A VERSATILE PHASE-FIELD FRACTURE MODEL FOR POLYMER COMPOSITES: CAPTURING THEIR MULTI-FACETED FRACTURE BEHAVIOR VIA GRADED INTERPHASES

Paras Kumar[1,2*], and Julia Mergheim[1]

[1] *Institute of Applied Mechanics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*
[2] *Competence Unit for Scientific Computing, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*
[*] *Presenting Author email: paras.kumar@fau.de*

Abstract

Accurate modeling of fracture in polymer nano-composites entails the consideration of numerous complex phenomena including the branching and coalescence of multiple cracks. This contribution employs a graded interphase enhanced phase-field fracture approach (PFF-GI) to capture a wide spectrum of experimentally observed fracture behaviors including particle debonding. Herein the overall fracture response of the composite material is controlled via the degree of grading, i.e. continuous variation in material properties, within an interphase region of finite thickness around the filler particle.

1 Introduction

Nanosized filler particles have been observed to be superior mechanical reinforcements for polymers in comparison to their microsized counterparts. The process of fracture in such heterogeneous materials, however, involves complex crack topologies emanating from various intricate microscale phenomena such as crack branching, coalescence, and particle debonding. Consequently, traditional sharp crack modeling approaches are of limited practical usage and hence, the phase-field approach (PFF) renders itself as a viable alternative. The standard PFF approach, however, cannot capture interfacial fracture and hence, appropriate enhancements are inevitable. This contribution explores the graded interphase enhanced phase-field fracture (PFF-GI) approach [1] which involves continuous grading or variation in the elastic and fracture properties, within an interphase region of prescribed thickness around the filler particle, by means of the power-law type interpolation function

$$P_i(r) = \alpha\, P_f + \left[1 - \left[\frac{r_m - r}{r_m - r_f}\right]^2\right]^n \left[P_m - \alpha\, P_f\right] \tag{1}$$

where, $P_i = P_i(r)$ is the value of a generic property P_i at a distance $r_f \leq r \leq r_m$ from the center of the filler particle and could represent the Young's modulus E_i or the critical fracture energy G_c^i within the interphase, cf. Figure 1. The subscripts f, m, and i in (1) stand for the filler, matrix, and interphase regions, respectively. The selected degree of grading, which is influenced by the grading exponent n and the scaling factor α, enables control over the composite material's fracture response and consequently facilitates the prediction of a wide variety of experimentally observed fracture behaviors as depicted in the next section by means of numerical examples.

2 Numerical examples and discussion

We consider, as the model problem, a square shaped specimen comprising of a circular filler particle and subjected to uni-axial tensile loading scenario, cf. the schematic in Figure 1. The silica filler particle is relatively stiffer and tougher w.r.t. the soft and weak epoxy matrix material into which it is embedded, i.e. $E_f > E_m$ and $G_c^f > G_c^m$ holds. In order to highlight the versatility of the PFF-GI approach, we study scenarios wherein the interphase material is tougher or weaker than the surrounding matrix material. The elastic grading exponent n_{el} and the elastic scaling factor α_{el} enable control over the elastic properties of the graded interphase, whereas n_{fr} and α_{fr} allow control over its fracture properties. The scaling factor α_{el} is chosen such that the graded interphase is never softer than the matrix material.

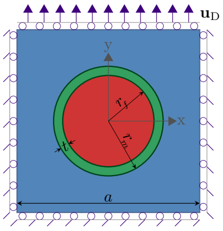
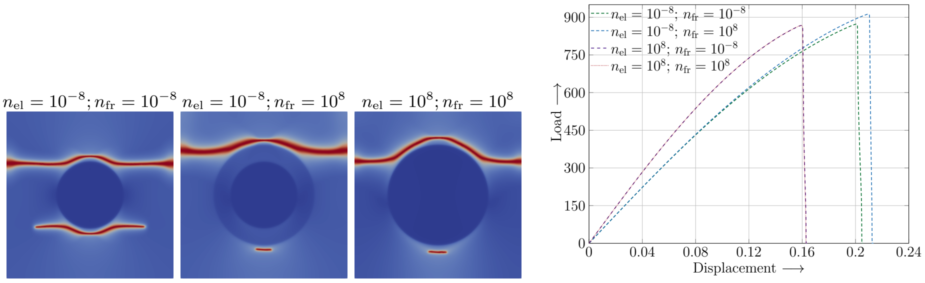


Figure 1: Specimen geometry and applied loading conditions.



(a) Crack phase-field contours at complete failure.

(b) Force-displacement curves.

Figure 2: Influence of interphase grading on fracture response in case of stiff and tough interphase, i.e. $E_i > E_m$ and $G_c^i > G_c^m$.

We first study the influence of interphase grading on the overall fracture behavior for the case of a tough and stiff interphase, i.e. $\alpha_{\text{fr}} = 1.0$ and $\alpha_{\text{el}} = 1.0$. Thus, in light of the relation (1), the dotted green-curve in Figure 2b corresponds to the standard case without any graded interphase effects, cf. the corresponding crack phase-field contour in Figure 2a. Next, keeping the interphase elastic properties fixed to that of the matrix, i.e. $n_{\text{el}} = 10^{-8}$, and increasing its critical fracture toughness to that of the filler material, i.e. setting $n_{\text{fr}} = 10^8$, a drastic change in the fracture pattern is observed as the damage zone now shifts to the matrix region outside of the graded interphase, cf. Figure 2a. Further, owing to the lower stiffness of the interphase w.r.t the filler, significant damage is observed therein. The high G_c^i leads to a higher peak load and a larger area under the force-displacement curve, and, therefore, a fracture superior response, in comparison to the one attained with the standard PFF model, cf. the two green curves in Figure 2b. Contrarily, having an interphase as stiff as the filler, i.e. $n_{\text{el}} = 10^8$, culminates in the failure occurring much earlier, regardless of the value of G_c^i. Such a behavior stems from the much higher stresses being set up in the neighboring matrix region due to the high stiffness of the interphase region. It is, thus, noteworthy that merely increasing the radius of the filler particle, i.e. setting $n_{\text{el}} = n_{\text{fr}} = 10^8$, does not lead to an improvement in the composite's fracture response.

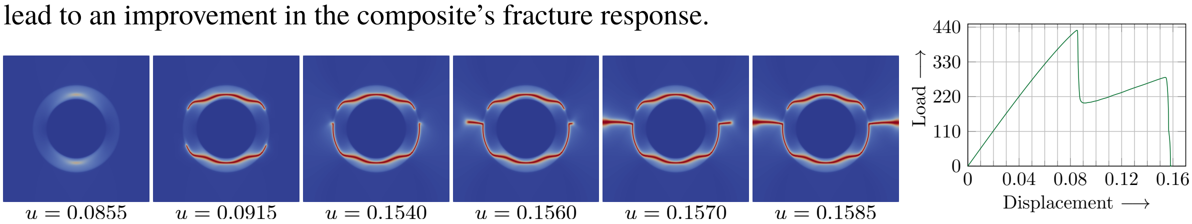


Figure 3: Evolution of diffuse crack in a specimen with weak interphase.

The second example deals with the case of a weak interphase, i.e. $G_c^i < G_c^m$ for the current study, in order to model cohesive failure between the filler particle and the matrix. For the sake of brevity, only one particular stiffness-toughness combination is presented here, cf. [1] for further details. Herein, we take $\alpha_{\text{fr}} = 0.125$ and $n_{\text{fr}} = 10^8$ such that $G_c^i = 0.25\, G_c^m$ holds for the silica-epoxy system considered in this study. Further, we fix $\alpha_{\text{el}} = 1.0$ and $n_{\text{el}} = 10^{-8}$ which culminates in the interphase region having the same stiffness as that of the matrix but much lesser fracture energy. Consequently, the crack nucleates within the interphase and then propagates into the matrix region before complete failure of the specimen occurs, cf. the phase-field contours and the force-displacement curve in Figure 3.

3 Conclusion and outlook

The PFF-GI approach studied in this work enables us to model, to certain extent, the multi-faceted fracture behavior of polymer composites with minimal modification of the standard PFF scheme. A wide variety of fracture behaviors, including a range of effective fracture responses, as observed in case of tough interphase, and the cohesive failure scenario, commonly observed in case of particulate composites, have been captured successfully. Further development extending the approach to model fracture in polymer composites undergoing large inelastic deformations is underway.

[1] P. Kumar, P. Steinmann and J. Mergheim, A graded interphase enhanced phase-field approach for modeling fracture in polymer composites, *Forces in Mechanics* **9**, 2022.