



PERGAMON

International Journal of Solids and Structures 38 (2001) 401–412

INTERNATIONAL JOURNAL OF
SOLIDS and
STRUCTURES

www.elsevier.com/locate/ijsolstr

Boundary element analysis of singular hygrothermal stresses in a bonded viscoelastic thin film

Sang Soon Lee *

Korea University of Technology and Education, School of Mechatronics Engineering, P.O. Box 55, Chonan, Chungnam 330-600, South Korea

Received 10 March 1999; in revised form 9 March 2000

Abstract

This paper deals with the stress singularity induced at the interface corner between the viscoelastic thin film and the rigid substrate subjected to the combined influence of temperature change and moisture absorption. A boundary element analysis is employed to investigate the behavior of interface stresses. The film is assumed to be thermorheologically simple. It is further assumed that moisture effects are analogous to thermal effects. Numerical results are presented for a given viscoelastic model, indicating the singular residual stresses induced during cooling down from the curing temperature, and how they can be altered by subsequent moisture absorption at room temperature. © 2000 Published by Elsevier Science Ltd.

Keywords: Viscoelastic film; Hygrothermal stress; Free-edge stress intensity factor; Boundary element method

1. Introduction

Polymeric films such as polyimide are extensively used in the electronic industry as dielectric insulating layers. Thin films deposited on a substrate can be subjected to residual stresses due to difference in the thermal expansion coefficients. The mismatch in thermal properties between a film and a substrate results in significant thermal stresses upon cooling down from the cure temperature. Thin films absorb moisture from the ambient environment, which induces swelling strains into films. Polyimide films are extremely hygroscopic and absorb large quantities of water. In the presence of water, adhesion of polyimide to substrates such as glass and aluminum tends to fall off rapidly. It is well known that the interface of bonded quarter planes suffers from a stress system in the vicinity of the free surface under external loading (Bogy, 1968). In such a region, two interacting free-surface effects occur, and singular interface stresses can be produced.

Polymeric films in general respond in a viscoelastic manner under loads and their time-dependent behavior is affected by temperature and moisture. Therefore, a time-dependent stress analysis of the

* Fax: +82-417-560-1360.

E-mail address: sslee@kut.ac.kr (S.S. Lee).

bimaterial system is essential in understanding and predicting failure in such systems. The aim of this paper is to study the time-dependent process of interface singular stresses developed in a viscoelastic thin film.

The viscoelastic interface problems have been studied by several investigators. Weitsman (1979) analyzed the mechanical behavior of an epoxy adhesive layer as the adhesive absorbs moisture from the ambient environment. Delale and Erdogan (1981) presented the viscoelastic behavior of an adhesively bonded lap joint. Lee (1998) performed the boundary element analysis of the stress singularity for the viscoelastic adhesive layer under transverse tensile strain. Because, the order of the singularity is material-dependent, it tends to change with time in viscoelastic materials.

In this study, the stress singularity at the interface corner between a substrate and a viscoelastic film subjected to the combined influences of temperature change and moisture absorption is investigated. The substrate is considered rigid as it is much stiffer than the viscoelastic film. The boundary element method (BEM) is employed to investigate the interface stresses in the viscoelastic thin film.

2. The stress singularity

The order of the stress singularity at the interface corner between the substrate and the viscoelastic film can be determined using a method similar to that described by Lee (1998). The substrate is assumed to be rigid. Fig. 1 shows the region near the interface corner between perfectly bonded viscoelastic and rigid quarter planes. The free surfaces are assumed to be traction free.

Polyimide films used in electronic packages are extremely thin, with the thickness rarely exceeding 50 μm . For sufficiently thin films it is possible to neglect the temperature gradient through the thickness and consider the transient case of uniform temperature $T(\mathbf{x}, t) = T(t)$. To simplify the problem, the additional assumptions are made as follows:

1. The film and the substrate are considered to be perfectly bonded, with no cracks or defects.
2. The film is linearly viscoelastic in tension but linearly elastic in bulk.
3. The film is thermorheologically simple. The coefficient of thermal expansion is constant.

In the following, a condition of plane strain is considered. A solution of

$$\nabla^4 \phi(r, \theta; t) = 0 \quad (1)$$

or, equivalently,

$$\nabla^4 \phi(r, \theta; \xi) = 0 \quad (2)$$

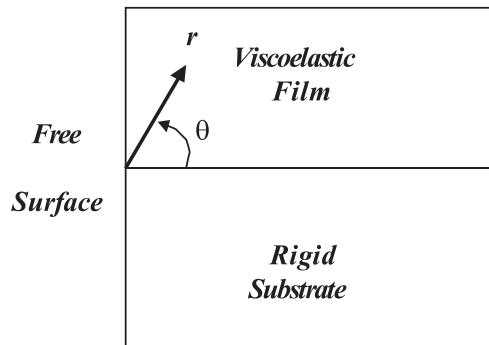


Fig. 1. Region near interface corner between the viscoelastic film and the rigid substrate.

is to be found such that the normal stress, $\sigma_{\theta\theta}$, and shear stress, $\tau_{r\theta}$, vanish along $\theta = \pi/2$. Further the displacements are zero across the common interface line $\theta = 0$. In Eq. (2), ξ is the *reduced time* defined as follows:

$$\xi = \xi(t) = \int_0^t \chi_T(T(\rho)) d\rho, \quad (3)$$

where χ_T is the shift function, a function of temperature history.

For a thin film and rapid rates of moisture diffusion, it is permissible to neglect the moisture gradient through the thickness and consider the transient case of uniform moisture content $m(x, t) = m(t)$. It is further assumed that moisture effects are analogous to thermal effects. Then, Eq. (3) can be rewritten in terms of a temperature and moisture shift function as follows:

$$\xi = \xi(t) = \int_0^t \chi_{Tm}(T(\rho), m(\rho)) d\rho. \quad (4)$$

In this paper, the shift function χ_{Tm} due to temperature T and moisture m is taken to be in the form

$$\chi_{Tm} = \chi_T(T)\chi_m(m). \quad (5)$$

In the present study, a constant temperature change $\Delta TH(t)$ and a constant moisture content $m(t) = m_\infty H(t)$ are considered. Here, m_∞ represents the equilibrium moisture uptake and $H(t)$ is the Heaviside unit step function. These simple fields are considered in order to allow the study to focus on the effects of viscoelastic behavior on the singular stress field. Under the constant temperature change $\Delta TH(t)$ and the constant moisture absorption $m(t) = m_\infty H(t)$, the reduced time ξ of Eq. (4) becomes

$$\xi = \chi_T \chi_m t. \quad (6)$$

The solution of this problem can be facilitated by the Laplace transform. With temperature change $\Delta TH(t)$ and moisture change $m(t) = m_\infty H(t)$ in the film, it is convenient to use the Laplace transform with respect to reduced time ξ , instead of *real time* t . Then, Eq. (2) can be rewritten as follows:

$$\nabla^4 \phi^*(r, \theta; s) = 0, \quad (7)$$

where ϕ^* denotes the Laplace transform of ϕ with respect to ξ and s is the transform parameter.

Using a method similar to that described by Williams (1952), the transformed characteristic equation is obtained as follows (Lee, 1998):

$$\frac{2\lambda^2}{s} - 8s[v^*(s)]^2 + 12v^*(s) - \frac{5}{s} - \left[\frac{3}{s} - 4v^*(s) \right] \cos(\lambda\pi) = 0, \quad (8)$$

where λ is the stress singularity parameter and s is the transform parameter. $v^*(s)$ is the Laplace transform of the viscoelastic Poisson's ratio $v(\xi)$.

The time-dependent behavior of the problem is recovered by inverting Eq. (8) into the time space. The film considered here is characterized by a standard solid tension relaxation modulus and an elastic bulk modulus as follows:

$$\begin{aligned} E(\xi) &= E_0 + E_1 \exp\left(-\frac{\xi}{t^*}\right), \\ K(\xi) &= K_0, \end{aligned} \quad (9)$$

where $E(\xi)$ is a tensile relaxation modulus, $K(\xi)$ is a bulk modulus, E_0 , E_1 and K_0 are positive constants, and t^* is the relaxation time. Introducing Eq. (9) into Eq. (8) and inverting the resulting equation, we have

$$2\lambda^2 - 8A_1(\xi) + 12A_2(\xi) - 5 - [3 - 4A_2(\xi)] \cos(\lambda\pi) = 0, \quad (10)$$

where

$$A_1(\xi) = \frac{1}{36K_0^2} \left[(3K_0 - E_0)^2 + E_1 \left(2E_0 + E_1 - 6K_0 - E_1 \frac{\xi}{t^*} \right) e^{-(\xi/t^*)} \right], \quad (11)$$

$$A_2(\xi) = \frac{3K_0 - [E_0 + E_1 e^{-(\xi/t^*)}]}{6K_0}. \quad (12)$$

The singularity at the interface corner has the form, $r^{1-\lambda}$. Roots of Eq. (10) with $0 < \text{Re}(\lambda) < 1$ are of main interest. The calculation of the zeros of Eq. (10) can be carried out numerically for given values of material properties. For $0 < v(\xi) < 0.5$, there is at most one root λ_1 with $0 < \text{Re}(\lambda) < 1$, and that root is real (Bogy, 1968).

3. Boundary element analysis of the interface stresses

A viscoelastic thin film bonded to an infinitely thick rigid substrate is shown in Fig. 2(a). The free surfaces of Fig. 2(a) are traction-free and the ingress of moisture provides the only loading. The film layer has thickness h and length $2L$. Due to symmetry, only one half of the layer needs to be modeled. Fig. 2(b) represents the two-dimensional plane strain model for analysis of the interface stresses between the film and the substrate. Calculations are performed for $L/h = 25$.

The external boundary conditions in the analysis model are given as follows:

$$\begin{aligned} \sigma_{xx} &= 0, & \tau_{xy} &= 0 \text{ along D-A,} \\ \sigma_{yy} &= 0, & \tau_{xy} &= 0 \text{ along A-B,} \\ \tau_{xy} &= 0, & u_x &= 0 \text{ along B-C,} \\ u_x &= 0, & u_y &= 0 \text{ along C-D.} \end{aligned} \quad (13)$$

A uniform temperature change $\Delta TH(t)$ in the film is equivalent to increasing the tractions by $\gamma(t)n_j$ (Lee and Westmann, 1995), where

$$\gamma(t) = 3K\alpha\Delta TH(t). \quad (14)$$

Here, K is the bulk modulus, n_j are the components of the unit outward normal to the boundary surface, and α is the coefficient of thermal expansion of the viscoelastic film.

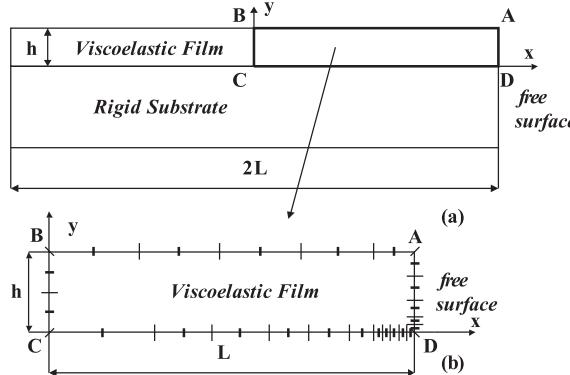


Fig. 2. Boundary element analysis model for determination of interface stresses developed in the viscoelastic film.

In Section 2, it was assumed that moisture effects are analogous to thermal effects. It is further assumed that the coefficient of hygroscopic expansion is constant. Then, Eq. (14) can be extended to the case of a uniform moisture change $\Delta mH(t)$ as follows:

$$\gamma(t) = 3K(\alpha \Delta T + \beta \Delta m)H(t). \quad (15)$$

Here, β is the coefficient of hygroscopic expansion of the viscoelastic film.

With a uniform hygrothermal change in the film, it is convenient to write the boundary integral equations with respect to *reduced time* ξ , instead of *real time* t . Then, the boundary integral equations without any other body forces are written as follows:

$$\begin{aligned} c_{ij}(\mathbf{y})u_j(\mathbf{y}, \xi) + \int_S \left[u_j(\mathbf{y}', \xi)T_{ij}(\mathbf{y}, \mathbf{y}'; 0+) + \int_{0+}^{\xi} u_j(\mathbf{y}', \xi - \xi') \frac{\partial T_{ij}(\mathbf{y}, \mathbf{y}'; \xi')}{\partial \xi'} d\xi' \right] dS(\mathbf{y}') \\ = \int_S \left[t_j(\mathbf{y}', \xi)U_{ij}(\mathbf{y}, \mathbf{y}'; 0+) + \int_{0+}^{\xi} t_j(\mathbf{y}', \xi - \xi') \frac{\partial U_{ij}(\mathbf{y}, \mathbf{y}'; \xi')}{\partial \xi'} d\xi' \right] dS(\mathbf{y}') \\ + \int_S \left[\gamma(\xi)n_jU_{ij}(\mathbf{y}, \mathbf{y}'; 0+) + \int_{0+}^{\xi} \gamma(\xi - \xi')n_j \frac{\partial U_{ij}(\mathbf{y}, \mathbf{y}'; \xi')}{\partial \xi'} d\xi' \right] dS(\mathbf{y}'), \end{aligned} \quad (16)$$

where u_j and t_j represent the displacement and traction, and S is the boundary of the given domain. $c_{ij}(\mathbf{y})$ is dependent only upon the local geometry of the boundary. For \mathbf{y} on a smooth surface, the free term $c_{ij}(\mathbf{y})$ is simply a diagonal matrix $0.5\delta_{ij}$. The viscoelastic fundamental solutions, $U_{ij}(\mathbf{y}, \mathbf{y}'; \xi)$ and $T_{ij}(\mathbf{y}, \mathbf{y}'; \xi)$, can be obtained by applying the elastic–viscoelastic correspondence principle to Kelvin's fundamental solutions of linear elasticity (see Appendix A).

A closed form integration of Eq. (16) is not possible and therefore numerical quadrature must be used. Eq. (16) can be solved in a step-by-step fashion in time by using the modified Simpson's rule for the time integrals and employing the standard BEM for the surface integrals. Eq. (16) can be rewritten in matrix form to give the global system of equations

$$[\mathbf{H}]\{\mathbf{u}\} = [\mathbf{G}]\{\mathbf{t}\} + \{\mathbf{B}_{Tm} + \mathbf{R}\}, \quad (17)$$

where \mathbf{H} and \mathbf{G} are the influence matrices, \mathbf{B}_{Tm} is the known input due to temperature and moisture content change, \mathbf{R} is the hereditary effect due to the viscoelastic history. Solving Eq. (17) under boundary conditions given by Eq. (13) leads to the determination of all boundary displacements and tractions. The solutions are obtained in terms of reduced time ξ . The final solutions are then obtained by converting to real time t .

4. Numerical examples

In order to examine the viscoelastic behavior along the interface line of the film, two examples are tested. The viscoelastic model characterized by Eq. (9) is employed.

4.1. Thermal residual stresses

The film is assumed to be stress-free at a temperature of 300°C, and is cooled suddenly from a cure temperature down to room temperature, i.e., 23°C. Purely dry conditions are assumed. The numerical values used in this example are as follows:

$$\begin{aligned}
E_0 &= 3.0 \times 10^3 \text{ MPa}, & E_1 &= 0.7 \times 10^3 \text{ MPa}, \\
K_0 &= 3.1 \times 10^3 \text{ MPa}, & \chi_T &= 1, & \chi_m &= 1, \\
\alpha &= 3.5 \times 10^{-5}/^\circ\text{C}, & t^* &= 10^2 \text{ min}, \\
\Delta T &= 277^\circ\text{C}.
\end{aligned} \tag{18}$$

The boundary element discretization consisting of 23 line elements was employed. The refined mesh was used near the interface corner. Quadratic shape functions were used to describe both the geometry and functional variations. The solutions were obtained in terms of reduced time. The final solution was then obtained by converting to real time. Viscoelastic stress profiles were plotted along the interface to investigate the nature of stresses. Figs. 3 and 4 show the distribution of normal stress σ_{yy} and shear stress τ_{xy} on the interface at nondimensional times $t/t^* = 0$ and 11.2. The numerical results exhibit the relaxation of interface stresses and large gradients are observed in the vicinity of the free surface. The normal stress σ_{yy} near the free edge is positive indicating that the viscoelastic film is under tension. Such residual tensile stress may cause interface debonding or delamination in the absence of applied external loads.

Fig. 5 shows the variation of the order of the singularity with the real time for the material properties given by Eq. (18). As the value of Poisson's ratio of the viscoelastic film becomes greater with time, the order of the singularity increases with time. For the comparison, it is interesting to consider solutions for two elastic films with elastic moduli $E(0)$ and $E(\infty)$, respectively. At the initial instant of time $t = 0$ the order of the singularity for the viscoelastic film is identical with that for the elastic film with modulus $E(0)$. As $t \rightarrow \infty$, the viscoelastic solution tends to that for the elastic material with elastic modulus $E(\infty)$. To characterize the singularity levels near the free edge, the free-edge stress intensity factor needs to be determined.

The free-edge stress intensity factor is normalized by the quantity $h^{1-\lambda}$, giving it stress unit, as follows:

$$K_{ij} = \lim_{r \rightarrow 0} \left(\frac{r}{h} \right)^{1-\lambda} \sigma_{ij}(r, \theta; t) \big|_{\theta=0}. \tag{19}$$

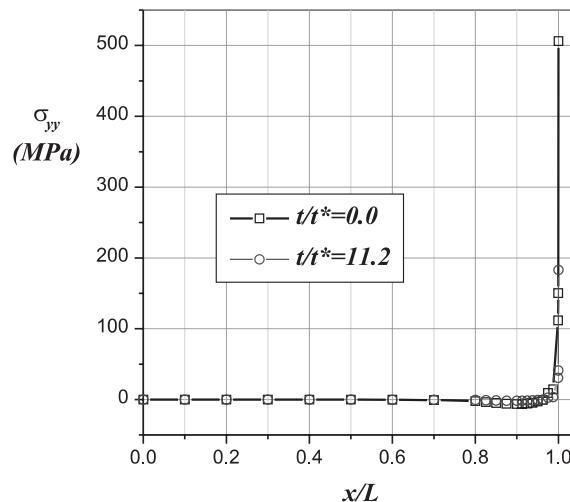


Fig. 3. Distribution of interface normal stresses at times $t/t^* = 0$ and 11.2.

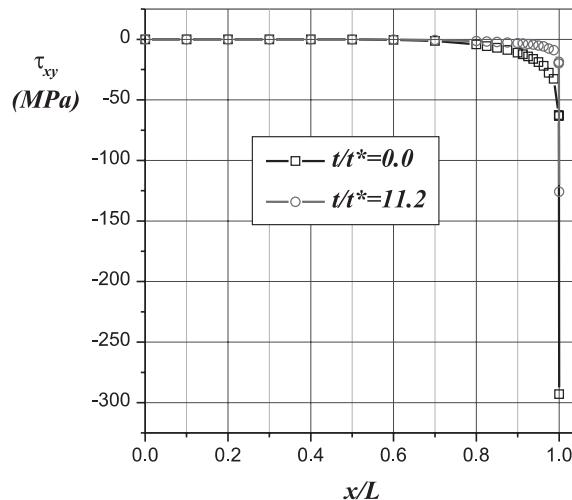
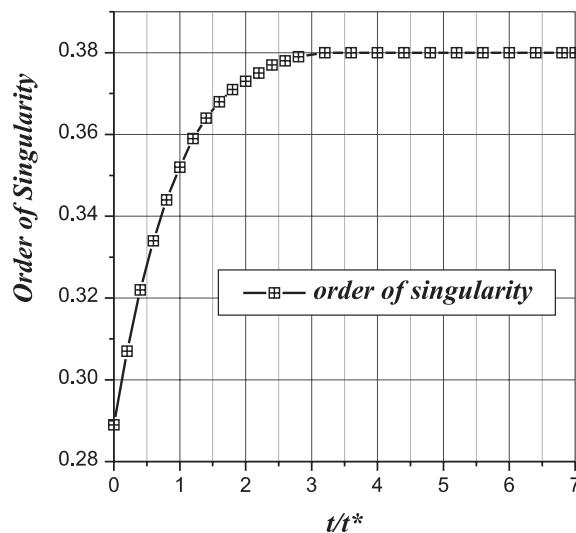
Fig. 4. Distribution of interface shear stresses at times $t/t^* = 0$ and 11.2.

Fig. 5. Variation of the order of the singularity.

Fig. 6 shows the variation of the free-edge stress intensity factor. It is shown that the free-edge stress intensity factor is relaxed with time while the order of the singularity increase with time. It is unclear how these competing effects will affect edge debonding or delamination.

4.2. Thermal residual and moisture-induced stresses

The film on a substrate is assumed to be stress-free at 300°C, and is cooled suddenly to room temperature (23°C). Then, the moisture concentration in the film is increased to the maximum saturation level. Moisture diffusion is assumed to take place almost instantaneously. The numerical values used in this example are as follows:

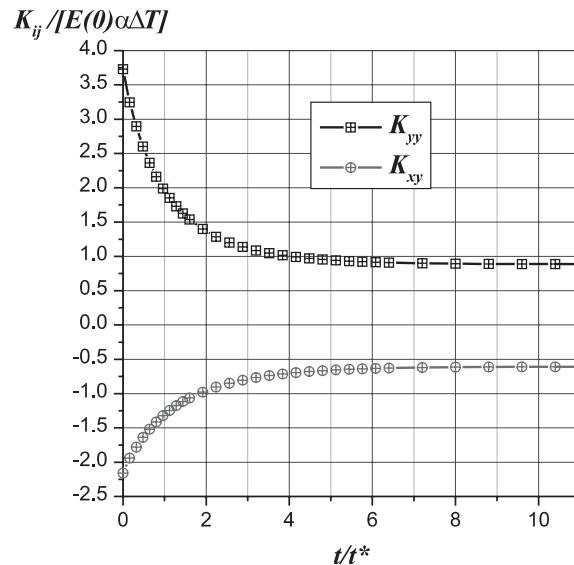
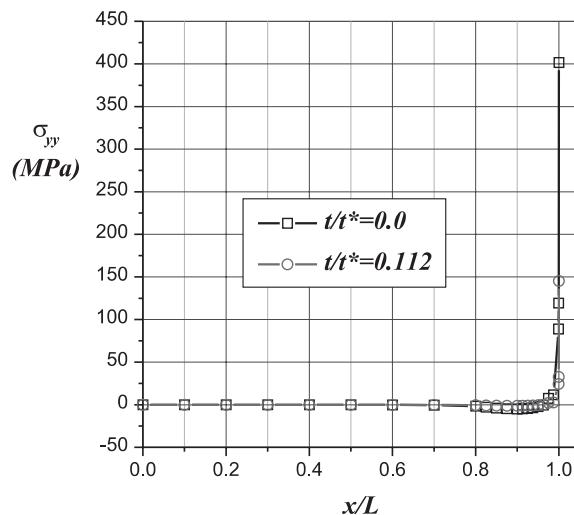


Fig. 6. Variation of the free-edge stress intensity factors.

Fig. 7. Distribution of interface normal stresses at times $t/t^* = 0$ and 0.112.

$$\begin{aligned}
 E_0 &= 3.0 \times 10^3 \text{ MPa}, & E_1 &= 0.7 \times 10^3 \text{ MPa}, \\
 K_0 &= 3.1 \times 10^3 \text{ MPa}, & \chi_T &= 1, & \chi_m &= 10^2, \\
 \alpha &= 3.5 \times 10^{-5} /^\circ\text{C}, & \beta &= 0.001 / \text{wt.\%} & t^* &= 10^2 \text{ min}, \\
 \Delta T &= 277^\circ\text{C}, & \Delta m &= 2\% \text{ (by weight).}
 \end{aligned} \tag{20}$$

Figs. 7 and 8 show the interface stress state in the film when exposed to the above stated conditions. Note that after moisture enters the film, the residual stresses induced by the thermal change (Figs. 3 and 4) are relieved. Fig. 9 shows the variation of the order of the singularity with the real time. In the presence of moisture, the order of the singularity increases faster. The free-edge stress intensity factor is shown in Fig. 10. It is obvious that moisture tends to reduce the magnitude of free-edge stress intensity factors, which can be viewed as an advantage of moisture absorption. However, it also reduces the critical free-edge stress intensity factor (K_{ij})_c by weakening the joint. Experimental evaluation is required to assess a trade-off between the advantageous and deleterious effects of moisture.

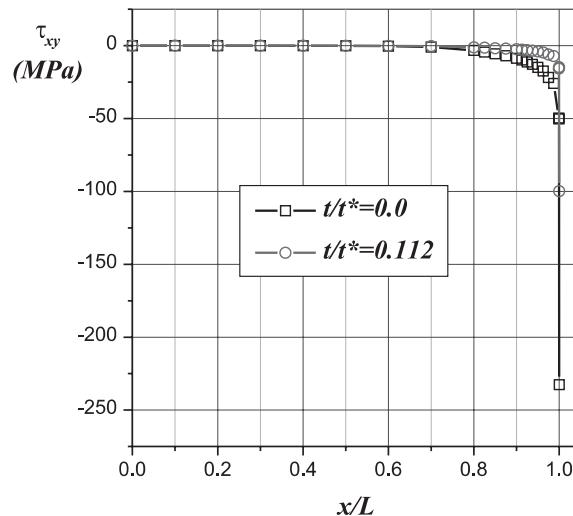


Fig. 8. Distribution of interface shear stresses at times $t/t^* = 0$ and 0.112.

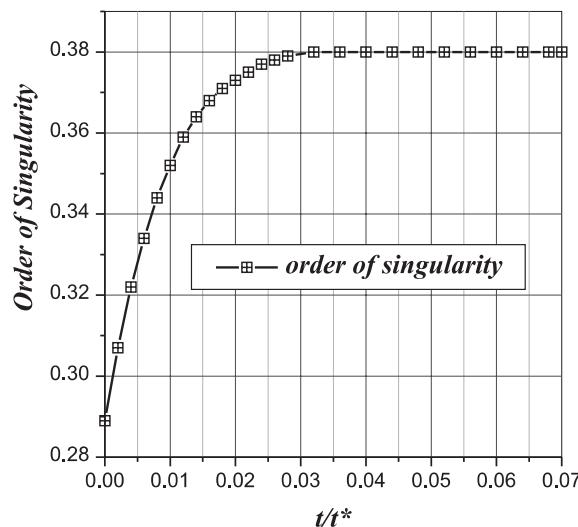


Fig. 9. Variation of the order of the singularity.

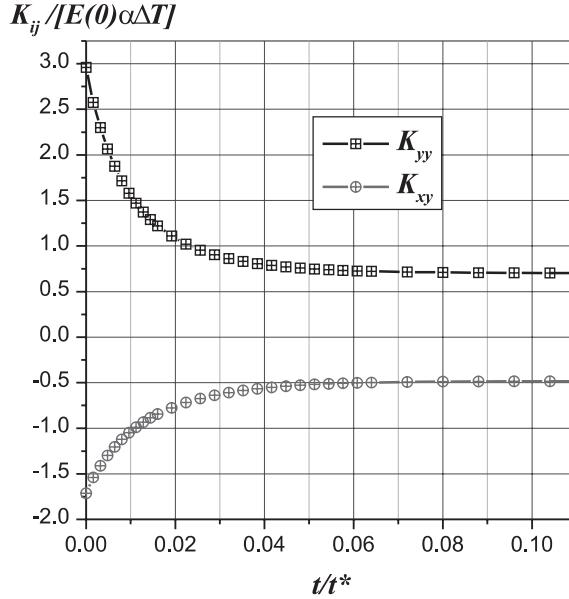


Fig. 10. Variation of the free-edge stress intensity factors.

5. Conclusions

The stress singularity induced at the interface corner between the viscoelastic film and the rigid substrate due to temperature and moisture change has been investigated. The interface stresses have been calculated using BEM. Thermal residual stresses developed during cooling from an elevated cure temperature down to room temperature are large enough to initiate edge cracks or delamination to relieve the residual stresses. Saturating the film with moisture tends to reduce the residual stresses induced by temperature change, since the film expands with absorbed moisture. The order of the singularity has been obtained numerically for a given viscoelastic model. In the presence of moisture, the order of the singularity increases faster. There is competition between the relaxation of the stress intensity and the increase of the order of the singularity. All results reported here are for $L/h = 25$, and are applicable to films that behave as if they are semi-infinite.

Appendix A. Viscoelastic fundamental solutions

The fundamental solutions for the viscoelastic model given by Eq. (9) are obtained as follows:

$$U_{ij}(\mathbf{y}, \mathbf{y}'; \xi) = \left[B_1(\xi) \ln \left(\frac{1}{r} \right) \delta_{ij} + B_2(\xi) r_{,i} r_{,j} \right] H(\xi), \quad (\text{A.1})$$

$$T_{ij}(\mathbf{y}, \mathbf{y}'; \xi) = -\frac{1}{r} \left\{ \begin{array}{l} B_3(\xi) [r_{,k} n_k(\mathbf{y}') \delta_{ij} + n_i(\mathbf{y}') r_{,j} - n_j(\mathbf{y}') r_{,i}] \\ + B_4(\xi) r_{,k} n_k(\mathbf{y}') r_{,i} r_{,j} \end{array} \right\} H(\xi), \quad (\text{A.2})$$

where $r_{,i} = \frac{r_i}{r}$,

$$r_i = y'_i - y_i \quad r^2 = r_i r_i, \quad (\text{A.3})$$

y_i is the coordinate of field point and y'_i is the coordinate of integration point.

$B_i(\xi)$ ($i = 1, 2, 3, 4$) are given as follows:

$$B_1(\xi) = \frac{M_1}{4\pi} (a_1 + a_2 e^{-c_3 \xi} + a_3 e^{-c_4 \xi}), \quad (\text{A.4})$$

$$B_2(\xi) = \frac{M_2}{4\pi} (a_4 + a_5 e^{-c_3 \xi} + a_6 e^{-c_4 \xi}), \quad (\text{A.5})$$

$$B_3(\xi) = \frac{M_3}{2\pi} (a_7 + a_8 e^{-c_4 \xi}), \quad (\text{A.6})$$

$$B_4(\xi) = \frac{M_4}{\pi} (a_9 + a_{10} e^{-c_4 \xi}), \quad (\text{A.7})$$

where

$$M_1 = \frac{[3K_0 + 2E(0)][9K_0 - E(0)]}{3K_0 E(0)[3K_0 + E(0)]}, \quad (\text{A.8})$$

$$M_2 = \frac{9K_0 - E(0)}{E(0)[3K_0 + E(0)]}, \quad (\text{A.9})$$

$$M_3 = \frac{E(0)}{3K_0 + E(0)}, \quad (\text{A.10})$$

$$M_4 = \frac{3K_0}{3K_0 + E(0)}, \quad (\text{A.11})$$

$$c_1 = \frac{3K_0 + 2E_0}{3K_0 + 2E(0)} \frac{1}{t^*}, \quad (\text{A.12})$$

$$c_2 = \frac{9K_0 - E_0}{9K_0 - E(0)} \frac{1}{t^*}, \quad (\text{A.13})$$

$$c_3 = \frac{E_0}{E(0)} \frac{1}{t^*}, \quad (\text{A.14})$$

$$c_4 = \frac{3K_0 + E_0}{3K_0 + E(0)} \frac{1}{t^*}, \quad (\text{A.15})$$

$$c_5 = \frac{1}{t^*} \quad (\text{A.16})$$

$$a_1 = \frac{c_1 c_2}{c_3 c_4}, \quad (\text{A.17})$$

$$a_3 = \frac{1}{c_3 - c_4} \left(c_1 + c_2 - c_4 - \frac{c_1 c_2}{c_4} \right), \quad (\text{A.18})$$

$$a_2 = 1 - a_1 - a_3, \quad (\text{A.19})$$

$$a_4 = \frac{c_2 c_5}{c_3 c_4}, \quad (\text{A.20})$$

$$a_6 = \frac{1}{c_3 - c_4} \left(c_2 + c_5 - c_4 - \frac{c_2 c_5}{c_4} \right), \quad (\text{A.21})$$

$$a_5 = 1 - a_4 - a_6, \quad (\text{A.22})$$

$$a_7 = \frac{c_3}{c_4}, \quad (\text{A.23})$$

$$a_8 = 1 - a_7, \quad (\text{A.24})$$

$$a_9 = \frac{c_5}{c_4}, \quad (\text{A.25})$$

$$a_{10} = 1 - a_9. \quad (\text{A.26})$$

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