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# Multiscale Simulation of Crack Growth in Silica/Epoxy Nanocomposites Using a Coupled XFEM–CZM Approach

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## Abstract

One of the fundamental challenges in the analysis of nanocomposites is the accurate prediction of crack initiation and propagation mechanisms. The incorporation of silica nanoparticles enhances fracture toughness, improves impact resistance, and reduces the brittleness of epoxy; these improvements are mainly attributed to crack deflection, the formation of localized plastic strain zones, and the proper distribution of stress within the matrix. In this study, the crack growth process is simulated using a multiscale approach at the micro-, meso-, and macro-scales. The simulations were carried out using the finite element method (FEM) in ABAQUS by combining the cohesive zone model (CZM), for interfacial debonding modeling, and the extended finite element method (XFEM), for predicting crack growth without the need for remeshing. At the microscale, two types of representative volume elements (RVEs), including a single-particle cell and a clustered-particle model, were analyzed, and the effect of the adhesive bonding type between the particle and the matrix was investigated. At the mesoscale, crack propagation in a heterogeneous medium containing nanoparticle was evaluated in order to identify the actual role of particles in altering the fracture path. At the macroscale, the composite was considered as a homogeneous medium, and the mechanical properties extracted from the lower scales were applied. Validation of the model against reliable available data shows that the proposed approach is capable of accurately predicting the mechanical behavior and fracture path of silica/epoxy nanocomposites.

**Keywords:** Composite materials, crack growth, multiscale modeling, extended finite element method, cohesive zone model, fracture mode, numerical method.

## 1.Introduction

Cracks are among the most important indicators of material degradation, with microcracks representing the initial stage of fracture. Their progressive growth can ultimately lead to catastrophic failure; therefore, accurate prediction of crack initiation and propagation is essential for structural integrity assessment [1]. In composite materials, this prediction is particularly challenging because of their heterogeneous microstructure and complex interactions between different phases. Crack evolution is strongly influenced by particle size, shape, volume fraction, spatial distribution, and particle–matrix interfacial bonding.

The use of representative volume elements (RVEs) provides an effective framework for investigating fracture mechanisms at the micromechanical scale. Combined with advanced numerical approaches such as the extended finite element method (XFEM) and cohesive zone modeling (CZM), RVE-based models can explicitly capture matrix cracking and interfacial debonding. The RVE size must be appropriately selected to represent the material heterogeneity and provide reliable predictions of effective properties and fracture behavior [2]. In silica/epoxy nanocomposites, particle–matrix interfacial damage is a critical fracture mechanism because interfacial debonding can induce stress concentrations and trigger subsequent matrix cracking. XFEM–CZM simulations have demonstrated that matrix cracking and interfacial debonding may occur simultaneously or sequentially, while particle geometry, size, and distribution can significantly affect crack initiation and deflection [3]. Therefore, realistic representation of the interface is essential for reliable prediction of fracture behavior.

Although homogenized macroscopic models efficiently describe effective material properties, they cannot fully capture the direct influence of individual nanoparticles on crack trajectories and microstructural damage evolution. Multiscale modeling can overcome this limitation by linking microstructural mechanisms to the macroscopic

structural response. In particular, two-scale approaches can identify critical regions at the structural level and subsequently analyze their microstructural behavior, providing a balance between computational efficiency and predictive accuracy [4]. Accordingly, the main objective of this study is to develop a physically consistent multiscale framework for predicting crack initiation and propagation in silica/epoxy nanocomposites. At the microscale, RVE models with single-particle and particle-cluster configurations are employed to investigate particle–matrix debonding and matrix cracking using CZM. At the mesoscale, nanoparticles are explicitly modeled within a representative structural domain to capture crack propagation, deflection, and crack–particle interactions. Finally, microscale RVE homogenization is coupled with explicit mesoscale crack-growth modeling to establish a link between microstructural damage mechanisms and structural behavior. The proposed framework aims to predict fracture evolution from damage initiation to crack propagation across multiple length scales while reducing the need for extensive experimental testing.

## 2.Methodology

The silica/epoxy nanocomposite was modeled as a two-phase heterogeneous material consisting of elastic, isotropic silica particles embedded in an epoxy matrix. The material properties used in the simulations are summarized in Table 1. The particle–matrix interface was modeled using a cohesive zone model (CZM) based on a bilinear traction–separation law. The interface initially exhibits linear elastic behavior, followed by damage initiation according to a maximum-stress criterion and progressive degradation until complete separation [4,5].

**Table 1. Material properties of the silica/epoxy nanocomposite [4,5].**

| **Property** | $E_P$ GPa | $V_p$ | $E_m$ GPa | $\nu_m$ | $\sigma_m^t$ MPa | $G_m$ J/m² |
|---|---|---|---|---|---|---|
| **Value** | 70 | 0.17 | 3.5 | 0.4 | 121 | 90 |

**Table 2. CZM parameters for the particle–matrix interface [4,6].**

| **Property** | K MPa/mm | $t_s^0$ MPa | $t_n^0$ MPa | $G_i$ J/m² |
|---|---|---|---|---|
| **Value** | $5 \times 10^7$ | 53 | 53 | 10 |

Here, (K) denotes the initial cohesive stiffness, ($t_n^0$) and ($t_s^0$) represent the normal and shear interface strengths, and ($G_i$) is the interfacial fracture energy. The cohesive parameters were adopted from previous experimental and numerical studies of silica/epoxy and similar particulate composites rather than independently calibrated experimentally in the present study [5].

Crack initiation and propagation were investigated using a three-scale framework comprising micro-, meso-, and macroscales. CZM was used to simulate particle–matrix adhesion, damage, and debonding, while XFEM was employed to model crack initiation and propagation in the matrix without remeshing. At the microscale, a representative volume element (RVE) with a single-particle unit-cell configuration was developed. Silica particles were embedded in an epoxy matrix, and the particle–matrix interface was modeled using CZM. Uniaxial tensile loading was applied to evaluate interfacial debonding and matrix cracking. The resulting effective mechanical and fracture properties were subsequently transferred to the higher-scale models. At the mesoscale, a larger representative domain containing multiple silica particles was modeled to investigate particle interactions and their influence on crack evolution. Particular attention was given to crack initiation, propagation and deflection, as well as the effects of particle distribution, volume fraction, and interfacial adhesion. Explicit representation of the particles at this scale allows their direct interaction with the propagating crack to be captured. At the macroscale, crack growth was simulated using XFEM in Abaqus. The effective properties and fracture parameters obtained from the lower scales were used as inputs. The model represents a two-phase composite subjected to uniaxial tensile loading under plane-strain conditions. Circular silica particles with a uniform distribution and an aspect ratio of unity were considered within a square representative domain. The effective stress–strain response was obtained from the applied loading, while the overall stress and strain were evaluated from the resultant boundary traction and applied displacement [6]. Both silica and epoxy were assumed to exhibit linear-elastic isotropic behavior before damage initiation. Nonlinear material behavior was not explicitly considered; instead, failure was represented through cohesive damage at the particle–matrix interface and crack propagation in the matrix. This assumption is appropriate for the small strains preceding damage initiation and is commonly used in micromechanical fracture modeling. The proposed multiscale framework enables the effects of silica nanoparticles on load transfer, stress redistribution, crack deflection, and fracture resistance to be evaluated consistently across different length scales. Strong particle–matrix adhesion promotes effective load transfer and delays damage initiation, whereas weak interfaces can cause premature debonding and reduce the reinforcing effect of the nanoparticles.

## 3. Results and Discussion

The interaction between interfacial debonding and matrix cracking was investigated using CZM for the particle–matrix interface and XFEM for matrix crack propagation. Damage initially developed through progressive interfacial debonding in regions of high stress concentration. With increasing deformation, local stress

redistribution promoted matrix crack initiation and subsequent propagation. The simulated crack evolution for different initial crack configurations is presented in Figure 1, demonstrating the progressive development and interaction of interfacial damage and matrix cracking.

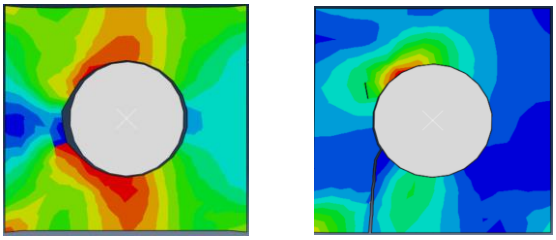


**Figure 1. Simulated crack propagation in the silica/epoxy nanocomposite RVE for different initial crack configurations.**

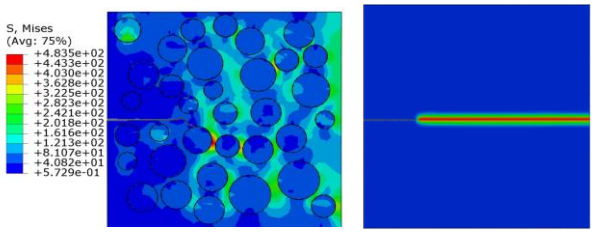



**Figure 2. Simulated crack propagation in the silica/epoxy nanocomposite at the meso and macro scale.**

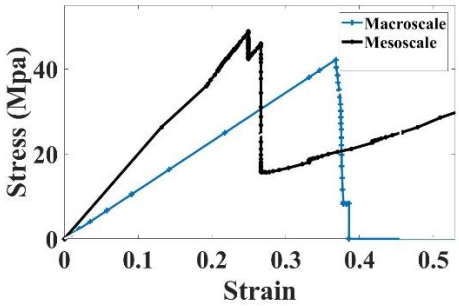



**Figure 3. Comparison of the stress–strain responses of the meso- and macroscale models with cohesive particle–matrix interfaces.**

Increasing the number of initial cracks from one to four reduced the RVE stiffness due to higher stress concentration and accelerated damage. In particle-cluster models, interfacial debonding initiated with increasing load, followed by matrix cracking, resulting in crack deflection, complex crack paths, stiffness degradation, and reduced load-carrying capacity. At the mesoscale, a reinforcement volume fraction of 31.15% was considered. Particle distribution and clustering significantly affected crack propagation through local stress concentration, crack deflection, and crack-tip shielding. As shown in Figure 2, clustered particles altered the local stress field and produced more complex crack paths, confirming the important role of particle dispersion and spatial topology in fracture resistance. The stress–strain responses in Figure 3 show that the cohesive interface strongly affects the mechanical response and post-peak softening, while the mesoscale model better captures particle distribution and interfacial damage. Using Mori–Tanaka–Eshelby homogenization, the effective Young's modulus, tensile strength, and fracture energy were approximately 3.75 GPa, 205 MPa, and 595 J/m², respectively, compared with 90 J/m² for neat epoxy. As shown in Figure 4, increasing particle content improves properties when dispersion is uniform; however, concentrations above approximately 15–20% may promote agglomeration and stress concentration, reducing the reinforcing efficiency.

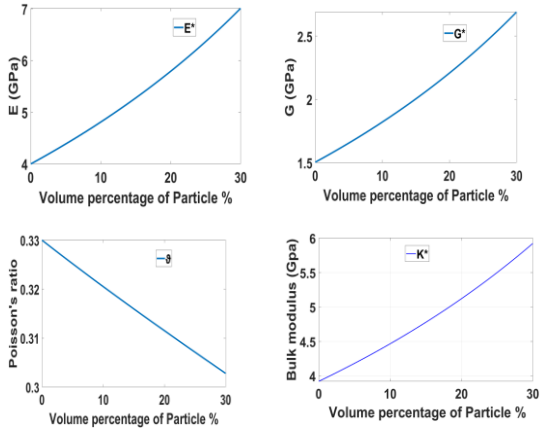



**Figure 4. Effect of silica particle volume fraction on the effective mechanical properties of the silica/epoxy nanocomposite.**

The stress–strain response further indicates that the cohesive interface plays a critical role in post-peak behavior. The maximum strength was approximately 45–47 MPa, followed by progressive softening associated with gradual interfacial debonding. This behavior confirms that the CZM formulation can effectively reproduce the transition from load-bearing behavior to progressive interfacial damage and final fracture.

Overall, the results demonstrate that fracture behavior in silica/epoxy nanocomposites is governed by the coupled effects of interfacial debonding, matrix cracking, particle distribution, clustering, and crack deflection. The combined results shown in Figures 1- 4 demonstrate that the proposed micro–meso–macro framework can effectively link microstructural damage mechanisms to the macroscopic fracture response.

## 4. Conclusion

This study investigated the fracture behavior of spherical particle-reinforced polymer composites using a multiscale XFEM–CZM framework. The coupled modeling of interfacial debonding and matrix cracking

enabled realistic prediction of damage initiation and crack propagation across different scales.

The microscale results showed that interfacial properties strongly affect crack growth, energy absorption, and strength, with debonding acting as a primary damage-initiation mechanism. At the mesoscale, particle distribution, clustering, crack deflection, and local stress concentrations significantly influenced fracture evolution, while increasing the number of initial cracks reduced stiffness and accelerated damage.

At the macroscale, homogenization successfully transferred the effective properties from lower scales to predict the overall structural response. Overall, interfacial strength, particle volume fraction and distribution, crack deflection, and the interaction between debonding and matrix cracking were identified as the main factors controlling fracture resistance. The proposed XFEM–CZM framework provides an efficient computational approach for predicting and optimizing the fracture performance of nanoparticle-reinforced composites with reduced reliance on extensive experimental testing.

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