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Temperature field in a multilayer assembly affected by a local laser heating

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Abstract—An analytical solution of a three-dimensional heat conduction problem is obtained for a multilayer thin coating–substrate assembly affected by both stationary and moving laser beams. For both cases analytical expressions for the temperature distributions in an assembly are obtained under the assumption that the ratio of coating thickness to laser beam radius is small. The obtained expressions can be employed for analysis of thermal reliability of multilayer assemblies used in microelectronics.

INTRODUCTION

The problem of thermal reliability of microelectronic devices has become important during the last decade due to trends towards large scale integration [1]. Modern electronic devices operate at a high power level. Thus a single chip which represents a multilayer thin coating–substrate assembly dissipates a heat flux of 0.1–1 MW m^{-2} [2]. Since the components of this assembly are made of different materials, such as ceramics, metal, semiconductors, an unavoidable mismatch of the thermal expansion coefficients in the heat generation can cause high thermal stresses and mechanical failure of the coating which make it unable to perform its function. Obviously the reliable operation of electronic equipment can be ensured by timely and precise detection of failure and its mode.

Recently a number of experimental methods that use pulsed laser irradiation of an assembly [3–5], such as photothermal, thermal imaging, thermoacoustic, etc., were employed for detection of failure modes and in particular for testing the integrity of bonding. These methods are based on the fact that the presence of subsurface defects affects the temperature distribution at the surface of an assembly irradiated by the focused laser beam. By comparing the measured temperature distribution and the predicted one on the basis of the solution of the heat conduction problem one can evaluate the performance of an assembly. Thus a solution of the heat conduction problem for a multilayer assembly is also of great interest in the problem of thermal reliability.

In the present investigation we derive an analytical solution of the heat conduction problem in a multilayer assembly based on the expansion of temperature distribution in a small parameter which is equal to the ratio of coating thickness to the laser beam radius. The advantage of this approach is that it leads to simple and explicit expressions for the three-dimensional temperature distribution which can be easily computed and are convenient for practical use. In particular they can be employed for determining the thermal stresses caused by the local laser heating of a multilayer assembly.

THERMAL ANALYSIS

Consider a heat conduction problem for a multilayer thin coating deposited on a substrate heated by laser radiation incident in the normal direction to the coating surface (Fig. 1). Determine the temperature distribution $T(x, y, z, t)$ in a multilayer slab $(-\infty < x < \infty, 0 \leqslant y < \infty, -d < z < \Delta)$ from the solution of the unsteady three-dimensional heat conduction equation with appropriate initial, boundary and continuity conditions for temperature and heat fluxes. Assume that laser radiation is absorbed completely at the surface of an assembly:

$$c_i\rho_i\frac{\partial T_i}{\partial t} = \lambda_i\left(\frac{\partial^2 T_i}{\partial x^2} + \frac{\partial^2 T_i}{\partial y^2} + \frac{\partial^2 T_i}{\partial z^2}\right)$$

$$T_0|_{t=0} = T_i|_{t=0} = \left.\frac{\partial T_i}{\partial y}\right|_{y=0,\infty} = \left.\frac{\partial T_i}{\partial x}\right|_{x=-\infty,+\infty} = \left.\frac{\partial T_0}{\partial z}\right|_{z=-d} = 0 \quad (1)$$

$$\lambda_k\frac{\partial T_k}{\partial z} = \lambda_{k+1}\frac{\partial T_{k+1}}{\partial z}, T_k = T_{k+1} \quad \text{at the interface } z = \sum_{i=1}^{k}\Delta_i \quad (2)$$

$$\lambda_n\frac{\partial T_n}{\partial z} = (1-\chi)q \quad \text{at the surface } z = \Delta = \sum_{i=1}^{n}\Delta_i. \quad (3)$$

Applying cosine Fourier and Laplace transforms to equation (1) we obtain for a substrate

NOMENCLATURE

- c specific heat
- d substrate thickness
- $\bar{d}$ dimensionless substrate thickness
- $erf(x)$ error function
- Fo Fourier number
- $H(x)$ Heaviside's function
- I_0 laser beam intensity
- $J_0(x)$ Bessel function of the first kind of zero order
- k thermal conductivity
- n number of layers in the coating
- p integration variable
- q heat flux absorbed by assembly
- r_b radius of the Gaussian laser beam
- s the Laplace transform parameter with respect to time
- t time
- T space-time distribution of the temperature in the assembly
- $\bar{T}$ Laplace–Fourier transforms of the temperature T
- $\mathbf{v}$ velocity of scanning of a laser beam
- $\bar{\mathbf{v}}$ dimensionless velocity
- x, y, z geometrical coordinates of the point in the assembly
- $\bar{x}, \bar{y}, \bar{z}$ dimensionless coordinates.

Greek symbols
- β_x, β_y the Fourier transform parameters with respect to x and y
- Δ coating thickness
- λ thermal conductivity
- ρ density
- τ dimensionless value of t
- χ reflectivity.

Subscripts
- 0 substrate
- i layer of the coating

Superscripts
- $+, -$ upper and lower surfaces of layer in the coating respectively

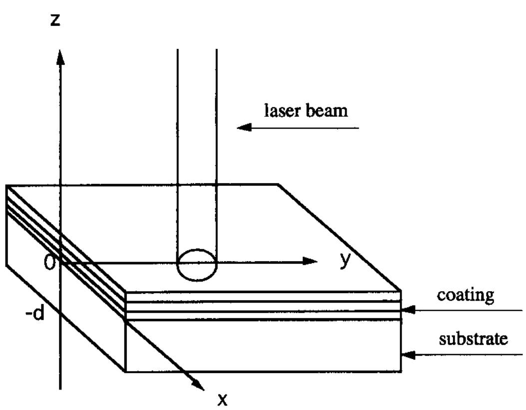

Fig. 1. Scheme of the multilayer assembly.

$$\frac{d^2\bar{T}_0}{dz^2} = \left(\frac{s}{k_0} + \beta_x^2 + \beta_y^2\right)\bar{T}_0 \quad (4)$$

where

$$\bar{T}_0(\beta_x, \beta_y, z, s) = \int_{-\infty}^{\infty} \cos(\beta_x x)\,dx \int_0^{\infty} \cos(\beta_y y)\,dy \times \int_0^{\infty} T_0(x, y, z, t) \exp(-st)\,dt. \quad (5)$$

The solution of equation (4) is

$$\bar{T}_0 = M \exp\left(-\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\,z\right) + N \exp\left(\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\,z\right) \quad (6)$$

where M and N are integration constants which can be determined from the boundary conditions.

Let us consider a limiting case of a thin coating and large Fourier number $Fo(\Delta_i) \equiv k_i t/\Delta_i^2 \gg 1$ which is of particular interest in practice. First of all we obtain the solution of a heat conduction problem for a coating which consists of one layer ($n = 1$). Equation (1) yields

$$\frac{d^2\bar{T}_1}{dz^2} = \left(\frac{s}{k_0} + \beta_x^2 + \beta_y^2\right)\bar{T}_1. \quad (7)$$

Integrating (7) over z we obtain

$$\left(\frac{d\bar{T}_1}{dz}\right)^+ - \left(\frac{d\bar{T}_1}{dz}\right)^- = \left(\frac{s}{k_0} + \beta_x^2 + \beta_y^2\right)\int_0^{\Delta_1} \bar{T}_1\,dz. \quad (8)$$

The dependence of temperature on the axial coordinate z can be represented in the following form:

$$\bar{T}_1 = (\bar{T}_1)^- + \left(\frac{d\bar{T}_1}{dz}\right)^- z + \frac{1}{2}\left(\frac{d^2\bar{T}_1}{dz^2}\right)^- z^2$$

or taking into account equation (7) one can obtain

$$\bar{T}_1 = (\bar{T}_1)^- \left[1 + \frac{1}{2}\left(\frac{s}{k_1} + \beta_x^2 + \beta_y^2\right) z^2\right] + \left(\frac{d\bar{T}_1}{dz}\right)^- z. \quad (9)$$

Using the latter expression for determination of the integral in the right-hand side of (8) one finds that

$$\left(\frac{d\bar{T}_1}{dz}\right)^+ = [1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2)\Delta_1^2]\left(\frac{d\bar{T}_1}{dz}\right)^- + \left(\frac{s}{k_1} + \beta_x^2 + \beta_y^2\right)(\bar{T}_1)^- \Delta_1. \quad (10)$$

In equation (10) the terms of order Δ_1^3 and $s\Delta_1^2/k_1$ can be neglected because of the above assumptions of small layer thickness and large Fourier numbers. In the same approximation one can obtain from (9) the following relation:

$$(\bar{T}_1)^+ = [1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2)\Delta_1^2](\bar{T}_1)^- + \left(\frac{d\bar{T}_1}{dz}\right)^- \Delta_1. \quad (11)$$

Combining the boundary conditions (2) at the interface $z = 0$ with expression (6) yields:

$$(\bar{T}_1)^- = M + N \quad \left(\frac{d\bar{T}_1}{dz}\right)^- = \frac{\lambda_0}{\lambda_1} \frac{d\bar{T}_0}{dz}\bigg|_{z=0} = \frac{\lambda_0}{\lambda_1} \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(M + N). \quad (12)$$

Substituting the latter expressions into (10), (11) we arrive at the following expressions:

$$(\bar{T}_1)^+ = \frac{\lambda_0}{\lambda_1} \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(-M + N)\Delta_1 + [1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2)\Delta_1^2](M + N)$$

$$\left(\frac{d\bar{T}_1}{dz}\right)^+ = [1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2)\Delta_1^2] \times \frac{\lambda_0}{\lambda_1} \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(-M + N) + \left(\frac{s}{k_1} + \beta_x^2 + \beta_y^2\right)(M + N)\Delta_1. \quad (13)$$

Repeating the same procedure for two, three and more layer assemblies one can determine the following general expressions for $(\bar{T}_n)^+$ and $(d\bar{T}_n/dz)^+$ in a multilayer coating composed of n layers with different thermophysical characteristics:

$$(\bar{T}_n)^+ = \alpha_n \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(-M + N) + \delta_n(M + N)$$

$$\left(\frac{d\bar{T}_n}{dz}\right)^+ = a_n \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(-M + N) + (b_n + c_n s)(M + N) \quad (14)$$

where

$$a_n = \frac{\lambda_0}{\lambda_n}\left[1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2) \sum_{i=1}^{n} \Delta_i^2\right] + (\beta_x^2 + \beta_y^2) \times \left\{\sum_{i=2}^{n-1}\left[\left(\prod_{m=i}^{n-1} \frac{\lambda_m}{\lambda_{m+1}}\right)\Delta_i \sum_{k=1}^{i-1} \frac{\lambda_0}{\lambda_k}\Delta_k\right] + \Delta_n \sum_{k=1}^{n-1} \frac{\lambda_0}{\lambda_k}\Delta_k\right\}$$

$$b_n = (\beta_x^2 + \beta_y^2) \sum_{i=1}^{n} \frac{\lambda_i}{\lambda_n}\Delta_i$$

$$c_n = \sum_{i=1}^{n} \frac{1}{k_i} \frac{\lambda_i}{\lambda_n}\Delta_i$$

$$\alpha_n = \sum_{i=1}^{n} \frac{\lambda_0}{\lambda_n}\Delta_i$$

$$\delta_n = 1 + \tfrac{1}{2}(\beta_x^2 + \beta_y^2)\left(\sum_{i=1}^{n} \Delta_i^2 + \sum_{i=2}^{n} \frac{\lambda_1}{\lambda_i}\Delta_1\Delta_i + \frac{\lambda_{n-1}}{\lambda_n}\Delta_{n-1}\Delta_n H(n-3)\right). \quad (15)$$

Let us determine integration constants M and N taking into account (2), (3), (14):

$$M = N \exp\left(-2\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\, d\right)$$

$$a_n \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(-M + N) + (b_n + c_n s)(M + N) = (1 - \chi)\frac{\bar{q}(s, \beta_x, \beta_y)}{\lambda_n}. \quad (16)$$

Solving equations (16) and substituting the determined values of M, N into (6) we obtain the following expression for the temperature distribution:

$$\bar{T}_0(\beta_x, \beta_y, z, s) = \frac{1 - \chi}{\lambda_n}\bar{q}\bar{\theta}_0 \quad (17)$$

where

$$\bar{\theta}_0(\beta_x, \beta_y, z, s) \equiv \cosh\left(\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}(d + z)\right) \times \left[a_n \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2} \sinh\left(\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\, d\right) + (b_n + c_n s)\cosh\left(\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\, d\right)\right]^{-1}. \quad (18)$$

In order to determine the inverse Laplace transform of (18) we employ a decomposition theorem (see, e.g. [6]) whereby the denominator of $\bar{\theta}_0$ is equated to 0:

$$a_n \sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2} \sinh\left[\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\, d\right] + (b_n + c_n s)\cosh\left[\sqrt{\frac{s}{k_0} + \beta_x^2 + \beta_y^2}\, d\right] = 0. \quad (19)$$

To solve this equation we introduce a new variable μ instead of s defined to the following relation

$$\mathrm{i}\sqrt{\frac{s}{k_0}+\beta_x^2+\beta_y^2}d = \mu \quad \mathrm{i}=\sqrt{-1} \tag{20}$$

Substitution of (20) into (19) after some algebra yields the characteristic equation for μ_m

$$\mu_m tg\mu_m = \varepsilon_1 - \varepsilon_2\mu_m^2 \tag{21}$$

where

$$\varepsilon_1 = \frac{d}{a_n}(\beta_x^2+\beta_y^2)\sum_{i=1}^{n}\left(1-\frac{k_0}{k_i}\right)\frac{\lambda_i}{\lambda_n}\Delta_i$$

$$\varepsilon_2 = \frac{1}{da_n}\sum_{i=1}^{n}\frac{k_0}{k_i}\frac{\lambda_i}{\lambda_n}\Delta_i.$$

It should be noted that the characteristic equation (21) is obtained from the solution of the heat conduction problem with boundary conditions of the second kind. The particular form of this equation for $\varepsilon_1 = 0$ and $\varepsilon_2 = 0$ was obtained previously for boundary conditions of the second and third kinds [6, 7]. Thus the characteristic equation derived above generalizes the known characteristic equations.

Equation (21) is a transcendental and therefore it is not feasible to obtain an exact analytical solution. However, the following approximate analytical expression for evaluation of roots μ_m can be used:

$$\mu_0 = \left(\frac{\varepsilon}{1+(4\varepsilon/\pi^2\delta)}\right)^{1/2} H(\varepsilon_1)$$

$$\mu_m = m\pi + \frac{\varepsilon_1}{m\pi+(2/\pi)|\varepsilon_1|} - m\pi\frac{\delta}{2m+(1/\varepsilon_2)} \tag{22}$$

where

$$\varepsilon = \frac{\varepsilon_1}{1+\varepsilon_2} \quad \delta = \frac{1+\tanh(2\varepsilon_2)}{1+\tanh(\varepsilon_2)} \quad m = 1,2,3,\ldots.$$

Evaluation of roots μ_m from expression (22) gives a satisfactory fit with the numerical solution of equation (21) for all values of ε_1 and ε_2 with relative error less than 3%. However, for values ε_1, $\varepsilon_2 \leqslant 0.2$, which are characteristic for thin coatings, the relative error does not exceed 1.5%.

Taking into account equation (21) and applying the decomposition theorem [8] for the calculation of the inverse Laplace transform and formula of the inverse Fourier transform, we determine from (17) the temperature distribution in a substrate

$$\bar{\theta}_0(\beta_x,\beta_y,z,t) = \frac{2k_0}{a_n d}\sum_{m=0}^{\infty}\Phi_m(z) \times \exp\left\{-\left[\frac{\mu_m^2}{d^2}+\beta_x^2+\beta_y^2\right]k_0 t\right\} \tag{23}$$

where

$$\Phi_m(z) \equiv \frac{\cos\mu_m(1+z/d)}{(\sin\mu_m\cos\mu_m+\mu_m)/(\mu_m\cos\mu_m)+2\varepsilon_2\cos\mu_m}. \tag{24}$$

The inverse cosine Fourier transform of $\bar{\theta}_0$ is

$$\theta_0(x,y,z,t) = \int_0^\infty\int_0^\infty \bar{\theta}_0(\beta_x,\beta_y,z,t) \times \cos\beta_x\cos\beta_y\,\mathrm{d}\beta_x\,\mathrm{d}\beta_y. \tag{25}$$

The dependence of the roots μ_m on parameters β_x, β_y given by expression (22) is relatively involved and it is not feasible to integrate (25) analytically.

Consider two special cases of temperature distribution within a multilayer coating–substrate assembly for which one can obtain convenient formulae for practical use.

1. The case of large Fourier numbers $Fo(r_b) = k_0 t/r_b^2 \gg 1$. The analysis of expressions (23) and (25) shows that integration in the vicinity of the point $\beta_x = \beta_y = 0$ constitutes the main contribution to the value of integral (25). Therefore the expression $(\beta_x^2+\beta_y^2)$ in (15) and (22) can be equated to 0. Then from (23) we obtain

$$\theta_0(x,y,z,t) = \frac{\lambda_n}{2\pi\lambda_0 td}\exp\left(-\frac{x^2+y^2}{4k_0 t}\right) \times \sum_0^\infty \Phi_m(z)\exp\left(-\mu_m^2\frac{k_0 t}{d^2}\right). \tag{26}$$

Employing (26) we can obtain a temperature distribution within a multilayer slab caused by the Gaussian laser beam of intensity q moving with a constant velocity $\mathbf{v}$ along the axis OY:

$$q = I_0\exp\left\{-\frac{x^2+(y-\mathbf{v}t)^2}{r_b^2}\right\} \tag{27}$$

Taking into account the boundary condition at $y = 0$ the temperature field can be represented in the form

$$T_0(x,y,z,t) = \frac{(1-\chi)I_0}{\lambda_n}\int_{-\infty}^{\infty}\mathrm{d}x_0\int_0^\infty\mathrm{d}y_0\int_0^\infty\mathrm{d}t_0 \times \exp\left\{-\frac{x_0^2+(y_0-\mathbf{v}t_0)^2}{r_b^2}\right\}[\theta_0(x-x_0,y-y_0,z,t-t_0) + \theta_0(x-x_0,y+y_0,z,t-t_0)]. \tag{28}$$

Substituting (26) in (28) after some algebra we have for the temperature field in a substrate

$$T_0(x,y,z,t) = \frac{(1-\chi)I_0 r_b}{\lambda_0\bar{d}} \times \int_0^\tau\left[\frac{1}{1+4\tau_0}\exp\left(-\frac{\bar{x}^2}{1+4\tau_0}\right)[F(\bar{y},\tau_0) + F(-\bar{y},\tau_0)]\times\sum_{m=0}^{\infty}\Phi_m(z)\exp\left(-\mu_m^2\frac{\tau_0}{\bar{d}^2}\right)\right]\mathrm{d}\tau_0 \tag{29}$$

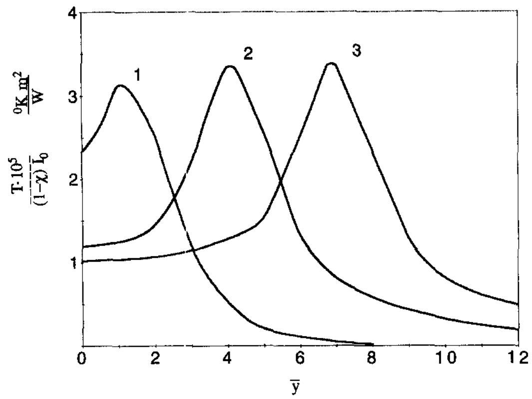

Fig. 2. Temperature profiles at a surface of assembly vs coordinate $\bar{y}$.

where

$$F(\bar{y},\tau_0) = \exp\left(-\frac{[\bar{y}-\bar{\mathbf{v}}(\tau-\tau_0)]^2}{1+4\tau_0}\right) \times \left[1+erf\left(\frac{\bar{y}+4\bar{\mathbf{v}}\tau_0(\tau-\tau_0)}{2\sqrt{\tau_0(1+4\tau_0)}}\right)\right] \quad (30)$$

$$\tau = \frac{k_0 t}{r_b^2} \quad \bar{v} = \frac{v r_b}{k_0} \quad \bar{d} = \frac{d}{r_b} \quad \bar{x} = \frac{x}{r_b} \quad \bar{y} = \frac{y}{r_b}.$$

The temperature field at the surface of the assembly $z = \Delta$ can be determined from (13) and (29) and has a form similar to (29) but with substitution $\bar{\Phi}_m$ instead of Φ_m defined by (24):

$$\bar{\Phi}_m = \frac{\cos\mu_m - (\alpha_n/d)\mu_m \sin\mu_m}{(\sin\mu_m \cos\mu_m + \mu_m)/(\mu_m \cos\mu_m) + 2\varepsilon_2 \cos\mu_m}. \quad (31)$$

Figure 2 shows the temperature profiles at the surface ($x = 0, z = 0$) of an assembly obtained from (29) and (31) for different values of time $t = 1$ s (curve 1), 3 s (2) and 5 s (3) for $\mathbf{v} = 10^{-3}$ m s^{-1}. The assembly consists of substrate (alumina, $d = 2000\mu$) and two layer coating (Pb, $\Delta_1 = 75\mu$ and SiO_2, $\Delta_2 = 10\mu$) which is irradiated by a laser beam of $r_b = 700\mu$. The maximum value of temperature T_m increases as the distance between the laser beam and the edge of a slab $y = 0$ increases and tends to some limiting value T_q depending on the velocity of scanning $\mathbf{v}$. Evaluation of the temperature field for different values of $\mathbf{v}$ reveals that the dependence T_q on $\mathbf{v}$ is weaker than the known one $T_q \propto 1/\sqrt{\mathbf{v}}$ for the moving point heat source ($r_b \to 0$).

2. The stationary ($\mathbf{v} = 0$) laser beam is far from the edge of slab $y = 0$ and therefore the temperature distribution is axially symmetric. Employing the cosine Fourier transform of the function q at $\mathbf{v} = 0$ and substituting expressions (23) and (27) in (17) after some algebra we obtain

$$T_0(x,y,z,t) = \frac{(1-\chi)}{\lambda_n} I_0 r_b^2 d \int_0^\infty \frac{1}{a_n} \times \sum_{m=0}^{\infty} \frac{\Phi_m(z)}{p^2 d^2 + \mu_m^2} \left\{1 - \exp\left[-\left(p^2 + \frac{\mu_m^2}{d^2}\right)k_0 t\right]\right\} \times \exp\left(-\frac{p^2 r_b^2}{4}\right) J_0(pr) p \, dp \quad (32)$$

where $p = \sqrt{\beta_x^2 + \beta_y^2}$. The temperature distribution at the surface of assembly is also expressed by (32) but with the function $\bar{\Phi}_m$ instead of $\Phi_m(z)$.

CONCLUSIONS

Expressions (29) and (32) are obtained for determination of the three-dimensional temperature distributions in a multilayer assembly irradiated by both stationary and moving laser beams. These expressions are represented in a closed analytical form and include only integration and summation. It should be noted that expression (29) can be employed also for determination of the temperature distribution in a region adjacent to the edge ($y = 0$) of a slab. This region is most prone to some modes of failures and therefore the thermal reliability testing of multilayer coating–substrate assemblies near the edges is a problem of great importance in microelectronics.

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