Characterization of Fiber Morphology and Its Effect on Mechanical Properties in Short Fiber Reinforced Rubber Composites: Postprint

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Abstract

To improve the performance prediction accuracy of short fiber-reinforced rubber composites, considering that fibers within such composites mostly exhibit random waviness, a discrete modeling approach was employed to establish a two-dimensional representative volume element (RVE) model of short fiber-reinforced rubber composites with wavy fibers. Uniaxial tensile simulations were performed on the numerical model and compared with experimental measurements, and the influence of fiber morphology on the mechanical properties of short fiber-reinforced rubber composites was analyzed. The results demonstrate that the numerical simulation results agree well with experimental measurements, indicating good model reliability; fiber waviness reduces reinforcement effectiveness; the mechanism by which fiber morphology affects the mechanical properties of short fiber-reinforced rubber composites is related to fiber content—under low volume fraction conditions, the modulus of SFRC (short fiber-reinforced rubber composite) decreases with increasing model curl ratio; under high volume fraction conditions, the modulus of SFRC exhibits a trend of first increasing then decreasing with increasing model curl ratio.

Full Text

Preamble

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Characterization of Fiber Morphology and Its Effect on Mechanical Properties of Short Fiber-Reinforced Rubber Composites

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Abstract: To improve the prediction accuracy of short fiber-reinforced rubber composite (SFRC) performance, this study considers that most fibers within SFRCs exhibit random wavy shapes. A discrete modeling method was employed to establish a two-dimensional representative volume element (RVE) model of SFRCs with wavy fibers. Uniaxial tensile simulations of the numerical model were conducted and compared with experimental measurements, and the influence of fiber morphology on the mechanical properties of SFRCs was analyzed. The results demonstrate that the numerical simulation results agree well with experimental measurements, indicating good model reliability. The wavy bending of fibers weakens their reinforcing capability. The influence mechanism of fiber morphology on SFRC mechanical properties is related to fiber content: at low volume fractions, the modulus of SFRC decreases monotonically with increasing model crimp percentage; at high volume fractions, the modulus of SFRC first increases and then decreases with increasing model crimp percentage.

Keywords: short fiber-reinforced rubber composite; short fiber; fiber morphological characterization; mechanical property; crimp percentage

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1. Finite Element Model

Short fibers in rubber matrices generally do not orient along the thickness direction, and SFRC products are essentially thin plate-like, which facilitates RVE model construction and allows simplification to a two-dimensional plane stress model.

1.1 Fiber Modeling Method

To establish wavy fibers with high aspect ratios, this study references methodologies from carbon nanotube composite research. As similar high-aspect-ratio fibrous reinforcements, carbon nanotubes also exhibit wavy geometries within matrices, making their modeling approaches applicable. While some studies model fibers as sinusoidal shapes or simpler arc shapes, using regular geometries to represent complex wavy fibers introduces deviations from reality. Therefore, a discrete modeling approach that considers fiber microstructure is more appropriate.

Based on discretization principles, each fiber can be divided into a series of fiber segments. The total number and length of segments are estimated from microscopic images. The starting point coordinate P_0 of the first segment is randomly selected within model boundaries with a random initial angle α_0. Using the preset segment length d, the starting coordinate P_1 of the second segment is calculated, generating the first fiber segment. A random deflection angle β_1 is then generated, and based on P_1 and β_1, the third segment' s starting coordinate P_2 is calculated to generate the second segment. This iterative process continues until a wavy short fiber is fully generated. [Figure 1: see original paper] illustrates the detailed algorithm logic, while provides parameter definitions. This operation can be implemented via PYTHON programming and imported into ABAQUS software.

To determine the fiber model geometry, the algorithm sets a maximum deflection angle between fiber segments, denoted as β , which characterizes the bending of the fiber microstructure. β is defined as the range for random deflection angle β , where β is a random value within (-β , β). As shown in [Figure 3: see original paper], fiber geometry varies significantly with β settings, with more pronounced waviness at higher β values.

Since the approach originates from discretization principles, obtaining reliable results requires determining a reasonable segment length related to fiber microstructure. This study estimated the appropriate segment length from SEM images of SFRC. The microscopic image shows that yellow dots represent fiber peak points, with approximately 12 segments in a 300 m length, yielding d = 0.025 mm. The total number of segments N is calculated as:

$$N_s = L_f / d$$

The overall fiber model construction employs the Random Sequential Adsorption (RSA) algorithm. Based on the non-intersecting fiber assumption, fibers satisfying the volume fraction V_f are generated sequentially within the model. The relationship between V_f and fiber number N_f is:

$$L^2 t V_f = \pi r^2 L_f$$

where L is the RVE model size, r is the fiber cross-section radius, and t is model thickness.

To avoid fiber intersection, the algorithm checks for intersections before generating each segment. If intersection occurs, the random deflection angle β is modified to automatically search for a viable path. For cases where no path can be found, this indicates strong fiber interactions requiring larger deflection angles. The algorithm employs staged parameters: maximum segment generation attempts C and maximum deflection angle β . Phase I parameters ($\beta\ _1$, C $_1$) and Phase II parameters ($\beta\ _2$, C $_2$) are preset. The algorithm first uses Phase I parameters. If no path is found within C_1 attempts within the β_1 range, it enters Phase II where β_1 is replaced with a larger β_2. If still unsuccessful after C_2 attempts, the fiber is abandoned and regeneration begins. The flowchart is shown in [Figure 4: see original paper]. In this study, β_1 serves as a variable discussed later, while $C_1 = 10$, $C_2 = 20$, and $\beta_2 = 60°$. Since Phase II is rarely entered, β hereafter refers to β_1.

1.2 Material Parameters

Short fibers are treated as linear isotropic elastic materials (aramid fibers) with elastic modulus 70,000 MPa, Poisson' s ratio 0.3, cross-section radius r = 0.006 mm, and lengths of 1.5 mm and 3.0 mm.

The rubber matrix is described using the Ogden N3 model:

$$W_{\text{Ogden}} = \sum_{i=1}^{3} \frac{\mu_i}{\alpha_i}(\lambda_1^{\alpha_i} + \lambda_2^{\alpha_i} + \lambda_3^{\alpha_i} - 3)$$

where and α are material parameters, and λ_1, λ_2, λ_3 are the first, second, and third principal stretch ratios. Rubber parameters from unfilled specimens are: ${}_1 = 8.116$ MPa, $\alpha_1 = 1.975$; ${}_2 = 5.725$ MPa, $\alpha_2 = 2.388$; ${}_3 = 5.467$ MPa, $\alpha_3 = -4.495$.

1.3 Model Parameters

RVE model size is critical for correctly representing material mechanical response. Generally, computational result convergence with increasing model size indicates satisfaction of RVE requirements. Through convergence analysis, the RVE model size was determined as L × L = 24 mm × 24 mm with thickness t = 2r = 0.012 mm.

1.4 Meshing

The rubber matrix uses 8-node quadrilateral elements (CPS8R) with 0.06 mm element size (160,000 elements total). Fibers use linear beam elements (B21H) with 0.025 mm element size, dividing a 1.5 mm fiber into 60 elements and a 3.0 mm fiber into 120 elements.

1.5 Constraints and Boundary Conditions

This study employs the embedded region constraint in ABAQUS to establish fiber-matrix contact, with the rubber matrix as the host region and short fibers as the embedded region.

RVE theory is based on continuum mechanics, requiring corresponding edges to satisfy continuous stress and displacement for deformation field compatibility. Periodic displacement boundary conditions are applied as:

$$u_{x=L} - u_{x=0} = \bar{u}_x$$
$$u_{y=L} - u_{y=0} = \bar{u}_y$$

where u represents nodal displacement with subscripts indicating node positions. These periodic boundary conditions are implemented using constraint equations.

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2. Numerical Simulation and Model Validation

2.1 Evaluation Parameters

This study focuses on fiber morphology effects on tensile modulus. Due to rubber' s nonlinear and incompressible nature, mechanical behavior is generally described using nominal stress. Based on periodic boundary conditions, surface average stress can be equivalently applied as concentrated nodal loads. Uniaxial tensile simulation is achieved by applying displacement loading at M1 while constraining M0 in both x and y directions and M2 in the x direction. Nominal stress is obtained from reaction force (RF) divided by initial surface area:

$$\sigma = \frac{\mathrm{RF}}{L \times t}, \quad \varepsilon = \frac{u}{L}$$

where RF is the sum of nodal reaction forces on the surface and u is nodal displacement.

2.2 Model Validation

Finite element models were established based on material formulations and compared with experimental data from our laboratory. Formulations are listed in . For each formulation' s fiber volume fraction and length, both straight-fiber models ($\beta = 0°$) and wavy-fiber models ($\beta = 7.5°, 15°, 22.5°, 30°$) were simulated and compared with experimental data, as shown in [Figure 6: see original paper].

The wavy-fiber models show good agreement with experimental data, with corresponding models listed in . Wavy-fiber models effectively reduce errors from straight-fiber models when predicting SFRC mechanical performance. Although simulations diverge from experiments at stresses of 1.5-2.0 MPa (primarily due to the ideal interface assumption, whereas actual debonding occurs at higher stresses), the results demonstrate wavy-fiber model reliability at stresses below 1.5 MPa.

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3. Effect of Fiber Morphology on SFRC Performance

Since wavy-fiber models established via the discrete method show good experimental agreement, but fiber morphology may vary under identical β conditions due to different modeling parameters (e.g., volume fraction, fiber length), this study uses crimp percentage to evaluate fiber geometry and investigates morphology effects on SFRC performance.

3.1 Fiber Geometric Morphology Characterization

In the fiber industry, crimp percentage (_c) is typically used to characterize fiber morphology, defined as (L_c - L_{in})/L_c × 100%, where L_c is extended length and L_{in} is crimped length. However, fibers in rubber matrices differ from natural fiber morphology, lacking distinct wave heights and numbers with irregular wave patterns. Therefore, this study defines a crimp percentage ( ) for rubber matrix fibers as (L_f - l)/L_f × 100%, where L_f is fiber length and l is the crimped length.

The crimped length l is calculated by fitting fiber nodes using least squares to determine a baseline representing fiber direction, with the projection length onto this baseline taken as l. Crimped width is characterized by the average distance (γ) and variance (δ) of fiber nodes from the baseline, as illustrated in [Figure 7: see original paper].

Overall model fiber morphology is characterized by representative parameters: average crimped length (l_r), average node distance from baseline (γ_r), variance (δ_r), and crimp percentage (_r), obtained by averaging across all fibers:

$$l_r = \frac{\sum_{i=1}^{N_f} l_i}{N_f}, \quad \gamma_r = \frac{\sum_{i=1}^{N_f} \gamma_i}{N_f}, \quad \delta_r = \frac{\sum_{i=1}^{N_f} \delta_i}{N_f}, \quad \rho_r = \frac{\sum_{i=1}^{N_f} \rho_i}{N_f} \times 100\%$$

3.2 Effect of Fiber Morphology on SFRC Modulus

Representative fiber morphology parameters (l_r, γ_r, δ_r, _r) were calculated for each model. [Figure 8: see original paper] shows the relationship between crimp percentage (_r) and maximum deflection angle (β). Based on this relationship, [Figure 9: see original paper] presents the correlation between fiber morphology parameters and _r across different models. The consistent curves indicate a one-to-one correspondence between _r and fiber morphology, enabling _r as an indicator for analyzing morphology effects on SFRC modulus.

[Figure 10: see original paper] compares stress at 10% strain for different volume fractions. The trend changes with increasing volume fraction: for L_f = 1.5 mm with V_f < 2.43% and L_f = 3.0 mm with V_f < 1.46%, stress decreases monotonically with _r, indicating that fiber crimp reduces modulus at low volume fractions where straight fibers provide optimal reinforcement. For L_f = 1.5 mm with V_f > 2.43% and L_f = 3.0 mm with V_f > 1.46%, stress first increases then decreases with _r, showing that moderately crimped fibers provide better reinforcement at high volume fractions.

[Figure 11: see original paper] compares stress at 10% strain for different fiber lengths. At equivalent crimp percentages, L_f = 3.0 mm models consistently show higher stress than L_f = 1.5 mm models, indicating longer fibers provide better modulus enhancement. However, when crimp percentage differences are large, shorter fibers at low crimp can match or exceed the performance of longer, highly crimped fibers, potentially explaining why some studies show negligible modulus improvement or even decreases with increasing fiber length.

Optimal crimp percentages were identified: approximately 10% for L_f = 1.5 mm at V_f = 3.4%, 15% for L_f = 3.0 mm at V_f = 2.43%, and 18% for L_f = 3.0 mm at V_f = 3.40%.

3.3 Mechanism of Fiber Morphology Effects

The differing mechanisms at low versus high volume fractions are analyzed using V_f = 0.49%, L_f = 3.0 mm and V_f = 3.40%, L_f = 3.0 mm models under periodic boundary conditions with concentrated force loading (0.432 N, σ = 1.5 MPa). [Figure 12: see original paper] shows von-Mises stress distributions for the low-volume-fraction case. The non-uniform stress distribution reveals low-stress zones near fiber load-bearing sections with stress concentration at fiber ends, indicating reinforcement depends primarily on individual fiber performance. As _r increases, the area of low-stress and stress concentration zones decreases, showing reduced load-bearing capacity. [Figure 13: see original paper] illustrates stress contours near fibers, showing discontinuous load-bearing regions along crimped fibers with frequent alternating low- and high-stress zones, which significantly weakens reinforcement.

[Figure 14: see original paper] shows stress distributions for the high-volume-fraction case. Compared to low-volume-fraction cases, more low-stress zones appear. As _r increases, low-stress area first increases then decreases. The straight-fiber model (β = 0°) shows distinct high-stress regions between low-stress zones, while the β = 7.5° model exhibits more uniformly distributed low-stress zones forming a framework structure. At higher _r values (e.g., β = 30°), high-stress regions increase and the framework structure disappears. At high volume fractions, overly straight fibers tend to align in the same direction within localized regions, creating high-stress zones where fibers are poorly oriented relative to the loading direction. Moderately crimped fibers provide more uniform distribution, and sufficient fiber quantity compensates for reduced individual fiber performance, enhancing SFRC modulus until crimp becomes excessive.

3.4 Effects of Fiber Length and Volume Fraction on Morphology

Since fiber morphology significantly impacts SFRC modulus and is difficult to observe experimentally, this study estimates in-situ fiber morphology by comparing numerical results with macroscopic experimental data. When simulation matches experimental data, the numerical geometry is considered representative of reality.

Based on matching results from [Figure 6: see original paper], the maximum deflection angles (β) of wavy models corresponding to different volume fractions were statistically analyzed. Using the β - _r relationship, the crimp percentages for different formulations were determined, as shown in [Figure 15: see original paper]. Crimp percentage generally increases with fiber content: from 0.49% to 3.40% V_f, _r increases from 3.3% to 16.5% for L_f = 1.5 mm and from 18.8% to 43% for L_f = 3.0 mm, consistent with experimental findings by Dong Zhixian.

Comparing L_f = 1.5 mm and L_f = 3.0 mm, the crimp percentage for longer fibers is 226.5%-556.7% higher at equivalent volume fractions, indicating longer fibers are more crimped within rubber. This aligns with Wang Jie et al.'s experimental results, as longer fibers experience greater bending forces during processing and are less likely to flow with the rubber. This explains why straight-fiber models show increasing error with fiber length—the actual fibers have excessive crimp that weakens reinforcement, validating the model' s predictive capability for fiber morphology.

Conclusions

1. Wavy-fiber models based on SEM analysis of fiber-reinforced rubber better represent actual fiber morphology. Numerical-experimental comparisons show good agreement, effectively reducing errors from straight-fiber models when predicting SFRC mechanical performance, particularly for longer fibers.
2. Fiber reinforcement capability decreases with increasing crimp percentage. Discontinuous load-bearing regions caused by fiber crimp are a primary reason for reduced reinforcement performance.
3. The influence mechanism of fiber morphology on SFRC modulus depends on volume fraction: at low volume fractions (L_f = 1.5 mm, V_f < 2.43%; L_f = 3.0 mm, V_f < 1.46%), fibers interact minimally and reinforcement depends mainly on individual fiber performance, showing monotonic modulus decrease with crimp percentage; at high volume fractions (L_f = 1.5 mm, V_f > 2.43%; L_f = 3.0 mm, V_f > 1.46%), fiber interactions occur and reinforcement also depends on fiber distribution, with moderately crimped fibers providing optimal enhancement, showing a non-monotonic trend where modulus first increases then decreases with crimp percentage.

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Note: Figure translations are in progress. See original paper for figures.