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Analysis of Crack Propagation in Carbon Nanotube Reinforced Magnesium Based Composites Under Tensile Load

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ABSTRACT

This article mainly conducts numerical simulations on the crack propagation of carbon nanotube reinforced magnesium based composites during uniaxial tensile failure. Selecting the cross-section of a representative carbon nanotube reinforced magnesium based composite material model as the research object, the model was loaded in multiple load steps using ANSYS finite element software, and the location and propagation path of cracks were discussed. It was found that cracks first appeared at the interface between carbon nanotubes and magnesium matrix; The direction of crack propagation is perpendicular to the direction of the load, which is called vertical crack propagation; As the load step gradually increases, the crack propagation speed gradually increases, especially when two parallel vertical cracks overlap, the crack propagation speed becomes more significant; Throughout the entire crack propagation process, the matrix has the most damaged units.

KEYWORDS

Magnesium based composite materials; Stretching; Crack propagation

1. INTRODUCTION

Magnesium based composite materials have excellent physical and mechanical properties [1-3], making them widely used in many fields. However, their low elastic modulus affects their application in the field of structural materials. However, the mechanical properties of magnesium based composite materials can be improved by adding reinforcing phases to compensate for their shortcomings. At present, scholars have extensively discussed carbon nanotubes, silicon nanotubes, and graphene as reinforcing phase materials [4, 5]. The application research of other reinforcement materials on metal matrix composites is also widely carried out. Li Xiaotong et al. [6] predicted the mechanical properties of hybrid SiC particle reinforced aluminum matrix composites through experiments, simulations, and convolutional neural network models. Han Dongya [7] discussed the interface microstructure and interface properties of Al based composites under the influence of interface modification layers, and studied the interface dominated fracture behavior through tensile and compression experiments on Al based composites. Ma Junchi [8] conducted a simulation study on the mechanical behavior of ultrafine grained particle reinforced aluminum/magnesium based composites, including an analysis of the mechanism of crack generation and propagation. The study found that fine cracks first appeared around the particles, and then gradually merged with other nearby fine cracks to form a main crack. The further propagation of the main crack led to macroscopic fracture of the composite material.

The elastic modulus of carbon nanotubes can reach about 1Tpa [9], which is about 5 times that of steel. Carbon nanotubes have high tensile and compressive strengths, ranging from 11-63 GPa and 100-170 GPa respectively [10], making them excellent reinforcing phase materials. Therefore, this papter uses carbon nanotube reinforced magnesium based composite materials to establish a three-dimensional random distribution model, and further discusses the crack propagation of the material during the failure process under axial tensile load. The discussion results of numerical simulation provide a theoretical basis for the application of nano reinforcement in the field of composite materials.

2. MODEL ESTABLISHMENT AND PARAMETER SELECTION

This paper presents a three-dimensional random placement program for hollow cylinders in microelements, developed using the APDL secondary development function of ANSYS software. Establish a model of carbon nanotube reinforced magnesium based composite material, simulate uniaxial tensile crack propagation on all surfaces, select single-walled carbon nanotubes with an inner diameter of 3nm, an outer diameter of 5nm, a length of 10nm, and a magnesium matrix size of 100nm. Select the cross-sectional view of a representative carbon nanotube reinforced magnesium based composite material model as the model for studying crack propagation, as shown in Figure 2.1. The parameter selection of the material is: Material 1 is Mg matrix parameter [11]: elastic modulus E_{Mg}=44GPa, Poisson's ratio V_{Mg}=0.35; Material 2 uses carbon nanotubes as reinforcement material with parameters [12]: elastic modulus E=523.4GPa, Poisson's ratio V=0.165.

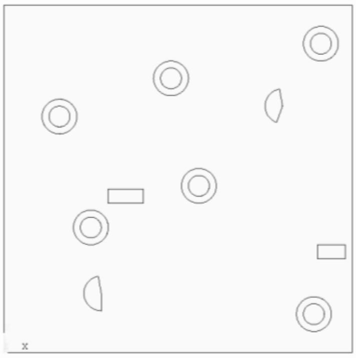


Figure 2.1. The model of carbon nanotubes in random distribution

3. RESULTS ANALYSIS

3.1. Loading Method

This paper uses the maximum tensile stress criterion to determine whether the element has failed and whether cracks have propagated. Assuming that the factor causing material fracture is the maximum tensile stress, when the maximum tensile stress σ_1 at any point in the material reaches the corresponding ultimate stress σ_b, the material will undergo brittle fracture. The condition for the hazardous point of the material to fracture and fail under complex stress states is that $\sigma_1 \geq \sigma_b$. The main application of ANSYS software's element birth and death function for structural analysis is to fix one side along the Y-axis direction in the X, Y, and Z directions, and apply uniaxial tension to the opposite side of that side. The simulation process uniformly and continuously loads the load onto the model, and in order to simulate the loading method of the experiment more realistically, a multi-step loading method is used. In order to achieve better simulation results, the Smartsize option is first used to control the accuracy to 1 for free mesh division, and then the Refine at option is applied to refine the mesh. The mesh division diagram is shown in Figure 3.1.

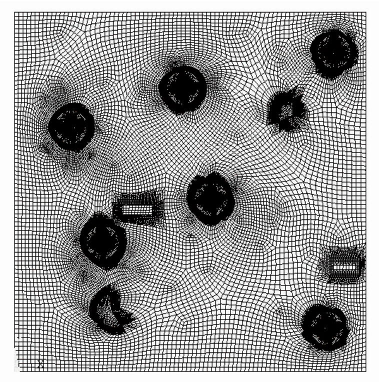
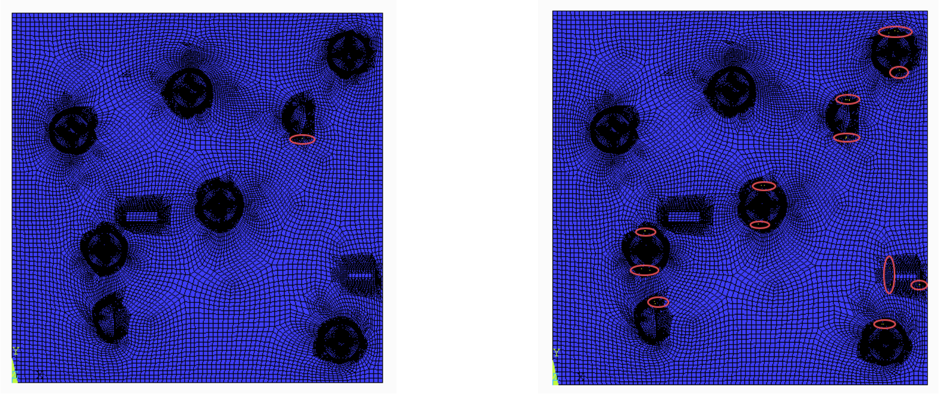


Figure 3.1. Grid partition

Based on reference [13], this article develops an APDL command stream to load the model and simulate crack propagation. In the program, load steps are used to implement loading, and Do loop statements are applied to achieve complex command repetition.

3.2. Result Analysis

In order to observe the crack propagation process more accurately, the analysis results of representative load steps in the simulated crack propagation process of various model sections of carbon nanotube reinforced magnesium based composite materials were selected. Figures 3.2, 3.5, and 3.6 show the crack nucleation stage, crack propagation stage, and crack fracture stage path diagrams of the model sections, respectively. During the tensile fracture process of composite materials, there are mainly two fracture modes: one is that the reinforcement body first experiences crack fracture, and the other is that the matrix first experiences crack fracture. When the crack propagates to the reinforcement body, the direction of crack propagation changes and deflects, resulting in interface separation between the reinforcement body and the matrix. According to reference [14], the stress distribution near carbon nanotubes is extremely uneven, and carbon nanotubes bear significant stress due to the different mechanical properties at the interface between carbon nanotubes and the matrix. During the tensile fracture process of carbon nanotube reinforced magnesium based composites, carbon nanotubes themselves have high elastic modulus and excellent mechanical properties, so carbon nanotubes are relatively less prone to fracture compared to magnesium matrix. Therefore, the fracture mode of carbon nanotube reinforced magnesium based composites is mainly in the form of debonding between the magnesium matrix and the interface.



(a) Step 5 unit

(b) Step 9 unit

Figure 3.2. Cloud diagram of the first principal stress during crack nucleation stage of model

From the crack nucleation stage of the model in Figure 3.2, it can be seen that when the load reaches step 5, a crack point is initiated, as shown in the circle in Figure 3.2 (a). When the load reaches step 9, the number of crack points gradually increases and all initiate near the interface between carbon nanotubes and magnesium matrix, indicating that the first principal stress is highest and most dangerous near the interface between the reinforcement and matrix.

To predict the crack propagation path and direction of the model, 10 key points were established on one side and set as paths based on the crack point initiated after the 9th loading step. The crack propagation was analyzed based on the distribution of the first principal stress on the path. Two paths were established on the model as shown in Figure 3.3, and the first principal stress distribution curve on the path is shown in Figure 3.4.

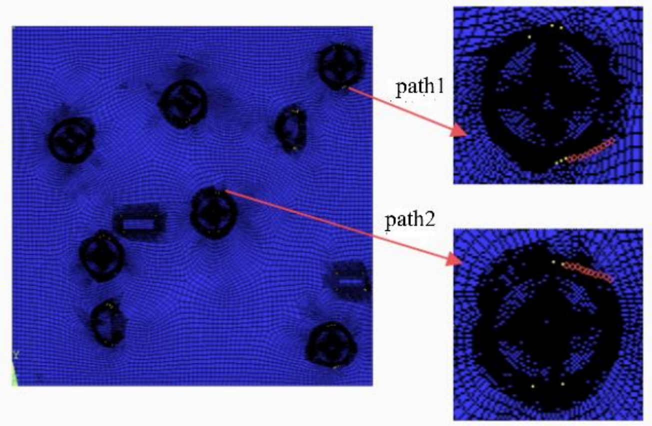
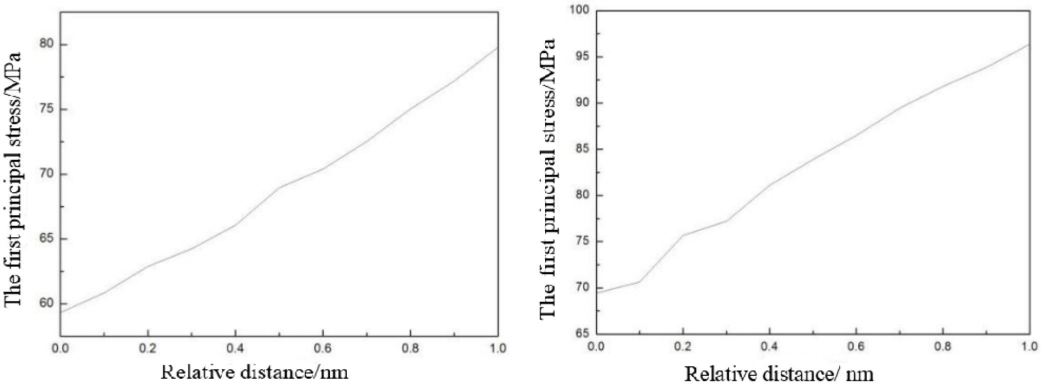


Figure 3.3. The two paths on model

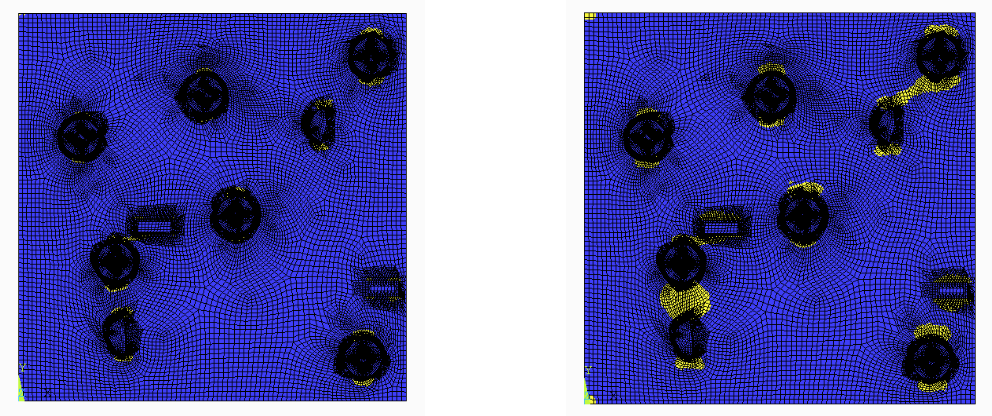


(a) Path1 (b) Path2

Figure 3.4. The first principal stress distribution corresponding to two paths on model

From Figures 3.3 and 3.4, it can be seen that both paths establish key points on one side of the crack initiation point. The first principal stresses at the initiation point are 59.34 MPa and 69.43 MPa, respectively. As the relative distance increases, the first principal stresses gradually increase linearly, reaching their maximum values of 79.79 MPa and 96.35 MPa at a relative distance of 1.0 nm. It can be inferred that near the interface between these two carbon nanotubes and the magnesium matrix, cracks are highly likely to propagate along the direction of these two paths until they break.

According to the crack propagation stage of the model in Figure 3.5 (a), it can be seen that when the load step reaches step 13, the crack propagates from the point of initiation to a single crack; When loaded to step 14, the cracks became clearer and were located near the interface between the carbon nanotubes and the reinforcement, and it was known that the direction of crack propagation was consistent with the previously predicted results. The crack propagation speed at this stage is significantly increased compared to the crack nucleation stage, and the crack propagation direction gradually expands on both sides perpendicular to the direction of the applied load, that is, the vertical crack. According to the crack fracture stage of the model in Figure 3.5 (b), it can be seen that when the load step reaches step 15, the two vertical cracks between the two carbon nanotubes that are closer together begin to coincide. By step 16, the cracks have completely overlapped and rapidly expanded, that is, the cracks near the interface between the carbon nanotubes and the magnesium matrix have expanded to cause material fracture and failure. It can be clearly seen that the crack propagation speed is faster in the fracture stage.



(a) Step 14 of crack propagation stage (b) Step 16 of Crack fracture stage

Figure 3.5. Cloud diagram of the first principal stress

The crack propagation criterion applied in this article is the first principal stress criterion. Based on the mode of crack propagation, it can be inferred that stress concentration is likely to occur on the upper and lower sides of the interface between the reinforcing body and the matrix perpendicular to the loading direction, as the crack undergoes vertical propagation during its formation. As the crack propagates, the stress distribution changes. When the crack begins to form, the stress distribution in the area near the crack is relatively small. When two vertically parallel cracks coincide, the range of the area with smaller stress distribution increases. This is because after the crack appears, the elements at the fracture site no longer transmit stress, so as the crack propagation intensifies, the area with smaller stress distribution gradually increases, the number of fractures in the matrix elements increases, and the cracks gradually overlap and penetrate, ultimately leading to material failure. This is consistent with the experimental conclusion obtained in reference[15] that the hindering effect of carbon nanotubes on cracks causes the matrix with lower diffusion resistance to turn and ultimately fracture. The model selection and simulation calculation in this article are reasonable.

From the perspective of micromechanics, when the carbon nanotube reinforced magnesium matrix composite material is subjected to a load as a whole, stress is transmitted to the carbon nanotubes through the magnesium matrix, and the material undergoes deformation in the tensile direction. However, due to the strong constraint effect of carbon nanotubes on the magnesium matrix as a reinforcing body, the deformation of the magnesium matrix containing the reinforcing carbon nanotube part is relatively small, while the deformation of the magnesium matrix without the reinforcing body is relatively large. As the load increases, the dislocation line at the crack begins to move. When the dislocation line moves to the carbon nanotube, due to the high elastic modulus of the carbon nanotube, it cannot pass through, resulting in dislocation loops around the carbon nanotube. As the load increases, stress concentration occurs near the interface between carbon nanotubes and magnesium matrix due to dislocation loops. At this point, cracks will debond at the interface, ultimately leading to interface detachment between carbon nanotubes and magnesium matrix, resulting in material failure and damage.

4. CONCLUSION

This article mainly studies the crack propagation during the uniaxial tensile failure process of carbon nanotube reinforced magnesium based composites. Select representative model cross-sections as research objects, use the element birth and death function in ANSYS finite element analysis software for finite element numerical simulation calculation, and adopt a multi-step loading method for crack initiation and crack propagation analysis. It was found that cracks first appeared at the interface between carbon nanotubes and magnesium matrix; The direction of crack propagation is perpendicular to the direction of applied load, which is called vertical crack propagation; As the load step gradually increases, the crack propagation speed gradually increases, especially when two parallel vertical cracks overlap, the crack propagation speed becomes more significant; The matrix is the unit that is most damaged during the entire crack propagation process.

When composite materials are subjected to load as a whole, stress is transmitted from the matrix to the reinforcement. The high elastic modulus of carbon nanotubes prevents dislocation lines from passing through them, resulting in dislocation loops around the carbon nanotubes. As the load increases, stress concentration occurs around the carbon nanotube due to dislocation loops. At this point, the crack will experience debonding at the interface, resulting in interface detachment between the carbon nanotube and the magnesium matrix, ultimately leading to material failure and destruction.

REFERENCES

[1] Liqin Yan, Yong Huang. Preparation and Properties Study of Carbon nanotube Toughened Al Mg Alloy Composite Materials [J]. Functional Materials, 2024, 55 (01): 1212-1216.

[2] Jiahong Wu, Wenguang Wang, Dingrui Ni, etc Microstructure and mechanical properties of TiB2 nano coating modified carbon fiber reinforced Mg based composites [J]. Materials Introduction, 2023, 37 (14): 126-131.

[3] Zewen Yan. Preparation and micromechanical behavior of Ti particle reinforced Mg based composites [D]. Yanshan University, 2022.

[4] Yan Jiang. Finite element analysis of stress field in carbon nanotube reinforced magnesium based composites [D]. Shenyang: Shenyang University of Technology, 2016.

[5] J F Li, L Zhang, J K Xiao, et al. Sliding wear behavior of copper-based composites reinforced with graphene nanosheets and graphite [J]. Transactions of Nonferrous Metals Society of China, 2015, 25(10):3354-3362.

[6] Xiaotong Li, Qianduo Zhuang, Zhiliang Niu, et al. Prediction of mechanical properties of hybrid SiC particle reinforced aluminum matrix composites based on neural networks [J]. Precision Forming Engineering, 2024, 16 (04): 95-100.

[7] Dongya Han. Study on the Interface Microstructure and Mechanical Behavior of Continuous Fiber Reinforced Al Matrix Composites [D]. Jilin University, 2024.

[8] Junchi Ma. Simulation study on the mechanical behavior of ultrafine grain particle reinforced aluminum/magnesium based composites [D]. Civil Aviation Flight Institute of China, 2024.

[9] Young H L, Seong G K, David T. Catalytic growth of single-wall carbon nano-tubes [J]. Physical Review Letters, 1997, 78(12):2393-2396.

[10] Wong E W, Sheehan P E, Liebert C M. Nanobeam mechanics: elasticity, strength, and toughness of nano-rods and nano-tubes [J]. Science, 1997, 277(26):1971-1975.

[11] Kun Jiao. Finite element numerical simulation study on stress-strain field of carbon nanotube reinforced magnesium based composites [D]. Lanzhou: Lanzhou University of Technology, 2010.

[12] Haijun Li. Finite element simulation of carbon nanotubes based on atomic potential [D]. Nanjing: Nanjing University of Aeronautics and Astronautics, 2006.

[13] Sun C T, Vaidya R S. Prediction of composite properties from a representative volume element [J]. Composites Science and technology, 1996, 56(2):171-179.

[14] Shuang Zhou, Yan Jiang, Yu Cui. Tensile Numerical Simulation of Carbon Nanotube Reinforced Magnesium Matrix Composites [J]. International Core Journal of Engineering, 2022, 8(3):407-419.

[15] Weixue Li, Yingge Xu, Yuan Hao, et al. Study on the mechanical properties of carbon nanotube reinforced AZ91D magnesium based composites [J]. Gansu Journal of Science, 2010, 22 (2): 34-37.