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Material Behaviour

Experimental investigation and constitutive modeling of the deformation behavior of Poly-Ether-Ether-Ketone at elevated temperatures

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ABSTRACT

The present study investigates the deformation behavior of Poly-Ether-Ether-Ketone (PEEK) at elevated temperatures and low strain rates through a combination of experiments and simulations. Uniaxial tension tests at elevated temperatures (293–543 K) and strain rates (8.3×10^{-3} to 3.3×10^{-1} s^{-1}) were performed, and the temperature- and rate-dependencies of the deformation behavior and mechanism of PEEK were discussed in detail. The Erichsen test was performed at temperatures varying from 473 to 533 K and a fixed speed of 1 mm/s. Based on an investigation of numerous constitutive models, a phenomenological model called DSGZ was employed in ABAQUS/Explicit to characterize the deformation behavior of PEEK at elevated temperatures, and the deviation between experimental and simulation data was less than 10% at large deformations. Moreover, the simulation results accurately predicted the necking and cold drawing phenomena in the tension test as well as the deformation in the Erichsen test.

1. Introduction

A customized Poly-Ether-Ether-Ketone (PEEK) cranial implant is a good option for patients and has the advantages of a matched elastic modulus with the cortical bone as well as good biocompatibility, radiation permeability and durability [1,2]. In general, PEEK cranial implants are fabricated by computer numerically controlled (CNC) milling [3–5]. However, this method suffers from some limitations. The cranial implant, which is a shell structure with a large curvature, is milled from a thick plate, resulting in a large amount of material waste. Moreover, the reliability of parts is also affected by microcracks caused by the milling process [5]. To overcome these disadvantages, some new methods need to be proposed. Thermoforming [6], which has been shown to be a low-cost and effective method of manufacturing polymer implants [7–10], is a better choice to form PEEK cranial implants compared with CNC. In this process, three-dimensional complex parts are net shaped from a thin sheet by using heat and pressure [11], and the voids or defects of the materials can be reconsolidated [12]. The processes used to form PEEK cranial implants are mainly carried out above the glass transition temperature T_g (416 K–438 K) and at a low strain rate. Hence, investigation of the deformation behavior of PEEK under elevated temperature and at a low strain rate is important for process optimization and implant quality control.

In the past two decades, the tensile and compressive properties of PEEK over a wide range of temperatures have been examined. Alberola et al. [13] investigated the tensile properties of PEEK films at room temperature over a wide strain rate range from 5×10^{-5} s^{-1} to 300 s^{-1}, and the results showed that the strain rate sensitivity significantly depended on the analyzed strain rate range. Subsequently, Rae et al. [14] conducted a comprehensive study of PEEK's mechanical properties. The tensile properties were measured at temperatures ranging from 223 to 423 K and strain rates ranging from 2.7×10^{-5} to 1.9×10^{-2} s^{-1}. The engineering stress-strain curves of PEEK only included the elastic and strain softening phase and temperature- and rate-dependences were discussed. More recently, Zakaria et al. [15,16] investigated the compressive yield stress of PEEK over a wide range of strain rates (1×10^{-4} to 10000 s^{-1}) and temperatures (143–433 K). The results showed that true stress was very sensitive to the temperature and strain rate, and the deformation of PEEK only included the elastic and strain softening phases. Although some research investigations have examined the mechanical properties of PEEK below or at T_g, few

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studies have investigated the deformation behavior and mechanism of PEEK above T_g. Dahoun et al. [17] studied large plastic deformations of PEEK under uniaxial tension under conditions of 453 K and 5×10^{-4} s^{-1} and discussed the deformation mechanism. However, this study was limited to a single temperature condition, and the temperature- and rate-dependences were not discussed.

Based on experimental investigations, many constitutive models have been proposed to characterize the nonlinear elastic deformation of polymers. The BPA model [18,19], a typical physical model, assumes that plastic resistance to flow can be decomposed into intermolecular and entropic resistances, which are related to strain softening and strain hardening, respectively. Glassy polymers must overcome these two resistances before undergoing strain hardening. However, physical models are difficult to calibrate and apply in practice because they involve numerous viscoelastic-plastic theories and utilize a large number of material parameters [20]. In contrast to physical models, phenomenological models [21] are more convenient for engineering applications because they use a brief equation or equations. The Johnson–Cook (JC) [21] model, which considers strain rate hardening and the thermal softening effect, has been successfully employed to simulate the mechanical properties of polymers [22,23], such as acrylonitrile butadiene styrene (ABS) and PEEK. As the temperatures has a great effect on the prediction of traditional JC model, Xu et al. [24] developed a modified JC model with the modification to combine the influence of processing thermal history to model the mechanical behavior of polycarbonate (PC). By using a damage model to describe the soften behavior, Xu et al. [25] further proposed a physically based constitutive model to describe the strain-rate dependent tension stress-strain responses of polycarbonate. Fei Chen et al. [26] developed a modified JC model with a new thermal softening equation to describe the plastic deformations of the compressive properties of PEEK at various strain rates and temperatures. However, the predictive results of the modified JC model were not accurate as the performance of PEEK changed dramatically when the temperature was above T_g. By summarizing several previous models and investigating the mechanical behavior of amorphous and semi-crystalline polymers, such as polycarbonate (PC), polymethyl-methacrylate (PMMA) and polyamide 12 (PA 12), a general model called DSGZ (Duan-Saigal-Greif-Zimmerman) [27] was developed that could better describe the deformation behavior of amorphous and semi-crystalline polymers at various temperatures. Our recent studies [28,29] have successfully applied this model to investigate the properties of polycarbonate under various conditions.

Although many experiments have been conducted and a series of constitutive models have been developed, most efforts have focused on the mechanical properties of PEEK below or at T_g, and few researchers have investigated the deformation behavior and mechanism of PEEK above T_g. In the present work, the tension behavior of PEEK is experimentally investigated over a wide range of temperatures from 293 to 543 K and at low strain rates of 8.3×10^{-3} to 3.3×10^{-1} s^{-1}. The temperature- and rate-dependences of the deformation mechanism of PEEK are discussed in detail. In addition, the Erichsen test is performed at temperatures varying from 473 to 533 K and at a fixed speed of 1 mm/s. Regarding modeling, the DSGZ model is employed to characterize the deformation behavior of PEEK at elevated temperatures and low strain rates, and the results are then implemented in ABAQUS/Explicit through a user material subroutine to simulate the uniaxial tension test and Erichsen test. Finally, a comparison between the experimental and predicted results is presented to evaluate the accuracy of the model.

2. Experimental

2.1. Material and specimen preparation

In this study, PEEK 450G supplied by the Victrex, Shanghai, China was used. The melting temperature of PEEK is 616 K and its glass transition temperature is 415 K. The specimens for the uniaxial tension test were ISO 527 IBA standard specimens, while the specimens for the Erichsen test were square sheets with a length of 120 mm and thickness of 5 mm. The specimens were kept at room temperature for three days before testing, and five samples were tested for each experimental condition. The mechanical and thermal properties of PEEK450G are presented in Table 1.

2.2. Uniaxial tension test

The temperature and strain rate have a significant impact on the tensile test results, so these two influencing factors were examined. As the thermoforming process for forming PEEK implants is mainly carried out above T_g and at a low strain rate, we selected temperatures ranging from 293 to 543 K and strain rates ranging from 8.3×10^{-3} to 3.3×10^{-1} s^{-1}. The conditions of the uniaxial tension test and Erichsen test are shown in Table 2.

A Zwick/Roell Z020 electronic universal material testing machine was used as the tensile test equipment, which was provided by the research laboratory platform of Die State Key Laboratory of Huazhong University of Science and Technology. The ISO 527-2 standard was selected as the test standard. The dimensions of the sample are shown in Fig. 1.

In this study, the force and displacement data obtained were converted into stress and strain data. The engineering stress σ_e and strain ε_e in the specimen were calculated as follows:

$$\sigma_e = \frac{F}{bh} \tag{1}$$

$$\varepsilon_e = \frac{L}{l} \tag{2}$$

where F and L are the force and displacement, respectively. b, h and l are the width, thickness and span of the test section of the specimen, respectively. Then, the true strain ε and true stress σ could be calculated according to the engineering strain and stress.

$$\varepsilon = \ln(1 + \varepsilon_e) \tag{3}$$

$$\sigma = \sigma_e(1 + \varepsilon_e) \tag{4}$$

2.3. Erichsen test

To validate the accuracy of the model, the Erichsen test was carried out in a self-developed thermoforming platform provided by the research laboratory platform of Die State Key Laboratory of Huazhong University of Science and Technology, as shown in

Table 1
Material properties of PEEK 450G.

Mechanical properties		Thermal properties	
Elastic modulus (GPa)	3.6	Thermal conductivity (W/mK)	0.25
Poisson's ratio	0.38	Specific heat (J/kg K)	2160
Density(kg/m^3)	1300	Glass transition temperature (K)	416
Yield stress (MPa)	100	Melt transition temperature (K)	616