Advances in Homogenization Methods for Low-Dimensional Functional Composite Materials (Postprint)

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Abstract

Low-dimensional functional composite materials have been widely applied in aerospace, energy industry, and other fields due to their excellent functional properties. This study focuses on the theoretical and numerical homogenization models for the effective functional properties of low-dimensional functional composite materials. First, the more widely used static, dynamic, and numerical homogenization methods are introduced, and the involved fillers, frequency-dependent electrical interface effects, and thermal interface effects are discussed in detail. Subsequently, the theoretical and numerical homogenization models for the functional properties of low-dimensional functional composite materials, including electrical properties, electromagnetic shielding properties, energy storage properties, thermal properties, and multi-field coupling properties, are presented. Finally, prospects for the future development of low-dimensional functional composite materials are discussed.

Full Text

Preamble

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Research Progress on Homogenization Methods for Low-Dimensional Functional Composite Materials

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Abstract: Low-dimensional functional composites have found extensive applications in aerospace, energy industries, and other fields due to their excellent functional properties. This study focuses on theoretical and numerical homogenization models for the effective functional properties of low-dimensional functional composites. First, widely used static, dynamic, and numerical homogenization methods are introduced, with detailed discussions on filler materials, frequency-dependent electrical interface effects, and thermal interface effects. Subsequently, theoretical and numerical homogenization models for functional properties of low-dimensional functional composites are presented, including electrical properties, electromagnetic shielding performance, energy storage performance, thermal properties, and multi-field coupling properties. Finally, future development directions for low-dimensional functional composites are discussed.

Keywords: low-dimensional functional composites; functional properties; homogenization methods; theoretical and numerical models

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1. Introduction

Low-dimensional functional composites, typically composed of low-dimensional nanomaterials and matrix materials such as polymers or metals, have attracted increasing attention due to their ease of processing, good flexibility, and low cost. These materials include two-dimensional materials such as graphene, transition metal dichalcogenides, MXenes, and silicene, which possess unique and excellent physicochemical properties but are not directly suitable for engineering applications. The macroscopic response of heterogeneous materials can be represented through homogenization, which replaces the average response of non-uniform materials, leading to the establishment of numerous homogenization models.

Since low-dimensional functional composites are formed by compounding low-dimensional fillers with matrix materials at the nanoscale, this design endows the composites with special functional characteristics such as high electrical conductivity and thermal conductivity, but also introduces challenges including interfacial defects and weak interfacial bonding. This study will focus on theoretical and numerical homogenization models for the effective functional properties of low-dimensional functional composites considering interface effects. Section 2 discusses the fillers, frequency-dependent electrical interface effects, and thermal interface effects of low-dimensional functional composites. Finally, Section 5 provides a summary and outlook on future development directions.

Homogenization generally refers to the transition from microscopic to macroscopic scales. In practical service conditions, low-dimensional functional composites face complex and variable environments, such as wide temperature ranges and high strain rates, posing severe challenges for research on their effective functional properties. The objective of composite homogenization methods is to calculate effective property parameters including mechanical, thermal, and electrical performance. Generally, homogenization methods can be categorized into theoretical homogenization methods and numerical homogenization methods.

1.1 Static Homogenization Methods

Widely used static homogenization methods include the Mori-Tanaka (MT) method, the Effective Medium Method (EMM), and the Hashin-Shtrikman (HS) method. The MT method is an explicit homogenization approach that can directly provide effective properties of composites. However, due to its inherent simplifications, the MT method cannot predict the percolation threshold and is not accurate for predicting percolation phenomena in low-dimensional functional composites. In contrast, EMM can reveal percolation behavior while ensuring predictions fall within or on the boundaries of HS bounds.

1.2 Effective Medium Theory

Effective medium theory was first developed around 1935 for calculating the effective dielectric constant of multiphase conductive media. Based on this assumption, Bruggeman established the Bruggeman Effective Medium Theory (B-EMT) using the Maxwell-Garnett relation in 1935. The B-EMT formulation is given by:

$$\sum_i f_i \frac{\epsilon_i - \epsilon^*}{\epsilon_i + 2\epsilon^*} = 0$$

where f_i and ϵ_i are the volume fraction and dielectric constant of phase i, respectively, and ϵ^* is the effective dielectric constant.

To address limitations, the Generalized Effective Medium Theory (GEMT) was developed, which is applicable to various filler volume fractions including high concentrations and provides percolation thresholds. Unlike B-EMT, GEMT does not exhibit dielectric anomalies. The implicit tensor equation from GEMT can be expressed as:

$$\frac{\epsilon_{eff} - \epsilon_m}{\epsilon_{eff} + 2\epsilon_m} = f_f \frac{\epsilon_f - \epsilon_m}{\epsilon_f + 2\epsilon_m}$$

This nonlinear implicit expression can be solved through iterative methods such as the Newton-Raphson method.

1.3 Mori-Tanaka Method

The Mori-Tanaka method is a classical analytical approach widely used for analyzing effective properties of composites. The effective stiffness tensor of a composite with Mori-Tanaka form can be expressed as:

$$\mathbf{C}_{eff} = \mathbf{C}_m + f_f(\mathbf{C}_f - \mathbf{C}_m)\mathbf{A}_f$$

where $\mathbf{C}_m$ and $\mathbf{C}_f$ are the elastic tensors of the matrix and inclusion phases, respectively, $\mathbf{A}_f$ is the strain concentration tensor, and f_f is the matrix phase volume fraction.

1.4 Dynamic Homogenization Methods

When composites are subjected to high-frequency vibration, impact, or wave propagation environments, the scale relationship between microstructure and wavelength/frequency makes dynamic homogenization far more complex than static cases. In the low-frequency regime, wave propagation exhibits non-dispersive characteristics, meaning wave velocity changes little with frequency, allowing characterization using quasi-static properties. In this case, traditional static homogenization can effectively describe material behavior. In the high-frequency regime, wave-material interactions become significant, requiring detailed microstructural modeling and scattering theory to capture heterogeneous features. The intermediate-frequency regime lies between these extremes, where wavelengths are insufficient to completely ignore microstructure effects but homogenization remains applicable.

Dynamic homogenization faces unique theoretical challenges due to its combination of quasi-static and high-frequency wave characteristics. For a long time, unified understanding has been lacking regarding equivalent principles, mathematical methods, and macroscopic characterization. The Willis theory has the following characteristics: (1) it introduces no assumptions about displacement patterns in the micro-macro transition and is therefore exact in this sense; (2) after homogenization, the influence of material heterogeneity is contained in macroscopic constitutive relations while macroscopic motion and geometric equations remain consistent with homogeneous media; (3) for elastic composites, the constitutive relations are local in time and space, while the homogenized macroscopic constitutive relations become non-local.

These assumptions simplify complex problems but also introduce limitations to self-consistent field methods. The first assumption neglects interactions between inclusions, making the method applicable only to low inclusion volume fractions. The second assumption ignores differences between average and effective wave fields, being valid only at lower frequencies. For low-dimensional nanocomposites, the relationship between wavelength and inclusion size requires wavelengths to reach at least the nanoscale for dynamic homogenization methods to be applicable, posing extremely high demands on both experimental measurement and the homogenization methods themselves.

The above homogenization methods can be applied not only to mechanical properties but also to functional properties of low-dimensional nanocomposites, with application examples detailed in subsequent sections.

1.5 Numerical Homogenization Methods

Numerical homogenization methods provide a reliable approach for analyzing materials with complex microstructures and nonlinear behavior. The primary advantage of numerical homogenization models lies in their ability to accurately describe complex microscopic features of materials. However, detailed calculations often entail extremely high computational costs, limiting their application.

Molecular Dynamics (MD) and Monte Carlo (MC) methods belong to molecular-scale numerical homogenization approaches. MD can predict the time evolution of interacting particle systems (such as atoms, molecules, or particles) and thereby predict relevant effective properties of composites. Based on interaction characteristics, appropriate potential functions are selected and simulation calculations are performed to obtain system evolution over time. The MC method, also known as the statistical sampling method, uses random numbers to generate system sample populations for calculating composite effective properties. Compared to MD, MC can only provide effective property information under steady-state conditions, while MD can predict effective properties during dynamic processes.

Finite Element Method (FEM) is one of the most commonly used numerical homogenization methods. Representative volume elements containing composite microstructure information are discretized into finite elements and solved under applied loads. FEM is suitable for multiscale nonlinear problems of composites with well-defined geometries, while MD offers significant advantages in considering atomic-scale interactions such as functional interface effects, and MC can effectively simulate macroscopic effective properties of composites with randomness or significant statistical features.

2. Interface Effects

Interface effects are key factors determining the excellent functional properties of low-dimensional functional composites. At the nanoscale, interfacial regions exhibit unique electrical and thermal properties that differ significantly from bulk materials. Due to the extremely high specific surface area of low-dimensional materials, the proportion of interfacial regions increases substantially, making them indispensable in functional property homogenization modeling of low-dimensional functional composites.

2.1 Electrical Interface Effects

Electron tunneling refers to the phenomenon where electrons in conductive materials can penetrate potential barriers with a certain probability, typically considered a static interface effect dependent on filler concentration rather than frequency. As the concentration of low-dimensional fillers increases, the height and width of potential barriers decrease significantly, facilitating electron penetration and making tunneling phenomena more pronounced.

2.2 Thermal Interface Effects

For enhancing composite thermal conductivity, interface thermal resistance plays a crucial role. For the Mori-Tanaka method, researchers have incorporated interface effects into the homogenization framework. In addition to EMM and MT methods, other theoretical models have been developed based on unit cell models combined with self-consistent homogenization schemes for analyzing thermal and electrical properties of rod-filled composites.

3. Homogenization Models for Functional Properties

3.1 Numerical Homogenization Models

Based on FEM, researchers have established multiscale methods to quantify parameters affecting the effective thermal conductivity of clay-reinforced polymer nanocomposites. Others have used FEM to study effective thermal conductivity of polymer composites containing heterogeneous nanofillers, proposing predictive models based on simulation results. Integral averaging methods combined with series and parallel models have been developed to comprehensively consider interface thermal resistance, porosity, and particle shape, with FEM validation. Multiscale homogenization schemes combining FEM and non-equilibrium MD have been developed to explore the influence of different nanoscale fillers on effective thermal conductivity of polymer nanocomposites. FEM studies have investigated the effects of contact thermal resistance, interface thermal conductivity, foam pillar length and diameter on effective thermal performance of graphene foam-filled nanocomposites, revealing that contact thermal resistance has a more significant impact than interface thermal conductivity for thermal conductivity.

MD simulations have systematically studied the influence of various defect types on effective thermal conductivity of graphene/polymer nanocomposites, revealing significant effects of structural defects on thermal transport. Research has shown the existence of percolation thresholds for thermal conductivity in graphene/polymer nanocomposites, providing theoretical guidance for optimizing filler volume fractions. MD simulations have evaluated thermal conductivity of hybrid nanocomposites to explore synergistic effects of multiple two-dimensional materials in composite systems. Considering size-dependent thermal transport mechanisms and environmental temperature effects, a multiscale homogenization model for effective thermal conductivity of graphene/polymer nanocomposites has been established by incorporating size-dependent mechanisms into Landau-like theory combined with EMM, subsequently validated through non-equilibrium MD simulations.

3.2 Theoretical Homogenization Models

For mechanical/electrical coupling properties, researchers have studied DC conductivity changes of carbon nanotube/polymer nanocomposites under strain based on EMM. The strain sensitivity coefficient of the overall nanocomposite can be defined as:

$$GF = \frac{\Delta R/R_0}{\epsilon}$$

where ΔR is resistance change, R_0 is initial resistance, and ϵ is material strain. Due to nanocomposite volume changes and progressive interfacial connection degradation, resistance change rate increases with applied strain.

A bottom-up electromechanical coupling homogenization model has been established to quantitatively predict dielectric loss and strain sensitivity coefficients of carbon nanotube nanocomposite sensors under AC loading. Similar to strain sensitivity coefficients, stress sensitivity coefficients can be defined. Research results show that stress sensitivity coefficients increase with loading time, with optimal aspect ratios for high sensing capacity increasing with carbon nanotube volume fraction.

FEM simulations have been used to model electromechanical responses of carbon nanotube/polymer nanocomposites, with MC methods studying representative volume element size effects on material property sensitivity. Homogenization models for frequency-dependent AC piezoresistive characteristics of self-sensing carbon nanotube/polymer nanocomposites have been proposed. Theoretical models for DC piezoresistive performance have been developed considering strain effects on volume fraction, critical volume fraction, percolation probability, and filler spacing, with FEM integration methods for validation.

Homogenization models considering different aspect ratios, volume fractions, inclusion sizes, interface thermal resistance, and electrical resistance have been developed to study effective thermoelectric properties of composites containing ellipsoidal inclusions, with FEM validation showing accurate prediction under temperature gradients. Multiscale statistical homogenization methods combining FEM and MD have been proposed to study filler size-dependent thermal expansion coefficients and thermoelastic properties of nanoparticle-reinforced polymer nanocomposites under thermomechanical coupling, where MD predicts nanoscale effective thermal properties and statistical homogenization introduces randomness parameters at the microscale.

4. Future Outlook

The development of multiscale homogenization models for low-dimensional functional composites is particularly crucial. Current research largely remains at the phenomenological description stage, with systematic understanding of the fundamental physical mechanisms of load-dependent interface effects still lacking. For complex multi-field coupling scenarios, significant scientific importance exists in establishing multiscale models. For example, interfacial atomic structures can be constructed based on density functional theory or molecular dynamics to analyze microscale force/thermal/electric field equilibrium relationships, with non-equilibrium Green’ s function methods used to extract local elastic, electrical, and thermal parameters of interfacial regions. These can then be incorporated into micromechanical homogenization methods at the macroscale to derive equivalent elastic moduli, dielectric constants, thermal conductivity, and other macroscopic performance parameters.

Future research should focus on: (1) systematic investigation of load-dependent interface effect mechanisms; (2) development of multiscale homogenization frameworks bridging quantum, molecular, micro, and macro scales; (3) integration of experimental validation with computational modeling; (4) exploration of novel low-dimensional materials and their hierarchical structures; (5) establishment of standardized protocols for characterizing interface properties in functional composites.

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