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FEM Simulation of the Effect of Coefficient of Thermal Expansion and Heat Capacity on Prediction of Residual Stresses of Compression Molded Glass Lenses

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Abstract. In this research, the effects of the coefficient of thermal expansion (CTE) and heat capacity on the prediction of residual stresses in BK7 compression molded glass lenses were studied. Three different groups of CTE and two different kinds of heat capacity, which are constant and proportional to temperature, were chosen to investigate the impacts of residual stresses. The simulation results show a big difference and suggest that the properties of glass materials determine the residual stresses and should be measured carefully.

1. Introduction

Compression molding as a hot pressing method is ideal for fabricating precision glass optical elements for its net-shape and high volume fabrication capability [1-3]. However, during cooling, residual stresses are eventually frozen in the molded lenses due to the structural relaxation phenomena when glass material goes through its transition temperature (T_g) region. Residual stresses, inside glass optical elements, can introduce refractive index variation, resulting unwanted light path deviation that may cause image quality deterioration. Therefore, residual stresses are important criteria for evaluating glass optical elements [4].

Finite element method (FEM) has been employed to study and optimize the compression molding process parameters [5-7]. The Tool-Narayanaswamy-Moynihan (TNM) model was applied to model the structural relaxation behavior of glass material during cooling [8, 9]. In this research, the structural relaxation behavior of an optical glass material was simulated by the FEM software MSC/MARC. Therefore, the residual stresses inside molded glass lenses can be predicted. In order to get realistic predictions of the residual stresses, the parameters used in FEM should be accurate. However, during the simulation, the CTE and heat capacity were measured with uncertainty. Different values may resulting variant prediction of residual stresses. Therefore, the effects of CTE and heat capacity on residual stresses were carefully studied.

2. Numerical simulation theory of glass molding

The compression molding process can be grouped into two major stages: heating and hot forming of the glass material, cooling. In the heating stage, the glass is heated to the molding temperature T_{molding}, which is slightly higher than the glass's T_g. In T_{molding}, the viscosity of glass will decrease and the glass can be modeled as a Newtonian fluid. During forming, the behavior of glass deformation is governed by a function of the stress σ_{ij} and strain rate $\dot{\varepsilon}_{ij}$, viscosity $\eta(T)$, shown in equation (1):

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$$\sigma_{ij} = 2\eta(T)\dot{\varepsilon}_{ij} \tag{1}$$

During cooling, the change of glass material's property is non-linear because it depends on current temperature and temperature history. A response function $M_v(t)$ is adopted to describe the change of a glass property, presented in equation (2) [9]:

$$M_v(t) = \sum_{i=1}^{n} \left(w_g\right)_i \exp\left(-\frac{t}{\tau_{vi}}\right) \tag{2}$$

where, $(w_g)_i$ are called weighting factors and τ_{vi} are the associated structural relaxation times. The structural relaxation times at a given temperature can be calculated using the TNM model, expressed in equation (3) [8]:

$$\tau_v = \tau_{v,ref} \exp\left(-\frac{H}{R}\left(\frac{1}{T_{ref}} - \frac{\mu}{T} - \frac{1-\mu}{T_f}\right)\right) \tag{3}$$

where $\tau_{v,ref}$ is structural relaxation time at reference temperature T_{ref}. H is activation energy, R is the ideal gas constant and μ is a fraction parameter. The value of μ lies between 0 and 1. Once the fictive temperature T_f is known, the property of glass material $p(T)$ can be calculated using equation (4) [9]:

$$\frac{1}{p(0)}\frac{dp(T)}{dT} = \alpha_g(T) + \left(\alpha_l(T_f) - \alpha_g(T_f)\right)\left(\frac{dT_f}{dT}\right) \tag{4}$$

where α_l and α_g are thermal expansion coefficients (CTE) of liquid and solid glass material, respectively. $p(0)$ represents the instantaneous value of the property of the glass material.

3. Numerical simulation

The numerical simulation was based on an aspherical glass lens. Figure 1(a) shows the schematic of the aspherical glass lens. The aspherical surface described by equation (5),

$$Z = \frac{-Cx^2}{1 + \sqrt{1 - (1+K)C^2x^2}} \tag{5}$$

where, x is the coordinate of the optical surface, K (4.3666) is the conic constant. C is surface curvature ($C = 1/R_1$, R_1 is the vertex radius of the aspherical surface).

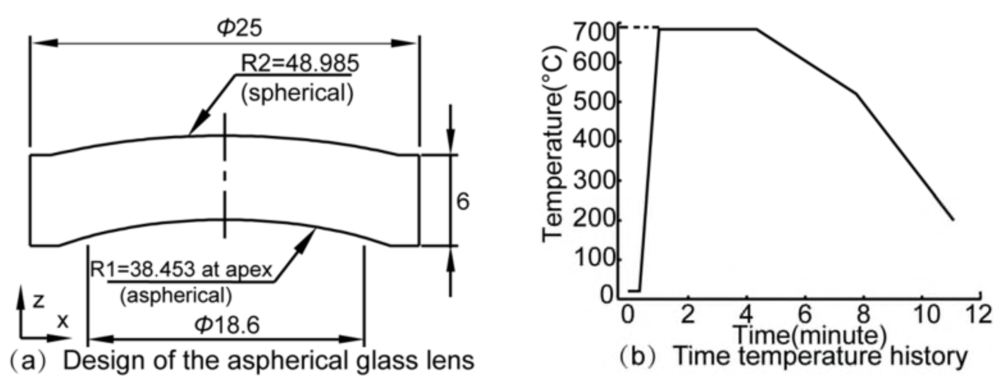

Figure 1. (a) Schematic of the aspherical lens (Units: mm),
(b) Time-temperature history of glass molding process.

Figure 1(b) shows the time-temperature history of the molding process. Molding was performed at 684 °C, and the temperature was kept until stresses due to forming were released. A two-steps cooling process was followed. First, the temperature was decreased to 520 °C at a rate of 0.8 °C/s, then to

200 °C at a rate of 1.6°C/s. When the temperature was decreased to 200 °C, the molded lens was taken out and cooled naturally.

In simulation, two dimensional (2D) axisymmetric models were applied because of the rotational symmetrical geometry of experiment settings. The glass and molds were meshed by four-node isoparametric quadrilateral element. Important mechanical and thermal properties of the glass (BK7) and molds (Tungsten carbide), are summarized in table 1. The parameters used in TNM model are summarized in table 2.

Table 1. Mechanical and thermal properties of BK7 glass [6] and Tungsten carbide [10].

Material Properties	BK7	Tungsten carbide
Elastic modulus, E [MPa]	82,500	570,000
Poisson's ratio, ν	0.206	0.22
Density, ρ [kg/m^3]	2,510	14,650
Thermal conductivity, κ_c [W/m °C]	1.1	63
Specific heat, C_p [J/kg °C]	858	314
Transition temperature, T_g [°C]	557	
Solid CTE, α_g [/°C]	5.6×10^{-6}	4.9×10^{-6}
Liquid CTE, α_l [/°C]	1.68×10^{-5}	--
Viscosity, η [MPa-sec] (at 685°C)	60	--

Table 2. Structural relaxation parameters used in numerical simulation [6].

Material properties	Value
Reference temperature, T_{ref} [°C]	685
Activation energy/gas constant, H/R [K]	47,750
Fraction parameter, μ	0.45
Weighting factor, w_g	1
Structural relaxation time, τ_v [sec] (at 685 °C)	0.019
Stress relaxation time, τ_s [sec] at 685 °C	0.0018

Figure 2 shows the model of deformed aspherical lens at the end of molding. The lens was meshed into 3,500 elements. Upper and lower molds were meshed into 381 and 365 elements, respectively.

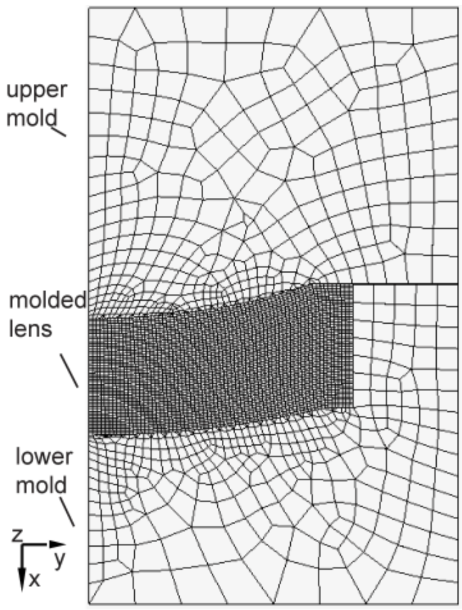

Figure 2. Deformed model of the aspherical glass lens.

Figure 3 shows the simulated distribution of the residual stresses inside the molded glass lens in cylindrical coordinates. The stress distribution displays half of the cross section of the aspherical lens viewed in the normal direction. In figure 3, negative value means compressive stress and positive value means tensile stress.

According to figure 3, the lens is mainly under tensile stress in the center and compressive stress at the top and bottom surfaces. Because the glass lost heat from its surfaces and the temperature of its center part was always higher than its surfaces. Therefore the center part will be under tensile stress as compared to the surfaces.

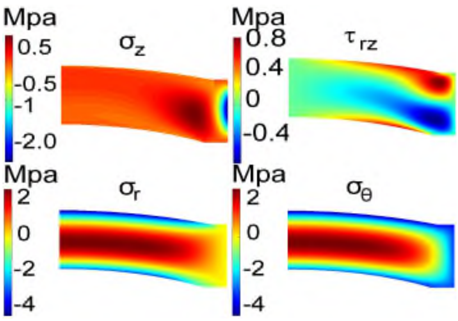

Figure 3. Numerical simulated residual stresses distribution in the aspherical glass lens in cylindrical coordinates: axial stress σ_z, shear stress τ_{rz}, radial stress σ_r, circumferential stress σ_θ.

4. Simulation results and discussion

4.1. Effect of coefficient of thermal expansion

Generally, the solid CTE of BK7 glass, in table 1, is an average CTE from 20 °C to 300 °C. And the CTE from 300 °C to T_g is unknown. Reference [6] measured the solid CTE of BK7 using Orton Dilatometer (Model 1000D), $\alpha_g = 8.3\times10^{-6}$ /°C. Then the liquid CTE α_l was calculated by using two different methods based on α_g and experimental data: $\alpha_l = 3.77 \times 10^{-5}$ /°C and 3.16×10^{-5} /°C. Reference [11], also mentioned that $\alpha_g = 5.6\times10^{-6}$/°C, $\alpha_l = 1.68\times10^{-5}$/°C by using α_l/α_g=3. Table 3 shows these three kinds of CTE.

Table 3. Coefficient of thermal expansion.

Solid CTE, α_g(/°C)	5.6×10^{-6}	8.3×10^{-6}	8.3×10^{-6}
Liquid CTE, α_l(/°C)	1.68×10^{-5}	3.77×10^{-5}	3.16×10^{-5}
$\alpha_l/\ \alpha_g$	3	4.54	3.81

Figure 4 shows the simulated radial stress σ_r based on CTE shown in table 3. The other parameters used in the simulation are shown in table 1 and 2. In figure 4, the radial stresses show the same trend, but with different magnitude. The maximum tensile stress shown in figure 4(b) is almost as twice as the stress shown in figure 4(a).

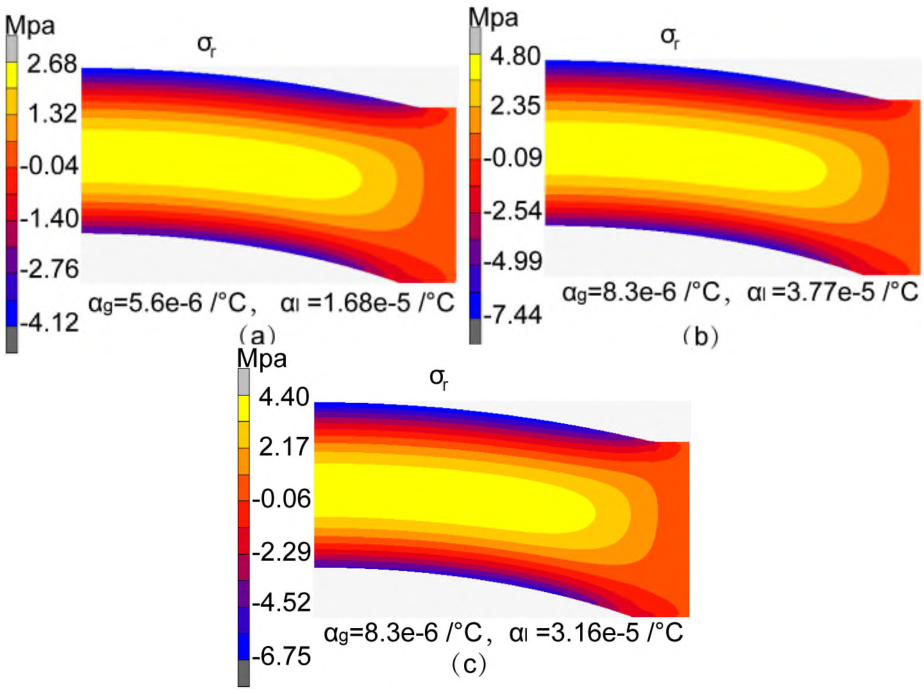

Figure 4. Numerical simulated radial stress σ_r under different CTE, (a) α_g=5.6×10^{-6} /°C, α_l=1.68×10^{-5} /°C, (b) α_g=8.3×10^{-6} /°C,α_l= 3.77×10^{-5} /°C, (c) α_g=8.3 ×10^{-6} /°C, α_l= 3.16×10^{-5} /°C. .

4.2. Effect of heat capacity

The heat capacity of the simulations shown in section 3 is set as a constant. However, in the region of T_g, due to structural relaxation, the volume of glass, elastic modulus, viscosity, heat capacity, etc. are related to temperature changes and temperature history. For poly-oxide, the relationship between liquid heat capacity C_{pl} and solid heat capacity C_{pg} is C_{pl} / $C_{pg} \approx 1.3$ [11] .

Figure 5 shows temperature-related heat capacity. The heat capacity is proportional to temperature until C_{pl} = 1.3 C_{pg} at T_g.

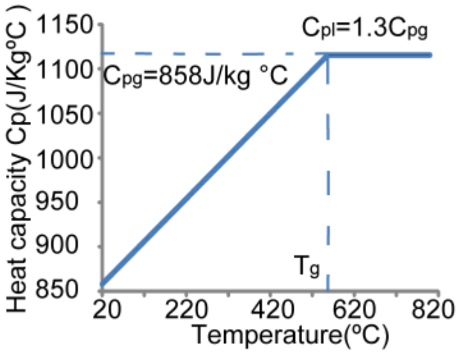

Figure 5. Heat capacity of BK7 changes with temperature.

Figure 6 (a) and (b) are the simulated radial stress of the fixed heat capacity and the temperature-related heat capacity, respectively. The corresponding maximum tensile stress and compressive stress are: (a) 2.68 Mpa, 4.12 Mpa; (b) 3.41 Mpa, 5.33 Mpa. It can be seen that the heat capacity has a certain effect on the residual stresses and can not be neglected.

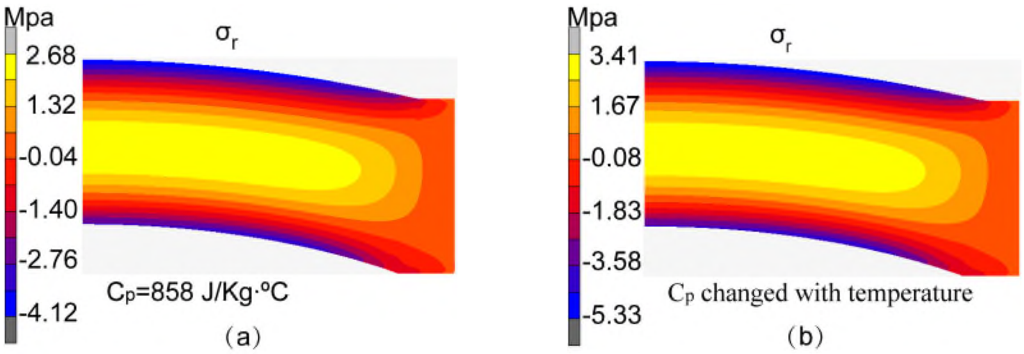

Figure 6. Finite element simulation of radial stress σ_r in the aspherical glass lens (a) C_p=858 J/Kg·°C, (b) C_p changed with temperature shown in figure 5

5. Conclusions

By using FEM with a structural relaxation model, it is able to predict the residual stresses inside compression molded glass lenses. Three types of CTE and two kinds of heat capacity were applied to investigate the influences on prediction of residual stresses. The results show that the simulated residual stresses have the same distribution. However the magnitude of residual stresses shows a big difference of the effect of CTE and heat capacity. Under different CTE (α_g, α_l), the maximum tensile stress of the radial stress at (8.3×10^{-6} /°C, 3.77×10^{-5} /°C) is almost as twice as the maximum tensile stress at (5.6×10^{-6} /°C, 1.68×10^{-5} /°C). For heat capacity, the heat capacity changed with temperature causes 20% larger than constant heat capacity in radial stress.Therefore, in numerical simulation, the parameters should be conform to reality in order to obtain accurate residual stresses.

References

[1] Allen Y Y and Jain A 2005 *J. Am. Ceram. Soc.* **88(3)** 579-86.
[2] He P, Wang F, Li L, Georgiadis K, Dambon O, Klocke F and Allen Y Y 2011 *J. Opt.* **13(8)** 085703.
[3] Li L, He P, Wang F, Georgiadis K, Dambon O, Klocke F and Allen Y Y 2011 *J. Opt.* **13(5)** 055407.
[4] Aben H and Guillemet C 1993 *Photoelasticity of Glass* (Springer Science & Business Media).
[5] Chen Y, Allen Y Y, Su L, Klocke F, and Pongs, G 2008 *J. Manuf. Sci. E.* **130(5)** 051012.
[6] Jain A, Firestone G C, and Allen Y Y 2005 *J. Am. Ceram. Soc.* **88(9)** 2409-14.
[7] Jain A 2006 *Experimental study and numerical analysis of compression molding process for manufacturing precision aspherical glass lenses* (Doctoral dissertation, The Ohio State University).
[8] Narayanaswamy O 1971 *J. Am. Ceram. Soc.* **54(10)** 491-8.
[9] Soules T F, Busbey R F, Rekhson S M, Markovsky A and Burkem A 1987 *J. Am. Ceram. Soc.* **70(2)** 90-5.
[10] Fujidie Co 2003 *Material: Cemented Carbide Alloys* (http://www.fujidie.co.jp).
[11] Scherer G W 1986 *Relaxation in glass and composites.*

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