

Constitutive modelling of polycarbonate at low, moderate and high strain rates

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Abstract. The objective of this paper is to experimentally investigate and predict the mechanical behavior of polycarbonate over a wide range of strain rate from 10^{-4} to 5000 s^{-1} . Considering the influences of the glass (α) transition and the second (β) transition on the mechanical behavior of polycarbonate, a new constitutive model is proposed, and it is decomposed into the α and β components. The α component dominates the low and moderate rate deformations, and the β component is related to the high rate deformation. In comparison with the experimental results, the model can accurately predict the mechanical behavior of polycarbonate at low, moderate and high strain rates.

1. Introduction

Polycarbonate has been extensively used as aircraft windows, eyeglasses and helmets, due to its low density, high impact strength and good transparency [1-3]. The mechanical behavior of polycarbonate is strongly dependent on strain rate, and a large number of studies on its mechanical behavior at low and high strain rates during the last few decades have been conducted. Its low rate ($< 10^0 \text{ s}^{-1}$) deformation behavior is readily captured with a MTS 810 servo-hydraulic machine [4] or an Instron servo-hydraulic testing machine [1], and its high rate deformation ($> 10^2 \text{ s}^{-1}$) behavior can be obtained with a split Hopkinson bar (SHP) [1-3, 5, 6]. Experimental results of polycarbonate indicate the bilinear relationship between the yield stress and the logarithm of the strain rate, and its yield stress at high rates increases more dramatically than that at low rates [1, 7]. However, its moderate rate ($10^0 \sim 10^2 \text{ s}^{-1}$) behavior is rarely investigated. Actually, polycarbonate experiences the low, moderate and high strain rate deformations in many impact accidents. Consequently, it is significant to investigate the low, moderate and high strain rate deformation behavior of polycarbonate.

With respect to the deformation mechanism of polycarbonate, the glass (α) transition and the secondary (β) transition of polycarbonate can be utilized to expound it. The Dynamic mechanical analysis (DMA) results and the bilinear relationship between the yield stress and the logarithm of the strain rate indicate that the α transition dominates the mechanical behavior of polycarbonate at low strain rates [1, 8], due to the non-activated β transition; the temperature of the β transition increases with an increasing strain rate, and the β transition is observed to be activated at high strain rates, which will have a dramatic influence on the mechanical behavior of polycarbonate in this case [1, 2, 9]. However, the deformation mechanism of polycarbonate at moderate strain rates is still in its infancy.



For the elastic–viscoplastic deformation behavior of polymers, a large number of constitutive models have been developed during the last few decades. Boyce, Parks and Argon [10] proposed a now-famous physical model called BPA for glassy polymers in 1988, and the BPA model employed two parallel resistances to describe the deformation of polymers, including an entropic resistance for strain hardening and an intermolecular resistance for strain softening. Subsequently, based on the BPA model, a large number of modified models were developed, such as the eight-chain Arruda-Boyce model [11], the full-chain model [12], the neo-Hookean approximation model [13] and the Mulliken-Boyce model [1]. Among these models, the Mulliken-Boyce model [1] expounded the deformation mechanism of polycarbonate with two rate-activated processes, namely, the α and β transitions, and the model was demonstrated to have an ability of accurately predicting the deformation of polycarbonate at low and high strain rates. However, there are a large number of material coefficients in these models, and some coefficients are difficult to solve, which makes these models difficult to calibrate and employ in practice.

There are also other models to predict the mechanical behavior of polymers, such as the G'Sell-Jonas [14], the DSGZ model [15] and the ZWT model [16]. The G'Sell-Jonas model [14] can capture initial elasticity, yield and strain hardening deformation features of polymeric materials, while it can not capture strain softening behavior. The DSGZ model [15, 17] compensates the shortcoming of the G'Sell-Jonas model, and it can accurately predict the large deformation of polycarbonate (PC), polymethyl-methacrylate (PMMA) and acrylonitrile-butadiene-styrene (ABS) at low strain rates for various temperatures, while it can not accurately simulate the deformation of polymeric materials at high strain rates. The ZWT model [16] employs a nonlinear spring and two Maxwell elements in parallel, and it can capture the deformation feature of PMMA at low and high strain rates, while the strain hardening deformation of PMMA has not been predicted with the ZWT model. To sum up, these phenomenological models can not expound the deformation mechanism of polymers, and they can not predict the large deformation of polymers from low to high strain rates.

The objective of this paper is to develop a new constitutive model to simulate the deformation of polycarbonate at low, moderate and high strain rates for room temperature. The new model is based on the Mulliken-Boyce model [1], the G'Sell-Jonas model [14] and the DSGZ model [15], and it allows for the deformation mechanism of polycarbonate at low, moderate and high strain rates. In addition, the new model is validated to have an ability to accurately predict the large deformation and the yield stress of polycarbonate from low to high strain rates for room temperature.

2. Experimental

In this study, the material was polycarbonate (EXL1414) from SABIC Innovative Plastics Company. An all-electric injection molding machine (JSW110AC) was utilized to produce cylindrical specimens. The specimens at low strain rates were 12.20 mm in diameter and 6.20 in length, and the specimens at moderate and high strain rates were 5.14 mm in diameter and 5.20 in length. Compressive tests at low, moderate and high strain rates were carried out with a Shimadzu universal testing machine, a Gleeble 3500 thermo-mechanical simulator and a split Hopkinson pressure bar (SHPB), respectively. The low rate tests were conducted at 10^{-4} , 10^{-3} and 10^{-2} s^{-1} , the moderate rate tests were conducted at 1 and 10 s^{-1} , and the high rate tests were conducted at 1600, 3000 and 5000 s^{-1} . All of the tests were conducted at room temperature. Prior to testing, all of the tested specimens were kept at room temperature for three days to eliminate the residual stress. Tests under the same conditions were repeated at least three times.

3. Constitutive model

According to the literatures [1, 18], the glass (α) transition of polycarbonate is related to low strain rates or high temperatures, while the secondary (β) transition of polycarbonate is associated with high strain rates or low temperatures. The activated temperature of the β transition of polycarbonate is quite low under the low strain rate loading. The temperature of the β transition increases

dramatically with an increasing strain rate, and it will shift to room temperature under the high strain rate loading. The bilinear relationship between the yield stress and the logarithm of strain rate indicates that the yield stress of polycarbonate at low strain rates is dominated by α transition, and that the yield stress at high strain rates is influenced by the α and β transitions. Consequently, the α transition dominates the mechanical behavior of polycarbonate at low strain rates, due to the non-activated β transition, whereas both the α and β transitions control the mechanical behavior at high strain rates, due to the activated β transition.

Considering the influences of the α and β transitions on the mechanical behavior of polycarbonate, a new constitutive model is proposed to accurately simulate the deformation of polycarbonate at low, moderate and high strain rates. The new model is on the basis of three previous models, including the Mulliken-Boyce model [1], the G'Sell-Jonas model [14] and the DSGZ model [15], as shown in Eqs. (1), (2) and (3),

$$\sigma = \begin{cases} K_{\alpha} \alpha(\varepsilon) \dot{\varepsilon}^{M_{\alpha}}, & \dot{\varepsilon} < 10^2 \text{ s}^{-1} \\ K_{\beta} \alpha(\varepsilon) \beta(\varepsilon) \dot{\varepsilon}^{M_{\beta}}, & \dot{\varepsilon} \geq 10^2 \text{ s}^{-1} \end{cases} \quad (1)$$

where,

$$\alpha(\varepsilon) = [\exp(-\alpha_1 \varepsilon) + \varepsilon^{\alpha_2}] [1 - \exp(C\varepsilon)] \exp(\alpha_3 \varepsilon) \quad (2)$$

$$\beta(\varepsilon) = [\exp(-\beta_1 \varepsilon) + \varepsilon^{\beta_2}] \exp(\beta_3 \varepsilon^2) \quad (3)$$

The new model is decomposed into the α and β components, as shown in Eq. (1). The α component dominates the low and moderate rate deformations owing to the non-activated β transition or the insignificant β -contribution, and the β component considers the contribution of the β transition under the high strain rate loading owing to the activated β transition. There are eleven material coefficients in this model, six (K_{α} , α_1 , α_2 , α_3 , M_{α} and C) related to the α transition and five (K_{β} , β_1 , β_2 , β_3 and M_{β}) related to the β transition. With regard to the deformation at low or moderate strain rates, $1 - \exp(C\varepsilon)$ and $\exp(-\alpha_1 \varepsilon)$ describe the initial nonlinear elastic deformation and the strain softening deformation, $\dot{\varepsilon}^{M_{\alpha}}$ shows the rate dependence of the deformation behavior, ε^{α_2} and $\exp(\alpha_3 \varepsilon)$ exhibit the strain hardening deformation; with regard to the deformation at high strain rates, $\exp(-\beta_1 \varepsilon)$ describes the strain softening deformation, $\dot{\varepsilon}^{M_{\beta}}$ shows the rate dependence of the deformation behavior, and ε^{β_2} and $\exp(\beta_3 \varepsilon^2)$ denote the strain hardening deformation.

Table 1. Material coefficients of polycarbonate.

Material coefficients	Value
α_1	4.378
α_2	0.918
α_3	0.276
M_{α}	0.0056
K_{α}	89.28 MPa · ms ^{M_{α}}
C	-17.62
β_1	12.88
β_2	0.0545
β_3	5.09
M_{β}	0.13
K_{β}	79.26 MPa · ms ^{M_{β}}

The new model has been implemented in ABAQUS/Explicit through a user subroutine VUMAT, to simulate the deformation of polycarbonate at low, moderate and high strain rates for room temperature. The corresponding coefficients were calculated and listed in Table 1. The Poisson's ratio and the density were set as 0.3 and 1200 kg/m³.

4. Experimental results vs. model precisions

Figure 1 shows the experimental results of polycarbonate from low to high strain rates. It is readily observed that all of the mechanical behavior of polycarbonate at low, moderate and high strain rates is decomposed into four parts: initial elasticity, yield, strain softening and strain hardening. The yield stress is found to increase with an increasing strain rate, and there is a small discrepancy between the increasing rate of the stress at low strain rates and that at moderate strain rates, whereas the increasing rate of the stress at high strain rates is much larger than that at low and moderate strain rates, which can be expounded by the two rate-activated processes, namely, the α and β transitions. The α transition dominates the low and moderate strain rate deformation, because the β transition has not been activated or the influence of the β transition on the mechanical behavior is insignificant under these conditions. However, the mechanical behavior of polycarbonate at high strain rates is different from that at low and moderate strain rates, and the stress at high strain rates is significantly influenced by the β transition, due to the activated β transition. Hence, the stress at high strain rates increases rapidly than that at low and moderate strain rates.

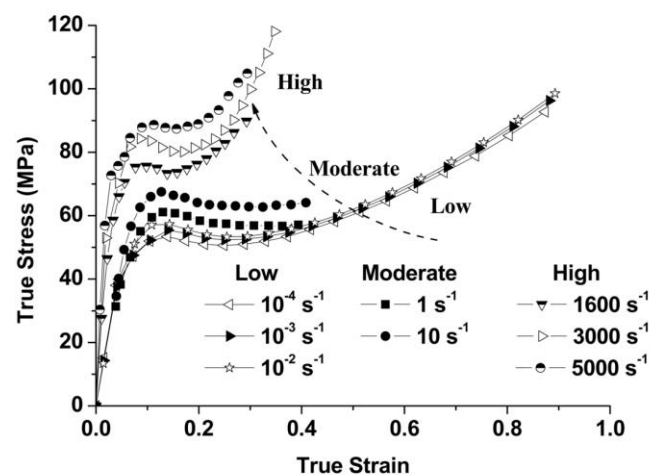


Figure 1. Experimental results of stress-strain responses at low, moderate and high strain rates.

Figures 2-5 show experimental and predicted stress-strain responses at low, moderate and high strain rates. It is observed that the model can capture the typical deformation features of polycarbonate over a wide range of strain rates, including initial elasticity, yield, strain softening and strain hardening. The model can show the same deformation feature as the experiment that the increasing rate of the stress at high strain rates is much larger than that at low and moderate strain rates (see Figure 5). This is attributed to the fact that the model considers the contribution of the β transition to the mechanical performance of polycarbonate at high strain rates. Hence, the model can accurately predict stress-strain responses at high strain rates. In addition, the model is validated that it can accurately simulate the large deformation of polycarbonate at low, moderate and high strain rates for room temperature.

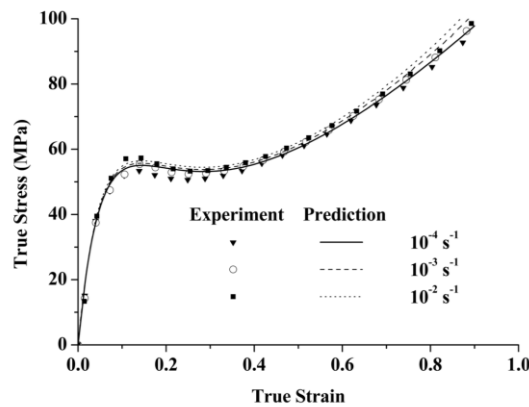


Figure 2. Experimental and predicted results of stress-strain responses at low strain rates.

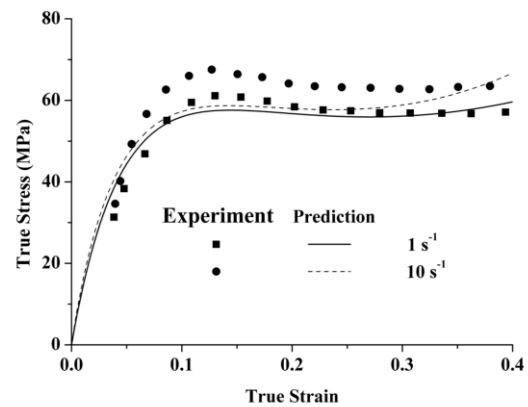


Figure 3. Experimental and predicted results of stress-strain responses at moderate strain rates.

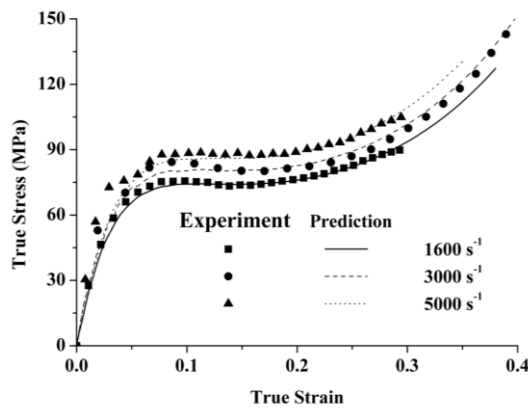


Figure 4. Experimental and predicted results of stress-strain responses at high strain rates.

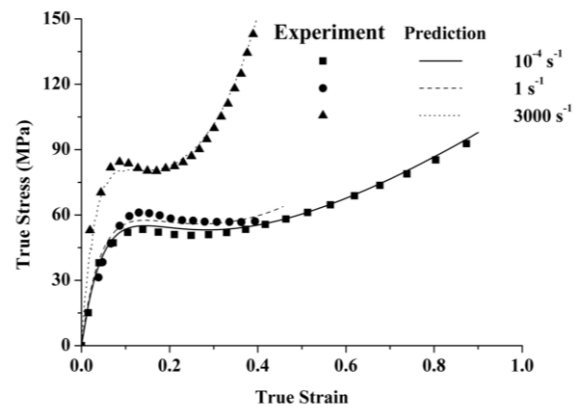


Figure 5. Experimental and predicted results of stress-strain responses at low, moderate and high strain rates.

Table 2. Errors between experimental and predicted true yield stresses.

Strain rate (s ⁻¹)	Experimental true yield stress (MPa)	Predicted true yield stress (MPa)	Error (%)
10 ⁻⁴	53.47	55.07	2.99
10 ⁻³	55.46	55.78	0.58
10 ⁻²	57.75	56.51	-2.15
1	61.47	57.58	-6.33
10	67.53	58.7	-13.08
1600	75.85	74.35	-1.98
3000	84.42	80.89	-4.18
5000	88.79	86.16	-2.96

Comparison between the experimental and predicted yield stresses under all of the service conditions is listed in Table 2. The error between the experimental and predicted yield stresses is utilized to evaluate our model's accuracy, which is expressed as

$$error = \frac{\sigma_{P,y} - \sigma_{E,y}}{\sigma_{E,y}} \quad (4)$$

where $\sigma_{E,y}$ and $\sigma_{P,y}$ are the experimental yield stress and the predicted yield stress. Seen from Table 2, the errors under all of the service conditions are less than 14 %, which indicates that there is only a small discrepancy between the experimental and predicted yield stress. Therefore, the model can accurately predict the yield stress over a wide range of strain rate from 10^{-4} to 5000 s^{-1} . In conjunction with the experimental results and the model predictions shown in Figures 2-5 and Table 2, it is validated that the model can accurately predict the stress-strain responses of polycarbonate at low, moderate and high strain rates.

5. Conclusions

The mechanical behavior of polycarbonate at low, moderate and high strain rates has been experimentally investigated and predicted. A new constitutive model was proposed to predict its mechanical behavior and to expound its deformation mechanism. The model allows for the influences of the α and β transitions on the mechanical behavior of polycarbonate, and it is decomposed into the α and β components. The α component dominates the low and moderate rate deformations, and the β component dramatically influences the high rate deformation, due to the activated β transition. Compared with the experimental results, the model predictions can characterize initial elasticity, yield, strain softening and strain hardening. In addition, the model predictions can represent the same experimental deformation feature that the increasing rate of the stress at high strain rates is much larger than that at low and moderate strain rates, and the model can accurately the yield stress and the large deformation of polycarbonate at low, moderate and high strain rates.

6. References

- [1] Mulliken AD and Boyce MC 2006 *Int. J. Solids Struct.* **43** p 1331-1356
- [2] Safari KH, Zamani J, Ferreira FJ, and Guedes RM 2013 *Polym. Eng. Sci.* **53** p 752-761
- [3] Fu S, Wang Y, and Wang Y 2009 *Polym. Test.* **28** p 724-729
- [4] Cao K, Wang Y, and Wang Y 2014 *Int. J. Solids Struct.* **51** p 2539-2548
- [5] Richeton J, Ahzi S, Vecchio KS, Jiang FC, and Makrady A 2007 *Int. J. Solids Struct.* **44** p 7938-7954
- [6] Cao K, Ma X, Zhang B, Wang Y, and Wang Y 2010 *Mater. Sci. Eng.: A* **527** p 4056-4061
- [7] Wang H, Zhou H, Huang Z, Zhang Y, and Zhao X 2016 *Mech. Time-Depend. Mater.* p 1-21
- [8] Siviour CR, Walley SM, Proud WG, and Field JE 2005 *Polymer* **46** p 12546-12555
- [9] Safari KH, Zamani J, Guedes RM, and Ferreira FJ 2015 *Mech. Time-Depend. Mater.* p 1-20
- [10] Boyce MC, Parks DM, and Argon AS 1988 *Mech. Mater.* **7** p 15-33
- [11] Arruda EM and Boyce MC 1993 *J. Mech. Phys. Solids* **41** p 389-412
- [12] Wu PD and Van der Giessen E 1995 *Int. J. Plast.* **11** p 211-235
- [13] Tervoort T, Smit R, Brekelmans W, and Govaert LE 1997 *Mech. Time-Depend. Mater.* **1** p 269-291
- [14] G'sell C and Jonas JJ 1979 *J. Mater. Sci.* **14** p 583-591
- [15] Duan Y, Saigal A, Greif R, and Zimmerman MA 2001 *Polym. Eng. Sci.* **41** p 1322-1328
- [16] Wang J, Xu Y, and Zhang W 2014 *Compos. Struct.* **108** p 21-30
- [17] Duan Y, Saigal A, Greif R, and Zimmerman MA 2002 *Polym. Eng. Sci.* **42** p 395-402
- [18] Richeton J, Ahzi S, Daridon L, and Rémond Y 2005 *Polymer* **46** p 6035-6043