Experimental testing and numerical modelling of ductile fracture of PEEK in incremental sheet forming process

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Abstract. This research investigates the use of Hooputra-based damage model to predict fracture of polyether-ether-ketone (PEEK) material and its application to single point incremental forming (SPIF) process under different conditions. Flat PEEK sheets are used to examine the influence of temperature changes on the Hooputra fracture strain-stress triaxiality damage curve and to verify the capability of the Hooputra ductile damage model in predicting fracture in uniaxial tensile tests and the SPIF process. The research showed that the formulas used to calculate stress triaxiality based on geometric dimensions are insufficient with notched samples because the radius of the notched sample is no longer circular after plastic deformation. Temperature alters the Hooputra damage curve; therefore, the Hooputra ductile damage formula should be developed to consider the effect of temperature. When the Hooputra damage curve is established according to the temperature effect, the uniaxial fracture is precisely predicted at different temperatures. Hooputra ductile damage model could be developed to capture the fracture initiation and propagation in SPIF process.

Introduction

Polyether-ether-ketone (PEEK) is a versatile thermoplastic polymeric material commonly used in industrial applications due to its excellent combination of physical and mechanical properties [1]. In addition, PEEK presents a viable option for medical implants since it has a comparable elastic modulus to cortical bone and is biocompatible [2]. PEEK's industrial and medical applications could be expanded by using novel forming processes such as single point incremental forming (SPIF). SPIF is a potential technique that could be developed as an alternative production solution for PEEK materials with significant lead time and cost benefits. To employ the SPIF to produce high-quality parts of PEEK, precise prediction of mechanical response and fracture behaviour of PEEK materials is important.

The stress triaxiality and plastic strain are considered to be the two most significant variables in crack initiation, growth, and coalescence in ductile fracture of materials [3]. As a result, various ductile fracture models based on stress triaxiality, and fracture strain were established. Johnson and Cook established a model to predict ductile fractures at high strain rates and temperatures, and the fracture strain is related to stress triaxiality [4]. A void growth model was developed by Kanvinde et al. to evaluate the ductile fracture in the range of high stress triaxiality [5]. Brünig et al. established a damage model as a function of stress triaxiality [6]. Peng et al. suggested an uncoupled ductile fracture model based on stress triaxiality and lode angle [7].

Based on the macroscopic strains and stresses a ductile fracture model was presented by Hooputra et al. [8]. The fracture strain in this model is a function of stress triaxiality. Many numerical investigations have been conducted based on Hooputra model. To select and calibrate the appropriate fracture criterion for a specific application, seven different fracture models were employed. Hooputra damage model was one of them. To achieve the goal, 15 different experimental tests on 2024-T351 aluminium covering a stress triaxiality range of -0.3 to 0.9 were performed. The Hooputra damage model was discovered to be very promising because it accurately predicts fracture in all types of experimental tests [9]. To determine which model could be used to predict the forming limits of 2024-T3 aluminium alloy, eight ductile fracture models were considered and calibrated. The Hooputra ductile damage model was shown to be more robust against over-fitting and could be used when the number of calibration data points is small [10]. The experimental tests required to determine the parameters of Hooputra ductile damage model of St14 steel could be neglected, and the parameters of Hooputra ductile damage model could be predicated using a forming limit diagram [11]. To analyse the impact of mechanical discontinuities on the crashworthiness performance of aluminium, the Hooputra damage model was combined with the Müschenborn-Sonne forming limit diagram. It was discovered that incorporating it led to more reliable crash simulations [12]. To predict the ductile fracture of metal alloys, a model based on stress triaxiality, and shear stress ratio was proposed. The proposed model was compared to the Hooputra ductile damage model, and there was a good correlation [13].

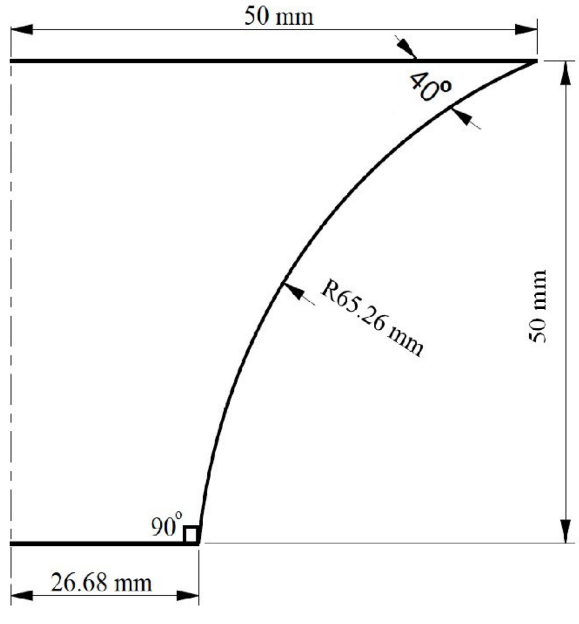
There are some research publications in the literature that illustrate the SPIF process's capacity to successfully deform PEEK material [14]. A novel incremental sheet forming (ISF) process was proposed to analyze the thermal formability of PEEK and investigate the geometric accuracy, twisting, and fracture mechanisms. The results showed that as the temperature increased, the accuracy of ISF part decreased and twisting angle increased. Striations marking is a common fracture mode in hot PEEK ISF [15]. An alternate spiral toolpath based on linear interpolation was developed to enhance the accuracy of SPIF of PEEK parts by reducing twisting in the deformed parts [16]. In comparison to traditional processes, the ISF process could be used to manufacture a customised product from PEEK, such as a cranial plate, with technological and economic advantages [2]. Cold SPIF of PEEK sheets was performed to evaluate the effect of ISF parameters on formability and to determine the best parameters for manufacturing the cranial plate and cheekbone. The findings of this study demonstrated the capability of the SPIF process in the biomedical field [17].

In this scientific context, precise selection of fracture strain and stress triaxiality values can improve the prediction of ductile fracture models that were established based on the plastic strain and stress triaxiality. The main motivation for this work is to evaluate the effect of temperature on the fracture strain and stress triaxiality of PEEK and to implement these values in the Hooputra ductile damage model to verify its accuracy to predict the ductile fracture of PEEK under different strain states e.g., uniaxial tensile test and the plane strain of SPIF process.

Material and experimental procedures

PEEK 450G extruded sheets with a thickness of 3 mm were used in this study's experimental testing. The glass transition and melting temperatures were determined using differential scanning calorimetry. PEEK has glass transition and melting temperatures of 149 ºC and 340 ºC, respectively. Tensile testing of standard samples (smooth) was performed by INSTRON testing machine in accordance with ASTM/D638/sample type V to determine the mechanical properties of PEEK sheets. The dimensions of the standard PEEK tensile sample were set to 63.5 mm total length, 9.53 mm gauge length, and 3.18 mm the narrow section width. All tests were performed at a constant strain rate of 1.75×10^{-3} S^{-1}. Four flat notched samples with varying notch radiuses (0.5, 1, 3, and 5 mm) were machined and tested to obtain different stress triaxialities. The gauge length width in smooth tensile sample and at notch root was designed to be 3.18 mm for each sample. Tensile tests on smooth and notched samples were performed at room temperature, 80 ºC, 120 ºC, and 150 ºC to examine the effect of temperature on fracture strain and stress triaxiality. Tensile samples were examined in a temperature chamber. Tensile samples were painted with a white and black stochastic pattern, and strains were captured using video measurement during the tensile tests. Table 1 reports the mechanical properties of PEEK sheet at room temperature.

To validate the accuracy of the Hooputra model in predicting ductile fracture in SPIF under plane strain conditions, an SPIF test of PEEK sheets was performed using a HURCO CNC milling machine equipped with a heating system to produce a hyperbolic truncated cone with varying angle (from 40º to 90º) (see Fig. 1). The PEEK blank has a size of 150 × 150 mm and a thickness of 3 mm. To improve the surface quality of the produced part, the ROCOL RDT grease compound was used as a lubricant between the high-speed steel forming tool and the PEEK sheet. The SPIF test was carried out with a tool diameter of 10 mm, a step size of 0.5 mm, a feed rate of 1000 mm/min, and a spindle speed of 100 rpm. An alternate spiral toolpath was used to reduce the twisting phenomenon in PEEK SPIF.



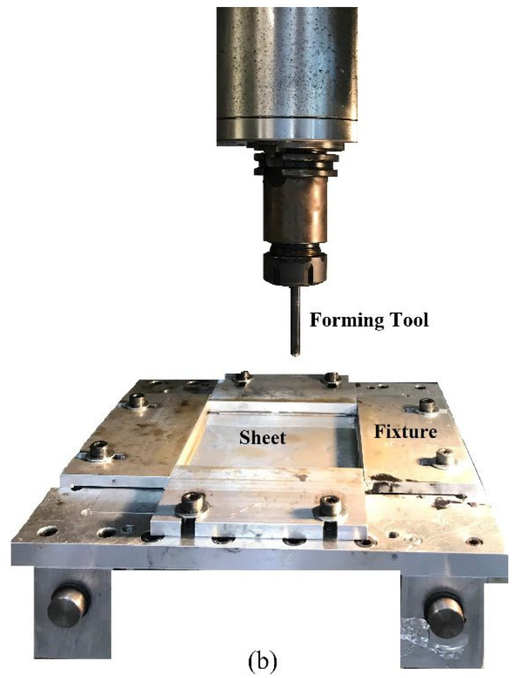


Fig. 1. (a) Geometric shape of the hyperbolic cone, and (b) SPIF experimental fixture.

Table 1. Mechanical properties of PEEK 450G at room temperature.

Elastic Modulus [GPa]	Poisson's ratio	Yield stress [MPa]	Density [kg/m^3]
3.6	0.38	84	1300

Finite element modeling

Abaqus/Explicit is used for estimating stress triaxiality and predicting crack initiation and propagation in uniaxial tensile samples and in the SPIF process. Tensile samples and the PEEK sheets in the SPIF process were modelled as deformable bodies, with isotropic elastic and plastic yielding, whereas the forming tool, blank holder, and backing plate were modelled as analytical rigid bodies. To predict stress triaxiality and fracture in the FE model, a 3D hexahedral element with 8 nodes and reduced integration (C3D8RT) was used. Due to the considerable deformation of PEEK materials at high temperatures, a small element size should be employed. The element size in this study is 0.15 mm in the tensile test and 0.25 mm in the SPIF test. In FE simulation, several friction coefficient values were investigated in order to determine the optimal friction coefficient. The results revealed that there is a good correlation between the FE and the experimental forming force with a coefficient of friction of 0.05.

The Hooputra ductile damage model is utilized in this study to predict fractures in both tensile and SPIF tests. The onset of fracture in the Hooputra ductile damage model is based on the nucleation, growth, and coalescence of voids. In this concept, fracture strain is only a function of stress triaxiality. The following is the Hooputra ductile damage model.

$$\varepsilon_{eq}(\eta) = a\, e^{-c\eta} + b\, e^{c\eta} \quad (1)$$

where the ε_{eq} is equivalent plastic strain at fracture; $\eta = {}^{\sigma_H}/_{\sigma_{eq}}$ is stress triaxiality; σ_H is the hydrostatic stress; σ_{eq} Von Mises equivalent stress; a, b, and c are materials parameters to be found from the tests. When the following condition is met in the FE model, the crack is initiated:

$$D = \int_0^{\varepsilon_{eq}} \frac{d\varepsilon_{eq}}{\varepsilon_{eq(\eta)}} = 1 \quad (2)$$

where D is the damage variable that ranges from 0 (virgin material) to 1 (fractured material). Crack initiation and propagation are modelled using element deletion. The element is eliminated from the FE model when the damage variable equals 1.

Results and discussion

Effect of plastic deformation and temperature on stress triaxiality

There are two approaches for determining the stress triaxiality of notched tensile samples. The first approach is based on the geometric dimensions of the specimen, and certain formulas were developed to compute the stress triaxiality, such as the Bridgman formula for rounded tensile samples and the Yuanli Bai formula [18] for flat samples. However, these formulas are no longer strictly relevant because the dimensions of tensile samples do not remain constant during the tensile test. Another approach is to use numerical simulation, where stress triaxiality is defined as the ratio of hydrostatic stress to Von Mises equivalent stress. The stress triaxiality in uniaxial tensile samples and in the SPIF process of a hyperbolic truncated cone is calculated using FE simulation in this work.

The position of stress triaxiality was measured using the minimum cross section of a flat tensile sample. As a result, the FE approach was used to examine the distribution of stress triaxiality on the minimum cross section through the thickness. To demonstrate that the empirical formulas that was used to capture stress triaxiality due to geometric dimensions are no longer strictly applicable, the FE simulation of smooth and notched samples (notch radius (R)=0.5, 1, 3, 5 mm) was run under the assumption that the material is elastic, then the simulation with elastic plastic properties was run. The stress triaxiality values are constant under the elastic condition because the dimensions of the tensile sample are not changed during the simulation and the sample returns to its original shape when the load is removed. As a result, the stress triaxiality under elastic condition is 0.33, 0.4, 0.43, 0.53, and 0.58 for smooth, R5 mm, R3 mm, R1 mm, and R0.5 mm samples, respectively. Fig. 2 (a) depicts the influence of plastic deformation at room temperature on the stress triaxiality distribution at the centre of an R5 mm notched sample. The stress triaxiality is uniform under elastic conditions because the dimensions of the notched sample are not changed, whereas under elastic-plastic deformation the radius of the notched sample is no longer circular after plastic deformation, so the stress triaxiality changes through the thickness of the sample and reaches its maximum value at the centre. The behaviour of all notched samples is the same, and the values of stress triaxiality at the centre of the other samples are presented in Table 2. The plastic deformation has no effect on the stress triaxiality of the smooth sample because in the tensile test of the PEEK smooth sample, the necking begins at the beginning of the test and extends throughout the gauge length of the tensile sample as shown in Fig. 2 (b), which means that the gauge length lines return to be parallel throughout the test and the fracture occurs when the molecular chains reach a certain length.

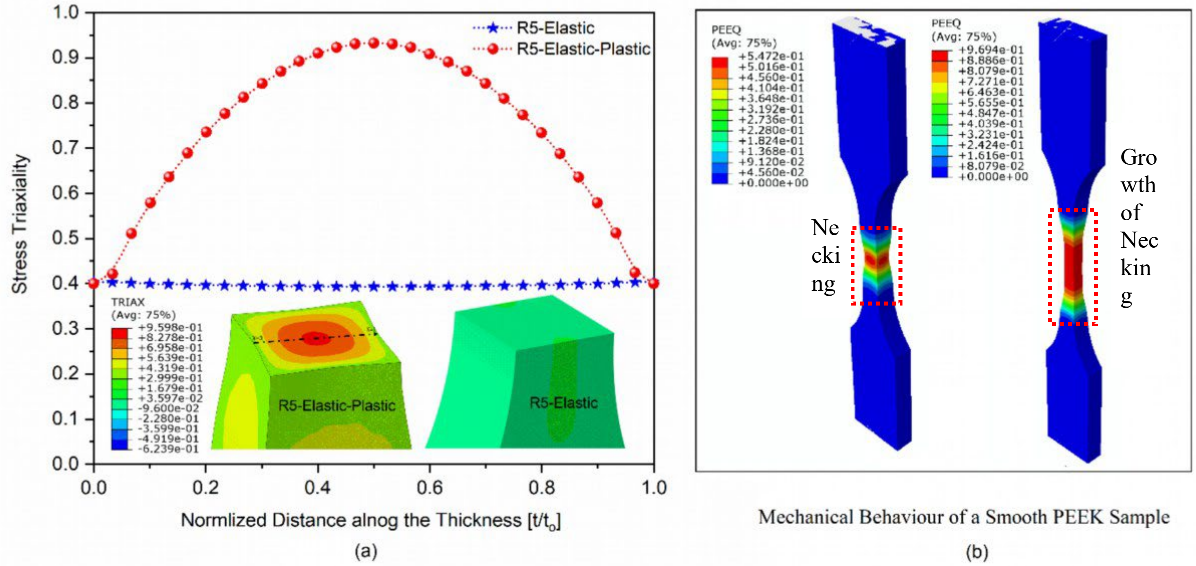


Fig. 2. (a) Stress triaxiality distribution over the thickness of a notched sample (R5 mm) under elastic and elastic plastic conditions and (b) mechanical behaviour of smooth sample.

PEEK is temperature sensitive, and raising the temperature below the glass transition temperature enhances its formability. To investigate the effect of temperature on stress triaxiality, tensile tests on smooth and notched samples were performed at various temperatures, including room temperature (22 ºC), 80 ºC, 120 ºC, and 150 ºC. The influence of temperature on the stress triaxiality of a notched sample (R5mm) is shown in Fig. 3 (a). It can be noted that the stress triaxiality decreases as temperature rises, which indicates that as PEEK formability increases with temperature, the stress triaxiality decreases. Temperature has the same effect on stress triaxiality in all notched samples, and the effect of temperature on smooth samples is identical to the effect of plastic deformation; the stress triaxiality of smooth samples does not change with temperature. Table 2 shows the experimental fracture strain and stress triaxiality results at various temperatures. To clarify why stress triaxiality decreases with rising temperature in notched samples, Fig. 3 (b) compares the FE results of stresses distribution at necking area of R5 mm notched sample at room temperature with one at 150 ºC. It is assumed that σ_1 is the tensile stress, which obtained from the experimental tensile test and decreases as the testing temperature rises. σ_2 and σ_3 denote the stress in the width and thickness directions, respectively. σ_2 and σ_3 are close to zero before necking and increase when necking begins. Because the yield stress of PEEK is greater at room temperature than at 150 ºC, high values of σ_2 and σ_3 are required to compress the sample and induce necking in the sample at room temperature, whereas the required stresses (σ_2 and σ_3) are decreased at 150 ºC as shown in the figure. When σ_2 and σ_3 are reduced, the hydrostatic stress decreases, resulting in a decrease in stress triaxiality.

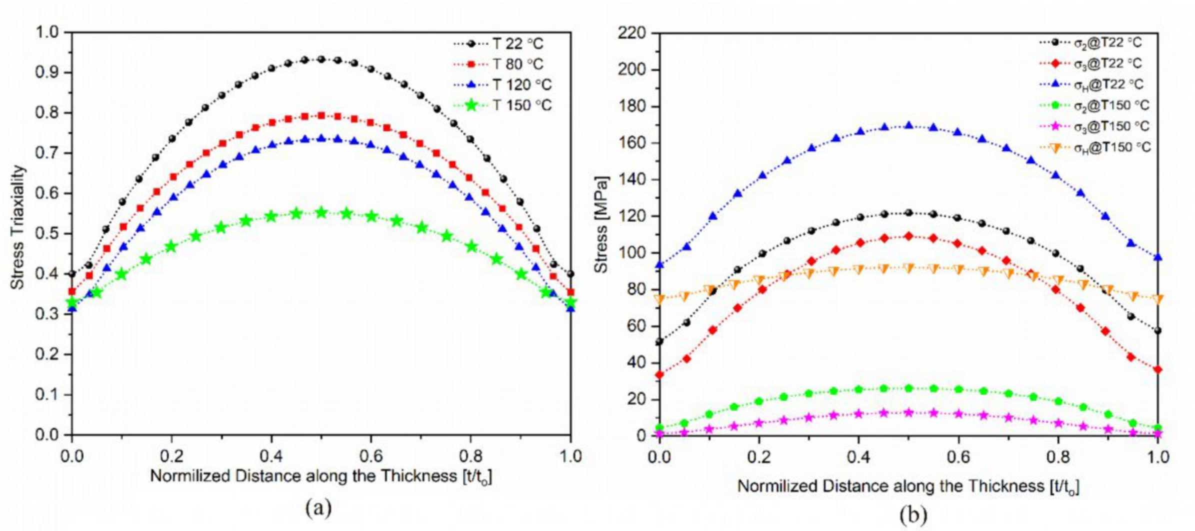


Fig. 3. Sensitivity of stress triaxiality (a) and stresses distribution (b) to temperature changes of R5 mm notched sample.

Table 2. Fracture strain-stress triaxiality (η) of PEEK at different notches temperatures.

Temp.	Smooth		R5		R3		R1		R0.5	
[ºC]	Strain	η	Strain	η	Strain	η	Strain	η	Strain	η
22	1.29	0.33	0.52	0.93	0.38	1.04	0.15	1.20	0.07	1.37
80	1.55	0.33	0.62	0.79	0.59	0.96	0.16	1.04	0.09	1.28
120	1.86	0.33	0.78	0.73	0.67	0.78	0.22	0.93	0.12	1.19
150	1.94	0.33	1.33	0.55	0.96	0.60	0.35	0.86	0.24	1.03

Determination of Hooputra ductile damage parameters

The Hooputra ductile damage model is utilised in this work to predict the fracture initiation and propagation in uniaxial tensile testing and the SPIF process. To calculate the Hooputra parameters at different temperatures the values of fracture strain and corresponding stress triaxiality from Table 2 are plotted as five isolated points at each temperature. To obtain the best match between Eq.1 and the five isolated points, a curve fitting procedure is carried out using MATLAB tools. The best-fitting values of a, b, and c represent the parameters of the Hooputra ductile damage model. Fig. 4 depicts the Hooputra damage curves at various temperatures based on data from Table 2, and Table 3 presents the relevant Hooputra parameters. According to Fig. 4 and Table 3, the temperature affects the Hooputra damage curve and Hooputra parameters; hence, the Hooputra ductile damage model should be modified to account for temperature impacts.

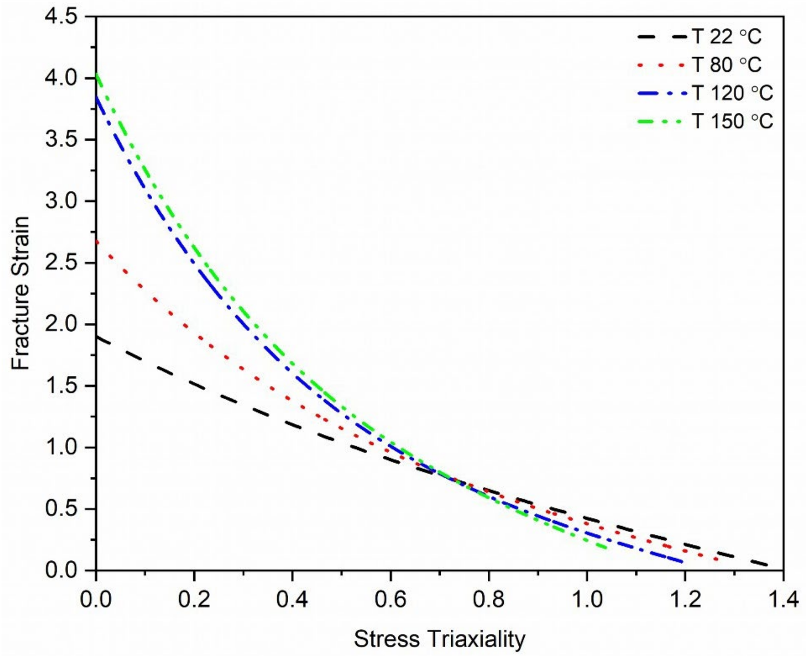


Fig. 4. Hooputra ductile damage curve at different temperatures.

Table 3. Hooputra parameters for PEEK at different temperatures.

Parameters	T 22 [ºC]	T80 [ºC]	T120 [ºC]	T150 [ºC]
a	2.034	2.715	3.863	4.063
b	-0.1318	-0.0389	-0.0181	-0.03111
c	0.97	1.567	2.133	2.099

Fracture prediction

To validate the potential of the Hooputra ductile damage model to accurately capture the PEEK fracture under different temperatures and strain states, such as uniaxial and plane strain states, the FE results of a smooth tensile sample at room temperature and 150 ºC, as well as the SPIF test at 80 ºC, were compared to the experimental results. Fig. 5 (a) depicts the predicted damage evolution of a smooth tensile sample at room and 150 ºC temperatures. The graphic clearly shows that the damage grows faster at ambient temperature than at 150 ºC. This is owing to PEEK's low formability and high stress triaxiality at room temperature as compared to150 ºC. Furthermore, when the deforming temperature is 150 ºC, the displacement to fracture is greater. Fig. 5 (b) shows a comparison of the experimental and numerical tensile stress-strain diagrams at room temperature and 150 ºC. The figure clearly shows that the mechanical response of PEEK changes with temperature, and fracture initiation is temperature sensitive. The FE prediction of PEEK fracture using Hooputra ductile damage model is comparable and closely matches the experimental data.

Fig. 6 depicts the damage evolution in the SPIF component under plane strain at 80 ºC. It is noted that during the early stages (low forming angles) of the SPIF process, the damage grows uniformly and close to zero, and when the stretching in the forming wall reaches a particular value at wall angle 58º, the damage begins to increase rapidly, leading to fracture in the transition region between the forming wall and the base of the truncated cone at wall angle 77.6º. The numerical forming angle were compared with the experimental one to validate the prediction results of the Hooputra ductile damage model to capture the fracture in the SPIF process of hyperbolic truncated cone shape. The primary results showed that the fracture occurred early according to Hooputra ductile damage at forming angle equal to 77.6º while the experimental fracture occurred at 88.24º (see Fig. 6). The possible explanation for this, the heat generated by the friction between the forming tool and the PEEK sheet and due to the plastic deformation is not taken into consideration in Hooputra damage model, which means the Hooputra ductile damage curve is constant in FE simulation, and according to the findings of this study, this curve changes with temperature and the safe region expands with increasing temperature. Particularly, in the SPIF FE model, the stress triaxiality-fracture strain values are compared with the Hooputra ductile damage curve, and if the value is below the curve, no damage occurs; however, if the value is above the curve, damage occurs in the FE model; however, the values of stress triaxiality-fracture strain change with increasing temperature (fracture strain increases and stress triaxiality decreases) due to the plastic deformation and friction. As a result, the Hooputra ductile damage model should be developed to account for the effect of temperature in order to be utilised to predict fracture in polymeric materials.

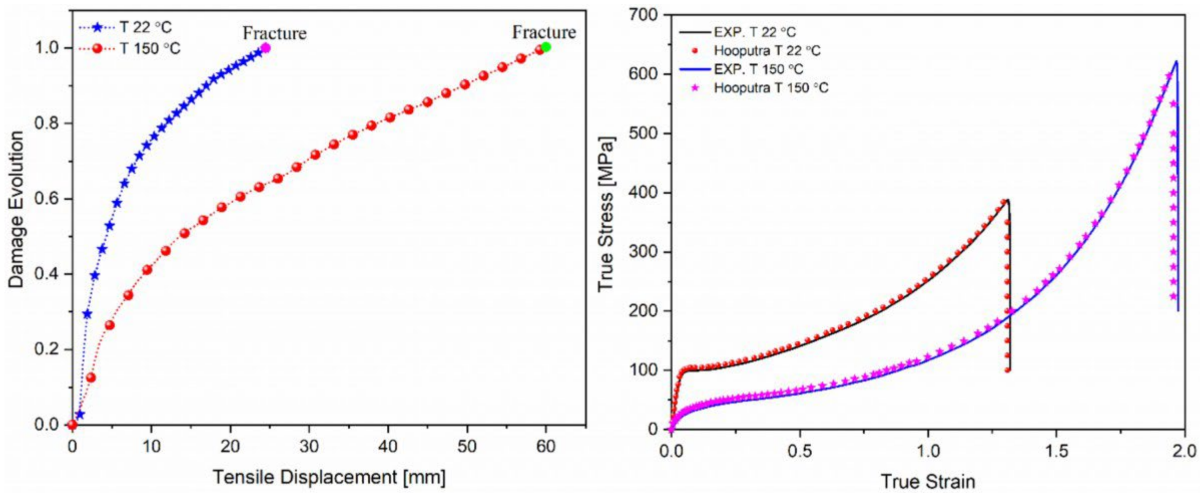


Fig. 5. (a) Uniaxial damage evolution at various temperatures, and (b) comparison of numerical and experimental stress-strain curves at various temperatures.

Conclusions

The influence of temperature on stress triaxiality and Hooputra ductile damage curve of PEEK was addressed in this work, and the Hooputra ductile damage results of fracture prediction of uniaxial tensile test and SPIF process were validated by the experimental work. The findings of this research can be summarised as follows:

- The stress triaxiality formulas based on geometric dimensions are not sufficient for notched samples because the radius of the notched sample is no longer circular after plastic deformation.
- The Hooputra ductile damage curve of PEEK material is temperature sensitive and changes with deformation temperature.
- When the influence of temperature is addressed in Hooputra parameter calculations, the uniaxial fracture is accurately predicted using the Hooputra ductile damage model. The fracture in the SPIF process is predicted with a percentage of error; this could be because the influence of friction-generated temperature was not taken into account in the FE model and the Hooputra ductile damage curve is constant throughout the FE simulation.
- According to this investigation, the Hooputra ductile damage model should be modified to take temperature into account in order to apply this model to predict fracture initiation and propagation in polymeric materials.

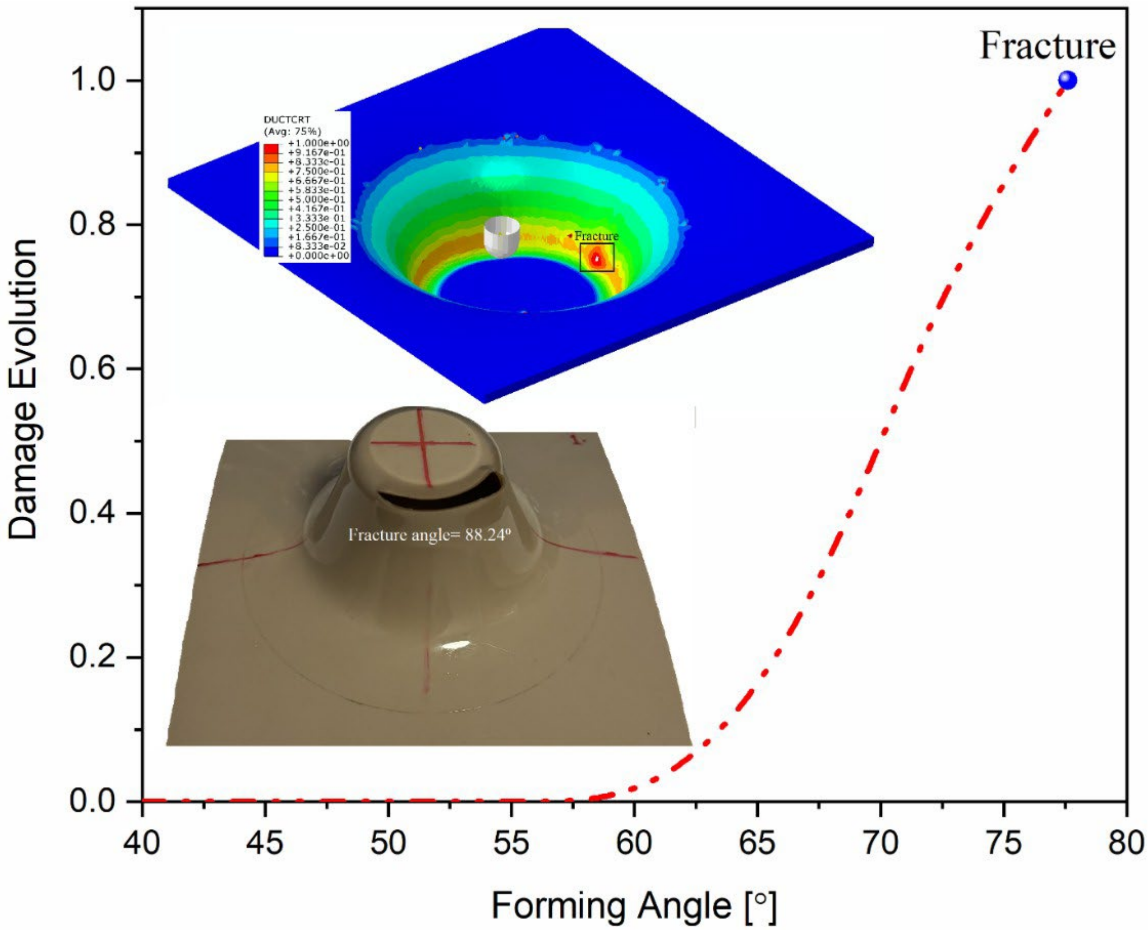


Fig. 6. Plane strain damage evolution at 80 ºC.

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