DE GRUYTER Nanotechnology Reviews 2023; 12: 20220522

Review Article

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Progress in FEM modeling on mechanical and electromechanical properties of carbon nanotube cement-based composites

https://doi.org/10.1515/ntrev-2022-0522
received October 11, 2022; accepted January 13, 2023

Abstract: Carbon nanotubes (CNTs) reinforced cementitious composite (CNRC) with excellent electrical and self-sensing properties, which enables it to serve as an intrinsic sensor for structural health monitoring (SHM). However, the requirements of modern industry for accurate calculation and performance design of engineering materials are not met by traditional experimental studies alone. The finite element method (FEM) has the advantages of simplicity of operation, accuracy, and cost-effectiveness, and it has been widely used in the property verification and prediction of various composite materials. In this article, the constitutive model, FEM modeling method, and simulation process of CNRC along with existing model types, innate relations, and model parameters are reviewed, and the corresponding mechanical, electrical, and electromechanical coupling properties of CNRC under different parameters are systematically analyzed by FEM method. By combining different uncertainty parameters and model types, the advantages and disadvantages of FEM for mechanical, electromechanical coupling, and SHM applications of CNRC modeling are explored. The results are in good agreement with those in the existing CNRC experiment, which effectively proves the reliability of the FEM method in CNRC research. This work is important to develop a sound theoretical model verification and performance prediction for early applications in SHM of CNRC.

Keywords: FEM modeling, CNT cement-based composite, performance simulation, SHM

1 Introduction

Modern infrastructure requires cement-based materials (CM) to be more mechanically tough and durable. Improvements in the performance of brittle CM are often achieved through the incorporation of ductile fibers, admixtures, or functional components [1]. However, the effect of micro-scale fibers on CM nanoscale defects is restricted, and at the same time, nanomaterials have many excellent properties that differ from those of conventional materials [2]. In recent years, nanomaterials have been used to improve some of the mechanical limitations of CM [3], including hardness, mechanical toughness, and durability, which have even been used to develop functional properties, such as electrical conductivity [4], thermal conductivity [5], electromagnetic wave absorption [6], and damping properties [7], which are used for specific applications. Commonly used nanomaterial includes cellulose [8], graphene [9], nanosilica [10], titanium dioxide [11], and carbon nanotubes (CNT) [12]. Among them, CNTs are favored by oversea scholars for their superior mechanical toughness [13], electrical [14], and thermal conductivity [15], as well as for their significant enhancements of durability to CM [16].

It is low cost-effective to incorporate CNTs into a large-quantity concrete structure to improve the overall performance of concrete due to the high price of CNTs. Allowing for the natural compatibility and durability of CNTs reinforced cementitious composite (CNRC) with concrete, self-sensing CNRCs can well be intrinsic sensors integrated with concrete elements applied in structure

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health monitoring (SHM) [17]. However, the nature of the variation in the mechanical and electrical signals of the sensors for the complicate structure as a whole is complex [18]. It is inefficient to test the performances of the sensors in the concrete by experimental methods alone, which is also a tremendous consumption of materials. In addition, the mechanical and self-sensing electrical performances of CNRC sensors measured with experimental methods are insufficient to enable the establishment of a complete theoretical system for CNRC sensors in SHM.

Computer simulations and modeling of material with appropriate experiment validation can provide access to a range of information that is difficult to obtain in traditional experiments, which saves significant costs and shortens research time [19]. Actually, within the engineering field, the finite element method (FEM) combines empirical formulas with a high degree of overlap with engineering design with a variety of special tools that are widely simulated in load-bearing and damage processes in materials to solve practical engineering problems [20]. Therefore, there are significant prospects for using FEM software to implement outline optimization design and coupling performance analysis of CNRC sensor materials, which provides effective material model analysis, parameters correction, and performance optimization [21].

Scholars from various countries have used FEM for the self-sensing property prediction of composite materials for SHM. Sivasuriyan *et al.* [22] argued that establishing a numerical model of SHM can be helpful in determining the structural response through various algorithms, to affirm the usefulness of FEM for SHM. Ghadhban *et al.* [23] proposed to use FEM to evaluate the change in resistance of a smart CM in detecting weight in perceived motion and apply it to traffic detection. Chalioris *et al.* [24] describe the utilization and validity of a customized portable low-cost SHM system that has been implemented as a PZT-based electromechanical conductivity (EMA) method for the detection and assessment of damage in bent reinforced concrete (RC) beams. Zacchei *et al.* [25] collected several data through SHM as well as the building information model of the real bridge and calibrated the bridge model by FEM. Based on that condition, monitoring techniques can be used for various industrial applications, especially for structural fault detection, El-Kafrawy [26] proposed a technique actually representing a non-destructive procedure with an immense benefit for SHM.

In recent years, the research studies on the use of FEM software to study CNRC have been increasing [27], but it is still necessary to fill this gap and to adequately understand the process of FEM modeling and performance analysis of CNRC. This article reviews model parameters, model types, and intrinsic constitutive relationships of CNRC from domestic to overseas, discusses the mechanical modeling methods, and analyzes their advantages and disadvantages in combination with uncertainty parameters. The testing methods and the degree of fit of the CNRC electromechanical coupling model to the existing conductivity theory are discussed to further verify the validity of the electromechanical coupling performance of CNRC in order to consider the feasibility and application of FEM in SHM. The limitations of FEM in modeling and directions for further research in the future are discussed with respect to the existing advances in CNRC models, which is important for establishing a reasonable theoretical constitutive validation and performance prediction for the early applications of CNRC.

2 FEM modeling of the CNRC

Based on the representation of the CNRC microstructure, the FEM is used to analyze the quantitative relationship between material properties and uncertain parameters by creating representative volume elements (RVE) to simulate the mechanical or electrical behavior of the cell under certain mechanical loads and boundary conditions [28]. This section introduces the establishment of RVE to explore the direction of the study of CNRC by models of different scales and also provides the selection of various literature for CNRC unit types and model parameters (as shown in Tables 1 and 2), considering the effects of different intrinsic structure relationships on the model, which provides a reference for the subsequent FEM study of CNRC.

2.1 RVE

In order to accurately characterize the behavior of a bulk object, it is desirable that the microscale properties of the object also be considered in the modeling.

Table 1: The simulation unit types of CNT and cement matrix selected for CNRC in varied literatures

Ref.	**Unit type**	
	CNT	**Cement matrix**
[35]	SOLID65	SOLID45
[45]	SOLID65	
[46]	SOLID65	
[43]	PLANE82	LINK1
[44]	PLANE42	
[47,48]	SOLID232	

Table 2: The simulation model parameters selected for CNRC in varied literatures

Ref.	Young's modulus (MPa)		Wall thickness of CNT (nm)	Poisson's ratio	
	CNT	Cement matrix		CNT	Cement matrix
[35]	1×10^6	3.1×10^4	0.34	None	None
[45]	5.234×10^5	3.773×10^4	0.1	0.165	0.22
[46]	1.026×10^6	3×10^4	0.34	0.165	0.2
[43]	5.5×10^6	2.89×10^4	0.066	0.19	0.2
[36]	1×10^6	3×10^4	None	0.35	0.2

A representative volume element (RVE) is generally used to model the structure and properties at the microscale [29,30]. The Mori–Tanaka theory proposes that the average stress in a composite matrix is uniformly distributed throughout the material [31], which provides a theoretical basis for the use of RVE in numerical simulations [32]. Suitable size for RVE can significantly improve the accuracy of FEM calculations. RVE is selected in the composite material, which cannot be too small; it needs to cover the complete physical properties of the composite material; RVE cannot be too large, and the size should be smaller than the one of the reinforcing phases so that the reinforcing phase should contain enough micro-elements and the stress and strain of the micro-elements can be advantageously equivalent to those of the reinforcing phase.

2.2 Model categories

At present, the establishment of the CNRC model can be roughly divided into the following three models according to the division of research scale: (1) CNT model based on nanoscale; (2) based on the micro-scale CNT and cement matrix interface bonding model; (3) overall CNRC model based on macro-scale.

The nano-scale model uses FEM to study the relevant characteristics of CNT (such as Young's modulus, tensile strength) at the nanoscale [33], and then, the simulation results are substituted into the CNRC model (Figure 1(a)). Due to the difference in order of magnitude between CNT and cement-based RVE model, the CNRC model is established by using a multi-scale analysis strategy, which can transmit information at different scales and avoid the influence of errors caused by model grid and material-related parameters on experimental results when using experimental data or other manuscript data. Eftekhari *et al.* [34] used a multi-scale method to study the fracture properties of CNRC. First, the influence of CNT chirality on the fracture properties of CNT was discussed, and the calculated CNT fracture parameters were reflected in the CNRC model.

The microscopic model is mainly used to study the interface problem between fiber and matrix at the microscopic scale. Two common methods are the XFEM model (Figure 1(b)) and the fiber pull-out model (Figure 1(c)). The XFEM model is a fiber–matrix interface connection

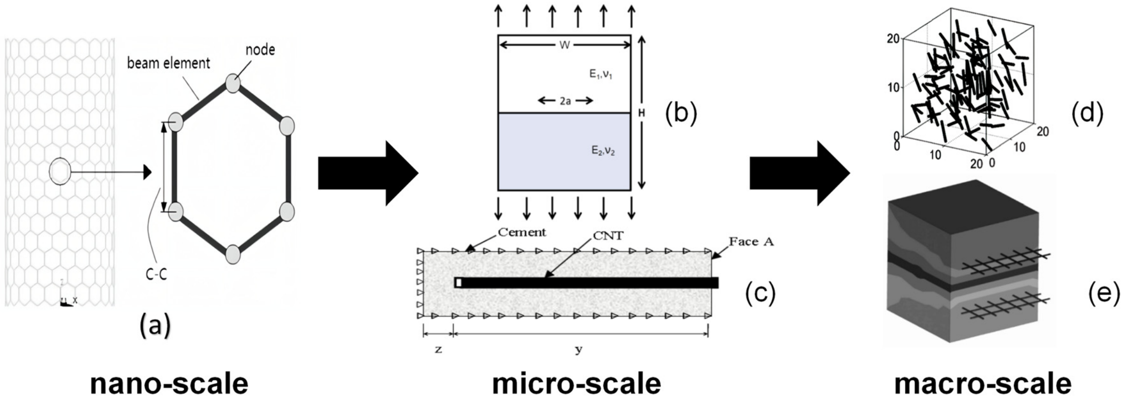

Figure 1: Typical multi-scale model of CNRC: (a) nanoscale model of the CNT [33]; (b) microscale XFEM model of CNRC [33]; (c) microscale model of fiber pulling-out from CNRC [35]; (d) macroscale mechanical model of CNRC [36]; and (e) macroscale electrical field model of CNRC [37].

model based on the horizontal enrichment function, which is generally used to describe the interfacial fracture properties of composite materials [38]. Eftekhari *et al.* [34] used the XFEM method to simulate the fracture behavior of CNRC with steel bars at the mesoscopic scale. The results confirmed that the XFEM method has an excellent contribution to the study of CNRC fracture performance. Another fiber drawing model is mainly used to study the bond–slip relationship between fiber and matrix. For example, Chan and Andrawes [39] established a CNRC mechanical RVE drawing model to study the effects of different mechanical parameters and interface parameters on the structural properties of the material.

The macroscale model is based on the continuous medium mechanics theory to study the influence of constituent materials through the average properties of composite materials [40], which not only provides a better simulation of the consistency and homogeneity of CNRC but also saves a lot of simulation time (Figure 1(d) and (e)). Unfortunately, the macroscopic model is unable to reflect the inhomogeneity and complexity of CNRC in real situations and the effects of local damage [41]. Attempts are being made to compensate for this shortcoming through multi-scale modeling or further optimization of macroscopic models.

2.3 Model parameters and types

2.3.1 Unit types

In FEM analysis, the choice of cell type directly determines the efficiency of the analysis and the accuracy of the results. The unit types are divided into point units: MASS, line units: LINK, BEAM, COMBIN, and surface units: PLANE, SHELL [42]. The units are divided into point units: MASS, line units: LINK, BEAM, COMBIN and surface units: PLANE, SHELL. When modeling CNRC, the CNRC model is divided into a plane model and a 3D model.

In the plane model, the CNT is simulated by the rod, and the unit type used is LINK1 [43] or BEAM4 [44]. LINK1 is a uniaxial compression unit, but it cannot withstand the bending moment. The CNT not only bears the tension and compression but also can withstand bending and torsion. Therefore, the BEAM4 unit can better simulate the C–C chemical bond in the CNT. To simulate the cement matrix by line, a four-node unit, PLANE42 [44] (which has creep, large deformation, plasticity and large strain capabilities and is generally used to study planar problems), or for higher accuracy, a more nodal unit such as the eight-node unit PLANE82 [43].

In the 3D model, the SOLID65 3D eight-node unit is chosen to simulate the cement matrix, which is not only able to better predict the cracks and fragmentation in the cement matrix [35] It is also more consistent with the fact that the compressive properties of the cement matrix are much greater than the tensile properties [45,46]; SOLID232 is a ten-node tetrahedral conduction cell with voltage freedom of 1 at each node and is commonly used to study the variation of conductivity of CNRC [47,48].

2.3.2 Parameter selection

FEM is based on two basic assumptions when analyzing materials: the small deformation assumption and the linear elasticity assumption. For the setting up of materials for CNRC linear elastic analysis, attention needs to be paid to the uniformity of the unit system of materials and the handling of parameters. The linear elastic analysis contains Young's modulus, Poisson's ratio, shear modulus, and bulk modulus, and only two of these parameters need to be determined in order to determine the other two. Here, in addition to the elastic modulus and Poisson's ratio of CNT, the research on the wall thickness of CNT is also added because the wall thickness of CNT must be considered when modeling, and the relevant CNRC parameters selected in the literature are shown in Table 2. The wall thicknesses chosen for CNT modeling are mainly 0.066 nm [49] and 0.34 nm [50].

The choice of Young's modulus and Poisson's ratio for CNT is more varied, although care should be taken to take appropriate values that do not exceed the applicable range of the FEM; otherwise, the experimental results will be biased too much. Although the Young's modulus of CNT was calculated to be 523.4 GPa and the Poisson's ratio to be 0.65 by establishing a CNT equivalent continuum model simulation, the Poisson's ratio obtained in this experiment was too high (greater than 0.5), resulting in an error in the calculation [44]. Tang [43] chose CNT with an elastic modulus of 5.5 TPa and a Poisson's ratio of 0.17 as the reinforcing phase for the study of CNRC; however, the elastic modulus of CNT obtained in the laboratory currently ranges from 0.92 to 1.05 TPa [51]; the CNT selected for this study does not fit the actual situation. In order to better fit the existing CNT research results, a CNT with a wall thickness of 0.34 nm, an elastic modulus of 1 TPa [42,52], and a Poisson's ratio of 0.165 [46] would be preferable. The selection of cement matrix parameters is similar to existing studies [47,53]; Wang *et al.* [52] modeled a cement matrix with Young's modulus of 30 GPa and Poisson's ratio of 0.2, which is more appropriate.

2.3.3 Constitutive relationships

2.3.3.1 Stress–strain constitutive relationships

CNRCs are mostly under complex stresses. In order to accurately describe the damage characteristics and mechanical behavior of CNRCs under complex loading, it is essential to select the appropriate constitutive relation of CNRC material for research and design [54]. The commonly used constitutive relationships of CNRC and their expressions are as follows.

1) Chan *et al.* [35,39] used the finite element program ANSYS for numerical simulation and modeling, to investigate the interfacial bond strength between CNT and CM using the RVE pull-out model and the extent of residual stresses on CM. The results demonstrate that the fiber pull-out model is more realistic for the study of the interfacial strength of the fiber and matrix. Typical constitutive relationships for the RVE pull-out model are shown below (Figure 2):

Before cracking:

$$\sigma_c = (E_m V_m + \alpha E_f V_f)\varepsilon_c = E_c \varepsilon_c, \tag{1}$$

After cracking:

$$\sigma_B(\delta) = V_f \int_0^{\frac{\pi}{2}} \int_0^{(L_f/2)\cos\theta} \sigma_b(\bar{\delta}, \theta) f(z) f(\theta) \mathrm{d}z \mathrm{d}\theta, \tag{2}$$

where σ_c is the stress in the composite; E_m and E_f are the moduli of elasticity of plain concrete and fibers, respectively; ε_c is the strain in the composite; V_f is the volume fraction of the fibers; L_f is the length of the fibers; θ is the angle of embedding of the fibers; z is the depth of embedding of the fibers. $\sigma_b(\bar{\delta}, \theta)$ is the load at fiber pull-out displacement function.

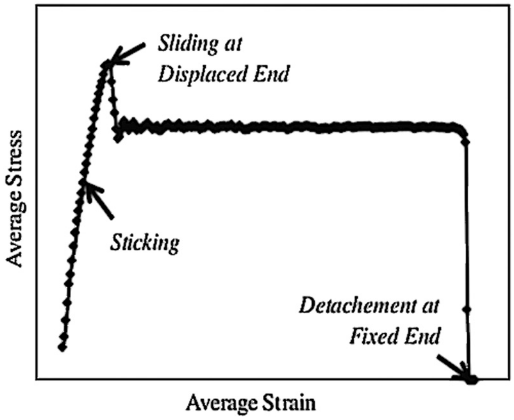

Figure 2: Typical constitutive relation of RVE pull-out model of CNRC [35].

2) Song [45] used the Hongnestand model to analyze the constitutive relationship between CNRC interface strength and crack propagation, and found that crack propagation was more obvious at the interface between fiber and CM. The Hongnestand constitutive relation is shown below:

Ascent stage:

$$\sigma_c = \left[2\frac{\varepsilon_c}{\varepsilon_0} - \left(\frac{\varepsilon_c}{\varepsilon_0}\right)^2\right]\sigma_0, \varepsilon_c < \varepsilon_0, \tag{3}$$

Descent stage:

$$\sigma_c = \left[1 - 0.15\left(\frac{\varepsilon_c - \varepsilon_0}{\varepsilon_{cu} - \varepsilon_0}\right)\right]\sigma_0, \varepsilon_0 < \varepsilon_c < \varepsilon_{cu}, \tag{4}$$

where σ_0 and ε_0 are the initial stress and strain of the composite, respectively; ε_{cu} is the peak strain of the rising section.

3) Tang [43] used Matlab software to input the compressive stress–strain constitutive relation of concrete found by Guo [55] into the finite software to investigate the effect of CNT dosing and aspect ratio on the strength of CM. The compressive stress–strain intrinsic structure relationship of Guo concrete is shown as follows [56,57]:

Ascent stage:

$$y = 1.2x - 0.2x^6, \quad x \le 1.0 \tag{5}$$

Descent stage:

$$y = \frac{x}{\alpha(x-1)^{1.7} + x}, \quad x \ge 1.0, \tag{6}$$

where $x = \varepsilon_c/\varepsilon_p$, $y = \sigma_c/f_t$; α is the parameter of the stress–strain curve in the descending section when uniaxial compressed; f_t is the representative value of the uniaxial compressive strength of the concrete; ε_p is the uniaxial compressive strength.

4) Wang [44] studied the interface separation between CNT and CM and the fracture of CNT in CM using finite element simulation software based on Wang Z M's theory of composite mechanics. The tensile stress–strain constitutive relationship of concrete deduced by Wang Z M is as follows [58,59]:

$$\sigma_c = \frac{1}{V\varepsilon_c}\sum_{k=1}^{n} \sigma_x^k \varepsilon_x^k V_k, \tag{7}$$

where σ_x^k, ε_x^k, and V_k represent the axial stress, strain, and volume of element k, respectively.

5) Wang *et al.* [52] modeled the variation patterns of clinker phase volume fraction and various hydration products with the degree of hydration. Based on the microstructural evolution of the cement hydration process, the mechanical properties of the cement paste were estimated using both autonomous and Mori–Tanaka^{34} methods, and the macroscopic mechanical properties of CNRC were predicted using a meshless approach based on a moving least squares approximation. The Mori–Tanake principal constructive relationship is shown below:

$$\sigma_c(x) = L_s : \varepsilon_c(x), \tag{8}$$

where L_s is the overall stiffness coefficient tensor of the material.

2.3.3.2 Electrical and electromechanical relationships

Dong *et al.* [47] effectively combined the GEM equation with the volume equation, from which the constructive relationship between CNT doping and resistivity of CNRC was derived to study the conductivity mechanism of CNCR and analyze its electromechanical coupling properties [48].

First, the constitutive relationship between ρ_{eff} and CNT content χ is determined by the GEM finite calculation equation of resistivity ρ_{eff}. The equation is as follows:

$$\chi_1 \frac{\rho_1^{-\frac{1}{t}} - \rho_{\text{eff}}^{-\frac{1}{t}}}{\rho_1^{-\frac{1}{t}} + A\rho_{\text{eff}}^{-\frac{1}{t}}} + (1 - \chi_1) \frac{\rho_2^{-\frac{1}{t}} - \rho_{\text{eff}}^{-\frac{1}{t}}}{\rho_2^{-\frac{1}{t}} + A\rho_{\text{eff}}^{-\frac{1}{t}}}, \tag{9}$$

$$A = \frac{1 - \chi_c}{\chi_c}, \tag{10}$$

where A and t are equation parameters, related to the size of the CNT and its spatial distribution in the CM; ρ_1 is the CNT resistivity, and ρ_2 is the CM resistivity; χ_c is the percolation threshold of the composite.

The relationship between the stress σ to which the CNRC is subjected and the CNT doping χ is derived from the volume equation (11)

$$\sigma_c = \frac{E}{1 - 2v}\left(1 - \frac{\chi_0}{\chi_1}\right), \tag{11}$$

where v is the Poisson's ratio; χ_0 is the volume content (%) of the CNT when initially added to the CM and χ_1 is the volume content (%) of the CNT in the CM after deformation in the same region of the CNRC.

Combining equation (9) with equation (11), the final electromechanical relationship between CNRC stress and effective resistivity can be obtained.

3 Influence of uncertain parameters on CNRC mechanical model

The optimization of the CNRC model is to make it more realistic and feasible. With this purpose, it is crucial to explore the sensitivity analysis of different models for uncertainty parameters [60]. According to the current status of research on CNRC at home and abroad, the content elastic modulus of CNT, the aspect ratio, the arrangement in the matrix, and the interface treatment with the matrix are chosen as uncertainty parameters in this section. The sensitivity of different CNRC mechanical models to uncertain parameters and the accuracy analysis of the FEM method for CNRC are mainly studied.

3.1 CNT dosage

The results of the current experimental study have proved that the effect of CNT content on CM is divided into three stages. First of all, when the content is excessively inexpensive, the mechanical strengthening effect of CNT on the substrate is almost ineffective [61]. Furthermore, with the increase of CNT content, the strength of CNRC also rises, and when the content reaches a certain value, the enhancement effect of CM reaches the maximum, which we call the CNT content at this time the optimal content. At the moment, the optimal results of FEM are between 0.4 and 0.6% [36,44,58,62] (the relationship between volume content of CNT and Young's modulus of CNRCis shown in Figure 3), which deviates slightly from the laboratory results of recent years and their own experimental results, but the

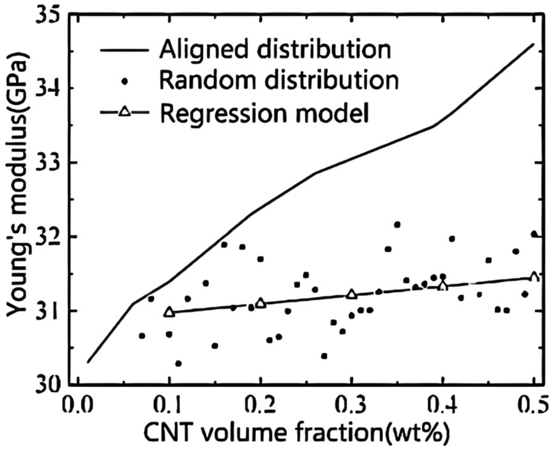

Figure 3: Relationship between volume content of aligned or random-distributed CNT and Young's modulus of CNRC [36].

margin of error is acceptable. Eventually, as the content continues to increase, the CNT will have a weakening effect on CM enhancement due to agglomeration caused by excessive van der Waals forces. However, the limitation of FEM in reflecting the effect of content on CM has led to the inability to simulate the real agglomeration of CNT in the cement base, which is one of the main reasons for the error between the current FEM results of optimal CNT content and the real experimental results [63]. In addition to improving the CM intrinsic properties, CNT incorporation can also enhance the seismic performance of the structure. Li and Sun [64] developed a FEM model of CNRC piers with 0.3% optimum content and investigated the seismic performance of CNRC piers under low circumferential repeated loads. It was shown that the load-carrying capacity and average stiffness of carbon nanotube concrete bridge piers were higher than those of ordinary concrete piers within the same cyclic load, while the ultimate load-carrying capacity was increased by 7.3% and the plastic deformation produced was smaller.

3.2 Young's modulus of CNT

For the study of the relationship between Young's modulus of CNT and CM strength, those two different approaches are proposed. Wang [36] adopted a multiscale approach to first establish a continuum equivalent model of CNT based on the molecular structure mechanics approach to predict the longitudinal and transverse elastic modulus constants of CNT and then established a fine-scale cellular model of CNRC planar stress with the influence of interfacial longitudinal and shear stresses based on the CNT simulation results; the proposed results proved that high modulus CNT is more effective for the strength enhancement of CM. Yet a large stiffness was chosen in the definition of the contact during modeling to prevent the matrix and fibers from penetrating each other, with the result that the final strength obtained differs too much from the existing results, which can be corrected by the reader by correcting the contact coefficient. Using a fiber pullout model to investigate the effect of CNT Young's modulus enhancement on the matrix, Chan [39] discovered that the strength of CNRC with an elastic modulus of 1.5, 1, and 2 TPa increased by 40, 75, and 100%, respectively, compared to a CNT Young's modulus of 500 GPa, while the toughness was substantially weakened. This is probably related to the fact that as Young's modulus of CNT increases, the cement matrix needs to provide a larger and more interfacial area to maintain the needle tip displacement of CNT, and then, the strength of CNRC increases with the fast pull-out velocity effect, for which the stress in the CNRC material decreases and the composite becomes brittle [65].

3.3 Aspect ratio of CNT

The effect pattern of CNT aspect ratio on CM is the same as that of content. In the range of minor strains, the strength of CNRC materials increases with increasing CNT aspect ratio [43] (the strength relationship between CNT length and the strength of CNRC is shown in Figure 4). Tang [46] compared the effect of CNT aspect ratio of 1, 2 and 3 on the CM, and it was in the maximum strength of 31.37 GPa for CNRC at aspect ratio of 3. The result that the aspect ratio has a positive effect on the enhancement effect of CM is unanimously accepted, but there are conflicting opinions on its influence agent. Chan and Andrawes [39] attribute the least effect of CNT aspect ratio on CM compared to other factors (*e.g.* content, Young's modulus, and interfacial bonding), whereas Al-Maharma *et al.* [66] commented that the length of CNT is the most critical factor affecting the fracture properties of CNRC. The reason for this disagreement may be that the XFEM model has a more prominent representation of the CNT length compared to the fiber pull-out model.

3.4 Arrangement of CNT

When dealing with the model, the arrangement and distribution of CNT in the matrix are the keys to modeling. First, CNT at different angles has an important effect on the model regarding the arrangement and distribution of

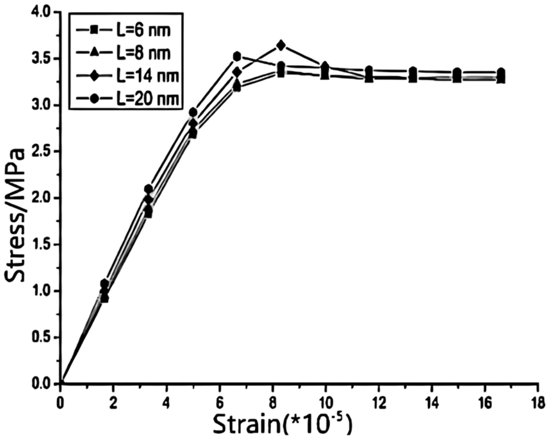

Figure 4: Strength–strain relationship of CNRC with varied CNT length [43].

fibers, as confirmed by the results of Chwał and Muc [67]. Therefore, consideration of fiber alignment is necessary for the modeling process of CNRC. Wang *et al.* [52] considered the effects of fiber orientation and random distribution in their study of CNRC (Figure 3); Chwał and Muc [67] also analyzed the effects of carbon nanotube alignment on the elastic properties of composites. In the treatment of fiber placement in the matrix, the use of the Monte Carlo method to generate fibers with random positions is unanimously considered to be the most effective treatment.

3.5 Interface bonding between CNT and CM

Interfacial peeling is an important cause of composite damage. The effective prediction of the nonlinear behavior between CNT and CM interfaces (including the nonlinear motion between interfaces and debonding behavior) with the help of FEM simulation method is the main means to quantify the mechanical properties of interfaces.

3.5.1 Interface theory model

For the study of the interfacial behavior between fibers and matrix, shear-lag and cohesion models are considered to be the two most effective methods used to characterize the stress transfer and damage evolution processes between materials.

The shear hysteresis model was first proposed for application in fiber composites in 1952 [68]. The model treats the interface between the fiber and the matrix as a perfect connection and assumes that the fiber receives only axial action, the matrix receives only shear action, and the elastic modulus of the fiber and the matrix does not change, at which time the relationship between the fiber axial stress and the interface shear stress satisfies the following equation.

$$\sigma_f^z(z) = \frac{\sigma_0}{\alpha}\left[1 - \frac{\cosh(\beta z)}{\cosh(\beta L)}\right], \tag{12}$$

$$\tau_i(a, z) = \sigma_0 \frac{a\beta}{2\alpha}\frac{\sinh(\beta z)}{\cosh(\beta L)}, \tag{13}$$

where α and β satisfy the following equation:

$$\alpha = \frac{E_\mathrm{m}}{E_\mathrm{f}}, \tag{14}$$

$$\beta = \left[\frac{\alpha}{a^2(1 + v_\mathrm{m})\mathrm{In}(b/\alpha)}\right]^{1/2}, \tag{15}$$

where E_m, E_f are the elastic modulus of the matrix and fiber; v_m is the matrix Poisson's ratio; a, b are the equivalent radii of the fiber and matrix in the monofilament system; σ_0 is the applied load.

The theory has a certain universality for composite materials, but the assumptions on materials and interfaces are too idealized, which is far from the actual conditions of composite materials. The accuracy of the model has been increased by modifying the shear-lag theory, such as Wang *et al.* [69], who first obtained the shear stress distribution between the fibers and the interface using the shear-lag theory and, on this basis, studied the relationship between the load and the fracture number of the material under non-uniform strength distribution using the Monte Carlo method; Zhang and Xu [70] found, based on the non-linear elastic properties of concrete, the stresses at the fiber ends and the temperature due to temperature changes on the shear stresses and the positive fiber stresses. The shear hysteresis theory of stress transfer in short fiber-reinforced concrete was improved based on the effects of non-linear elastic properties of concrete, the stresses at the fiber ends, and the temperature due to temperature changes on shear stresses and positive fiber stresses.

The fracture mechanics-based cohesion model takes into account the elastic–plastic behavior of the matrix and is widely used to calculate the interfacial damage and fracture processes of materials. Hillerborg [71] first applied the cohesion model to finite element calculations and proposed a virtual cracking model for concrete. The cohesion model can better simulate the crack extension behavior and the interfacial mechanical behavior of composite materials because it introduces the cohesive region and cohesive force, thus avoiding the problem of stress singularity at the crack tip as in the linear elastic fracture mechanics. Since the calculation process is more complicated, it is not introduced too much in this article.

3.5.2 Interface multiscale model

CNRC interface simulation can be divided into nanoscopic, microscopic, and macroscopic in terms of scale. Macroscopic interface model is a numerical analysis method that divides the solution domain into a grid and uses a weighted residual method in the form of equivalent integrals or a variation method for solving generalized stationary values to establish approximate differential equations to predict structural performance based on the assumption of approximate functions in the partition [72]. This model is computationally efficient but does not reflect local damage. Microscopic and nanoscopic interface models are based on the atomic or molecular level to locally study the microscopic or nanoscopic structure of the interface and the interactions between them, and then calculate the properties of the interface, and the main methods are molecular dynamics methods and Monte Carlo methods. This model can reflect the local damage process of the material, but it is difficult to simulate the boundary conditions of the material. In addition, there is a lack of theoretical basis for the intrinsic parameters of the macroscopic model. Therefore, the top-down multiscale approach of predicting parameters from microscopic or nanoscopic models for the interfacial properties of the model and then bringing the predicted parameters into the macroscopic model is widely used in interfacial studies [73,74]. The representation of interfacial strength is mainly divided into two categories. One is bond strength, and the literature studies [46] and [45] first used molecular dynamics methods at the nanoscopic scale to study CNT bonding to CM. The other category is bond slip, where Chan [35] used the fiber-pulling model to find out the bond–slip relationship between CNT and CM at the microscopic scale and carried the calculated intrinsic structure related to the macroscopic model of CNRC (Figure 5). In fact, although the bond strength model has a simpler calculation process, its essence is to give an ultimate peel-bearing capacity to the composite material, which cannot explain the process of interface peeling. On the contrary, the bond–slip model can reflect the intrinsic relationship of debonding between composites in more detail. Therefore, the bond–slip model has more theoretical significance for the study of interfacial strength.

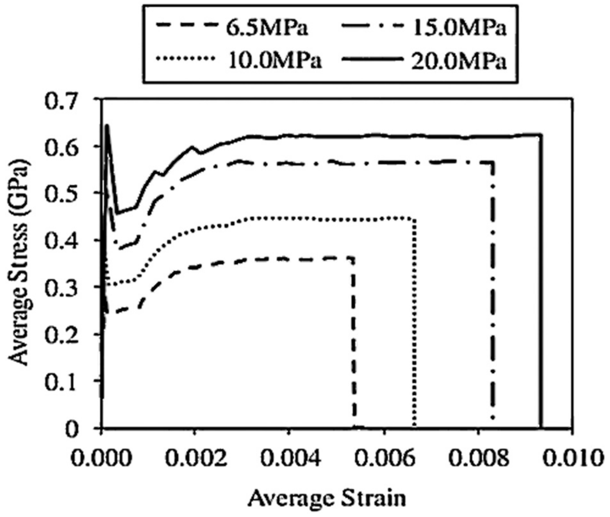

Figure 5: Constitutive relationship of RVE pull-out model of CNRC under varied shear strength [35].

4 FEM Analysis of electrical properties and electromechanical coupling properties of CNRC

A conventional cement-based material is almost insulating, which makes it difficult to attempt their direct use for structural failure and damage monitoring. In recent years, conductive carbon nanotubes have been used to modify the electrical conductivity and electromechanical sensing properties of CNRC oversea [75]. This has resulted in the evolution of intrinsic electromechanical sensors with higher sensitivity and superior performance for SHM applications. By summarizing the current status of FEM research on the electrical and electromechanical coupling properties of CNRC, the section analyzes the advantages and disadvantages of FEM for analyzing the electrical and electromechanical properties of CNRC, which aims to optimize the parameters and performance of the electromechanical coupling properties of CNRC models to help the SHM applications of CNRC.

4.1 Electromechanical coupling performance

The key to putting CNRC into realistic application in SHM is to be able to make an accurate prediction of its electromechanical coupling performance. The main means is to deduce the relationship between mechanical stress or strain and the overall resistivity of CNRC through theory, verify it using experimental or modeling methods, find the percolation threshold of CNRC, further analyze its sensing mechanism in depth, and realize the prediction of CNRC sensing performance. In fact, the FEM method can only select the specified CNT doping amount for the corresponding calculation, which is not sufficient to obtain the percolation threshold of CNRC and the corresponding electromechanical coupling relationship. Therefore, we need to choose a suitable resistivity theory model to fit the numerical results of the FEM method to get the resistivity calculation equation of CNRC. At present, the commonly used conductivity theories mainly include percolation theory, effective medium theory, and tunneling effect theory [76].

Dong *et al.* [47] and Niu *et al.* [48] modeled CNRC using Monte Carlo methods and explored the fit of the model to the GEM equation and Simmons tunneling equation and found that the best fit to the GEM equation was achieved when the CNT doping was 1.5%, while the Simmons tunneling equation was satisfied for all CNT doping between 0.31 and 1.33%. Both studies confirm that the FEM method is feasible for the study of the electromechanical coupling performance of CNRC, but the accuracy of the model is not high. On the one hand, the authors only consider the relationship between compressive stress and resistivity, but the actual stress state is much more than that; on the other hand, the model does not take into account the tunneling effect of the conducting material, which is also related to the performance limitation of ANSYS software for electric field calculation.

In contrast, the hybrid fine-scale mechanics and FEM approach for CNRC proposed by Garcia-Macias *et al.* [37] not only considers the contribution of electron hopping and conductive networks to the conductivity of CNRC (Figure 6), but also enables the analysis of resistivity changes in arbitrary strain states. The results show that the longitudinal and transverse piezoresistive coefficients of CNRC have some similarities, and the CNRC sensor can be approximately modeled as a volumetric strain sensor with a single piezoresistive coefficient. Embedding the simplified simulations into concrete structural members to explore the practical applications of the sensors could be a future research direction.

The aforementioned literature only considered the influence of the intrinsic properties or content of CNT on the electromechanical properties of CNRC; in fact, the porosity of CM itself also greatly affects the formation of conductive pathways in CNRC. Xiao [77] and Wang *et al.* [78] established a three-dimensional random field model of CNRC based on Mori–Tanake and tunneling effect theory, increased the effect of pore water ions on CNRC resistivity with the change of pore connectivity under strain, proposed a prediction model of piezoresistive effect, and compared it with experimental results (Figure 7). The results show that the connectivity of the CNRC conductive network is found to be better with the increase of CNT doping, but after reaching the percolation threshold, the conductivity of the material decreases due to the ionic effect on the piezoresistance effect becomes smaller.

The FEM model for the electromechanical properties of CNRC needs to be improved gradually. First, the existing literature simplifies the CNT as a cylinder, and thus, the CNT doping in the model is larger compared to the real case (CNT should be a hollow tubular structure [79]), resulting in a lower percolation threshold. Second, only uniform distribution is still considered for the CNT distribution, resulting in slightly larger overall resistivity results for the CNRC than the experimentally obtained resistivity results. Finally, the dynamic simulation of the conductive network inside the CNRC can be further realized, which is important for the analysis and prediction of the microstructure of the conductive network [80].

4.2 SHM applications

The fundamental purpose of studying the electromechanical coupling performance of CNRC is to enable its application in SHM. The principle is to add CNRC into concrete

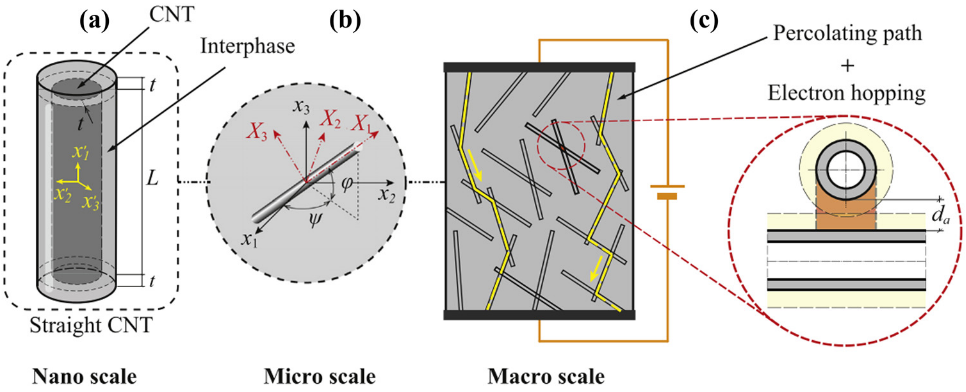

Figure 6: (a) Nanoscale RVE outline of straight CNT; (b) microscale the contribution of electron transition; (c) macroscale conductive network mechanism to the overall conductivity of CNTRC [37].

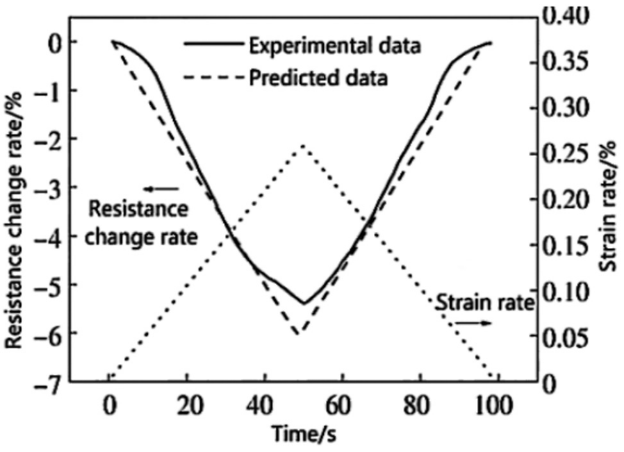

Figure 7: Numerical simulation and experimental results comparison between piezoresistive behaviors of CNRC [78].

structures by coating or embedding, *etc*., and obtain the stress and strain inside the concrete through electrical signals to obtain the internal damage state of the structure. Some scholars have tried to simulate the stress state and strain compatibility of CNRC sensors embedded in concrete structures through FEM, such as Cui *et al.* [81]. The optimally designed CNRC sensors were embedded in concrete for health monitoring and their stress state was investigated, and it is believed that the simulation results can predict the stress–strain relationship in concrete more accurately, but it still needs to be corrected for the corresponding influencing factors to ensure the accuracy of the model. In fact, there are mean reports on the applications of CNRC sensors in concrete structures for SHM using FEM, and they are worthy to further study.

5 FEM limitations of CNRC and future prospects

In order to improve the accuracy of the calculation and to correspond directly to reality, the limitations of CNRC simulations at the present stage are presented, for which the recommendations are made for future prospects:

1) Simulating the effect of CNT agglomeration on CNRC. It is well-known that as the number of fibers increases, it is difficult to play a role in CM due to CNT's own properties, but it is still a great challenge to realistically simulate the agglomeration effect of CNT in CNRC. For solving this problem, the study of Romanov *et al.* [63] is a wonderful inspiration. They investigated the degree of agglomeration from fully discrete to partially discrete and finally fully agglomerated states for the size and density of CNT agglomerates and developed a double-scaled model capable of realistically simulating the aggregation of CNT in composites.
2) Simulation of CNRC electromechanical performance in different environments. FEM has significant advantages in studying nonlinear problems under complex conditions (*e.g.*, static, dynamic, different humidity and temperature), and its application to SHM under different harsh conditions has a significant effect on future structural safety improvement [82]. Li [83] used ABAQUS software to study the seismic performance of bridge piers containing CNRC, and the structure showed that the seismic performance of bridge piers containing CNRC was superior compared to plain concrete. Liu *et al.* [84] proposed a combined FEM and computational fluid dynamics approach to evaluate the fire performance of bridges and concluded that the multi-scale modeling approach was more effective for localized fires.
3) Simulation of the inhomogeneity of CNT in CM. The uniformity assumption is widely used in FEM, which is obviously unrealistic. To further consider the inhomogeneous distribution of CNT in CM, the following method can be used for reference. Lu and Leung [85] proposed to calculate the bridging law for each different section, which contributes to simulating the strength dispersion and unsaturated cracking phenomena in fibrous concrete; Elnekhaily and Talreja [86] calculated the degree of inhomogeneity of fibers in the matrix by statistical data and developed a related algorithm; Song *et al.* [87] used a modified A&A (Andreasen & Andersen) model to design a densely compacted UHPFRC cement matrix, which optimized some key parameters of fiber orientation and distribution; Ghasemi *et al.* [88] optimized the distribution of short fibers in a continuous media structure made of fiber-reinforced composites by an efficient gradient-based optimization method, which maintained the accuracy of the model while greatly reducing the computational time by increasing the mesh size.

6 Conclusion

Since the CNT greatly improves the mechanical and electrical properties of the CM and gives it a good electromechanical coupling performance, it helps to realize the SHM of CNRC sensors. Yet, the experimental method alone is not sufficient to support the establishment of a theoretical system for the electromechanical coupling performance of CNRC, and FEM can be used as a supplement and extension of the experimental study to obtain some data and conclusions that are difficult to obtain from the experimental study. Therefore, this article investigates and analyzes the CNRC model and performance analysis based on FEM.

1) The multiscale approach can combine the advantages of different models for CNRC analysis, which can substantially improve the accuracy of CNRC simulation.
2) The fiber pullout model is currently the optimal method for the study of composite interfaces, reflecting the bond–slip relationship between fiber and matrix debonding of CNRC.
3) The FEM of the mechanical and electrical properties of CNRC has been gradually developed and optimized, which has a non-negligible role in the improvement of the electromechanical coupling theory of CNRC.
4) The method of probing the stress–strain distribution of CNRC sensors embedded in concrete using FEM is feasible, and the sensing performance under different environmental conditions can be discussed in the future.

Funding information: This study was financially supported by the National Natural Science Foundation of China (No. 51878364), Projects from China Construction Eighth Division (No. JM20191030, QUT-2022-FW-0192, and QUT-2022-FW-0028), and the National “111” project, and Gaofeng discipline project funded by Shandong Province.

Author contributions: Conceptualization, supervision, and resources: Jianlin Luo, Jigang Zhang, Liqing Zhang; data curation, formal analysis, and methodology: Xuejun Tao and Jianlin Luo; funding acquisition, investigation, and project administration: Jianlin Luo and Min Zhu; validation, visualization, and writing – original draft: Xuejun Tao, and Jianlin Luo; writing – review and editing: Xuejun Tao, Jianlin Luo, Liqing Zhang. All authors have accepted responsibility for the entire content of this manuscript and approved its submission

Conflict of interest: The authors state no conflict of interest.

Data availability statement: Some or all data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

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