Proceedings of the 4th International Conference on Functional Materials and Civil Engineering
DOI: 10.54254/2755-2721/2026.34474

Multiscale Investigation on Interfacial Bonding and Interlaminar Shear Behavior of PAI-Modified CF/PEEK Composites

Linzhe Feng

School of Civil Engineering, Wuhan University, Wuhan, China
2023302101148@whu.edu.cn

Abstract. Carbon fiber reinforced polyether ether ketone (CF/PEEK) composites commonly suffer from weak interfacial bonding and susceptibility to interlaminar shear failure in service. Based on existing experimental and simulation data, this study establishes a multi-scale research framework combining molecular dynamics (MD) for interfacial analysis and mesoscopic finite element method (FEM) for shear simulation. Systematic analysis and discussion are conducted to explore the effects of polyamide-imide (PAI) interfacial modification, fiber volume fraction and ply angle on the interfacial bonding state and interlaminar shear performance of CF/PEEK composites. Molecular dynamics results reveal that the overall interfacial bonding energy of the CF-PAI-PEEK system is higher than that of the CF-PEEK system at various temperatures. At 350 °C under compressive load, shear load and combined load, the interfacial interaction is continuously strengthened with the addition of PAI, and the optimal interfacial bonding performance is achieved under combined loading. Following the loading specifications for specimens stipulated in GB/T 1450.1, a mesoscopic equivalent model consisting of fibers, resin and interfacial cohesive elements is established. By adopting the transversely isotropic constitutive model for carbon fibers, isotropic elastic constitutive model for PEEK and quadratic stress damage criterion for interfaces, the shear responses of laminates with ply angles of 0°, 20° and 90° under different fiber volume fractions are simulated. The simulation results indicate that the equivalent shear strength of the composites increases as the fiber volume fraction rises from 0.60 to 0.70. PAI modification can significantly raise the threshold of interfacial damage and effectively delay delamination failure. Among the three ply structures, the 20° laminate possesses the highest shear strength, while the 90° laminate has the lowest. Only the PAI-modified structures with fiber volume fractions of 0.65 and 0.70 achieve a shear strength of 60 MPa or above, which meets the relevant standard requirements. The findings of this study provide valuable references for the interfacial design and ply optimization of high-performance CF/PEEK composites.

Keywords: CF/PEEK composite, PAI interfacial modification, molecular dynamics, mesoscopic finite element, interlaminar shear, cohesive zone model

© 2026 The Authors. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (https://creativecommons.org/licenses/by/4.0/).

DOI: 10.54254/2755-2721/2026.34474

1. Introduction

Carbon fiber reinforced polyether ether ketone (CF/PEEK) composites combine the high strength and high modulus of carbon fibers with the excellent heat resistance, chemical corrosion resistance and damage tolerance of PEEK resin. Therefore, they have broad application prospects in aerospace, rail transit, lightweight structures of high-end equipment and other fields [1, 2]. Nevertheless, the inherent interfacial compatibility between carbon fibers and PEEK resin is unsatisfactory, leading to poor load transfer capacity at the interface. Under shear loading, interfacial debonding, interlaminar delamination and local failure tend to occur easily, which impair the service reliability of structural components. Previous studies have demonstrated that the failure behaviors of thermoplastic composites are governed not only by the intrinsic properties of fibers and matrix, but also closely related to the bonding quality of interfacial layers, local stress redistribution and ply configurations [3, 4].

Polyamide-imide (PAI) is a polymer with superior heat resistance and high polarity. It can modify the chemical properties of carbon fiber surfaces and optimize the interfacial interaction between carbon fibers and PEEK matrix [5, 6]. Previous experimental results show that adding PAI into the CF/PEEK system brings significant changes to thermal conductivity, dynamic mechanical analysis (DMA) performance and interfacial bonding characteristics, which proves that the interfacial layer exerts a critical impact on the overall performance of composites. However, macroscopic experiments alone can hardly clarify the microscopic mechanism of interfacial enhancement, nor quantitatively elaborate how ply angle and fiber volume fraction affect the shear failure path [7, 8].

Against this research background, this paper develops a multi-scale analysis method integrating molecular dynamics and mesoscopic finite element simulation based on reported experimental phenomena and simulation data. At the molecular scale, the effects of PAI modification on the interfacial bonding energy and structural stability of CF/PEEK are analyzed. At the mesoscopic scale, a finite element model considering the damage evolution of fibers, resin and interfaces is established to compare the interlaminar shear responses and damage evolution laws under different ply angles and fiber volume fractions. On the basis of the above analysis, the mechanism by which PAI interfacial modification improves the shear bearing capacity of CF/PEEK composites is further revealed.

2. Research methods and model establishment

2.1. Multi-scale research scheme

This study adopts a multi-scale approach combining interfacial mechanism identification and mesomechanical response prediction. Molecular dynamics is employed to construct interfacial models of CF/PEEK and CF/PAI/PEEK systems. Interfacial bonding energy is calculated under various temperatures and loading conditions to evaluate the modification effect of PAI on interfacial interaction. Based on the laws of interfacial enhancement, a mesoscopic equivalent finite element model is established on the Abaqus platform. Cohesive elements are used to characterize the behaviors of fiber-resin and fiber-fiber interfaces, and the equivalent stress-strain curves as well as shear strength of different ply structures are obtained.

DOI: 10.54254/2755-2721/2026.34474

2.2. Molecular dynamics model

In accordance with the reported molecular simulation protocols, CF/PEEK and CF/PAI/PEEK models are established respectively. The NVT and NVE ensembles are applied to conduct heating, relaxation and stabilization processes at eight different temperatures, so as to analyze the temperature effect on interfacial bonding conditions. Furthermore, sandwich interfacial models of CF/PEEK/CF and CF/PAI/PEEK/PAI/CF are built at 350 °C. After heating and stabilization, compressive load, shear load and combined compressive-shear load are applied sequentially. Configurations with equivalent pressures around 0.5 MPa, 1.0 MPa and 2.0 MPa are selected to calculate the interfacial bonding energy.

Interfacial bonding capacity is quantified by bonding energy. A higher bonding energy indicates stronger interaction between fiber surface and resin, as well as greater potential for interfacial load transfer. Comparative analysis of bonding energy variations across different systems, temperatures and loading states provides a solid basis for defining interfacial parameters and analyzing failure mechanisms in the mesoscopic model.

2.3. Mesomechanical model

Referring to the loading mode of interlaminar shear specimens specified in GB/T 1450.1, this study adopts a mesoscopic equivalent modeling strategy. Given the extremely small thickness of single carbon fiber plies in actual laminates, direct layer-by-layer macroscopic modeling would result in excessive computational cost. Hence, a representative unit cell is abstracted for the shear-dominated central region of the specimen. The overall model is a cuboid structure (see Figure 1), which is stacked alternately with 10 fiber layers and 10 resin layers along the thickness direction. To investigate the influence of ply angles, three models with typical fiber orientations of 0°, 20° and 90° are established separately (see Figure 2).

In mesh generation, three-dimensional hexahedral solid elements are adopted for fibers and resin matrices. Zero-thickness cohesive elements are arranged at fiber-resin interfaces and between adjacent fiber bundles. Opposite displacement loads are applied on the top and bottom surfaces of the model to simulate interlaminar shear (see Figure 3), which is equivalent to the stress state of the central region with the most significant deformation of standard specimens. Equivalent stress-strain curves of each model are acquired by monitoring the overall reaction force and average strain.

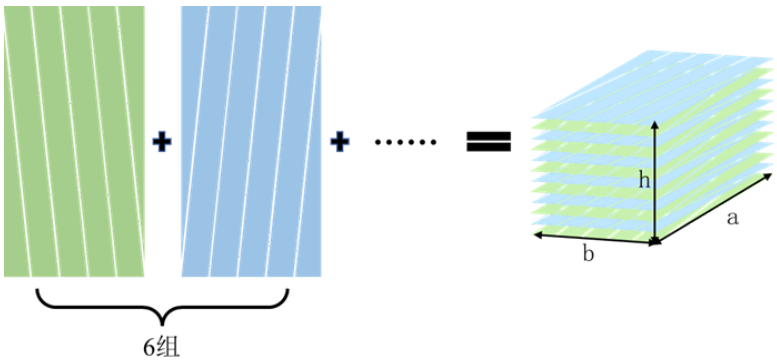

Figure 1. Overall configuration of the model

DOI: 10.54254/2755-2721/2026.34474

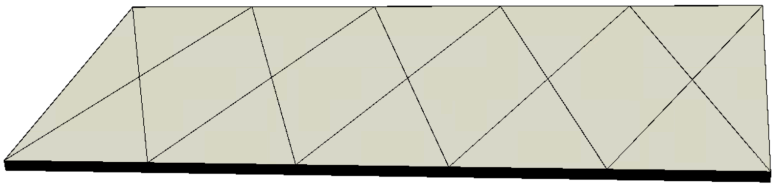

Figure 2. Schematic diagram of ply angles

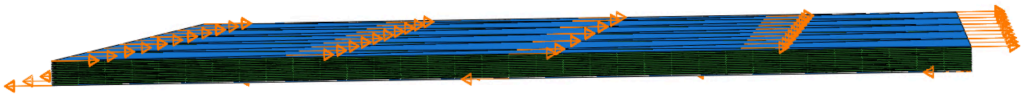

Figure 3. Schematic diagram of applied displacement loads

2.4. Constitutive models and material parameters

PEEK resin is regarded as an isotropic linear elastic material at the macroscopic scale, with an elastic modulus of 3.8 GPa and a Poisson's ratio of 0.40. Carbon fiber is defined by a transversely isotropic constitutive model combined with bilinear plasticity and progressive damage evolution. The three-dimensional Hashin failure criterion is adopted in the post-elastoplastic stage to characterize the failure modes of fibers and matrix. The elastic parameters of the representative carbon fiber applied in the mesoscopic model are listed in Table 1.

The cohesive zone model is adopted to describe interfacial behaviors. The initiation of interfacial damage is judged by the quadratic nominal stress criterion, and linear softening is used to simulate damage propagation. To improve the convergence of numerical calculation, element deletion is realized via secondary development when the interfacial stiffness decreases to a relatively low level. According to reference parameters, the nominal interfacial modulus is set to approximately 2.7 GPa, and the strength parameters related to interfacial damage range from 60 MPa to 110 MPa, which conforms to the empirical feature that the interfacial performance accounts for 70% to 80% of that of the resin matrix. Models with and without PAI modification are distinguished by different interfacial properties and surface characteristics of carbon fibers.

Table 1. Representative material parameters in mesoscopic model

Parameter	Value
E1 / GPa	340
E2 / GPa	15
E3 / GPa	15
υ_{12}	0.20
υ_{13}	0.20
υ_{23}	0.25
G12 / GPa	24
G13 / GPa	24
G23 / GPa	5.03

DOI: 10.54254/2755-2721/2026.34474

3. Results and discussion

3.1. Molecular-scale modulation effect of PAI on interfacial bonding

Molecular dynamics simulation results indicate that the interfacial bonding behaviors of both CF/PEEK and CF/PAI/PEEK systems are highly sensitive to temperature, while their variation trends differ significantly. For the CF/PEEK system, the interfacial bonding energy remains relatively stable when the temperature is below the melting point of PEEK. Once the temperature exceeds the melting point, the mobility of PEEK molecules increases and the interfacial contact becomes more sufficient, leading to a temporary rise in bonding energy. As the temperature further rises beyond the decomposition temperature, partial PEEK molecules escape, resulting in a gradual decline of interfacial bonding energy. In contrast, before the temperature reaches the decomposition temperature of the CF/PAI/PEEK system, new chemical bonds are gradually formed between PAI and PEEK, which strengthens the interfacial interaction. Consequently, the bonding energy increases steadily with rising temperature. Even at higher temperatures, the interfacial bonding energy maintains a relatively high level with only minor fluctuations.

The advantages of PAI modification become more prominent under different loading conditions at 350 °C. For the CF/PEEK/CF system, the interfacial bonding energy rises when the load increases from 0.5 MPa to 1.0 MPa, yet the growth slows down as the load continues to increase to 2.0 MPa, suggesting a plateau effect for interfacial contact enhancement. By comparison, the interfacial bonding energy of the CF/PAI/PEEK/PAI/CF system keeps increasing within the load range of 0.5 MPa to 2.0 MPa, proving that the PAI interlayer can maintain stable interfacial coordination under loading. Moreover, the interaction between interfacial atoms and molecules is more intensive under combined compression and shear loading, and the corresponding bonding energy is higher than that under pure compression or pure shear. The above results demonstrate that PAI not only improves the initial interfacial bonding strength, but also enhances the interfacial stability under complex thermo-mechanical coupling conditions.

3.2. Mesoscopic shear damage evolution under different ply angles

Mesoscopic simulation results show that all models present typical interlaminar shear deformation after reverse displacement loads are applied on the top and bottom surfaces. The displacement distributes in a gradient along the thickness direction: positive displacement gradually decreases in the upper layers, while the absolute value of negative displacement increases in the lower layers. Due to the adoption of interfacial cohesive elements, obvious relative slip occurs between fiber layers and resin layers. After interfacial damage initiates, independent deformation and dislocation take place among fiber bundles.

For the 0° ply structure, stress concentration first emerges at the edges at the initial loading stage, where the stress and strain of outer fibers near boundaries reach the maximum (see Figure 4). With the continuous increase of load, shear stress accumulates rapidly at the fiber-resin interface due to the large difference in elastic modulus between fibers and resin. Eventually, the interfacial elements at the outer interlaminar boundaries fail first. It reveals that although the 0° ply structure can bear shear loads effectively, the interfacial mismatch effect is prominent and tends to induce delamination at boundaries.

At the initial loading stage of the 20° ply structure, high stress is mainly distributed around the boundaries. The fibers are arranged alternately at ±20°, enabling loads to be fully transferred to the intermediate resin layers and adjacent fiber layers (see Figure 5). Strain distribution results show

DOI: 10.54254/2755-2721/2026.34474

that local stress concentration still exists in outer regions, whereas the internal strain field is more uniform and the propagation of interfacial damage is relatively slow. This structure achieves effective collaborative load bearing between rigid fibers and ductile resin, thus delivering higher shear strength and more stable damage evolution.

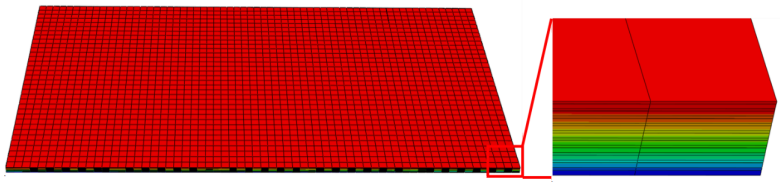

Figure 4. Schematic diagram of loaded specimen with 0° ply angle

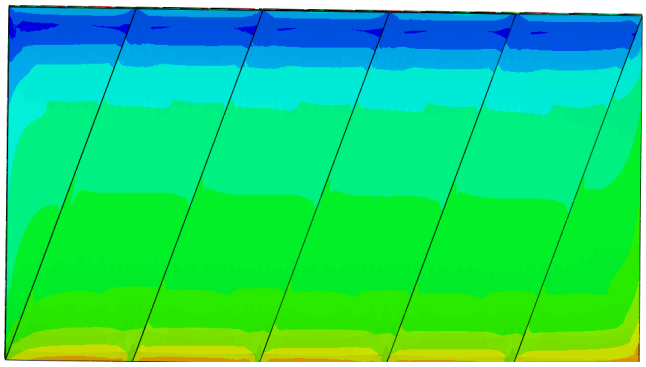

Figure 5. Schematic diagram of loaded specimen with 20° ply angle

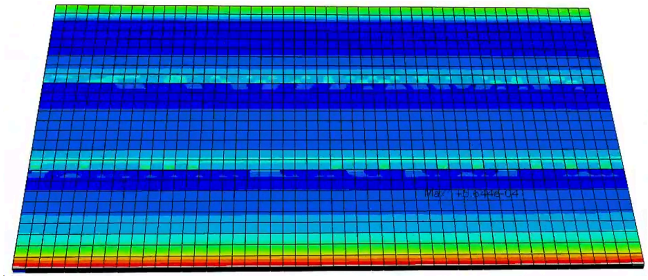

Figure 6. Schematic diagram of loaded specimen with 90° ply angle

For the 90° ply structure, fibers share similar stress levels at the initial loading stage. As deformation develops, interfacial deformation between fibers aligned in the same direction within a single layer increases sharply, and the stress of boundary elements rises continuously. Large lateral deformation of fibers along the loading direction triggers the initiation and gradual propagation of interfacial damage at boundaries, which eventually leads to complete interfacial failure and interlaminar delamination (see Figure 6). Compared with 0° and 20° ply structures, the 90° configuration is more prone to early interfacial failure between fibers, resulting in the lowest overall shear bearing capacity.

3.3. Effects of fiber volume fraction and PAI modification on equivalent shear strength

A comparative analysis of models with fiber volume fractions of 0.60, 0.65 and 0.70 shows that the equivalent shear strength of the composites increases with the rise of fiber volume fraction regardless of ply angles. This trend is fundamentally attributed to the much higher elastic modulus

DOI: 10.54254/2755-2721/2026.34474

of carbon fiber compared with PEEK resin. A higher fiber content improves the overall stiffness of the composite, enabling it to withstand greater stress under equivalent shear strain.

Comparisons between specimens with and without PAI modification verify that PAI can effectively enhance the equivalent shear strength of all ply structures. The main reason is that PAI optimizes the interfacial compatibility between carbon fiber surface and PEEK matrix, increases interfacial fracture strength and damage resistance, and delays interfacial failure until a higher strain level is reached. The equivalent stress-strain curves indicate that modified and unmodified groups share similar variation trends. Nevertheless, the PAI-modified group presents obvious advantages in peak stress and damage initiation threshold. In addition, the simulated curves are well consistent with experimental ones in overall trends, which proves that the established mesoscopic model can accurately reflect the actual loading process of the composite.

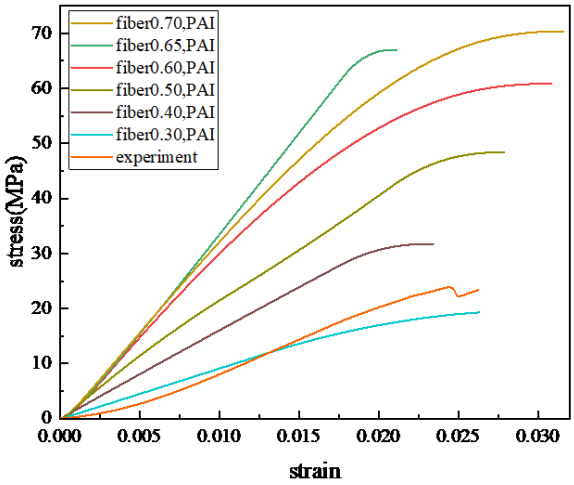

Figure 7. Comparison diagram of 0° ply structure with PAI modification

3.4. Mechanism analysis and engineering implications

Combined with the results from molecular and mesoscopic analyses, the performance improvement of CF/PEEK composites via PAI modification follows a progressive mechanism: enhanced interfacial bonding, delayed damage propagation and elevated overall load-bearing capacity. Molecular dynamics results confirm that PAI increases interfacial bonding energy and improves interfacial stability under high temperature and loading conditions. Mesoscopic simulation further verifies that the reinforced interface restrains relative slip and delamination failure, allowing the high-modulus characteristic of carbon fibers to be fully exerted.

Ply structure exerts a remarkable effect on shear performance. The 20° ply structure achieves the highest shear strength, indicating that a moderate fiber deflection facilitates coordinated energy dissipation and load redistribution between fibers and resin. The shear strength of the 0° ply structure is relatively lower, while the 90° ply structure is most likely to suffer overall failure due to local interfacial damage. For engineering applications, moderate-angle ply combined with interfacial enhancement is recommended on the premise of manufacturability, so as to balance structural strength and damage tolerance.

DOI: 10.54254/2755-2721/2026.34474

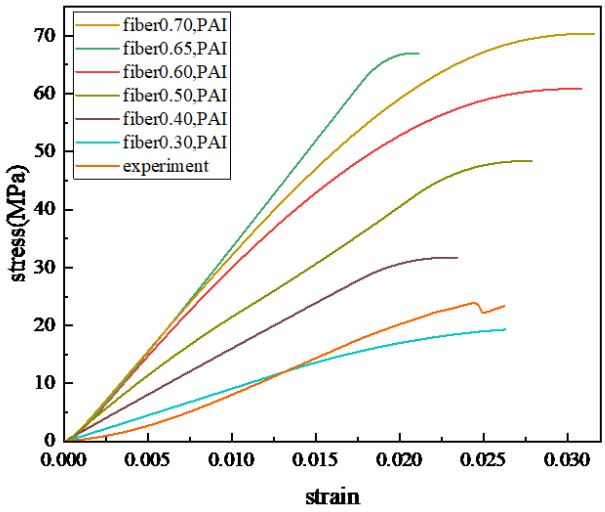

Figure 8. Comparison diagram of 20° ply structure with PAI modification

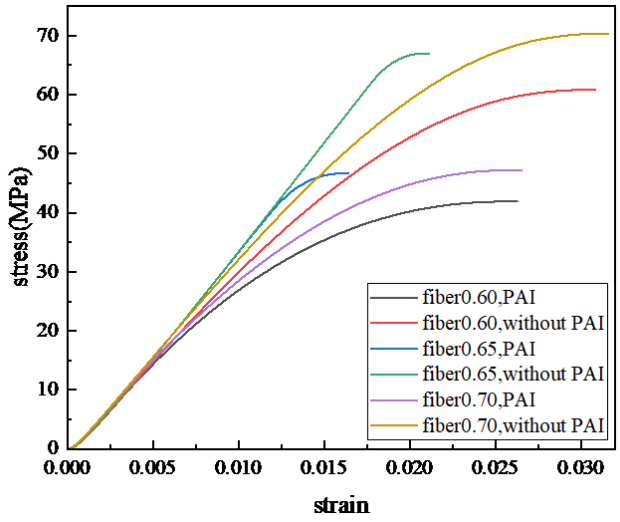

Figure 9. Comparison of 90° layup angles with and without PAI

It is worth noting that only the PAI-modified models with fiber volume fractions of 0.65 and 0.70 attain a shear strength of 60 MPa or above that complies with relevant standards, as illustrated in Figure 7, Figure 8 and Figure 9. Therefore, for the design of CF/PEEK structures dominated by interlaminar shear performance, both the minimum fiber volume fraction and interfacial modification strategy should be taken into consideration. Performance improvement cannot rely merely on increasing fiber content.

4. Conclusion

1. Molecular dynamics results show that the CF-PAI-PEEK system has higher overall interfacial bonding energy than the CF-PEEK system. At 350 °C under various loading conditions, the PAI-modified interface maintains stronger and more stable interfacial interaction, with the most prominent bonding performance observed under combined compression and shear loading.

DOI: 10.54254/2755-2721/2026.34474

2. Mesoscopic finite element simulation reveals that the equivalent shear strength of laminates with ply angles of 0°, 20° and 90° rises continuously as the fiber volume fraction increases from 0.60 to 0.70. PAI modification raises the threshold of interfacial damage and delays delamination failure, thereby improving the overall shear bearing capacity.

3. Among the three typical ply structures, the 20° laminate presents the highest shear strength, followed by the 0° laminate, and the 90° laminate has the lowest value. The 20° ply structure facilitates the synergistic effect of fiber stiffness and resin ductility, and reduces the risk of premature local interfacial failure.

4. In accordance with relevant standard requirements, only the structures with fiber volume fractions of 0.65 and 0.70 after PAI modification achieve a shear strength of 60 MPa or above. It demonstrates that PAI interfacial modification and rational ply design are effective approaches to enhance the interlaminar shear performance of CF/PEEK composites.

References

[1] Hashin Z. Failure criteria for unidirectional fiber composites [J]. Journal of Applied Mechanics, 1980, 47(2): 329-334.

[2] Chamis C C. Simplified composite micromechanics for predicting microstresses [R]. NASA Technical Memorandum 87295, 1986.

[3] Naghipour P, Bartsch M, Voggenreiter H. Simulation and experimental validation of mixed mode delamination in multidirectional CF/PEEK laminates under fatigue loading [J]. International Journal of Solids and Structures, 2011, 48(6): 1070-1081.

[4] Hojo M, Ochiai S, Gustafson C G, et al. Effect of matrix resin on delamination fatigue crack growth in CFRP laminates [J]. Engineering Fracture Mechanics, 1994, 40(1): 35-47.

[5] Aymerich F, Found M S. Response of notched carbon/PEEK and carbon/epoxy laminates subjected to tension fatigue loading [J]. Fatigue and Fracture of Engineering Materials and Structures, 2000, 23(8): 675-683.

[6] Shrestha R, Simsiriwong J, Shamsaei N. Mean strain effects on cyclic deformation and fatigue behavior of polyether ether ketone (PEEK) [J]. Polymer Testing, 2016, 55: 69-77.

[7] Sobieraj M C, Murphy J E, Brinkman J G, et al. Notched fatigue behavior of PEEK [J]. Biomaterials, 2010, 31(35): 9156-9162.

[8] Standardization Administration of China. (2005). GB/T 1450.1–2005: Test method for interlaminar shear strength of fiber-reinforced plastics [Standard]. Standards Press of China.