula has been conveniently used for the last few decades, the original single-layer assumption of the formula has limited its applications mostly to single-layered structures like spin-coated polyimides or deposited metal thin film on substrates.

In today's microelectronics, as multilayer substrates have become widely available, a ''modified version'' of Stoney's formula has become necessary. One important example of multilayer substrates in today's microelectronics is the lamination-based multichip module (MCM) substrates shown in Fig. 1.[12,13] In the lamination process, a polymeric overlay film is overlaid on a silicon substrate using a polymeric adhesive, so the process involves at least double-layered composite films consisting of the overlay film and adhesive. When it comes to the thermal behavior of metal thin film interconnections not only on silicon wafers[7–11] but also on multilayer substrates, a correct understanding of the thermal behavior of the multilayer substrates themselves is a necessary first step.

While the majority of reports in the literature have focused on single-layer analysis using Stoney's formula, we examined an extended usage of Stoney's formula for multilayer analysis. A few useful closed-form expressions have been developed for the multilayer analysis under certain sets of assumptions and using different approximations, but most of them have rarely been supported by experimental investigation.[1–5] In this study, a simple model, the multilayer-modified Stoney's formula, which predicts the stress contribution of each individual layer was proposed and verified through experiments and numerical analysis. Using various kinds of materials employed in a typical lamination-based MCM–D technology, the thermomechanical behavior of the lamination-based multilayer substrates was measured by a laser profilometry during thermal cycling. The measured values were compared with calculated values using the multilayer-modified Stoney's formula.

II. THEORY

The first theoretical formula for the evaluation of stresses, arising in a thin film prepared on a thick substrate, was suggested by Stoney[6] and is still widely used for stress calculation from the measured deformation of the substrate. This formula can be written as follows:

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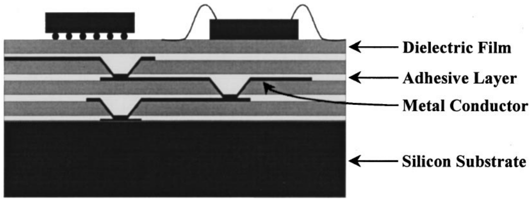

FIG. 1. Schematic diagram of the lamination-based silicon monolithic MCM–D substrates.

$$\sigma_f = \frac{E_s}{6R}\frac{t_s^2}{t_f}, \tag{1}$$

where σ_f is the stress in the film, $E_s = E_s^o/(1-\nu_s^o)$ is the biaxial Young's modulus for the substrate material where E_s^o and ν_s^o are the elastic modulus and the Poisson's ratio of the substrate material, respectively, t_f and t_s are the thickness of the substrate and the film, respectively, and R is the radius of curvature. Note that Stoney's formula allows one to calculate the film stress directly from measured deflections without knowledge of the properties of the film. The factor $1/(1-\nu_s^o)$ did not appear in Stoney's original results but was added in order to properly account for the biaxial stress field as discussed by Kinosita[14] and more recently by Suhir.[1]

Stoney's formula can be used, as long as the mechanical properties of the film material are unavailable. Otherwise the formula

$$\sigma_f = E_f \Delta\alpha \Delta T \tag{2}$$

can be used, where E_f is the biaxial Young's modulus and $\Delta\alpha = \alpha_f - \alpha_s$, where α_f and α_s are the CTEs for the film and substrate, respectively, and ΔT is the temperature excursion.

Meanwhile, the formulas for the curvature, R, can be obtained by equating formulas (1) and (2) as

$$R = \frac{1}{E_f t_f \Delta\alpha}\left(\frac{E_s t_s^2}{6\Delta T}\right). \tag{3}$$

Furthermore, from formula (3) and the geometrical consideration of the curvature, i.e.,

$$B = \frac{L_s^2}{8R} \tag{4}$$

the maximum bow value, B, can be obtained as

$$B = \frac{3L_s^2}{4}\left(\frac{E_f t_f \Delta\alpha \Delta T}{E_s t_s^2}\right), \tag{5}$$

where L_s is the scan length of laser profilometry and is 8 cm in this study.

According to formulas (1) and (5), the level of stress in a film is proportional to the maximum bow value as[15]

$$\sigma_f = \left(\frac{4}{3L_s^2}\right)\left(\frac{E_s t_s}{t_f}\right) \times B. \tag{6}$$

Note that formulas (1) through (6) are only for single-layered structures. For multilayer structures, we suggest the formula, $B = \Sigma B_i$, as the multilayer-modified Stoney's formula, where B is the maximum bow value of a multilayer structure as a whole at a certain temperature, and B_i is the amount of bowing caused by ith layer at the same temperature and is calculated from the original Stoney's formula, formula (1). Formula (6) implies that when multiple thin films are deposited sequentially onto a much thicker substrate, each film causes a fixed amount of bowing to occur irrespective of the order in which the films are deposited, i.e., $B = \Sigma B_i$. From this concept and formula (5), we obtain

$$B = \sum_{i=1}^{n} B_{fi} = \frac{3L_s^2}{4}\sum_{i=1}^{n}\left(\frac{E_{fi}\alpha_{fi}t_{fi}\Delta T_{fi}}{E_s t_s^2}\right), \tag{7}$$

where E_{fi}, α_{fi}, t_{fi} and ΔT_{fi} are the biaxial Young's modulus, coefficient of thermal expansion, thickness, and thermal excursion of the ith-layer film, respectively. If formula (7) is differentiated with respect to temperature and rearranged, the result is the slope of the thermal cycling curve

$$\frac{dB}{dT} = \frac{3L_s^2}{4}\sum_{i=1}^{n}\left(\frac{E_{fi}\alpha_{fi}t_{fi}}{E_s t_s^2}\right). \tag{8}$$

Note that formula (8) is readily applicable for the lamination-based multilayer MCM–D substrates using a la-

TABLE I. Physical constants for the lamination-based MCM–D substrate materials; room temperature property values.

Materials	Symbol	E (GPa)	ν	α (10^{-6}/°C)	t (μm)
Silicon	Si	141	0.22	2.6	525
Coverlay®[a]	E25KH25	0.5	0.37	60	50.8
Ultem®[b] 1000	U17	3.9	0.35	31	17.3
Ultem®[b] 1000 film	U50	3.9	0.35	31	50.8
Kapton®[c] type 100 HN	KH25	2.6	0.34	20	25.4
Kapton®[c] type 200 HN	KH50	2.6	0.34	20	50.8
Kapton®[c] type 300 HN	KH75	2.6	0.34	20	76.2
Kapton®[c] type 500 HN	KH125	2.6	0.34	20	127.0
Apical®[d]	AP25	8.8	0.34	12	25.4

[a] Coverlay® is the registered trademark of Toray, which consists of 25 μm epoxy thermoset and 25 μm Kapton film, hence, the symbol E25KH25.
[b] Ultem® is the registered trademark of GE.
[c] Kapton® is the registered trademark of DuPont.
[d] Apical® is the registered trademark of Allied-Apical.

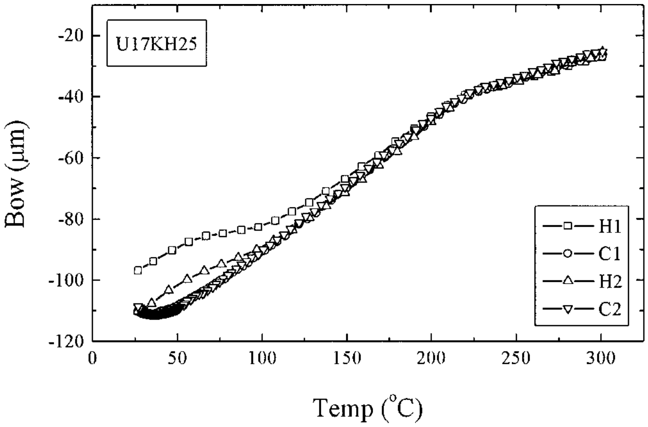

FIG. 2. Thermal behavior of the Ultem/Kapton composite consisting of 17.3 μm Ultem thermoplastic and 25.4 μm Kapton polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

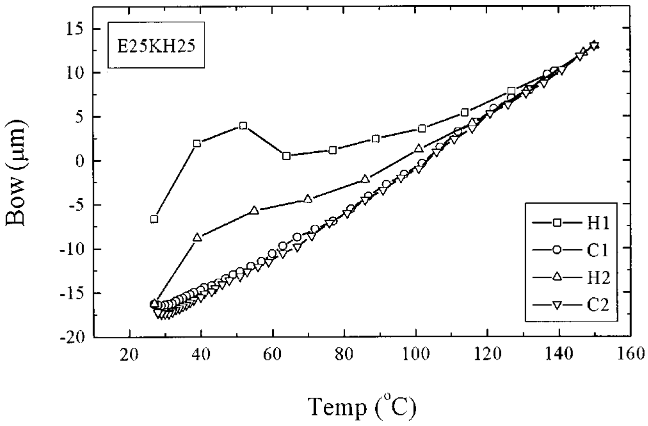

FIG. 3. Thermal behavior of Coverlay film consisting of 25.4 μm epoxy thermoset and 25.4 μm Kapton polyimide film on a silicon substrate. H1 =1st heating cycle, C1=1st cooling cycle, etc.

ser profilometry. Formulas (7) and (8), the multilayer-modified Stoney's formulas, imply that the composite stress and bowing of multilayer structures are due to the individual contribution of each individual layer.

III. EXPERIMENT

Thermal cycling was performed on the laminated substrates composed of various kinds and thickness of adhesives and overlay films (Table I). Stress test structures were fabricated on 10 cm diameter by 525-μm-thick (001) single crystal silicon wafers. Materials used in a typical lamination-based MCM–D substrate were applied to the substrate: 17.3 and 50.8 μm of Ultem 1000 as thermoplastic adhesives, 25.4 μm epoxy as a thermoset adhesive, 25.4, 50.8, 75.2 and 127.0 μm Kapton polyimide films as overlay films, and 25.4 μm Apical polyimide film as an alternative overlay film of Kapton film. Physical constants of the substrate, adhesive polymers and overlay polymers are summarized in Table I. Note that the epoxy thermoset adhesive was provided in Coverlay film consists of the 25.4 μm epoxy thermoset and 25.4 μm Kapton film, and the physical properties of Coverlay film, the epoxy/Kapton composite, were given in Table I.

The composites were laminated to the silicon substrate by heat and pressure at 310 °C/55 psi/60 min for the Ultem thermoplastic adhesive and at 150 °C/50 psi/40 min for the epoxy thermoset adhesive. The maximum bow values were measured during thermal cycling by a laser profilometry.[9] The test structures were thermally cycled between room temperature and 300 °C for the Ultem thermoplastic adhesive, and between room temperature and 150 °C for the epoxy thermoset adhesive. The commercial software MSC/NASTRAN (Ref. 16) was implemented as a simulation tool where plane strain element was utilized for the expression of the composite films. The other conditions were: the number of elements was 800, the maximum aspect ratio was 23.1, boundary conditions were pinned and simply supported, and loading condition was thermal loading.

TABLE II. Comparison of the slopes of the Ultem/Kapton and epoxy/Kapton composites on a silicon substrate.

Composite	Measured μm/°C)	Modified-Stoney (μm/°C)	Numerical (μm/°C)
U17KH25	0.4069	0.4936	0.4170
E25KH25	0.2429	0.2104	0.1918

TABLE III. Comparison of the slopes of the Ultem/Kapton and Ultem/Apical composites on a silicon substrate.

Composite	Measured (μm/°C)	Modified-Stoney (μm/°C)	Numerical (μm/°C)
U17KH25	0.4069	0.4936	0.4170
U17AP25	0.4694	0.5730	0.4869

IV. RESULTS AND DISCUSSION

Figure 2 shows the thermal cycling result for the Ultem/Kapton composite consisting of 17.3 μm Ultem thermoplastic and 25.4 μm Kapton film on a silicon substrate. The maximum bow value at room temperature after fabrication and storage for 48 h was about 110 μm and was due to both intrinsic and thermal stresses.[17,18] The intrinsic stress (or bowing) relaxed during the initial stage of the first heat cycle (H1), then the bow value increased by about 10% on cooling (C1) as a result of the CTE mismatch. Reproducible hysteresis was obtained during further cycles. The curve deflected somewhat above 217 °C reflecting the presence of the Ultem layer whose viscoelastic behavior would be expected to relax the stress above the glass transition temperature, T_g. The T_g of Ultem 1000 is approximately 217 °C, so low elastic modulus and viscoelastic behavior are expected above T_g. A small amount of hysteresis and linear slopes indicate that the deformation was primarily elastic below T_g. No other transitions were observed since the T_g for Kapton is above 400 °C.

Figure 3 shows the thermal cycling result for Coverlay film consisting of 25.4 μm epoxy thermoset and 25.4 μm Kapton film on a silicon substrate. The maximum substrate bow value at room temperature after fabrication and storage for 48 h was about 15 μm. Intrinsic stress relaxed during the first half of the heating cycle (H1), then the bow value increased by almost 80% on cooling (C1) as a result of the CTE mismatch. The intrinsic stress during the first heating cycle was presumably due to moisture absorption,[19] because polymer dielectric materials absorb some level of moisture depending on the relative humidity of storage. Reproducible hysteresis was obtained during further cycles.

Table II compares the measured values of the slope (dB/dT) with the calculated values from the multilayer-modified Stoney's formula and numerical analysis. The cool-

TABLE IV. Comparison of the slopes of the Ultem/Kapton composite with different adhesive thickness on a silicon substrate.

Composite	Measured (μm/°C)	Modified-Stoney (μm/°C)	Numerical (μm/°C)
U17KH25	0.4069	0.4936	0.4170
U50KH25	1.0329	1.0783	0.9703

TABLE V. Comparison of the slopes of the Ultem/Kapton composite with various overlay film thickness on a silicon substrate.

Composite	Measured (μm/°C)	Modified-Stoney (μm/°C)	Numerical (μm/°C)
U50KH25	1.0329	1.0783	0.9703
U50KH50	1.1083	1.2586	1.1561
U50KH75	1.2053	1.4375	1.3526
U50KH125	1.5124	1.7911	1.7745

ing portions of the first cycles (C1) were taken from Figs. 2 and 3 to measure the slope to minimize the intrinsic stress effect. The analysis assumed linear elastic behavior and used room temperature physical property values (Table I). It is generally assumed that the physical properties of polymer materials are constants in a low and small temperature range below the glass transition temperatures, so the slopes were measured in the temperature range below the T_g. Insignificant hysteresis and linear slopes imply predominantly elastic deformation. Table II shows that regardless of adhesive types, whether thermoplastics or thermosets were used as a lamination adhesive, the proposed multilayer-modified Stoney's formula was well applied in the temperature range below T_g.

In all cases using Ultem thermoplastic, as we will see from Tables II through V, the calculated values using the multilayer-modified Stoney's formula as well as the numerical model exceeded by a small amount the measured values with constant deviation. This was mainly due to the dependence of physical properties of Ultem thermoplastic on the measurement environment, or the slightly imperfect elastic behavior of Ultem thermoplastic even below T_g.

Figure 4 shows the thermal cycling result for the Ultem/Apical composite consisting of 17.3 μm Ultem thermoplastic and 25.4 μm Apical film on a silicon substrate, where Apical polyimide film was used as an alternative overlay film of Kapton film. The thermal behavior was much the same as that of the Ultem/Kapton composite on a silicon substrate in Fig. 2. The curve deflected somewhat above 217 °C reflecting the presence of Ultem thermoplastic as did for the Ultem/Kapton composite. The maximum substrate bow value at room temperature after fabrication and storage for 48 h was about 120 μm. Table III summarizes the measured values of the slope (dB/dT) from Figs. 2 and 4. The comparison of the measured values and the calculated values from the multilayer-modified Stoney's formula and numerical analysis indicates that the proposed formula could be applied to the overlay films with different physical properties.

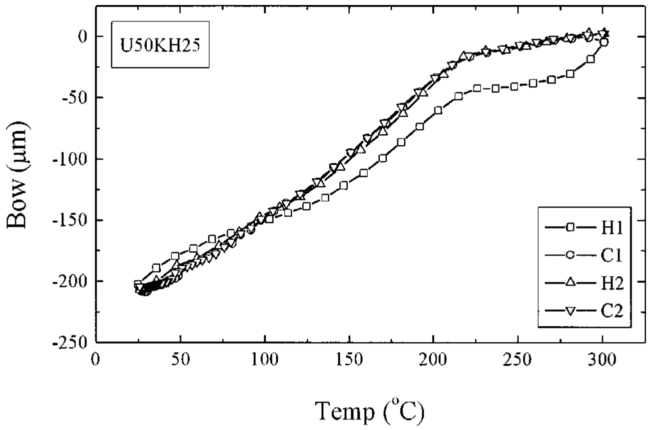

FIG. 5. Thermal behavior of the Ultem/Kapton composite consisting of 50.8 μm Ultem thermoplastic and 25.4 μm Kapton polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

Figure 5 shows the thermal cycling result for the Ultem/Kapton composite consisting of 50.8 μm Ultem thermoplastic and 25.4 μm Kapton film on a silicon substrate. The thermal behavior was much the same as that of 17.3 μm Ultem thermoplastic case in Fig. 2, except the increased size of hysteresis loop at high temperature region above T_g. This is mainly due to the viscoelastic behavior of Ultem thermoplastic above T_g, now that the amount of Ultem thermoplastic was increased from 17.3 to 50.8 μm in Fig. 5. Also, the maximum substrate bow value at room temperature after fabrication and storage for 48 h increased to about 210 μm because of the increased amount of Ultem thermoplastic. Table IV summarizes the measured values of the slope (dB/dT) from Figs. 2 and 5 to see the adhesive thickness

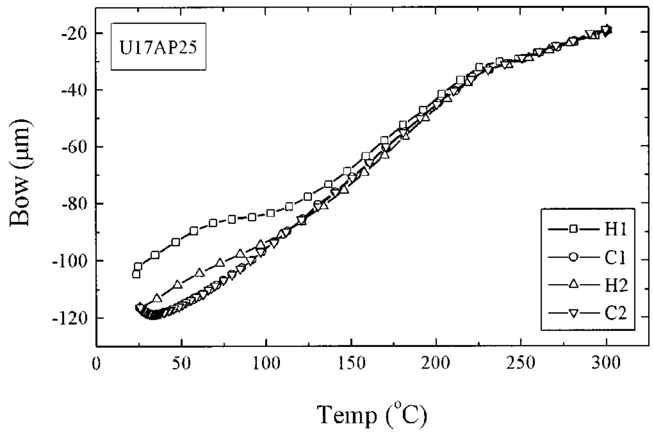

FIG. 4. Thermal behavior of the Ultem/Apical composite consisting of 17.3 μm Ultem thermoplastic and 25.4 μm Apical polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

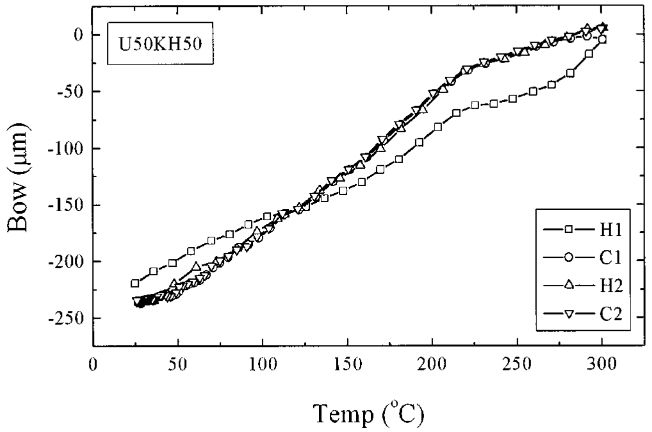

FIG. 6. Thermal behavior of the Ultem/Kapton composite consisting of 50.8 μm Ultem thermoplastic and 50.8 μm Kapton polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

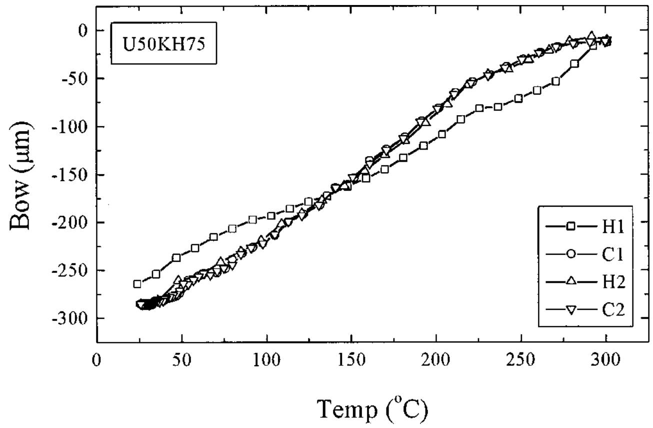

FIG. 7. Thermal behavior of the Ultem/Kapton composite consisting of 50.8 μm Ultem thermoplastic and 76.2 μm Kapton polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

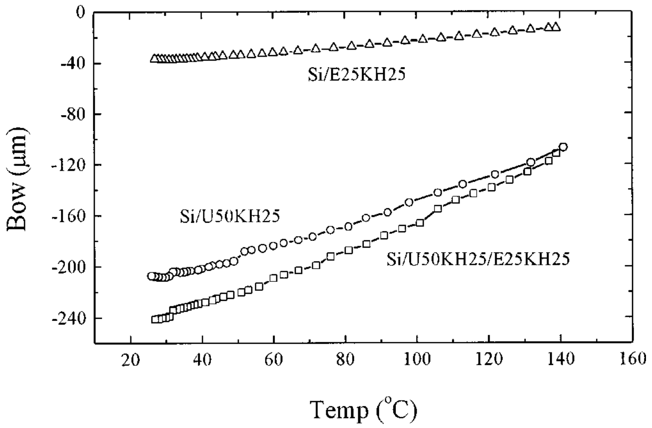

FIG. 9. Thermal behavior of the silicon/Ultem/Kapton (Si/U50KH25), silicon/epoxy/Kapton (Si/E25KH25), and silicon/Ultem/Kapton/epoxy/Kapton (Si/U50KH25/E25KH25) structures. Only the first cooling curves (C1) are presented.

effect. The comparison of the measured values and the calculated values from the multilayer-modified Stoney's formula and numerical analysis suggests that the proposed formula can be used regardless of adhesive thickness.

Figures 5 through 8 show the thermal cycling results for the Ultem/Kapton composite on a silicon substrate with various Kapton film thickness. The 25.4, 50.8, 75.2, and 127.0 μm Kapton films were overlaid using 50.8_μm Ultem adhesive. As summarized in Table V, the agreement was well established between measured and calculated values regardless of the overlay film thickness.

For more realistic modeling of the lamination-based MCM–D substrates, where the fabrication of upper-layer dielectrics must be accomplished at the temperatures below the temperatures of low-layer dielectrics,[13] the Ultem/Kapton composite and Coverlay film were laminated sequentially on a silicon substrate at 310 and 150 °C, respectively. Figure 9 shows the thermal behavior of such a multilayer structure, a silicon/Ultem/Kapton/epoxy/Kapton (Si/U50KH25/E25KH25) structure, where the 50.8 μm Ultem thermoplastic and the 25.4 μm epoxy thermoset were used as lamination adhesives, and the 25.4 μm Kapton films were used as overlay films. Only the first cooling curves are presented in Fig. 9. Figure 9 also shows the thermal behavior of the silicon/Ultem/Kapton (Si/U50KH25) and silicon/epoxy/Kapton (Si/E25KH25) structures. At each temperature, it is obvious that the relation, $B = \Sigma B_i$, was well established, i.e., each individual composite layer contributes independently a fixed amount of bending to the multilayer structure as suggested by the multilayer-modified Stoney's formula.

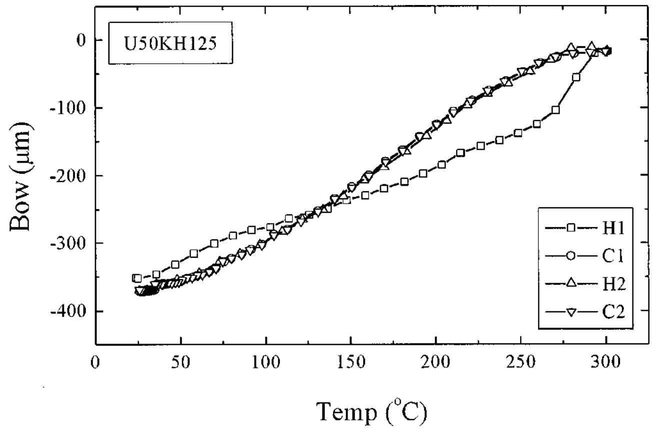

FIG. 8. Thermal behavior of the Ultem/Kapton composite consisting of 50.8 μm Ultem thermoplastic and 127.0 μm Kapton polyimide film on a silicon substrate. H1=1st heating cycle, C1=1st cooling cycle, etc.

Note that one of the key thermomechanical issues during the MCM–D substrate fabrication is substrate bowing, and the other important concern is the thermal stress caused by the CTE mismatch. While the thermal stress causes mechanical failure of films, such as adhesion reduction, contact peel-off, and variations in electrical properties,[11,20] substrate bowing makes the fabrication process difficult, for example, vacuum mounting for handling and substrate sawing after fabrication.[20] It also causes a misregistration problem during photolithography and fine-pitch wire bonding, a stress concentration problem in internal structures such as via,[15] and flip chip bump failure due to repeated thermal loading. The agreement between the experimental results and formulas (7) and (8) suggests that the amount of multilayer substrate bowing can be properly understood when the contribution of each layer is combined through the multilayer-modified Stoney's formula.

V. CONCLUSION

While the majority of reports in the literature have focused on single-layer analysis using the original Stoney's formula, in this study, we examined the extended usage of Stoney's formula for the multilayer analysis. A simple model, the multilayer-modified Stoney's formula, which predicts the stress contribution of each individual layer was proposed and verified through experiments and numerical analysis. Using various kinds of materials employed in a typical lamination-based MCM–D technology, the thermomechanical behavior of the lamination-based multilayer substrates was measured by a laser profilometry during thermal cycling. The agreement between the experimental and calculated results suggests that the amount of multilayer substrate bowing can be correctly described when the contribution of each layer is combined through the multilayer-modified Stoney's formula.

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