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REVIEW

A Short Review of the Literature on the Multiscale Modeling of Nanoparticle-Reinforced Composites

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Abstract

In recent years, various nanocomposites based on the inherent properties of nanofillers have been actively investigated. When nanoparticles are incorporated into a polymeric matrix, such as nylon, polyurethane, or polypropylene, lightweight composites with excellent strength can be fabricated. Given the rapid developments in nanotechnology, nanocomposites with enhanced performance are expected to be adopted in various industrial fields. This short review analyzes the literature on multiscale analysis of particle-reinforced nanocomposites published over the past decade. We aim to contribute to the growth of related technologies by providing prospective readers with an opportunity to review multiscale trends. Multiscale modeling is expected to contribute to the development of nanomaterials and their associated applications by reliably predicting the properties of inhomogeneous materials.

Keywords Multiscale modeling · Nanoparticle · Spherical reinforcement · Composite · Research trends

Introduction

The materials industry is among the most critical industries in the global economy [1–3]. Recently, studies that aim to improve the functionalities of existing polymers by mixing them with nanofillers have been actively conducted worldwide to overcome the limitations of traditional materials [4–6]. Advanced composites are crucial technological elements for electric vehicles, aerospace applications, and semiconductors, and the application fields of nanocomposites are gradually expanding (see Fig. 1) [7–10]. However, an accurate mechanism analysis has not yet been achieved owing to the different physical and chemical properties of each component.

Currently, most nanoparticle-reinforced composites are only partially verified on the laboratory scale [11–14]. The fact that experimental results vary significantly among researchers lowers the interest of companies in promoting development and investment in this field [15–17]. The use of materials that do not present consistent performance reproducibility via trial-and-error leads to unreliability in terms of composite stability and long-term durability, which are essential for commercialization [18–20]. This constitutes a significant obstacle for industrial applications.

For the successful development and mass production of next-generation composites, it is essential to identify reliable material mechanisms, define performance evaluation methods, and establish a theoretical analysis methodology for practical composite designs. The research subject of nanocomposites constitutes a technical field wherein physicochemical characteristics are not sufficiently identified; hence, various research approaches are required [21, 22].

With the development of material theory and the progress in computer hardware performance, the volume of research based on computer-based multiscale analysis has increased [23–25]. This short review analyzes research papers that focused on multiscale analyses of nanoparticle-reinforced composites published over the past decade. Through this, we aim to contribute to the growth of related technologies by providing prospective readers with an opportunity to review multiscale trends. Multiscale modeling is expected to contribute to the development of nanomaterials and their

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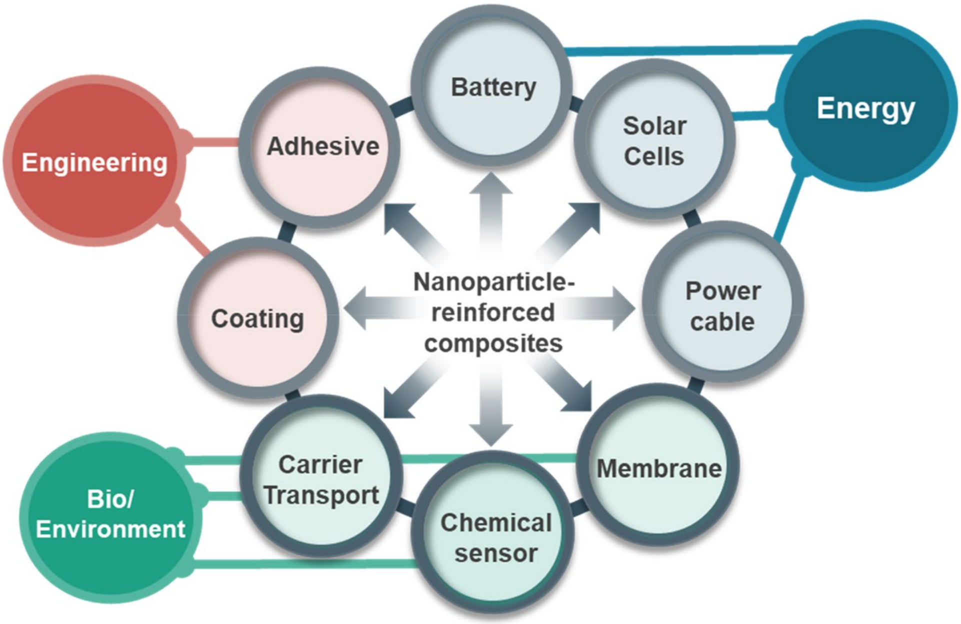


Fig. 1 Representative examples of applications of nanoparticle-reinforced composites

related applications by reliably predicting the properties of inhomogeneous materials [26].

Statistical Research Trends of in the Modeling of Nanoparticle-Reinforced Composites

To analyze the trends of published journal papers statistically while focused on the multiscale modeling of nanoparticle-reinforced composites, related papers were collected using the following main keywords: (1) multiscale modeling, (2) nanoparticle, and (3) composites [27]. The analysis targets were papers indexed in SCOPUS published between 2013 and 2022. The SCOPUS search engine was employed for collecting and analyzing the data; data mining was performed based on the year, country, institution, and field.

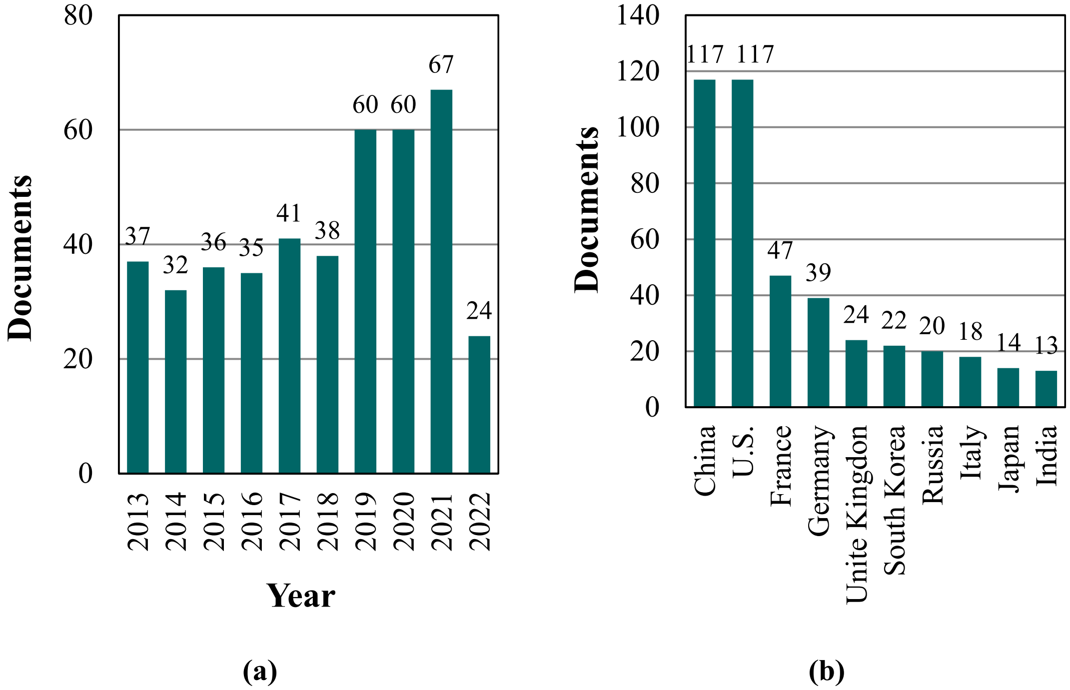
As presented in Fig. 2a, 430 research papers in total focusing on the multiscale modeling of nanoparticle-reinforced composites were published between 2013 and 2022. As can be observed, the number of papers gradually increased in 2013 and demonstrated steady growth after 2018 [28, 29]. In particular, most papers that focused on multiscale modeling of nanoparticle-reinforced composites were published in 2021. The reason for the low number of publications in 2022 is that the latest unpublished papers are not included here.

The countries with the most active research on the multiscale modeling of nanoparticle-reinforced composites over the past ten years are China and the United States (U.S.), each with a total of 117 published papers (Fig. 2b). Related technology development has also been actively carried out in France, Germany, and the United Kingdom [30]. In addition, researchers in Korea, Russia, Japan, Italy, and India have been steadily producing results on related research topics.

Research institutes that have published most papers on multiscale modeling are the Ministry of Education of China, the Chinese Academy of Science, and the Centre National de la Recherche Scientifique (CNRS) in France, each with 12 papers published over the past ten years (Fig. 3a). Northwestern Polytech University and Purdue University in the U.S. published eight papers each, and Seoul National University in Korea and Sapienza University di Roma in Italy published seven papers each. It can be seen that papers have been published by major research institutions belonging to various countries, including China, France, and the U.S.

As can be observed from Fig. 3b, materials science is the primary field in which papers on the multiscale modeling of nanoparticle-reinforced composites have been published, accounting for approximately 30%. Engineering is the second most popular field, slightly behind materials science. As a whole, the majority of technical papers related to the multiscale modeling of nanoparticle-reinforced composites appear to be focused on materials science and engineering.

In this chapter, papers addressing the multiscale modeling of nanoparticle-reinforced composites were selected and a quantitative analysis was then conducted to analyze the underlying technological trends. The number of papers was found to have increased continuously from 2013 to 2022. In total, 430 international papers were published during this period. The analysis revealed a gradual increase in the number of papers from 2013 to 2017, followed by significant growth from 2018 onwards. The highest growth rate was found in the past four years. The primary countries that



(a) **(b)**

Fig. 2 Summaries of research papers by **a** year and **b** country

published papers on multiscale modeling were China and the U.S., each with 117 papers, followed by France, with 47 papers.

The U.S. and China appear to be conducting joint research with most of the other countries that publish in this area. Therefore, they can be considered as hub countries for research on the multiscale modeling of nanoparticle-reinforced composites. The Ministry of Education of China, the Chinese Academy of Science, and the CNRS in France are the research institutes that have published most papers on multiscale modeling worldwide. Moreover, most research papers have been published in the fields of materials science and engineering. In particular, over 60% of the published articles on multiscale modeling are focused on materials science and engineering.

Recapitulation of Multiscale Modeling Based on Molecular Dynamics, Micromechanics, and the Finite Element Method

When a multiscale system is configured using molecular dynamics (MD), micromechanics, and the finite element method (FEM), more accurate predictions of the mechanical properties of nanoparticle-reinforced composites can be realized by effectively simulating the interfacial properties between nanofillers and the matrix (Fig. 4) [31–33]. To achieve this, it is necessary to derive a modified micromechanical-based stiffness equation as a link between the nanoscale and macroscale [34–36]. Such a modified micromechanical stiffness equation considers the elastic modulus of the material as it is and sets the interfacial properties, which are simultaneously affected by the mechanical properties of the material and its molecular structure, as the model constant [17, 37–39].

The model described in one study [40] can be derived by applying Eshelby's tensor to an existing micromechanical model [41]. The derived equation is as follows [42, 43]:

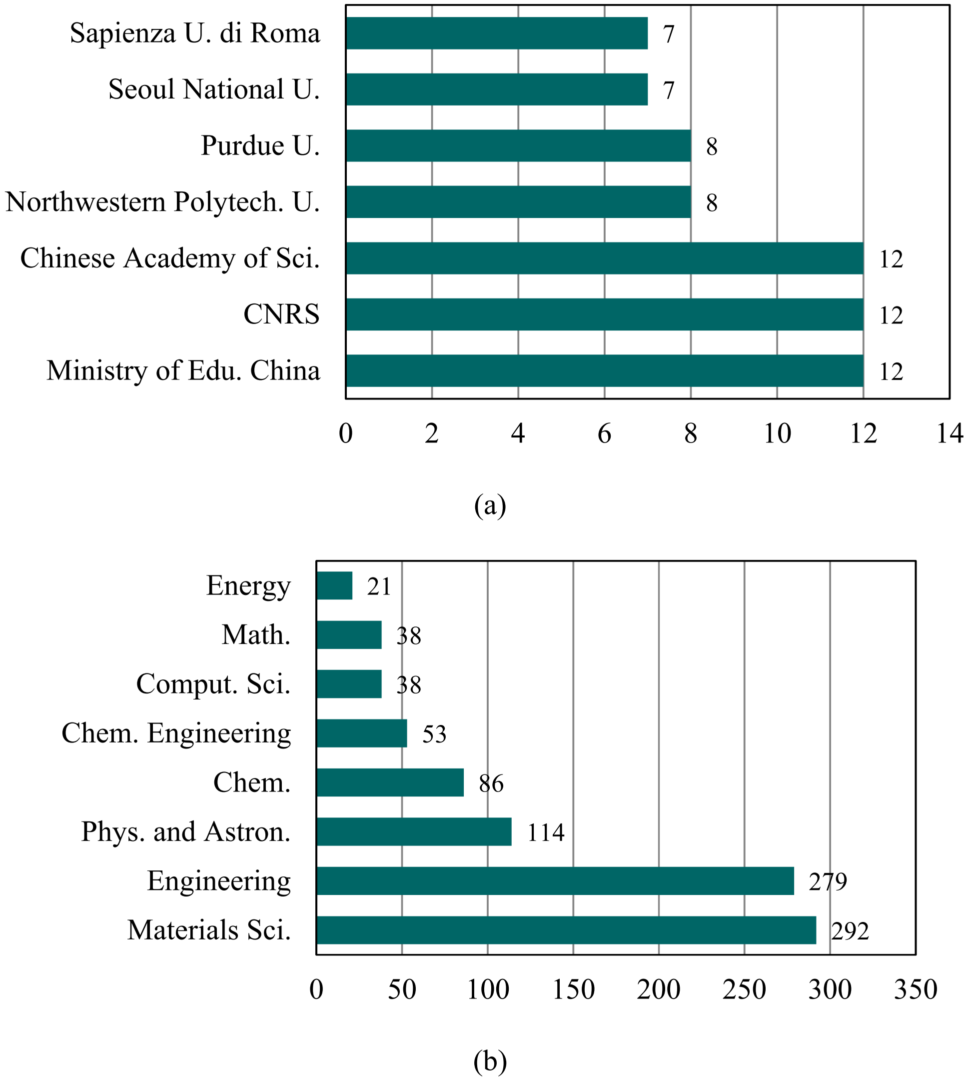
$$C^* = \lambda^*_{IK}\delta_{ij}\delta_{kl} + \mu^*_{IJ}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) = \begin{bmatrix} \lambda^*_{11} + 2\mu^*_{11} & \lambda^*_{12} & \lambda^*_{13} & 0 & 0 & 0 \\ \lambda^*_{21} & \lambda^*_{22} + 2\mu^*_{22} & \lambda^*_{23} & 0 & 0 & 0 \\ \lambda^*_{31} & \lambda^*_{32} & \lambda^*_{33} + 2\mu^*_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu^*_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu^*_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu^*_{12} \end{bmatrix} \quad (1)$$

where

$$\lambda^*_{IK} = 2\lambda_0\chi^{(2)}_{KK} + 2\mu_0\chi^{(1)}_{IK} + \lambda_0\sum_{n=1}^{3}\chi^{(1)}_{nK},\ \mu^*_{IJ} = \mu_0\left(\chi^{(2)}_{IJ} + \chi^{(2)}_{JI}\right) \quad (2)$$

with

Fig. 3 Summaries of research papers by **a** affiliation and **b** subject area



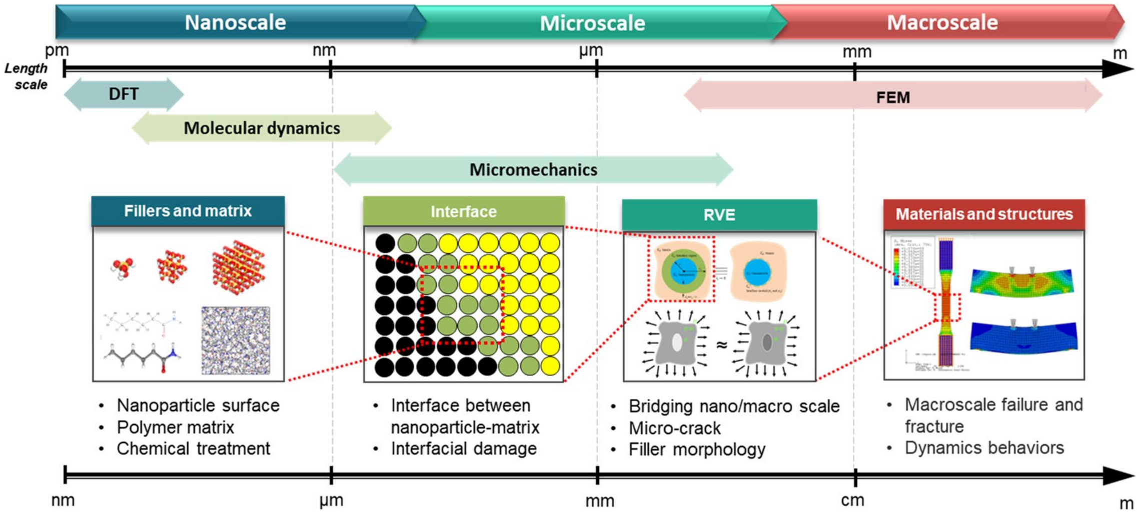
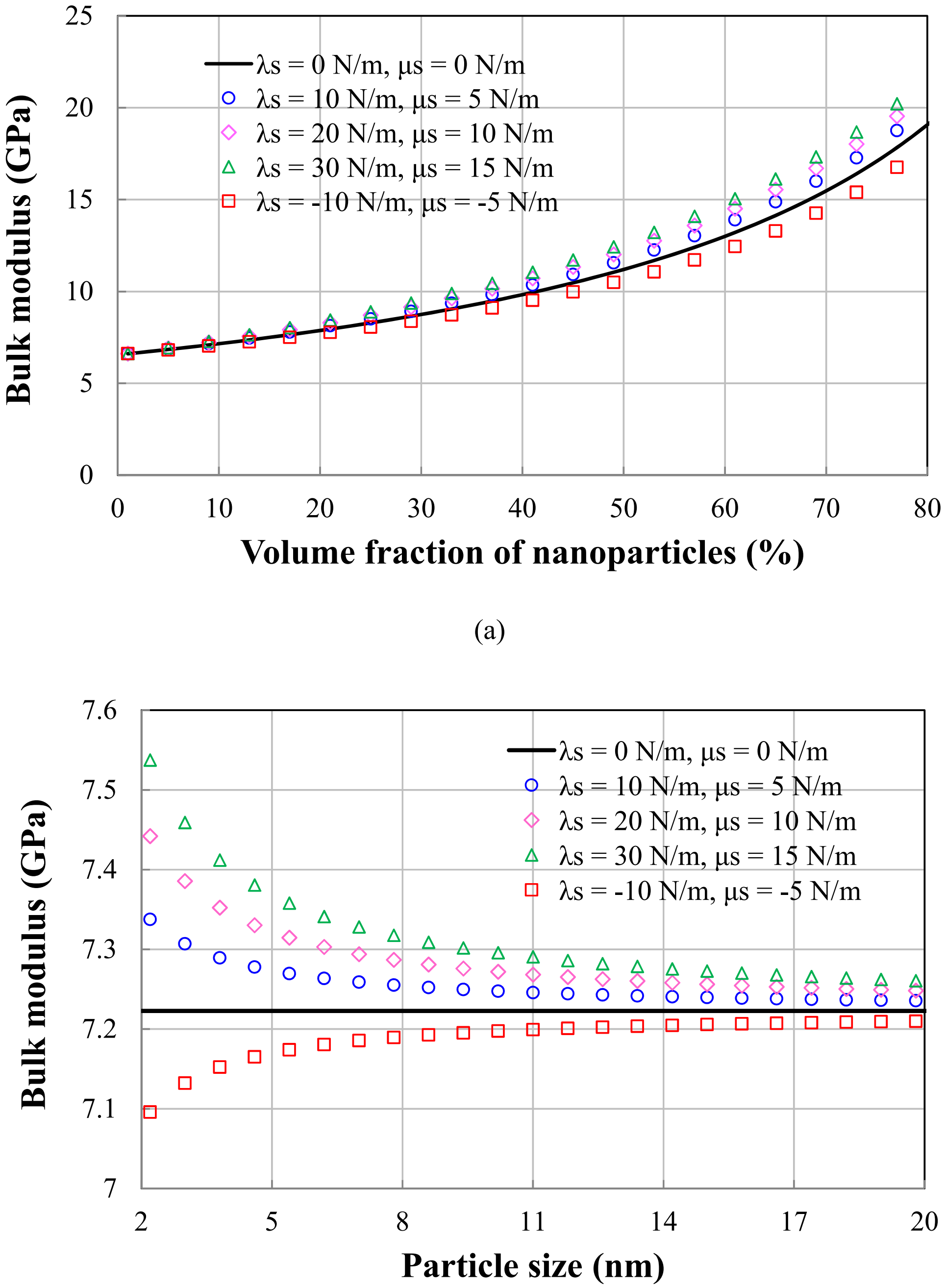


Fig. 4 Scheme for multiscale modeling based on MD, micromechanics, and FEM

$$\chi_{IK}^{(1)} = \Lambda_1 + \Lambda_{IK}^{(3)},\ \chi_{IJ}^{(2)} = \frac{1}{2} + \Lambda_2 + \Lambda_{IJ}^{(4)} \tag{3}$$

In Eq. (3), the interfacial properties between two phases and microcracks caused by external loads are considered. The definitions of the constants Λ_1, Λ_2, $\Lambda_{IK}^{(3)}$, and $\Lambda_{IJ}^{(4)}$ in Eq. (3) and their derivation processes are comprehensively described in the Appendix B of [43].

Further, a numerical analysis of a silica nanoparticle-reinforced epoxy composite conducted on the basis of Eq. (1) reveals that the influence of the interfacial properties is greater when the particle size is small and the nanoparticle content ratio is large (Fig. 5) [44]. However, as the particle size increases, the effect of the interface between the two phases on the nanocomposite decreases. Specifically, when the nanoparticle size is 15 nm or larger, the effect is expected nearly to disappear.



(a)

(b)

Fig. 5 Effects of interface parameters on the effective bulk modulus of nanoparticle-reinforced composites with varying **a** contents of nanoparticles and **b** different nanoparticle sizes

MD calculations can be performed using an open-source code, such as the LAMMPS (Large-scale Atomistic Modeling Massively Parallelized Simulation) or with commercial software such as Materials Studio [45]. The total energy value of a nanocomposite, calculated using MD, can be estimated by a comparison with the equation of state (EoS) [46]. The MD calculation results can be used for interfacial constant estimations through an inverse analysis with micromechanics-based calculations. This calculation process is described in greater detail in two studies [43, 47].

The completed micromechanical-based constitutive equation can be incorporated into the FEM to solve the boundary condition problems of materials and/or structures. The predicted analysis results can be directly compared with experimental results under the same boundary conditions. The von Mises stress distribution of the 3D modeled specimen can be estimated through the FEM [48]. Through these processes, it is possible to estimate local influences on the nanoscale effectively during the macroscale characterization of nanocomposites [26, 49, 50].

In addition, data-driven research based on artificial intelligence (AI) for designing new materials has been very actively conducted [51]. The data-driven analysis has the strength to increase the accuracy of material property prediction; however, it also has the disadvantage of being too data-dependent. In addition, this method has a limitation in that it is difficult to predict the material characteristics outside the range of the trained data [52, 53]. Recently, in order to overcome these problems, an improvement of the deep neural network and the multiscale convergence model have been studied [54].

Summary

Predicting the performance of nanoparticle-reinforced composites via a single-scale analysis is often difficult and thus multiscale analysis techniques are required to overcome various limitations [55–57]. Through multiscale simulations, it is possible to conduct more accurate regional analyses on the nanoscale level and predict material/structural behaviors on the macroscale level [58]. In addition, multiscale simulations can help to predict the maximum strength and stability of nanocomposites according to various material combinations and mixing ratios.

Precluding unnecessary experiments and concentrating on research that focuses on nanocomposites with a high probability of success can both save time and preserve funds while also ultimately promoting better research efficiency and stability [59, 60]. In future, we expect that more nanomaterials will be developed and that their utilization will increase. However, for nanocomposite materials to be used more widely in industries, establishing reliable simulation approaches is essential [61].

In the future of multiscale technology for nanocomposites, three challenges are anticipated to be overcome: First, it is necessary to converge time-series prediction technology that can consider the complex durability and fatigue of heterogeneous materials over time. Second, the development of an AI-based data fusion multiscale analysis is required. Data-based interpretation has been widely applied in the past, but it is increasing more rapidly in recent years. Third, a high-efficiency analysis processing method that can perform calculations quickly should be developed. The current method requires a relatively large amount of hardware capacity. It is believed that multiscale modeling will be able to accurately simulate and predict the physical/chemical properties of more diverse materials in the future by overcoming the above challenges.

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Declarations

Conflict of interest The authors have no conflicts of interest to declare.

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