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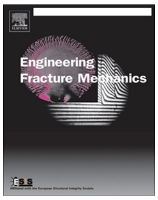

Fracture properties prediction of clay/epoxy nanocomposites with interphase zones using a phase field model

Mohammed A. Msekh [c,d], N.H. Cuong [c], G. Zi [e], P. Areias [f], X. Zhuang [c], Timon Rabczuk [a,b,*]

[a] *Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*
[b] *Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*
[c] *Institute of Structural Mechanics, Faculty of Civil Engineering, Bauhaus-University Weimar, Germany*
[d] *Civil Engineering Department, College of Engineering, University of Babylon, Babylon, Iraq*
[e] *School of Civil, Environmental and Architectural Engineering, Korea University, Republic of Korea*
[f] *Departamento de Física, Universidade de Évora, Portugal*

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ABSTRACT

We predict the macroscopic tensile strength and fracture toughness of fully exfoliated nano silicate clay epoxy composites accounting for the interphase behavior between the polymeric matrix and clay reinforcement. A phase field approach is employed to model fracture in the matrix and the interphase zone of the polymeric nanocomposites (PNCs) while the stiff clay platelets are considered as linear elastic material. The effect of the interphase zones, e.g. thickness and mechanical properties (Young's modulus and strain energy release rate) on the tensile strength, and fracture parameters of the composite is studied in detail. The dissipation energy due to fracture in the PNCs is extracted for different thicknesses and properties of the interphase zones. We show through numerical experiments that the interphase thickness has the most influence on the tensile strength while the critical strain energy release rate of the interphase zones affects the dissipation energy depending on the interphase zone thickness.

1. Introduction

Clay morphology along with other factors such as the nano clay Young's modulus and clay volume fraction/weight content is one of the most important factors in enhancing the stiffness of polymer nanocomposites. Hbaieb et al. [1] reported excellent mechanical properties of PNCs for fully exfoliated clay. Depending on the degree of dispersion of the clay, other benefits can be garnered from the composite such as temperature transition and electrical properties [2]. Finally, the clay nanofillers play a significant role in enhancing the polymeric nanocomposite's durability, properties, and the thermal stability.

The interfacial interaction between any heterogeneous components is an important factor that determines the properties of the composite [3]. In composite materials, the interface is the surface boundary between any homogeneous phases in thermodynamic equilibrium [4]. On the other hand, the intermediate phase formation between the joint surfaces of the neat epoxy and the silicate clays is referred to as *interphase*. In other words, the interphase (IP) is a zone with a finite thickness. The IP zone has different properties from the composite components. The IP properties depend on the processing and

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[*] Corresponding author.
E-mail address: timon.rabczuk@tdt.edu.vn (T. Rabczuk).

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Nomenclature

E_{IP}	Young's modulus of the interphase zone
E_c	Young's modulus of the clay
E_m	Young's modulus of the matrix
m and n	material parameters
$\mathbf{F}$	deformation gradient
$g(\phi)$	stress degradation function
k	system condition parameter
B	thickness of the sample
dU	change in total energy
a	initial crack length
da	change in initial crack length
ℓ_0	length scale parameter
$\mathcal{G}_c$	critical energy release rate
$\mathcal{G}_{cIP}$	critical energy release rate of the interphase zone
$\mathcal{G}_{cm}$	critical energy release rate of the matrix
Ψ^s	surface energy
Ψ^b	bulk energy
Ψ	total energy
γ	crack surface density
γ_{IP}	crack surface density in the interphase zones
γ_m	crack surface density in the matrix
$\phi(x)$	phase field parameter
λ and μ	Láme constants
RVE	representative volume element

reaction conditions of PNCs [5]. Clay platelets may have morphological variations near their surfaces in the IP zone. Note that the surface area of defect-free platelets will be smaller than the surface area of platelets containing pores and cracks on their surface area. The molecular and atomic structure of the platelet surface can differ from the bulk of the platelets themselves. This structure can be changed or broken down by chemical surface treatments. Besides, during the creation of the composite, an increase or decrease in the temperature during composite processing may eliminate certain useful surface reactivity and change the interface properties. The interaction between the clay and the matrix is influenced by the chemical and physical bonds at the interface, while the matrix composition in the IP is affected by the platelets surface. The non-interactive components and impurities of the epoxy can set the IP zone and change the local structure. The thickness of the IP zone may extend from a couple of nanometers to several nanometers. The mechanical strength as well as chemical and thermal properties of the composite can be significantly affected by the structure of this zone [6–9]. In conclusion, the IP zone in nanocomposites cannot be ignored due to the high ratio of the IP volume to total volume.

Fracture in polymer layered silicate (PLS) commonly occurs either in the matrix or the interphase/interface [10]; the latter one might promote debonding the silicate from the epoxy matrix [11]. Accordingly, the properties of the composites depend on the matrix and the filler adhesion. The IP zone properties, its thickness and volume can affect the PNCs properties considerably due to the major role of the clay nanofillers. Experiments attempting to measure the IP zone thickness and its mechanical properties were done by Zita [5] and Zita et al. [12]. They show that estimating the contact surface between the silicate and the matrix is difficult. Some models account for the formation of the IP, either by assuming a finite thickness and homogeneous IP zone properties or assuming that the properties are changing continuously from one phase to another [13]. Models accounting for the IP zone were proposed for instance by Ji et al. [14], Pukanszky [15] and Zare et al. [16,17]. Models for PNCs accounting also for their parameter uncertainties were developed in [18–23]. Mortazavi et al. [24] investigated the IP effects on the elastic modulus and the thermal conductivity of PNCs by using a three-dimensional finite element with linear elastic material modeling. Samandari and Khatibi [25] extracted the elastic modulus of PNCs through the nanoclay inclusion modulus and its shape using analytical models. Similar studies were carried out by Fertig and Garnich [26]. Chia et al. [27,28] studied the influence of interfaces on the mechanical properties of nanocomposites. They also modeled the clay gallery failure with a cohesive zone model [29].

The mechanical properties of interface layers have been predicted using different methods including molecular dynamics and analytical estimations [30] with contradictory results. For instance, Odegard et al. [31] and Adam et al. [32] reported the IP is softer than the epoxy matrix while the opposite conclusion was drawn in Qiao and Brinson [33], Mesbah et al. [34], and Liu and Brinson [35].

The experimental determination of the IP thickness is difficult. For organically modified montmorillonite clay immersed in different epoxies (such as Polyamide 6, Polylactic Acid, High-Density Polyethylene, Polypropylene, and Polyamide 12), the relationship between the IP thickness to the clay platelets thickness varies between 1 and 4.5 nm [16]. Akay [36] and

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