Warpage Prediction of Optical Media

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ABSTRACT

A numerical simulation of the warpage of injection-compression molded optical media such as CD’s and DVD’s due to asymmetric cooling is developed. A thermal viscoelastic constitutive model is employed to calculate the thermally induced stress. The stress is not symmetric with respect to the mid-plane of the disk because of the differential mold temperatures employed. Before demolding, the out-of-plane deformation is constrained by the mold walls. After ejection, the disk is quenched in the air, and is free to deform, causing warpage to develop in the disk. A finite element analysis code is developed using axisymmetric plate elements to simulate the warpage of the disk after demolding. The complete finite element formulation is described. Simulation results of warpage for CD-R moldings are compared with experimental observations under different processing conditions such as melt temperature, mold temperature, and packing pressure using an optical grade of polycarbonate. Good agreement of the simulation results and experimental observations is obtained. The comparison of the simulation and experiment reveals that the processing conditions have complicated effects on the warpage, and mold temperature has the greatest effect on the warpage in the current study.

INTRODUCTION

Optical media such as CD’s and DVD’s are typically injection-compression molded using optical grade of polycarbonate (PC). One critical quality of the mass produced optical media is warpage caused by internal residual stresses, which reduces the dimensional stability of the disks, and is particularly detrimental for DVD’s because it hinders the bonding of multiple substrates. There are many causes of the warpage of injection/injection-compression molded parts. Paro, et al. offers various reasons for warpage such as uneven cooling, flow orientation effect, uneven packing, and gate effect, with schematic illustrations [1]. In the current study, the warpage induced by asymmetric thermal stress due to differential mold temperatures is studied, and simulation results of CD-R moldings are compared with experimental observations under different processing conditions.

There are two types of residual stresses [2]: flow induced stress and thermally induced stress. The first is due to the shear flow during the filling and packing stages, and the shear and normal stresses developed are partly frozen-in due to the rapid cooling of the melt. The second type of residual stresses arises during the cooling process of the injection-compression molding. As illustrated in Fig. 1, when the hot polymer melt is injected into the relatively cold mold cavity under high pressure, a thin layer of the melt solidifies. As the part experiences further cooling, the solidification develops inward. Along the thickness direction of the part, the temperature distribution is highly non-uniform. Consequently, each material point through the thickness solidifies at a different time, under different pressure, and experiences different shrinkage. The temperature and pressure history, coupled with the viscoelastic properties of the polymer during the rapid cooling process results in the development of the thermally induced residual stresses. While the flow induced stresses are the main sources of molecular orientations and hence the sources of anisotropic mechanical and optical properties between the flow and cross-flow directions, they are generally lower than the thermally induced stresses by one to two orders of magnitude [3]. As such, the warpage of the disk is mainly caused by the thermally induced stresses.

Fig. 1. Schematic of polymer flow during mold filling

Ideally, if the temperatures of the mold walls of the stationary and moving mold halves are exactly the same, the stress distribution across the thickness direction will be symmetric over the mid-plane of the disk, and there will be no warpage in the molded disk. However, it is common to find a temperature difference between the two mold halves in practice due to the location of the gates, the difference of the coolant temperatures of both sides, or the stochastic deviation of the actual temperature from the control parameters set on the machine. As a result, the gapwise distribution of the residual stress will no longer be symmetric. Before ejection of the disk, the out-of-plane deformation is constrained by the mold walls. After ejection, the disk experience free quench in the air, and is free to deform. Due to the asymmetry of the internal stress, the disk will tend to warp in order to achieve a lower energy state.

PROCESS SIMULATION

The simulation of the injection-compression molding process is previously described [4]. The energy equation for the process before ejection is:

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\[ \rho C_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + \eta \dot{\gamma}^2 \]  

(1)

where \( \eta \) is the viscosity, \( P \) is the pressure, \( T \) is the temperature, \( \dot{\gamma} \) is the shear rate, \( C_p \) and \( k \) are the specific heat and thermal conductivity of the polymer respectively. After ejection, the energy equation simplifies to:

\[ \rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \]  

(2)

The energy equation is solved by a finite difference method to obtain the transient temperature along both the radial direction and the thickness direction throughout the whole process.

### CONSTITUTIVE MODELS

Assuming that time-temperature superposition applies, a linear thermo-viscoelastic constitutive model [5] is given by:

\[ \sigma = -P I + \sigma^d \]  

(1)

\[ p^h = -\frac{1}{3} tr(\sigma) = \int \left( \frac{\alpha}{\kappa} \frac{\partial T}{\partial t} - \frac{1}{\kappa} tr(\epsilon) \right) d\tau \]  

(2)

\[ \sigma^d = \sum_{i=1}^{m} 2 \int g_i e^{-\xi_i(r)\theta_i/\kappa} \epsilon^d d\tau \]  

(3)

where \( \sigma^d \) and \( \epsilon^d \) are the deviatoric stress and strain tensors; \( g_i \) and \( \Theta_i \) are the shear moduli and the corresponding relaxation times, and \( m \) is the number of modes; \( T \) is the temperature; \( p^h \) is the hydrostatic pressure and \( I \) is the unit tensor. The temperature dependent thermal volume expansion coefficient, \( \alpha \), and the isothermal compressibility coefficient, \( \kappa \), in the expression of hydrostatic pressure are defined as:

\[ \alpha = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_p, \quad \kappa = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T \]  

(4)

which are obtained from the \( p-v-T \) relationship. The pseudo-time \( \xi \) is defined as:

\[ \xi(\tau) = \int_0^\tau \frac{1}{a_T(T)} d\tau \]  

(5)

where \( a_T \) is the shift factor of the time-temperature superposition principle.

The shear modulus of the polymer is modeled by a set of discrete moduli \( g_i \) and relaxation times \( \Theta_i \), determined from dynamic mechanical testing. The material behavior and model parameters were characterized and found consistent, as previously described [6].

### FINITE ELEMENT FORMULATION

After demolding, the warpage of the disk is modeled by a finite element analysis (FEA). The elements chosen are 2-node 1-D axisymmetric thin plate elements discretized along the radial direction as shown in Fig. 2. A cylindrical coordinate system \( (r, \theta, z) \) is employed. There are 3 degrees of freedom for each node:

\[ D = [u \ w \ \phi]^T \]

corresponding to radial and vertical displacement as well as rotation.

![Fig. 2. Schematic of disk discretization. From [7]](image)

Each element along the radial direction of the disk is divided into a number of layers along the thickness direction to calculate the displacements and thermal stresses as a function of \( z \). The thickness discretization is the same as in the calculation of the gapwise temperature distribution by the finite difference method. Due to the mold filling process, the temperature distribution of the disk is not homogeneous along the radial direction. Therefore, temperature and thermal stress are both functions of \( r \) and \( z \).

### MAIN ASSUMPTIONS OF FEA

1. There is no transverse shear deformation. Therefore, normals to the mid-plane before deformation remain straight and normal to the mid-plane after deformation. This assumption is from the classical Kirchhoff thin plate theory. Since the radius to thickness ratio of CD’s and DVD’s is generally greater than 50, the thin plate assumption is justifiable.
2. \( u = \bar{u} - z\bar{\phi} \), where \( \bar{\phi} = \frac{dw(r)}{dr} \) is the rotation, \( \bar{u} \) and \( \bar{w} \) are the displacements of the mid-plane of the disk.
3. \( v = 0 \), which is the axisymmetric condition.
4. \( w = \bar{w}(r) \).
STRAIN-DISPLACEMENT RELATIONSHIP

Since there are six degrees of freedom in each element, six coefficients have to be taken in the displacement interpolation polynomials. Assuming radial displacement varies linearly in \( x \), and vertical displacement varies as a cubic in \( x \), where \( x \) is the local coordinate of the radial direction, the displacement within an element is described as [8]:

\[
\begin{bmatrix}
\epsilon_x \\
\epsilon_z \\
\epsilon_{xz} \\
\kappa_r \\
\kappa_z \\
\kappa_{rz}
\end{bmatrix} =
\begin{bmatrix}
1-x \\
1-3x^2+2x^3 \\
ax - 2x^2 + x^3 \\
\xi f(x) \\
\xi^2 f(x) \\
\xi^3 f(x)
\end{bmatrix}
\begin{bmatrix}
u_i \\
\nu_j \\
\nu_k \\
\nu_l \\
\nu_m \\
\nu_n
\end{bmatrix}
\]

where \( \xi = x/s \), \( s \) is the length of the element, and \([\nu_i \nu_j \nu_k \nu_l \nu_m \nu_n]^T\) is the nodal displacement vector.

The strain-displacement relationship in cylindrical coordinate system is derived to be:

\[
\begin{bmatrix}
\epsilon_r \\
\epsilon_\theta \\
\epsilon_z \\
\kappa_r \\
\kappa_\theta \\
\kappa_{rz}
\end{bmatrix} =
\begin{bmatrix}
-1 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{r} & 0 & \frac{1}{r} & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
v_i \\
v_j \\
v_k \\
v_l \\
v_m \\
v_n
\end{bmatrix}
\]

(7)

where \( \epsilon_r \) and \( \epsilon_\theta \) are the radial and hoop strains respectively, \( \kappa_r \) and \( \kappa_\theta \) are the radial and hoop curvatures respectively, and \( r \) is the radius. Eq. 7 can be written in matrix form:

\[
\epsilon = \sum_{i=1}^{n} \mathbf{B}_i \mathbf{v}_i
\]

where \( \mathbf{B}_i \) is the strain-displacement matrix.

The incremental strain-displacement relationship can be derived in a similar manner as:

\[
\Delta \epsilon = \sum_{i=1}^{n} \mathbf{B}_i \Delta \mathbf{v}_i
\]

(9)

The detailed derivation of the strain-displacement relationship is listed in the Appendix.

STRESS-STRAIN RELATIONSHIP

The viscoelastic constitutive equation is solved by a finite difference method in the time domain consistent with [5, 9]. In this method, at time \( t_{n+1} \), the stresses are evaluated based on the stress state at time \( t_n \), plus the temperature and pressure history up to \( t_{n+1} \). The stress in matrix form is found to be:

\[
\sigma = \mathbf{H} \Delta \epsilon + \mathbf{h}
\]

(10)

where \( \sigma \) is the stress tensor, \( \Delta \epsilon \) is the strain increment tensor, \( \mathbf{H} \) is the rigidity matrix, and \( \mathbf{h} \) is the history vector. Detailed derivations of \( \mathbf{H} \) and \( \mathbf{h} \) can be found in [9].

STIFFNESS MATRICES AND LOAD VECTORS

Derived from the principle of virtual work, the set of linear equations to be solved can be written as:

\[
\mathbf{K} \Delta \mathbf{D} = \mathbf{R}
\]

(11)

where \( \mathbf{K} \) is the global stiffness matrix, \( \Delta \mathbf{D} \) is the displacement increment vector to be solved, and \( \mathbf{R} \) is the right-hand side vector.

The element stiffness matrices can be written as:

\[
\mathbf{K}^e = \int_A \int_{d/2} \int_{d/2} \mathbf{B}^T \mathbf{H} \mathbf{B} \mathbf{d}z \mathbf{d}p
\]

(12)

\[
= \int_{d/2} \int_{d/2} \int_{d/2} \mathbf{B}^T \mathbf{H} \mathbf{B} \mathbf{d}z \mathbf{d}p = 2\pi \int_{d/2} \int_{d/2} \mathbf{B}^T \mathbf{H} \mathbf{B} \mathbf{d}z \mathbf{d}p
\]

where \( \mathbf{B} \) is the strain-displacement vector defined in Eq. 8, \( \mathbf{H} \) is the viscoelastic rigidity matrix defined in Eq. 10, \( d \) is the thickness of the disk, and \( r_1 \) and \( r_2 \) are the radii of the two nodes respectively.

The element right-hand side vector can be written as:

\[
\mathbf{R}^e = \int_A \int_{d/2} \int_{d/2} \mathbf{N}^T \mathbf{f} \mathbf{d}z \mathbf{d}p
\]

(13)

\[
= \int_{d/2} \int_{d/2} \int_{d/2} \mathbf{N}^T \mathbf{f} \mathbf{d}z \mathbf{d}p = 2\pi \int_{d/2} \int_{d/2} \mathbf{N}^T \mathbf{f} \mathbf{d}z \mathbf{d}p
\]

where \( \mathbf{N} \) is the shape function matrix, \( \mathbf{f} \) is the body force vector, and \( \mathbf{h} \) is the history vector defined in Eq. 10.

The numerical integration over the thickness is implemented by the trapezoidal rule, and the numerical integration over the radial direction is implemented by the Gauss quadrature for both element stiffness matrices and element right-hand side vectors.

BOUNDARY CONDITIONS

In-mold:

1. \( \sigma_{zz} = -p \), where \( p \) is the pressure in the mold cavity.
2. \( \Delta \epsilon_r = \Delta \epsilon_\theta = 0 \). There only non-zero strain increment is the one in the thickness direction.

Condition 2 is equivalent to a no slip boundary condition on the mold walls. The radial and hoop strains are zero, only the displacement in the thickness direction is allowed. This condition is especially true for injection-compression molding, where the compression is in the \( z \) direction. In fact, any radial displacement would harm the micro-replication of the features on the disks.

The condition can be obtained directly, there is no need to calculate the displacements by the finite element analysis. The stress components are directly calculated by \( \sigma = \mathbf{h} \). Free quench:

1. \( \sigma_{zz} = 0 \), which is the plane-strain condition.
2. $\Delta\varepsilon_{rr} \neq 0$, $\Delta\varepsilon_{\theta\theta} \neq 0$, $\Delta\varepsilon_{zz} \neq 0$. All strains are non-zero, and the disk is free to deform.

The displacement field is solved by the finite element method. No boundary conditions should be applied during free quenching except the displacement constraints to prevent rigid body movement.

RESULTS AND DISCUSSION

The simulation of injection-compression molding process, as well as related $p$-$v$-$T$, rheological, thermal, and viscoelastic models have been previously described [4, 6]. Briefly,

- The flow rate is controlled by the screw speed, which is profiled to be slow at the start of injection and increase with the disk radius so as to best maintain constant melt front velocity during the filling stage. A 4-stage screw speed profile is listed in Table 1.

<table>
<thead>
<tr>
<th>Position (mm)</th>
<th>Speed (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.50</td>
<td>80.0</td>
</tr>
<tr>
<td>29.00</td>
<td>100.0</td>
</tr>
<tr>
<td>25.00</td>
<td>120.0</td>
</tr>
<tr>
<td>6.00</td>
<td>80.0</td>
</tr>
<tr>
<td>3.50</td>
<td></td>
</tr>
</tbody>
</table>

- A 3-step packing pressure profile is used, which gradually decreases the packing pressure in the cavity as the melt solidifies. The profile is listed in Table 2. Note that the value of the packing pressure is the hydraulic pressure. The melt pressure at the nozzle is calculated by the hydraulic pressure multiplied by an intensity factor, which is 12.36 for the machine used in this study.

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Pressure (kgf/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>40.0</td>
</tr>
<tr>
<td>0.10</td>
<td>20.0</td>
</tr>
<tr>
<td>0.25</td>
<td>10.0</td>
</tr>
</tbody>
</table>

- A 3-step clamp force profile is used to allow the mold to open (breathe) during the filling to promote flow then close during the packing to promote pressure uniformity and feature replication. The profile is listed in Table 3.

<table>
<thead>
<tr>
<th>Clamp Force (ton)</th>
<th>Clamp Time (s)</th>
<th>Change Time(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td>22.0</td>
<td>1.50</td>
<td>0.10</td>
</tr>
<tr>
<td>15.0</td>
<td>1.00</td>
<td>0.50</td>
</tr>
</tbody>
</table>

The experiments also investigated the effects of melt temperature (between 300°C and 320°C) and mold temperature (between 100°C and 114°C) with a 3 level design of experiments.

In order to study the warpage of injection-compression molded disk due to asymmetric cooling, the temperature of the stationary side of the mold in the simulation is set to be 5°C lower than that of the moving side, which is the nominal mold coolant temperature. Zero vertical displacement constraint is applied for the finite element analysis at the circular stack bump of the disk ($r = 18$ mm), where the disks are in contact when stacked in a spindle. The warpage of the molded disks is measured at every millimeter of the radius from $r = 27$ mm to $r = 57$ mm. Five disks are measured for each DOE run, and the experimental data shown in the following results are the average of the five disks.

The gapwise distributions of the thermal stress at a radial location of $r = 35$ mm just before demolding and after 20 seconds of quench in the air at room temperature when the temperature of the whole disk has dropped to the room temperature are shown in Fig. 3. Before demolding, the stress is dominantly compressive because of the high cavity pressure during the filling and packing stages. The gapwise distribution of the thermal stress is not symmetric with respect to the mid-plane because of the differential mold wall temperatures. The stress in the left hand side of the thickness is more compressive than that in the right hand side since the pressure decay of the left hand side is slower than the right hand side due to the higher temperature of the left hand side. After demolding, the disk is free to deform, and the asymmetric internal stress causes the warpage of the disk to develop. The stress distribution is less asymmetric after 20 seconds of free quench compared with just before demolding, and more tensile stress develops in the core region of the disk during the free quench in the air. The final disk has tensile stress at the surfaces and in the core, and compressive stress near the surfaces. The integration of the stress over the thickness is zero, indicating that the stress is in a self-equilibrium state.

![Fig. 3. Thermal stress gapwise distribution under median processing conditions](image-url)
EFFECT OF MELT TEMPERATURE

In order to study the effects of melt temperature on the warpage of the molded disks, low and high melt temperatures are used with other processing conditions the same as the median values. The experimental and simulated vertical displacements are shown in Fig. 5 (a) and (b). As is observed from the figure, the simulation results compare very well with the experimental data. The main effect of melt temperature on warpage is shown in Fig. 6. In the simulation, the trend is that the higher the melt temperature, the higher the value of the warpage, but in the experiment, the median melt temperature has the lowest warpage.

EFFECT OF MOLD TEMPERATURE

The experimental and simulated vertical displacements with low and high values of the mold temperature are shown in Fig. 7 (a) and (b). Other conditions are the median values. The main effect of mold temperature on the warpage is shown in Fig. 8. Both simulation and experiment show that higher mold temperature leads to higher value of warpage.
EFFECT OF PACKING PRESSURE

The experimental and simulated vertical displacements with low and high packing pressures and median values for other conditions are shown in Fig. 9 (a) and (b). The main effect of packing pressure on the warpage is shown in Fig. 10. In the experiment, the warpage at low and median packing pressures has almost the same values, and as the packing pressure increases to the high value, the warpage increases significantly. While in the simulation, the median pressure has the highest value of warpage. Higher and lower packing pressure both result in decreased warpage compared with median value. This phenomenon is different from the observations in [10] for injection molding, where it is observed that the higher the packing pressure is, the lower the warpage will be.
as a cubic in \( x \), where \( x \) is the local coordinate of the radial direction, and taking advantage of the relationship \( \overline{\varphi} = \frac{d\overline{w}(x)}{dx} \):

\[
\begin{align*}
\pi & = \alpha_1 + \alpha_2 x \\
\overline{w} & = \alpha_3 + \alpha_4 x + \alpha_5 x^2 + \alpha_6 x^3 \\
\frac{d\overline{w}}{dx} & = \alpha_4 + 2\alpha_5 x + 3\alpha_6 x^2
\end{align*}
\]

The last equation in Eq. 14 comes directly as the derivative of the second equation. Writing Eq. 14 in matrix form:

\[
\begin{bmatrix}
\pi \\
\overline{w} \\
\frac{d\overline{w}}{dx}
\end{bmatrix} =
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & x & x^2 & x^3 \\
0 & 0 & 1 & 2x & 3x^2
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4 \\
\alpha_5
\end{bmatrix}
\]

By substituting the values of \( \pi, \overline{w} \), and \( \overline{\varphi} \) at node 1 and node 2 of an element, the coefficients are solved to be:

\[
\begin{align*}
\alpha_1 &= \pi_1 \\
\alpha_2 &= \overline{w}_1 - \pi_1 \\
\alpha_3 &= \overline{w}_1 \\
\alpha_4 &= \overline{\varphi}_1 \\
\alpha_5 &= -\frac{\overline{\varphi}_1}{s^2} - 2\frac{\overline{w}_1}{s^2} + 3\frac{\overline{w}_2}{s^2} - 3\frac{\overline{w}_3}{s^2} \\
\alpha_6 &= \frac{s^2}{s^2} + 2\frac{\overline{w}_1}{s^2} + 2\frac{\overline{w}_2}{s^2}
\end{align*}
\]

where \( s \) is the length of the element.

Substituting the coefficients \( \alpha_i \) to \( \alpha_6 \) into Eq. 14, one obtains:

\[
\begin{bmatrix}
\pi \\
\overline{w} \\
\overline{\varphi}
\end{bmatrix} =
\begin{bmatrix}
1 - \xi & 0 & 0 & 0 & 0 \\
0 & 1 - 3\xi^2 + 3\xi^3 & s(\xi - 3\xi^2 + \xi^3) & 0 & 3\xi^2 - 3\xi^3 & s(\xi^2 - \xi^3)
\end{bmatrix}
\begin{bmatrix}
\pi_1 \\
\overline{w}_1 \\
\overline{\varphi}_1
\end{bmatrix}
\]

or

\[
\begin{bmatrix}
\pi \\
\overline{w} \\
\overline{\varphi}
\end{bmatrix} = \sum_{i=1}^{s}
\begin{bmatrix}
N_\pi(\xi) & 0 & 0 \\
0 & N_\pi(\xi) & N_\omega(\xi)
\end{bmatrix}
\begin{bmatrix}
\pi_i \\
\overline{w}_i \\
\overline{\varphi}_i
\end{bmatrix}
\]

where \( \xi = x/s \), \( N_\pi(\xi) \), \( N_\omega(\xi) \), and \( N_\varphi(\xi) \) are the shape functions for \( \pi \), \( \overline{w} \), and \( \overline{\varphi} \) respectively, and \( [\pi_1 \overline{w}_1 \overline{\varphi}_1 \pi_2 \overline{w}_2 \overline{\varphi}_2]^T \) is nodal displacement vector.

By taking the relationship:
are the radial and hoop curvatures respectively, and ρ is the radius. Eq. 22 can be written in matrix form:

$$
\left[ \begin{array}{c}
\Delta \epsilon_r \\
\Delta \epsilon_\theta \\
\Delta \kappa_r \\
\Delta \kappa_\theta
\end{array} \right] =
\left[ \begin{array}{cccc}
-1 & \frac{6 \xi}{r} & \frac{2}{r} & 0 \\
\frac{6 \xi}{r} & \frac{2}{r} & \frac{2}{r} & 0 \\
0 & \frac{2}{r} & \frac{2}{r} & 0 \\
0 & 0 & 0 & \frac{2}{r}
\end{array} \right]
\left[ \begin{array}{c}
\Delta \pi_r \\
\Delta \pi_\theta \\
\Delta \sigma_r \\
\Delta \sigma_\theta
\end{array} \right]
$$

(24)

In matrix form:

$$
\Delta \epsilon = \sum_{i=1}^{n} \mathbf{B}_i \Delta \mathbf{u}_i
$$

(25)

REFERENCES