

A COMBINED MOLECULAR DYNAMICS AND FINITE ELEMENT STUDY ON PARTICULATE-REINFORCED POLYMER NANOCOMPOSITES

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Abstract. This study introduces a multiscale modeling approach that combines Molecular Dynamics (MD) and the Finite Element Method (FEM) to evaluate the mechanical behavior of polymer composites reinforced with nanoparticles, using functionally graded interphase modeling. At the atomic scale, MD simulations explore interfacial adhesion, the characterization of the perturbed zone (called “interphase”) between the matrix and the nanoparticle, and the mechanical behaviors of each phase in the heterogeneous material. As deduced from the MD simulations when computing the mean squared displacement, the interphase can be modeled as a functionally graded zone. These findings are then integrated into FEM to assess the local mechanical fields as well as the macroscopic properties of the nanocomposite, through different boundary conditions. Different types of functionally graded interphases are simulated, including linear, exponential, and power law. The effects of the reinforcement fraction and the functionally graded interphase are investigated accordingly. The main novelty of the current study is a physics-informed MD-FEM multiscale framework in which the interphase properties are not assumed but directly extracted from Molecular Dynamics simulations. Overall, the proposed methodology offers a physics-informed and computational strategy for investigating the mechanical behavior of nanoparticle-reinforced composites.

Keywords: multiscale modeling, molecular dynamics (MD), finite element method (FEM), polymer nanocomposites, computational mechanics, interphase.

1. INTRODUCTION

Polymer nanocomposites reinforced with nanoparticles have emerged as a class of advanced materials with superior mechanical, thermal, and electrical properties (Choi et al., 2015). For instance, particulate reinforcements like silica or graphene oxide can significantly improve stiffness, toughness, and thermal stability in polymer matrices such as epoxy or polyethylene (Choi et al., 2015). Despite these advantages, the effective performance of particulate-reinforced polymer nanocomposites is heavily influenced by the interphase region—a transitional zone between the reinforcement and the matrix (Brown et al., 2003). This interphase arises due to interactions at the nanoscale, including chemical bonding, potential forces, and polymer chain mobility near the particle surface (Berriot et al., 2002; Brown et al., 2003).

Molecular Dynamics (MD) simulations have proven invaluable for capturing atomic-scale phenomena in nanocomposites, including interphase formation and nanoparticle-polymer interactions (Hossain et al., 2010). Conversely, Finite Element (FE) methods excel at mesoscale and macroscale analyses, enabling the simulation of Representative Volume Elements (RVEs) and the overall nanocomposite response (Pfaller et al., 2016). Hybrid approaches combining MD and FE have been explored to bridge these scales, where MD informs FE models with nanoscale parameters (Amraei et al., 2018; Bazmara et al., 2021; Chang et al., 2015; Charitos & Kontou, 2024; Chen et al., 2024; Eghbalian et al., 2023; Muhammad et al., 2023; Pfaller et al., 2016; Seidel et al., 2006; Uthale et al., 2021; Vu-Bac et al., 2018; Zakaria & Shelesh-Nezhad, 2014). Many existing MD-FEM coupling approaches model it as a homogeneous layer with arbitrarily assumed properties. In particular, the gradual transition of mechanical properties across the polymer-particle interface has not been sufficiently captured in prior studies.

In the present study, instead of assuming a homogeneous interphase, we extract interphase characteristics from MD simulations via the mean squared displacement and represent this perturbed zone as a functionally graded region. To the best of our knowledge, this is the first work to integrate functionally graded interphase laws (linear, exponential, power law) into FEM simulations of polymer nanocomposites. Next, by incorporating graded interphase models into FEM, we investigate both local stress/strain fields and macroscopic mechanical properties under different loading conditions. We also study the combined effects of the reinforcement fraction and functional gradation, which have not been systematically explored in previous MD-FEM coupling works. The paper is organized as follows: Section 2 details the microstructure, MD simulation setup, and homogenization procedure; Section 3 presents the results and discussions, including the characterization of the interphase, mesh convergence analysis, local strain and stress fields, and parametric study; and Section 4 concludes with implications and future work.

The novelties of the current study are as follows. The first novelty is a physics-informed MD-FEM multiscale framework in which the interphase properties are not assumed but directly extracted from Molecular Dynamics simulations. The second novelty is the identification of the polymer-nanoparticle interphase as a functionally graded region, rather than a homogeneous layer, based on atomistic evidence. The third novelty is the systematic incorporation of different functional grading laws (linear, exponential, and power-law) for the interphase into the FEM framework.

2. MATERIALS AND METHODS

2.1. Description of microstructure

We examine a composite microstructure consisting of 3 phases: a matrix, a nanoparticle, and a perturbed zone of the matrix surrounding the nanoparticle, called the interphase. The matrix has a length L , while the nanoparticle has a radius R_p . The nanoparticle is placed at the center of the domain, with its reinforcement fraction represented by f_i . From a mechanical perspective, the matrix and the nanoparticle are assumed to follow linear isotropic elasticity, while the interphase is revealed as a functionally graded material by using MD simulations, as shown in the following.

At the lower scale, Molecular Dynamics simulations are used to characterize the structural and mechanical behavior of the polymer matrix, nanoparticle, and interphase region. The extracted atomistic information is then upscaled and incorporated into a continuum-scale FEM model.

2.2. Molecular dynamics simulation

The dynamics of a particulate system at the atomic or molecular scale can be described by the Molecular Dynamics (MD) approach, which is based on Newton's laws of motion (Allen & Tildesley, 1989). Initialization, calculating potential energy, calculating forces, calculating

accelerations, integrating equations of motion, and updating locations, velocities, etc., are the primary steps in MD. Since MD is a proven technique, further information can be obtained from the work of Allen and Tildesley (1989).

2.2.1. Polymer system

In this study, a Monte Carlo-based method known as the "Self-Avoiding Random Walk" was used to construct the initial configuration of the polymers (Hossain et al., 2010). The polymer system's relaxation state satisfying the force field shown above at 100 K (under Nosé-Hoover NPT control (Nosé, 1984)) was then obtained by MD simulations. Because it is significantly lower than the glass transition temperature of polyethylene, which is approximately 250 K (Hossain et al., 2010), 100 K was used as the equilibrium temperature in this work in order to acquire a typical elastic behavior of polymeric materials. According to Brown et al. (2008), a time step of 2 fs was employed in this study for coarse-grained simulations.

2.2.2. Nanoparticle

In this study, silica nanoparticles are used to reinforce the polymer. The crystalline structure of silica, α -quartz, the most prevalent polymorph of silica crystals, was converted to the amorphous structure via a melt-and-quench process (Brown et al., 2008). For additional information about the MD simulation of the silica system, readers may refer to the work of Brown et al. (2008).

2.2.3. Nanocomposite system

Once the polymer and silica systems have been obtained, the nanocomposite unit cell can be virtually built, as shown below. First, the MD box containing the polymer is expanded by a volume equal to the one occupied by the particle. Second, a soft repulsive potential is progressively placed into the middle of the box. Finally, once the target hole diameter has been obtained, the silica particle is introduced, forming the nanocomposite's initial structure. This generating phase is followed by an MD relaxation method. Using this method, MD simulations might be used to characterize both the interphase and the mechanical behavior.

2.3. Homogenization

The homogenization approach calculates the apparent mechanical characteristics of particulate composite materials by averaging the microstructural response over a representative volume element (RVE) (Yvonnet, 2019). Consider a microstructure composed of N phases, the domain is denoted by $\Omega \subset \mathbb{R}^D$ where $D = 2$ in this case for simplicity. The boundary is denoted by $\partial\Omega$. The elasticity tensor $\mathbf{C}(\mathbf{x})$ is written such as:

$$\mathbf{C}(\mathbf{x}) = \sum_{i=1}^N \chi_i(\mathbf{x}) \mathbf{C}^i, \quad (1)$$

where $\mathbf{C}^i$, $i = 1, 2, \dots, N$ is the elasticity tensor of each phase in the heterogeneous material. From the local properties of the phases and the corresponding geometries, the goal of the problem is to determine the effective elastic tensor $\bar{\mathbf{C}}$ for the equivalent homogeneous structure. It should be noted that the interfaces between the phases (in particular, between the matrix and the interphase, and between the interphase and the nanoparticle) are assumed to be continuous. In the case of elasticity, this means that the displacements $\mathbf{u}$ and the normal force fields $\sigma \cdot \mathbf{n}$ are continuous across the interfaces.

According to the Kinematic Uniform Boundary Condition (KUBC), the homogenization problem is set as follows: given the strain field $\bar{\epsilon}$ on the boundary $\partial\Omega$, the displacement field $\mathbf{u}(\mathbf{x})$ in the domain Ω is such as:

$$\nabla \cdot \sigma(\mathbf{u}(\mathbf{x})) = 0 \quad \forall \mathbf{x} \in \Omega, \quad (2)$$

where

$$\sigma(\mathbf{u}(\mathbf{x})) = \mathbf{C}(\mathbf{x}) : \varepsilon(\mathbf{u}(\mathbf{x})), \quad (3)$$

and

$$\varepsilon(\mathbf{u}(\mathbf{x})) = \frac{1}{2} \left(\nabla \mathbf{u}(\mathbf{x}) + \nabla^T \mathbf{u}(\mathbf{x}) \right), \quad (4)$$

satisfying

$$\langle \varepsilon \rangle = \bar{\varepsilon} \quad (5)$$

It should be noted that in this study, the Static Uniform Boundary Condition and the Periodic Boundary Condition are not considered for simplicity. To solve the problem of finding the effective elasticity tensor in 2-dimensional space, 3 separate problems were posed including 2 cases of a tensile test at the center along x - and y -directions, and 1 corresponding shear test. The displacement field $\mathbf{u}(\mathbf{x})$ is then given by:

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}^{(11)}(\mathbf{x})\bar{\varepsilon}_{11} + \mathbf{u}^{(22)}(\mathbf{x})\bar{\varepsilon}_{22} + 2\mathbf{u}^{(12)}(\mathbf{x})\bar{\varepsilon}_{12}, \quad (6)$$

where $\mathbf{u}^{(ij)}(\mathbf{x})$ is the solution according to:

$$\bar{\varepsilon} = \frac{1}{2} (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i), \quad (7)$$

where $\mathbf{e}_i$, $i = 1, 2$ are unit matrices. The KUBC for the 2 tensile tests are given such as:

$$\bar{\varepsilon} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \bar{\varepsilon} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \quad (8)$$

Similarly, the KUBC for the shear test is given by:

$$\bar{\varepsilon} = \begin{bmatrix} 0 & 1/2 \\ 1/2 & 0 \end{bmatrix}. \quad (9)$$

3. RESULTS AND DISCUSSION

3.1. Identification of interphase from Molecular Dynamics simulation

Using the simulation procedure described previously, the polymer, the silica nanoparticle, and the nanocomposite system are obtained, ready for the characterization of the interphase and the mechanical behavior of each phase in the domain. Fig. 1 provides images of MD simulations for the nanocomposite system at 0% of strain, at about 25% of strain in a tensile test, and stress-strain curves for a tensile test along x -, y - and z -directions. As introduced previously,

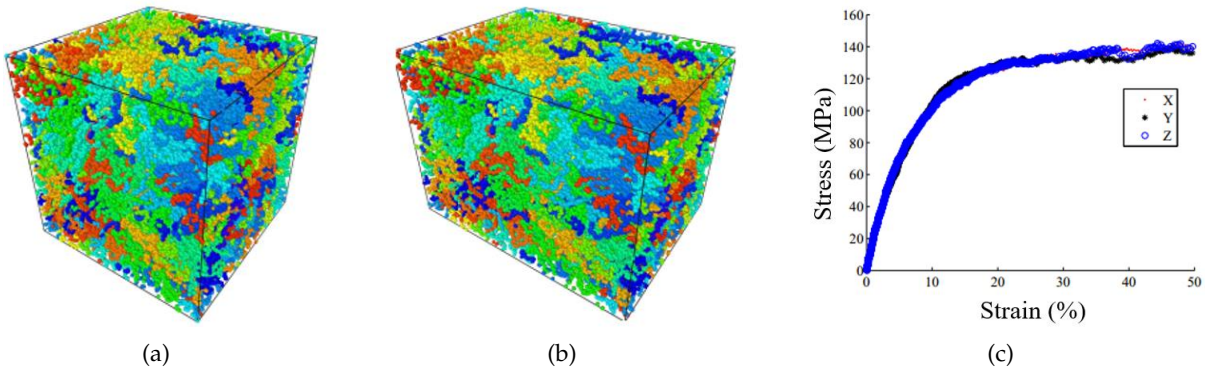


Fig. 1. MD simulations for nanocomposite system: (a) simulation box at 0% of strain, (b) simulation box at about 25% of strain in a tensile test and (c) stress-strain curves for tensile test along x -, y - and z -directions (Le, 2020)

this study considers only the linear isotropic elasticity of the matrix and the nanoparticle. Thus, as deduced from MD simulations, the bulk and shear moduli of the matrix are 5.16 and 0.93 GPa, respectively. Similarly, the bulk and shear moduli of the nanoparticle are 36.8 and 30.5 GPa, respectively. This information is then integrated into the Finite Element simulation in the next sections.

In order to identify the modified zone of the matrix surrounding the nanoparticle, the mean squared displacement (MSD) of the polymer units is computed. The graph of mean squared displacement of the polymer surrounding the nanoparticle is shown in Fig. 2. It is clearly seen in Fig. 2 that there are decreases of the mean squared displacement in the neighborhoods of the nanoparticle. We also observe that the decrease of mean squared displacement occurs for a distance of 2 nm from the surface of the nanoparticle. From these remarks, the interphase can be modeled as a functionally graded material.

The choice of 2 nm for the interphase thickness is directly obtained from the mean squared displacement profile of polymer chains in the vicinity of the silica nanoparticle. We observed that polymer mobility is significantly perturbed within ~ 2 nm from the nanoparticle surface, beyond which the mean squared displacement converges to the bulk polymer behavior. This 2 nm thickness is consistent with experimental results reported in the literature. For instance, Berriot et al. (2002) reported an interphase thickness in the same range by using Nuclear Magnetic Resonance. In the case of polyethylene reinforced by nanosilica, the interphase thickness is relatively independent of particle size (Brown et al., 2008), as it is governed mainly by interactions at the particle-polymer interface. However, the interphase thickness is dependent on the temperature, as shown by Berriot et al. (2002) when varying the temperature from 60 °C to 120 °C.

The characterization of the interphase in the nanocomposite allows for the following hypotheses for further studies, i.e., the modelling of the interphase in a multiscale framework:

- In this case of polyethylene reinforced by a silica nanoparticle, the interphase is identified as a shell of thickness 2 nm surrounding the nanoparticle;
- The mean squared displacement surrounding the nanoparticle is gradually increased to the MSD of the normal polymer matrix, allowing the assumption that the interphase can be modeled as a functionally graded material.

3.2. Functionally graded interphase modeling

It is interesting to notice that the interphase is a modified zone of the matrix surrounding the nanoparticle. Thus, the bulk and shear moduli of the functionally graded interphase (assumed to be locally isotropic), are modeled as a function of the bulk and shear moduli of the matrix, respectively, as shown in the equation below.

$$\begin{cases} \kappa_{\text{int}} = f(r) \times \kappa_m \\ \mu_{\text{int}} = f(r) \times \mu_m \end{cases} \quad (10)$$

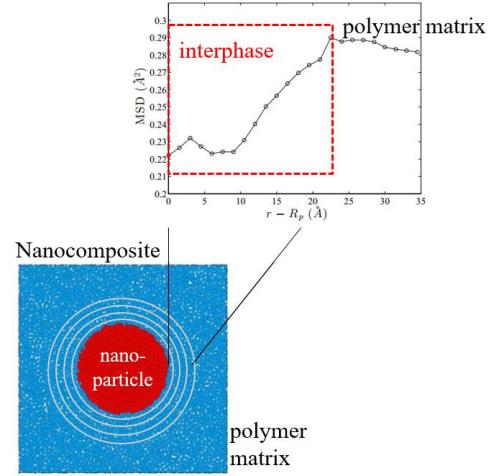


Fig. 2. Identification of interphase: mean squared displacement of particles at the vicinity of the nanoparticle surface

where $f(r)$ is the functionally graded law and r is the radial distance from the surface of the nanoparticle. In this study, different types of functionally graded interphases are considered, including linear, exponential, power law type 1, power law type 2, and power type 3, as detailed in the equation below as a function of the radial distance:

$$\left\{ \begin{array}{l} f(r) = 1, \text{ without interphase} \\ f(r) = \frac{1-A}{t}r + A, \text{ linear law} \\ f(r) = A \exp\left(-\frac{\log(A)}{t}r\right), \text{ exponential law} \\ f(r) = A \left(\frac{r+1}{1}\right)^{\left(\frac{\log\left(\frac{1}{A}\right)}{\log\left(\frac{1}{1}\right)}\right)}, \text{ power law type 1} \\ f(r) = A \left(\frac{r+0.2}{0.2}\right)^{\left(\frac{\log\left(\frac{1}{A}\right)}{\log\left(\frac{1}{0.2}\right)}\right)}, \text{ power law type 2} \\ f(r) = A \left(\frac{r+0.01}{0.01}\right)^{\left(\frac{\log\left(\frac{1}{A}\right)}{\log\left(\frac{1}{0.01}\right)}\right)}, \text{ power law type 3} \end{array} \right. \quad (11)$$

where t is the thickness of the interphase, determined as $t = 2$ nm from Molecular Dynamics simulations; A is the amplitude and r is the radial distance from the surface of the nanoparticle. Fig. 3 introduces an illustration of the polymer particle surrounding the nanoparticle in the MD simulation and an illustration of the functionally graded interphase with different laws.

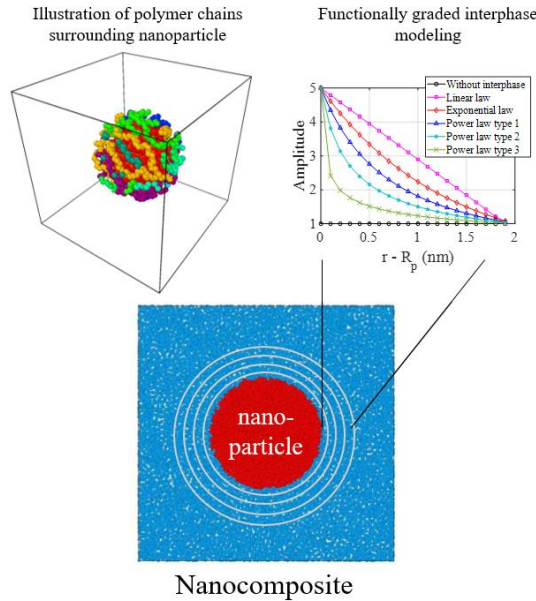


Fig. 3. Illustration of polymer particle surrounding the nanoparticle in MD simulation and illustration of functionally graded interphase with different laws

3.3. Finite element simulation and parametric study

Three variables are parametrically considered, including the laws for the functionally graded interphase, the amplitude A , and the reinforcement fraction f_i , as detailed in Table 1 below. It should be noted that the case of no interphase (the interphase is the same as the matrix) is also considered for reference.

Table 1. Parametric study

Nr	Variable	Variation
1	Reinforcement fraction f_i	$f_i^{\min} = 0.05$, $f_i^{\max} = 0.3$ (corresponding length L from 22.5 to 10 nm)
2	Law for functionally graded interphase	6 types included: Without interphase, Linear law, Exponential law, Power law type 1, Power law type 2, Power law type 3
3	Amplitude A	$A^{\min} = 1$, $A^{\max} = 10$

3.3.1. Mesh convergence analysis

Fig. 4 introduces the mesh convergence analysis for the study. The value of the first component of the effective elasticity tensor C_{11}^{eff} is evaluated with a different number of nodes in the FE mesh. It is seen that from a value of 400,000 nodes in the domain, the convergence is obtained, for all types of functionally graded interphases.

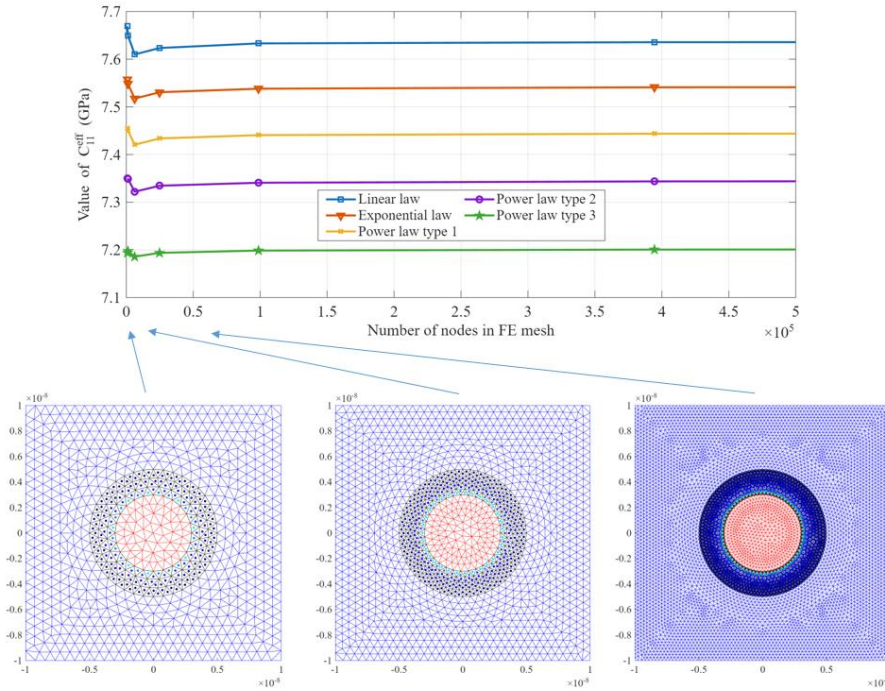


Fig. 4. Mesh convergence analysis

3.3.2. Local stress and strain fields

Fig. 5 introduces the local fields in a shear test with different configurations, for the case $A = 2$, $R_p = 3$ nm, $L = 15$ nm. Six cases of the interphase, including without interphase, linear law, exponential law, power law type 1, power law type 2, and power law type 3, are considered. Similarly, Fig. 6 shows local fields in a tensile test with different configurations, for the case $A = 2$, $R_p = 3$ nm, $L = 15$ nm (approximately $f_i = 12\%$). In terms of reinforcement fraction, Fig. 7 provides local fields in a shear test when decreasing the reinforcement fraction from $f_i = 12\%$ to $f_i = 6\%$. It is clearly seen that thanks to the existence of an interphase, the load transfer mechanism is much better than in the case of no interphase (i.e., smaller strain and

higher stress to reach the same boundary conditions). We also remark the difference between each type of functionally graded interphase in the local strain and stress fields.

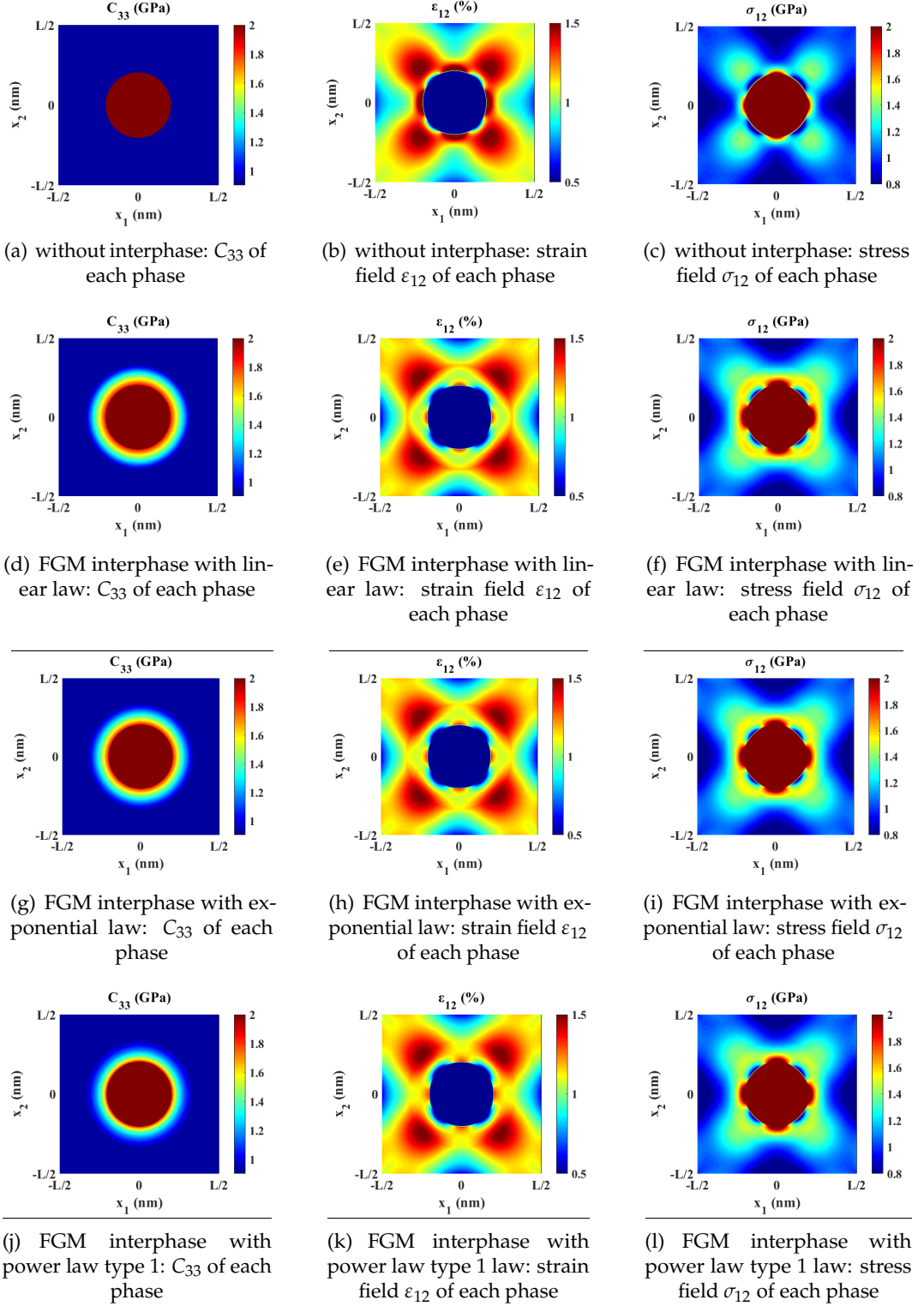


Fig. 5. Local fields in a shear test with different configurations, for the case $A = 2, R_p = 3$ nm, $L = 15$ nm (approximately $f_i = 12\%$). All figures are plotted with same colorscale

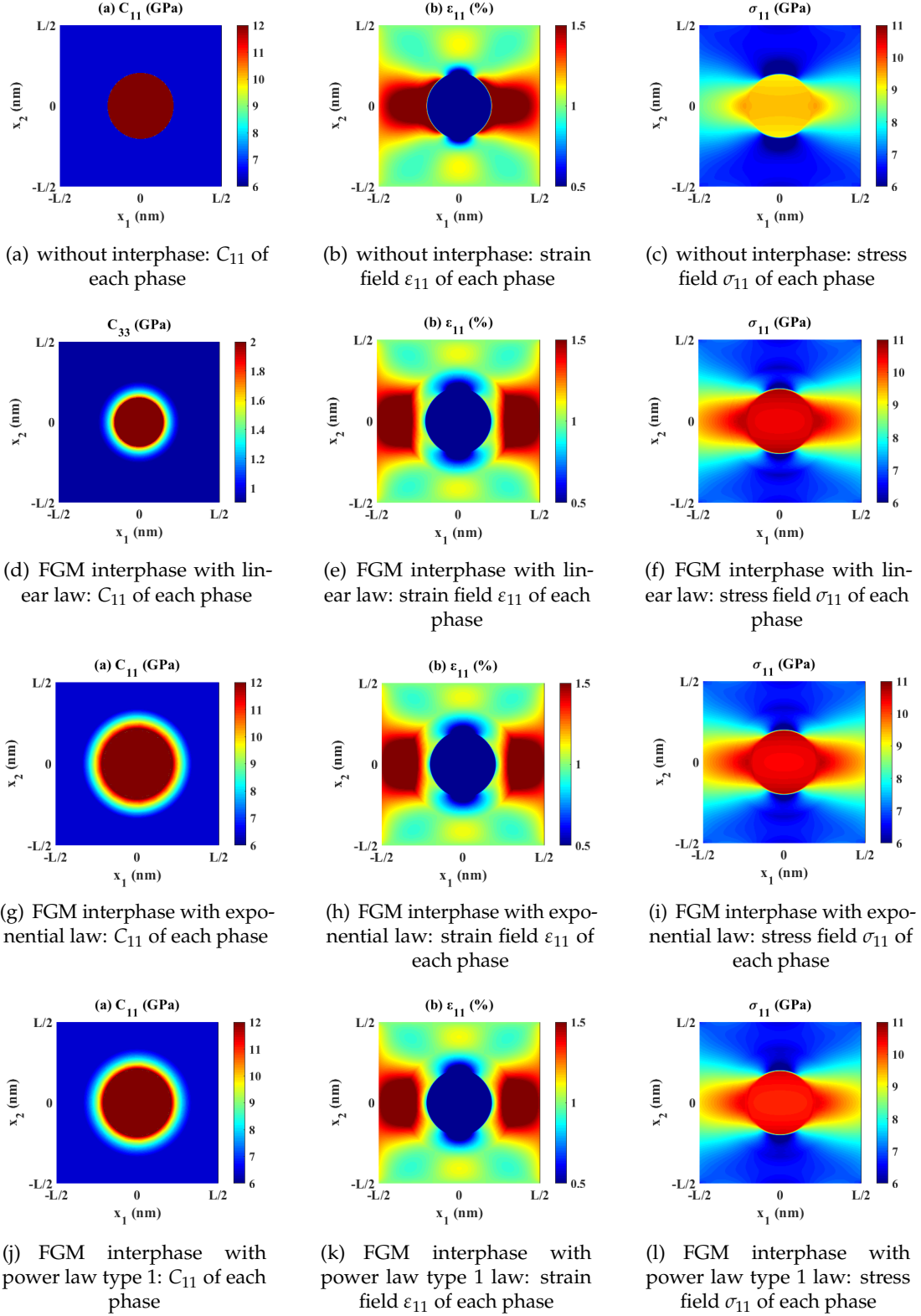


Fig. 6. Local fields in a tensile test with different configurations, for the case $A = 2$, $R_p = 3$ nm, $L = 15$ nm (approximately $f_i = 12\%$). All figures are plotted with same colorscale

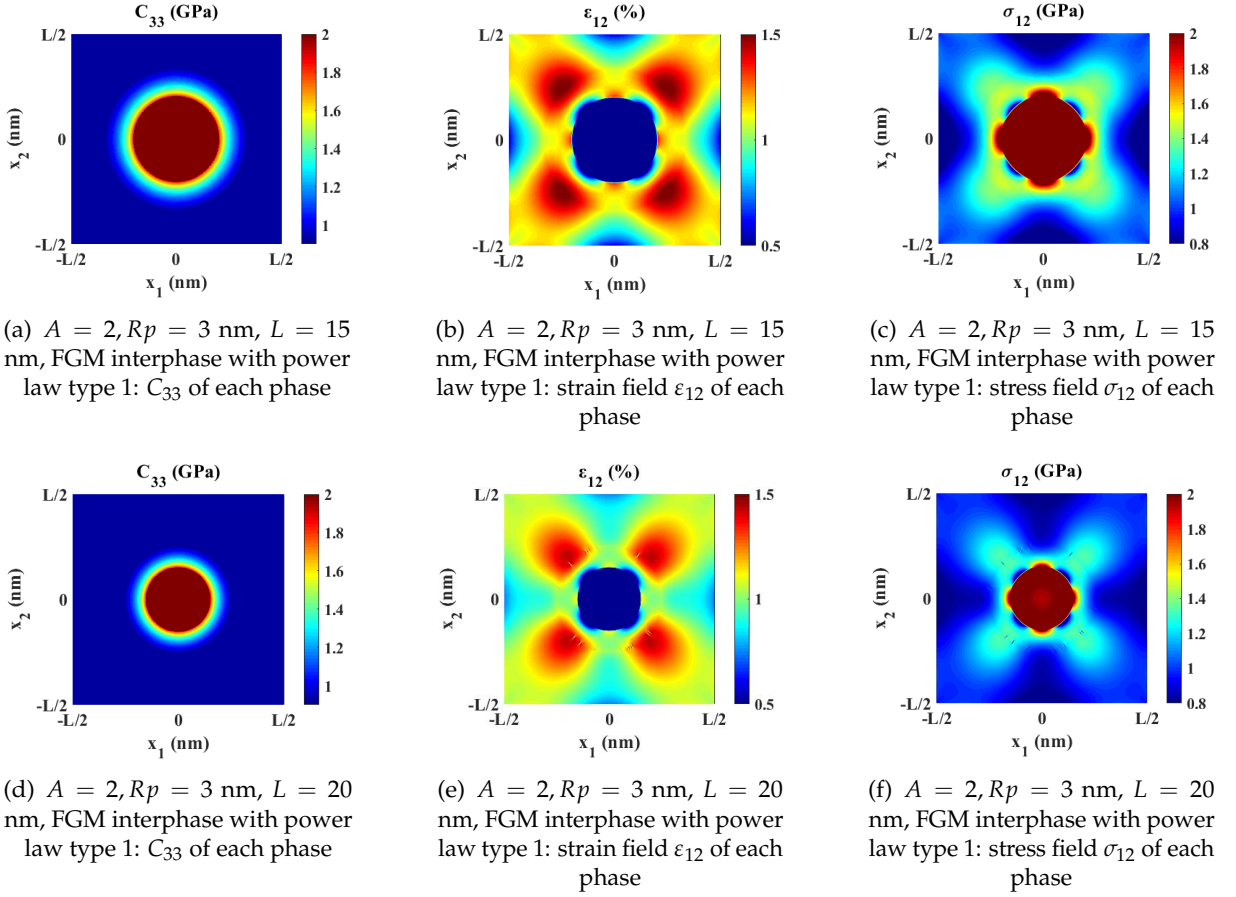


Fig. 7. Local fields in a shear test when decreasing the reinforcement fraction from $f_i = 12\%$ to $f_i = 6\%$. All figures are plotted with same colorscale

3.3.3. Parametric study on effective properties

In this section, the effects of the reinforcement fraction and the type of functionally graded interphase on the effective properties of the nanocomposite are analyzed. Fig. 8, Fig. 9 and Fig. 10 introduce such effects for C_{11}^{eff} , C_{12}^{eff} and C_{33}^{eff} , respectively. The effect on C_{22}^{eff} is the same as C_{11}^{eff} . It is seen in Fig. 8, Fig. 9 and Fig. 10 that the effective properties of the nanocomposite increase as the reinforcement fraction increases. This is an expected trend, as the added reinforcement material contributes to the overall stiffness of the nanocomposite.

Next, the presence of a functionally graded interphase significantly increases the effective properties compared to the case "Without interphase". This highlights the importance of the interphase region in the mechanical properties of the nanocomposite. The interphase acts as a transition zone that improves the load transfer between the reinforcement and the polymer matrix.

The type of FGM law used for the interphase has a noticeable impact on the composite's stiffness, particularly at higher reinforcement fractions. The interphase modeled with the linear law, power law type 1, and exponential law provide the highest effective stiffness. This suggests that these specific grading profiles are most effective at enhancing the overall mechanical performance. The curves for these 3 laws are very close, indicating similar stiffening effects. On the other hand, the power law type 3 results in the lowest effective stiffness among all the

FGM interphase models. While it still performs better than the no interphase case, its stiffness enhancement is the least pronounced.

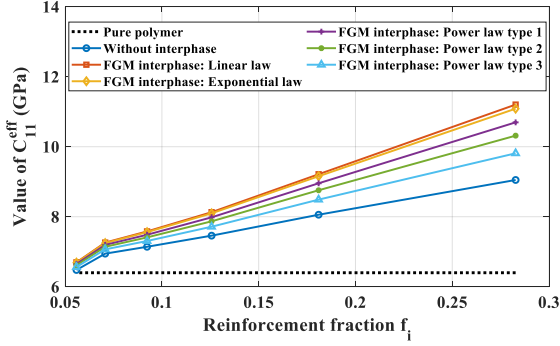


Fig. 8. Parametric study: C_{11}^{eff} in the function of reinforcement fraction and functionally graded interphase

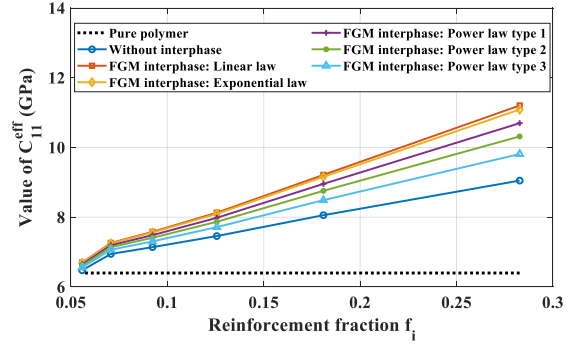


Fig. 9. Parametric study: C_{12}^{eff} in the function of reinforcement fraction and functionally graded interphase

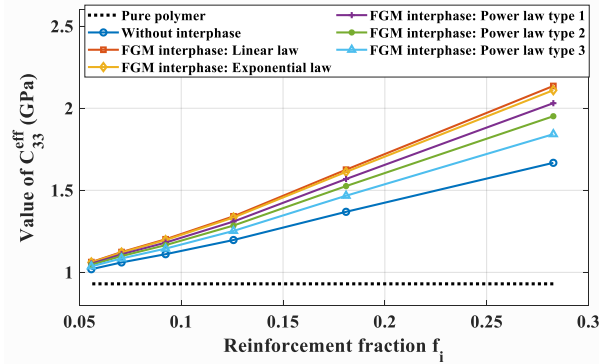


Fig. 10. Parametric study: C_{33}^{eff} in the function of reinforcement fraction and functionally graded interphase

4. CONCLUSIONS

This study introduces a combined MD and FE approach for modeling particulate-reinforced polymer nanocomposites with a focus on the functionally graded interphase. The primary objectives are: (1) to use MD simulations to characterize the atomic-scale interphase geometry and properties; (2) to implement these in an FE framework for investigating the effective mechanical properties under different boundary conditions. The main conclusions are listed below:

- The mean squared displacement surrounding the nanoparticle is gradually increased to the MSD of the normal polymer matrix, allowing the assumption that the interphase can be modeled as a functionally graded material.
- The presence of a functionally graded interphase significantly improves the nanocomposite's stiffness compared to a nanocomposite without an interphase. This highlights the interphase's critical role in facilitating efficient load transfer.
- The functional form of the functionally graded interphase is a key parameter. The "Power law type 1", "Linear law", and "Exponential law" consistently yield the highest stiffness.

However, this study is still limited to the effect of the functionally graded interphase on the effective properties of the nanocomposite, and no inverse identification is carried out. Besides, the current study focuses primarily on elastic behavior under small deformations, and the interphase properties are derived under quasi-static conditions. In future studies, the most appropriate functionally graded interphase should be identified based on experimental data or MD simulation results for better understanding and application. Additionally, future studies may consider temperature and strain-rate effects on the functionally graded interphase, as well as more complex nanoparticle geometries and distributions.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CREDIT AUTHOR STATEMENT

Tien-Thinh Le: *Conceptualization, Methodology, Formal analysis, Investigation, Writing – original draft, Writing – review & editing, Supervision, Project administration.*

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