



A multi-scale and multi-mechanism approach for the fracture toughness assessment of polymer nanocomposites



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ARTICLE INFO

Article history:

Received 8 August 2013

Received in revised form 13 November 2013

Accepted 15 November 2013

Available online 28 November 2013

Keywords:

A. Nanoparticles

B. Fracture toughness

B. Interphase

ABSTRACT

In the present work, a multi-scale modelling strategy to assess the fracture toughness of nanoparticle filled thermosetting polymers is presented. The model accounts for the main damaging mechanisms arising in this kind of materials, i.e. nanoparticle debonding, plastic yielding of nanovoids and plastic shear banding of the polymer. Further, the proposed analytical framework considers the influence of an interphase around nanoparticles, a particular feature of nanocomposites.

Comparison of the theory to a bulk of experimental data from the literature shows a very good agreement.

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1. Introduction

Nanotechnology has recently emerged as a suitable tool to optimise properties of materials by designing their internal structure at the very nanoscale thus assisting in the achievement of desirable combinations of physical and mechanical properties [1–3]. However, to fully exploit the potential benefits of nanomodification, appropriate models able to soundly predict the macroscale mechanical properties from material structure need to be developed.

With the aim to explain the significant improvements of polymer toughness achievable with low nanofiller contents and considering the importance of the several damaging mechanisms that might take place at the nanoscale, some authors have recently suggested to use a “multi-mechanism” modelling strategy [4–8].

However, modelling the effects of nanoscale damaging mechanisms on macroscale properties is far from easy, essentially because at that length scale classical micromechanics is no longer valid. Instead, the adoption of a multi-scale strategy is necessary in order to describe the nanocomposite material behaviour, physically and mathematically, in each individual scale of interest.

In the recent literature several authors dealt with the analysis of toughening mechanisms in nanocomposites.

Chen et al. [9] carried out a theoretical study on the amount of energy dissipated by interfacial debonding of nanoparticles and provided a close form solution for the critical detachment stress. The size distribution of particles and the debonding probability

were included into the analytical formulation using a logarithmic normal distribution and the Weibull distribution function, respectively.

Some years later, the present authors refined the analysis carried out in [9] studying the effects of a small interphase zone embedding the nanoparticle [10] and of surface elastic constants [11] on the critical debonding stress. In both cases, the range of the nanoparticle radii where those effects are significant was proved to be limited to the nanoscale [10,11].

The energy dissipation phenomena due to particle debonding, voiding and subsequent yielding of the polymer have been analysed by Lauke [4] who used a simple geometrical model of particle–particle interaction in a regular particle arrangement. By further applying a critical stress criterion, Lauke found a dissipation zone which was independent of the particle diameter and justified the increase of crack resistance with decreasing particle size by the increase in the specific debonding energy [4].

Williams [5] re-analysed in detail the toughening of particle filled polymers assuming that plastic void growth around debonded or cavitated particles is the dominant mechanism for energy dissipation. He assumed a tri-axial state of stress around the spherical particle and supposed the debonding and cavitation conditions to be controlled by either surface energy or the cohesive energy of the particle. Williams further noted that, even if the debonding process is generally considered to absorb little energy, it is essential to reduce the constraint at the crack tip and, in turn, to allow the epoxy polymer to deform plastically via a void-growth mechanism. A similar result was found also by the present authors [12].

Hsieh et al. [6,7] studied the fracture toughness improvements resulting from nanomodification of epoxy resins with silica nanoparticles. Based on experimental observations, they identified

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two dominant mechanisms responsible of toughening improvements, namely localised shear banding of the polymer and particle debonding followed by subsequent plastic void growth. They finally adapted a previous model due to Huang and Kinloch [13] for rubber modified epoxy polymers to predict the fracture toughness improvements resulting from nanomodification.

The investigations in [4–7] support the idea, recently formulated also by the present authors [8], that the most effective approach to predict the nanocomposite toughness is a “multi-mechanism” modelling strategy, in which the contribution of each mechanism is appropriately determined and weighted according to the specific case (accounting for the type, the morphology and the functionalisation of the nanofiller). Accordingly the nanocomposite fracture toughness can be written as the summation of the fracture toughness of the unloaded matrix, G_{im} , and the fracture toughness improvement due to the each i -th damaging mechanism, ΔG_i .

Great efforts have been recently devoted by the present authors to develop analytical formulations for ΔG_i contributions due to the most relevant toughening mechanisms occurring in nanoparticle filled polymer resins. Among these, debonding of nanoparticles followed by plastic yielding of nanovoids [12] and plastic shear banding of the polymer [14] have been analysed. The major novelty of these recent works, with respect to those in the previous literature dealing with the same subject [4–7], lays on the fact that the effect of an interphase zone surrounding the nanoparticle, characterised by mechanical properties different from those of the constituents, is explicitly considered.

Starting from the analytical models developed in previous works [12,14], the main aim of the present paper is to provide a multiscale analytical procedure useful to evaluate the overall fracture toughness of a polymer/nanoparticle nanocomposite.

The proposed multiscale-multimechanism model accounts for particle debonding, plastic yielding of nanovoids and shear banding of the polymer, thus allowing to quantify the effect of the associated energy dissipation phenomena on the overall fracture toughness of the material. Theoretical predictions for the nanocomposite fracture toughness are compared with a large bulk of experimental data taken from the literature, showing a satisfactory agreement.

2. Description of the multiscale strategy adopted for the analysis

Nanocomposites are endowed with a hierarchical structure, which encompasses the nano and the macro length-scales. A successful prediction of the mechanical properties of these materials thus requires models able to account for the phenomena peculiar of each length-scale and to bridge their effects from the nano scale to the macroscale.

According to [8] it can be stated that, generally speaking, three stages should be addressed in nanocomposite modelling, each stage being referred to a specific length scale and to be tackled with the aid of dedicated models. Basic models can be finally assembled to build a multiscale modelling strategy.

The present authors have recently proposed a hierarchical multiscale strategy according to which the nanocomposite material is mathematically decomposed into three systems of interest.

Briefly:

- the macroscale system is thought of as an amount of material over which all the mechanical quantities (such as stresses and strains) are regarded as averaged values [15] and are supposed to be representative of the overall material behaviour;
- the micro-scale system is thought of as being sufficiently small to be regarded, mathematically, as an infinitesimal volume of

the macro-scale one. At the same time it has to be, by definition, large enough to be statistically representative of the properties of the material system (described by a *Representative Volume Element*, RVE);

- the nanoscale system represents a single unit cell of those compounding the micro-scale system and it accounts for the material morphology at the nanoscale.
- The link between different system is obtained through the combined use of the Mori–Tanaka theorem and the Global Concentration Tensors of Eshelby dilute solution (see Fig. 1). Accordingly, the stress acting on the boundary of a single nano-inhomogeneity (nanoscale) is approximated as:

$$\sigma_n = \mathbf{H} : \left\{ \frac{1}{V} \int_V \hat{\sigma} dV \right\} = \mathbf{H} : \sigma \quad (1)$$

where \mathbf{H} is the Global Concentration Tensors of Eshelby dilute solution [10], and $\frac{1}{V} \int_V \hat{\sigma} dV$ is the mean value for the stress fields over the RVE which, thanks to Mori–Tanaka theorem equates the macro-scale stress field.

The system under investigation at the nanoscale, shown in Fig. 2a, is constituted by:

- a spherical nanoparticle (nanovoid) of radius r_0 ;
- a shell-shaped interphase of external radius a and thickness t ($a = t + r_0$) and uniform properties;
- a volume of matrix of which the size are much greater than a and r_0 .

This system accounts for molecular interactions at the nanoscale through the size and elastic properties of the interphase layer [10]. Unfortunately there is a lack of reliable data about the law of variation of the interphase properties across its thickness [16]. This urged some authors [10,12,14,16–19] to assume that a through-the-thickness average is representative of the overall property distribution within the interphase. Consequently, the interphase is supposed to be homogeneous and isotropic.

The system at the macro-scale is constituted, instead, of a cracked nano-modified matrix (see again Fig. 2b) under mode I loadings. It is assumed that the macroscopic stress fields due to the crack, given by Irwin’s solution (see [14] for more details) enhances the formation of a process zone containing all the nanoparticles subjected to damage, thus promoting energy dissipation at the nanoscale, and resulting, in turn, in an overall fracture toughness improvements of the nanocomposite.

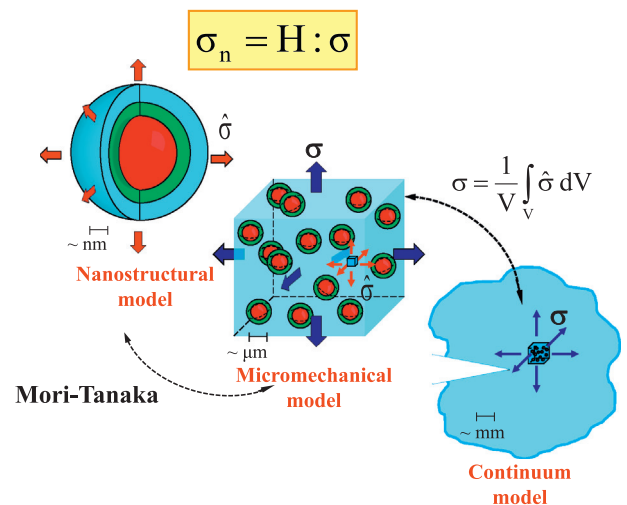


Fig. 1. Multiscale strategy and systems of interest.

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