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ARTICLE

Experimental and Statistical Analysis of Fatigue Behavior in Zr-based Bulk Metallic Glass

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Abstract: Three-point bending fatigue experiments were conducted on a typical Zr-based bulk metallic glass (BMG) at ambient temperature to investigate the fatigue behavior under cyclic loading conditions. Results show that the stress amplitude-cycles to failure (*S-N*) curve of the Zr-based BMG is determined, and the fatigue endurance limit is 442 MPa (stress amplitude). To evaluate the probability-stress amplitude-cycles to failure (*P-S-N*) curve, an estimation method based on maximum likelihood was proposed, which relies on statistical principles to estimate the fatigue life of the material and allows for a reduction in the number of samples required, offering a cost-effective and efficient alternative to traditional testing methods. The experimental results align with the American Society for Testing and Materials (ASTM) standard, indicating the reliability and accuracy of this estimation method in evaluating the fatigue behavior of Zr-based BMG.

Key words: bulk metallic glass; *P-S-N* curve; fatigue test; statistical analysis

Bulk metallic glasses (BMGs) have been considered as candidate materials for the structural applications due to their special mechanical properties[1–5]. However, the fatigue performance of these materials often exhibits a significant drop compared to their static mechanical properties, which limits their practical applications as engineering materials[5–7]. Menzel[8–10] reported that damage initiation changes orientation abruptly after reaching a critical length, which has little contribution to the total fatigue life. Fatigue experiments were conducted on the BMGs under different conditions[11–21], including frequencies[13], environments[14–17], loading modes[18–21] and other fatigue enhancement factors[22–25]. Additionally, cyclic accumulated deformation in nano-sized[26] and micro-sized[27] metallic glass was conducted to reveal the origin of the fatigue mechanisms. Highly fatigue-resistant BMGs were obtained with different compositions[28–29]. Obtaining accurate fatigue life is often costly and time-consuming due to numerous complex factors involved in fatigue failure[1–3]. With increasing the complexity and diversity of materials, traditional fatigue testing methods, which often require large sample numbers, may not be feasible or economical. This has led to a growing need for accurate fatigue life prediction methods that can be applied to small samples. Therefore, probability and statistics analysis have been widely utilized in the reliability and life durability estimations of materials[1–2]. These methods enable the consideration of various factors that can affect the fatigue behavior of materials, thereby enabling more accurate predictions and estimations[30–31]. The fatigue life of conventional materials is inherently statistical and influenced by numerous sensitive factors[31–32]. Therefore, accurate prediction of fatigue life requires consideration of these factors and their interactions, which can be challenging. For instance, size effect on the fatigue life has been modeled based on the Weibull distribution for BMGs. The results show that the statistical predictions are consistent with the

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experimental results[33–34]. In order to obtain relatively accurate probability-stress amplitude-cycles to failure (*P-S-N*) curves with fewer samples, some investigations have been conducted on the statistical method. The stress amplitude-cycles to failure (*S-N*) curves of BMGs have been predicted by statistical methods for a series of BMGs[35].

In this study, comprehensive fatigue experiments were conducted on the $Zr_{40}Ti_{25}Cu_8Be_{27}$ BMG[36–40] to assess its fatigue life. To evaluate the *P-S-N* curve, an estimation method based on maximum likelihood (ML) was proposed to estimate the fatigue life of the material relied on statistical principles, which can reduce the number of samples required and offer a cost-effective and efficient alternative to traditional testing methods. The *P-S-N* curve estimation method has been optimized through the experimental analysis, utilizing a three-parameter non-linear function of the *S-N* curves and fatigue life data[41].

1 Experiment and Statistical Methods

1.1 Fatigue test experiments

The $Zr_{40}Ti_{25}Cu_8Be_{27}$ BMG plates (2 mm×10 mm×70 mm) were developed with glass transition temperature T_g=578 K and wide supercooled liquid region ΔT=129 K, as reported in Ref.[36−40]. The amorphous characteristic of specimens was verified by X-ray diffraction (XRD, D8, Bruker AXS Gmbh, Germany) and differential scanning calorimetry (DSC, Pekin Elmer, DSC-7). Specimens for fatigue testing were machined directly from these ingots. Rectangular smooth beams, with thickness B=2 mm and width W=2 mm, were tested by three-point bending test with the span S_L=16 mm. Specimens were polished carefully on the four surfaces and the corners were slightly rounded to reduce the stress concentration. Stress life fatigue tests were performed on the Bose ElectroForce 3330 fatigue testing machine in air to obtain the *S-N* curve and 10^7-cycle fatigue endurance strength for the BMG. Loads were applied under load control at a constant frequency of 25 Hz (sine wave) and a fixed stress ratio R of 0.1 ($R=\sigma_{min}/\sigma_{max}$). Stresses ($\sigma$) on the tensile surface were calculated by the beam mechanics theory dependent on the applied stress $\sigma = 3PS_L/(2BW^2)$. The loading cycles to failure N_f were plotted as a function of the stress amplitude σ_a, defined as the average stress between the maximum and minimum values, i. e., $\sigma_a=(\sigma_{max}-\sigma_{min})/2$, at a fixed stress ratio R of 0.1.

1.2 *P-S-N* curve estimation method

The maximum likelihood estimation (MLE) method is a commonly used parameter estimation method in statistics[31]. It estimates the values of unknown parameters by maximizing the likelihood function of the target variables. The MLE method has many advantages, for example, it is a relatively simple and intuitive estimation method that can be applied to various statistical models. It also possesses good statistical properties such as consistency and asymptotic normality. In practical applications, the MLE method is widely used in various fields, including regression analysis, survival analysis, time series analysis, etc. Drawing from experimental results, a ML method for estimating *P-S-N* curves was proposed in this work. As shown in the inset of Fig.1, at each stress level σ_i (i=1, 2, ⋯, n), fatigue life N_i can be obtained. The fatigue limit of the BMG, defined as the endurance strength at 10^7 cycles with R=0.1, is approximately 442 MPa. This exceptional fatigue resistance highlights its potential for structural applications where durability and longevity are crucial.

A group of specimens were tested under the reference stress σ_r, which is chosen in the range of 10^3–10^5 cycles. The fatigue life data obtained from tests were then used to estimate the *P-S-N* curve. This curve estimation method is based on a three-parameter non-linear function of the *S-N* curves and utilizes fatigue life data to provide a more accurate and robust estimate. Then the logarithms of fatigue life of the group specimens could be estimated from the mean and standard deviation of the reference group, $\bar{\mu}_r = \frac{1}{n}\sum \lg N_i$ and $\bar{S}_r = \sqrt{\frac{1}{n-1}\sum(\lg N_i - \bar{\mu}_r)^2}$, respectively. Three-parameter expression for *P-S-N* curves at survival probability p was adopted:

$$\lg N_p = \lg A_p - m_p \lg(\sigma - \sigma_{0p}) \tag{1}$$

where A_p, m_p and σ_{0p} are material constants and N_p is the life with survival probability of p. For p=0.5, the following equation is proposed:

$$\mu(\sigma) = \lg N_{0.5} = \lg A - m \lg(\sigma - \sigma_0) \tag{2}$$

where $\mu(\sigma)$ represents the mean of logarithm of fatigue life at stress level σ. Assuming that the fatigue life is normally distributed, $\lg N_p$ can be calculated by Eq.(3):

$$\lg N_p = \mu(\sigma) - \mu_p S(\sigma) \tag{3}$$

where $S(\sigma)$ is the standard deviation of the $\lg N_p$ under stress level σ; μ_p is the standard normal deviate with survival probability p. μ_p can be determined as the normal distribution when p is given. Combining Eq.(1–3), $S(\sigma)$ can be calculated as follows:

$$S(\sigma) = \frac{1}{\mu_p}\lg\left(\frac{A}{A_p}\right) - \frac{m}{\mu_p}\lg(\sigma - \sigma_0) + \frac{m_p}{\mu_p}\lg(\sigma - \sigma_{0p}) \tag{4}$$

Considering the reference case and assuming $\sigma = \sigma_r$, Eq.(2) and Eq.(4) can be written as follows:

$$\bar{\mu}_r = \lg A - m \lg(\sigma_r - \sigma_0) \tag{5}$$

$$\bar{S}_r = \frac{1}{\mu_p}\lg\left(\frac{A}{A_p}\right) - \frac{m}{\mu_p}\lg(\sigma_r - \sigma_0) + \frac{m_p}{\mu_p}\lg(\sigma_r - \sigma_{0p}) \tag{6}$$

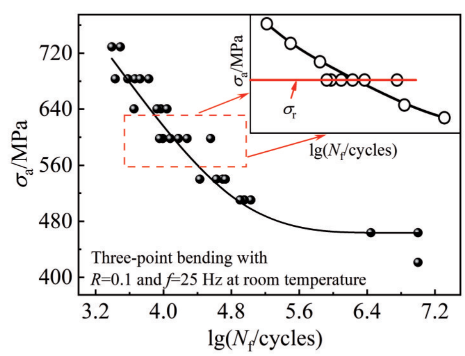

Fig.1 *S-N* curve of the $Zr_{40}Ti_{25}Cu_8Be_{27}$ BMG obtained through three-point bending test at room temperature

Combining Eq.(2), Eq.(5), Eq.(4) and Eq.(6), the following equations can be given:

$$\mu(\sigma) = \bar{\mu}_r + m \lg\left(\frac{\sigma_r - \sigma_0}{\sigma - \sigma_0}\right) \tag{7}$$

$$S(\sigma) = \bar{S}_r + \frac{m}{\mu_p} \lg\left(\frac{\sigma_r - \sigma_0}{\sigma - \sigma_0}\right) + \frac{m_p}{\mu_p} \lg\left(\frac{\sigma - \sigma_{0p}}{\sigma_r - \sigma_{0p}}\right) \tag{8}$$

For the normal distribution, when p=0.841 and μ_p=1.0, replace the subscript p by 1. Eq.(8) can be rewritten as:

$$S(\sigma) = \bar{S}_r + m \lg\left(\frac{\sigma_r - \sigma_0}{\sigma - \sigma_0}\right) + m_1 \lg\left(\frac{\sigma - \sigma_{01}}{\sigma_r - \sigma_{01}}\right) \tag{9}$$

Assuming that the fatigue life under any stress level is normally distributed, the probability density function of the fatigue life can be expressed as:

$$f(\lg N_f) = \frac{1}{\sqrt{2\pi}\, S(\sigma_i)} \exp\left\{ -\frac{\left[\lg N_i - \mu(\sigma_i)\right]^2}{2S^2(\sigma_i)} \right\} \tag{10}$$

The likelihood function with n independent events can be written as:

$$L = \prod_{i=1}^{n} f(\lg N_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\, S(\sigma_i)} \exp\left\{ -\frac{\left[\lg N_i - \mu(\sigma_i)\right]^2}{2S^2(\sigma_i)} \right\} \tag{11}$$

Taking the natural logarithms of the both sides of Eq.(11), Eq.(12) is given:

$$\ln L = -\sum_{i=1}^{n} \left\{ \ln\sqrt{2\pi} + \ln S(\sigma_i) + \frac{\left[\lg N_i - \mu(\sigma_i)\right]^2}{2S^2(\sigma_i)} \right\} \tag{12}$$

Substituting Eq.(7) and Eq.(9) into Eq.(12), an explicit form of ln L can be obtained. The ML estimates of m, m_1, σ_0 and σ_{01} can be determined corresponding to the maximum point of ln$L$. Therefore, $\mu(\sigma)$, $S(\sigma)$ and P-S-N curves can be determined from Eq.(7), Eq.(9) and Eq.(3), respectively.

2 Results and Discussion

The stress-life fatigue data (S-N) of the $Zr_{40}Ti_{25}Cu_8Be_{27}$ metallic glass under three-point bending at ambient temperature is shown in Fig. 1. Under three-point bending cyclic loading, shear bands will be formed in amorphous alloys. In these shear bands, the accumulation of free volume leads to the creation of voids. Under tensile stress, voids grow, resulting in stress concentration in these void regions and promoting the initiation of fatigue cracks. As cyclic loading continues, fatigue cracks will propagate. A small plastic zone will form at the crack tip, which serves to blunt the crack tip. However, numerous shear bands and secondary cracks will expand around the crack tip. As a typical case, Fig. 2 shows the fractography results observed by SEM for a specimen fractured at σ_a=640.52 MPa and N_f=8400 cycles. The fractured surface shows three distinct regions: zone I represents the crack initiation, zone II represents the stable crack propagation, and zone III denotes the final unstable fracture, as shown in Fig.2a. The fatigue crack initiates from the tensile-stressed-side surface of the specimen, i. e. zone I. Fig. 2b shows the tension stressed and compression stressed side coexisted in the fractured surface. As shown in Fig. 2c, representative uniform fatigue striations, vertical to the crack growth direction, are observed on the fracture surface, which indicates the stable crack growth. When the crack is propagated, the deformation is accumulated on the surface of specimen. If the deformation increases to a critical size,

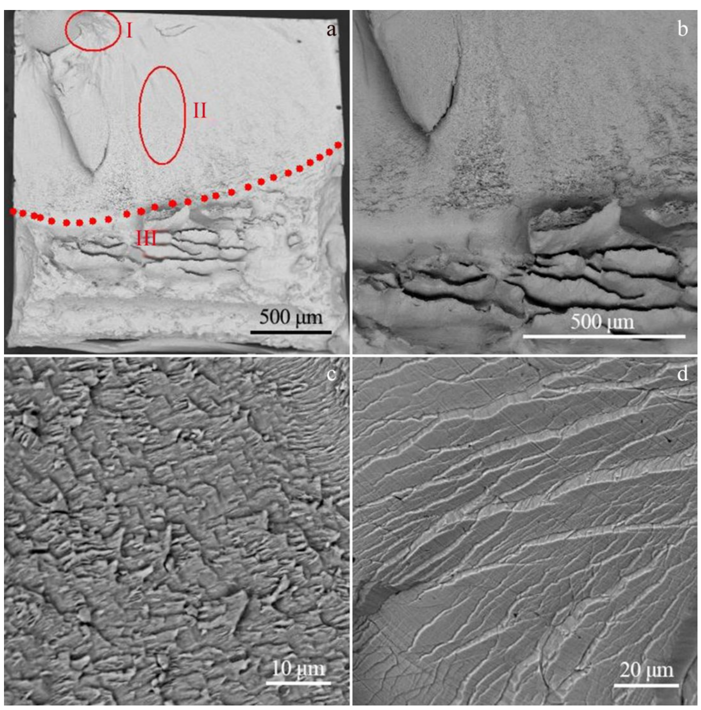

Fig.2 SEM micrographs of the fatigue morphologies of BMG at a stress amplitude of σ_a=640.52 MPa after 8400 cycles: (a) entire fatigue fractography including fatigue crack initiation site (zone I), stable fatigue crack growth (zone II) and fast fracture (zone III); (b) tension and compression regions; (c) close-up view of zone II; (d) accumulated deformation from the side perspective

catastrophic fracture occurs, as shown in Fig.2d.

For the purpose of comparison between the developed ML method and direct method from American Society for Testing and Materials (ASTM)[43], the test data are divided into two sets. One set is arranged according to the direct method from ASTM, and the other is arranged by the proposed ML method. Both sets of fatigue data are listed in Table 1 and Table 2, which are the same as results given in Fig.1.

P-S-N curves can be obtained directly from the test results in Table 1 according to the ASTM[40]. When p=0.841,

Table 1 Stress and fatigue life data of the $Zr_{40}Ti_{25}Cu_8Be_{27}$ metallic glass tested under three-point bending with R=0.1 and f=25 Hz

σ_a/MPa	Test number	N_f/cycles	$\lg N_f$	Mean	Standard deviation
729	2	3 100	3.49	3.44	0.07
		2 460	3.39		
683.5	5	6 700	3.83	3.64	0.15
		2700	3.43		
		4 600	3.66		
		5 300	3.72		
		3 800	3.58		
640.5	4	4 500	3.65	3.90	0.17
		9 300	3.97		
		8 400	3.92		
		11 000	4.04		
598.2	6	9 800	3.99	4.17	0.22
		9 000	3.95		
		36 000	4.56		
		19 000	4.28		
		15 000	4.18		
		12 000	4.08		
540.2	4	49 800	4.70	4.62	0.14
		53 600	4.73		
		42 000	4.62		
		26 800	4.43		
510.6	3	107 000	5.03	4.97	0.06
		89 600	4.95		
		80 000	4.90		
463.8	2	2.787×10^6	6.45	6.72	0.39
		10^7	7		
421.4	1	10^7	7	7	0

Table 2 Stress and fatigue life data of the $Zr_{40}Ti_{25}Cu_8Be_{27}$ metallic glass with the proposed ML method

σ_a/MPa	Test number	Cycles to failure	Logarithm of fatigue life
729	1	2 460	3.39
683.5	1	6 700	3.83
640.5	1	4 500	3.65
598.2 (σ_r)	6	9 800	3.99
		9 000	3.95
		36 000	4.56
		19 000	4.28
		15 000	4.18
		12 000	4.08
540.2	1	49 800	4.70
510.6	1	107 000	5.03

$\lg N_{0.841}(\sigma) = \mu(\sigma) - S(\sigma)$, in the ASTM[42–43], the double log scale of the linear *S-N* curve is recommend as follows:

$$\lg N = a + b \lg \sigma \tag{13}$$

where a and b are materials constants. Linearly fit Eq.(13) to evaluate $\lg N_{0.5}$ and $\lg N_{0.841}$:

$$\lg \mathrm{N}_{0.50} = 29.3182 - 9.05 \lg \sigma \tag{14}$$

$$\lg N_{0.841} = 29.4194 - 9.17 \lg \sigma \tag{15}$$

Because the logarithm of fatigue life obeys a normal distribution:

$$S = \lg N_{0.50} - \lg N_{0.841} \tag{16}$$

The standard deviation of the fatigue life with the stress amplitude can be determined by Eq.(14–16).

As described in the previous section, in Table 1 and Table 2, σ_r=598.2 MPa, $\bar{\mu}_r$=4.17263 and $\bar{S}_r$=0.22263 are abtained based on the ML method. Combining Eq.(7), Eq.(9) and Eq.(12), the maximum point of Eq. (12) can be obtained by the genetic algorithm with m=3.2039, m_1=1.9972, σ_0=424.74 and σ_{01}= 453.74. Substituting the values into Eq. (7) and Eq. (9), the following equations can be obtained:

$$\mu(\sigma) = 11.3471 - 3.2039\lg(\sigma - 424.74) \tag{17}$$

$$S(\sigma) = 3.0834 - 3.2039\lg(\sigma - 424.74) + 1.9972\lg(\sigma - 453.74) \tag{18}$$

The mean and standard deviation of the fatigue life can be determined from Eq. (17) and Eq. (18). The fatigue life with arbitrary survival probability p can be obtained by Eq.(3), for instance, when p=0.841, $\lg N_{0.841}(\sigma) = \mu(\sigma) - \mu_{0.841}\sigma(\sigma) = \mu(\sigma) - S(\sigma)$, i.e., $\lg N_{0.841}(\sigma) = 8.2637 - 1.9972\lg(\sigma - 453.74)$.

Corresponding the two statistical methods and experimental results, Table 3 and Table 4 show a comparison of the fatigue life with survival probability p=0.50 and p=0.841, respectively. It is noteworthy in Fig. 3 and Fig. 4 that despite the smaller test specimen number for the developed ML approach, reasonably accurate results are still obtained compared to both experimental data and the ASTM method. This finding highlights the potential of the developed ML method as a valid and efficient alternative for determining *P-S-N* curves, especially at both ends of the S-N curve. As shown in Fig. 3 and Fig. 4, the difference between the ASTM method and experimental results is close to the predictions of the proposed method. It is mentioned that ML method exhibits the correct asymptotic behavior at the extremes compared with ASTM method. When the fatigue life approaches 0, the strength predicted by the ML method aligns closely with the uniaxial strength. In contrast, the strength predicted by the ASTM method falls significantly below the ultimate strength, regardless of the survival probabilities. This observation highlights the superiority of the ML method in capturing the material's behavior under fatigue conditions. The more accurate predictions of ML method enable a more precise assessment of material performance and reliability, which is crucial for ensuring the durability and safety of structures, as can be seen in Fig. 3 and Fig. 4. In addition, when the fatigue life tends to infinite cycles, the ASTM shows no endurance limit stress and ML method asymptotically reaches the endurance limit stress, as shown in Fig. 3 and Fig. 4. From Table 3, Table 4, Fig. 3 and Fig. 4, it indicates that the developed ML and the ASTM methods give similar *P-S-N* curve in the range from 10^3 to 10^5 cycles. In terms of practical applications, the ML method excels beyond the limitations of the ASTM method. Specifically, the fatigue endurance limit, which is common among most materials, can be more accurately determined by ML approach. Similarly, the ultimate strength, another critical material property, can also

Table 3 Comparison of the logarithm of fatigue life obtained through two theoretical methods and experimental results at p=0.50

σ_a/MPa	Test results	ASTM	Error for ASTM/%	MLE	Error for MLE/%
729	3.44	3.41	-0.89	3.39	−1.46
683.5	3.64	3.66	0.53	3.62	−0.77
640.5	3.90	3.92	0.57	3.87	−0.71
598.2	4.17	4.19	0.36	4.17	-5.2×10^{-4}
540.2	4.62	4.59	−0.67	4.74	2.58
510.6	4.97	4.81	−3.05	5.15	3.83

Table 4 Comparison of the logarithm of fatigue life obtained through two theoretical methods and experimental results at p=0.841

σ_a/MPa	Test results	ASTM	Error for ASTM/%	MLE	Error for MLE/%
729	3.37	3.27	−3.10	3.39	0.62
683.5	3.49	3.52	0.77	3.54	1.50
640.5	3.73	3.78	1.44	3.73	2.4×10^{-4}
598.2	3.95	4.05	2.60	3.95	3.0×10^{-4}
540.2	4.48	4.46	−0.56	4.39	−1.98
510.6	4.89	4.68	−4.36	4.76	−2.82

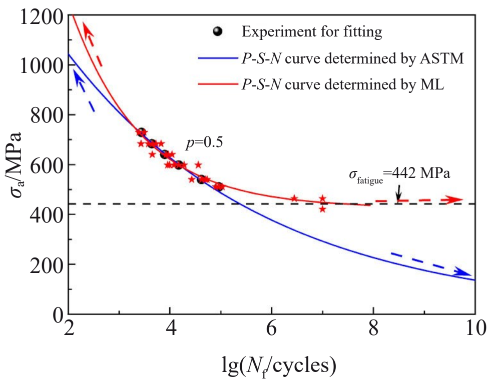

Fig.3 Comparison of *P-S-N* curves determined by the ASTM and developed ML methods under survival probability p=0.50 (the red star marks the experimental data for verification)

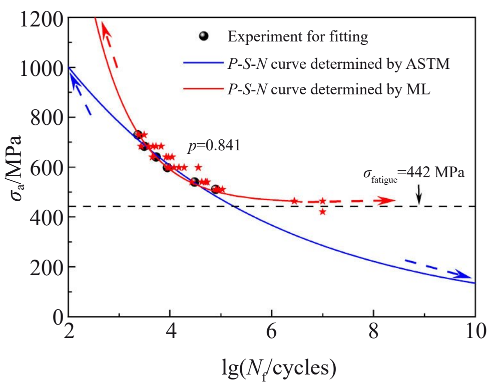

Fig.4 Comparison of *P-S-N* curves obtained by the ASTM method and the developed ML method under survival probability of p =0.841 (the red star marks the experimental data for verification)

benefit from the predictive capabilities of ML method. The reduction in specimen number offers significant cost savings and allows for a more comprehensive analysis of material behavior across a broader range of stress levels and conditions. Overall, the ML method offers a versatile and efficient tool for materials scientists and engineers, enabling them to make informed decisions in material selection, design and application[44].

In practical scenarios, constrained by experimental conditions and time, it is often limited to small sample sizes for fatigue test data, posing significant challenges for accurate fatigue life prediction. To address this problem, statistical methods such as MLE are integrated into this fatigue life prediction framework. MLE is a powerful technique that leverages sample data to estimate model parameters by maximizing the likelihood function. In the context of fatigue life prediction, MLE is used to estimate the parameters of the fatigue life distribution, enabling the establishment of the relationship between reliability and lifespan at a given stress level. Specifically, a likelihood function is constructed based on the small sample fatigue test data. Through steps such as logarithmization and derivation, the parameter values are identified as the ones that maximize the likelihood function. These parameter values not only reflect the distribution characteristics of fatigue life but also provide a basis for plotting fatigue life curves.

The significance of small sample fatigue life prediction lies in its ability to deliver relatively accurate predictions with limited experimental data. This is crucial for guiding the design, optimization and maintenance of mechanical components. Additionally, this approach reduces experimental and time costs and enhances efficiency. The advantages of MLE are particularly noteworthy in this study. By leveraging the ML principle, it enables us to extract meaningful information from even small datasets, providing robust and reliable parameter estimates. This, in turn, enhances the accuracy and precision of fatigue life predictions, which are crucial for making informed decisions in mechanical engineering applications.

Moreover, it should be mentioned that the ASTM method requires at least 27 specimens, whereas the ML approach only utilizes 11 specimens. This significant reduction in the number of specimens required for the ML method results in considerable experimental cost savings. It is essential to point out that the proposed ML method assumes that the statistical nature of fatigue life data remains consistent across various stress levels in the experiments. Therefore, further validation is essential for different failure modes and various statistical distributions to ensure the generality of the method. In conclusion, this study demonstrates the potential of MLE method for efficiently predicting the fatigue behavior of Zr-based BMG. The developed method offers a cost-effective and accurate alternative to traditional testing methods, such as the ASTM standard. However, further research is required to validate the method across different materials and failure modes, as well as to investigate its application in other material systems.

3 Conclusions

1) With the help of the experimental and statistical technique, the fatigue behavior of $Zr_{40}Ti_{25}Cu_8Be_{27}$ BMG is investigated. The fatigue endurance limit of this BMG is determined to be impressive 442 MPa. The fatigue morphology features signatures of accumulated plastic deformation, fatigue striation, fatigue crack initiation, propagation and ultimately fast fracture.

2) ML method is introduced to analyze the fatigue behavior. This method utilizes statistical techniques to predict the *P-S-N* curve, which represents the relationship between stress, cycle number and failure probability. The prediction of the ML method is in good agreement with the experimental data. A significant advantage of this approach is the reduced number of specimens required, offering a more efficient and cost-effective alternative to the standard ASTM method.

3) The current work contributes to an understanding of the fatigue behavior of BMGs, especially the potential of ML methods in predicting material behavior under cyclic loading conditions.

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Zr基大块金属玻璃疲劳实验与概率寿命预测

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摘　要：对Zr基大块金属玻璃（BMG）进行了室温下三点弯曲疲劳实验，旨在探究其在循环载荷下的疲劳行为。结果表明，根据确定的应力幅度-破坏循环（*S-N*）曲线，Zr基BMG的疲劳极限为442 MPa。为评估*P-S-N*曲线，提出了一种基于最大似然原理的估算方法，利用统计原理预测材料疲劳寿命，减少了所需样本数量，降低了实验成本。实验结果与美国测试和材料协会（ASTM）标准相符，证明了估算方法的可靠性和准确性。

关键词：金属玻璃；PSN曲线；疲劳测试；统计分析

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