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Micromechanical modeling of nanocomposites considering debonding of reinforcements

J. Nafar Dastgerdi [a,b,*], G. Marquis [a], M. Salimi [b]

[a] Department of Applied Mechanics, Aalto University school of science and technology, P.O. Box 14300, FIN-00076 Aalto (Espoo), Finland
[b] Department of Mechanical Engineering, Isfahan University of Technology, Isfahan 8415683111, Iran

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ABSTRACT

This paper deals with a constitutive model of particulate-reinforced nanocomposites which can describe the debonding damage, elasto-plastic behavior of matrix and particle size effects on deformation and damage. An incremental damage model of particulate-reinforced composites based on the Mori–Tanaka's mean field concept, considering the particle size in nanoscale is further developed to consider the debonding of reinforcements in nanocomposites. The applicability of the proposed theory is investigated for nanocomposites consisting of Al_2O_3 nanoparticles with different size embedded in magnesium alloy (AZ31 and ZK60A) and pure magnesium (Mg) matrix. Based on the present model, analysis of stress–strain response for Al_2O_3–AZ31 nanocomposite under uniaxial tension is carried out. The effects of particle size and adhesive energy of nanoparticles at interface on stress–strain response of Al_2O_3–AZ31 nanocomposite is obtained. Moreover, in this paper the effect of debonding of reinforcements on effective Young's modulus and toughness of the particulate reinforced nanocomposites is demonstrated. When the debonding damage starts to occur, the stress–strain curve for the damaged nanocomposite deviate to lower stress from those for the perfect composite. The influences of adhesive energy at interface and particle size on the stress–strain curve are considerable. Composites with lower adhesive energy at interface and larger particle size have poor toughness due to lower area under the stress–strain curve. In addition, Progressive debonding leads to a loss of stiffness in nanocomposites.

1. Introduction

Nanocomposites have been widely studied and employed in diverse fields of science and engineering applications in the past decade. Compared with many conventional materials (such as metals, alloys, and polymers), fiber or particle reinforced nanocomposites offer prominent features such as low density, high strength to weight ratio, high stiffness, high toughness, improved creep resistance, enhanced wear resistance, superior environmental durability, and so on. Typically, a low modulus matrix is combined with high stiffness and high modulus inclusions, which carry the external loads transferred by the matrix through the interfaces. The interface behavior can significantly affect the mechanical properties of nanocomposites. Theoretical predictions on effective mechanical properties of fiber or particle reinforced nanocomposites are usually made under the assumption of high interfacial strength (with perfect bonding). Hence, an assumption of strong or perfect interface would be inadequate for those types of composites.

The debonding process in composites has been widely studied in the literature. Nicholson [1] considered a rigid spherical inclusion embedded in and completely adhered to a much larger sphere of matrix. Assuming that the adhesive bond was weak and the matrix sphere is subjected to a uniform fixed radial stress on its outer surface, Nicholson found a criterion for detachment. Gent [2,3] studied the interfacial debonding for a rigid spherical inclusion under uniaxial tension by both experiments and theory. He studied the process of debonding and suggested an approximate expression of the critical stress required for debonding. Lauke published results of stress concentration calculations of a coated particle within a linear elastic polymer matrix under multiaxial applied load [4] and a particle in a non-linear polymer matrix of a cylindrical specimen under uniaxial load [5]. He also investigated the effect of particle size distribution on debonding energy and crack resistance of polymer composites [6]. The volume specific debonding energy was calculated as a function of the position in front of a crack for different debonding stress criteria. The contribution of particle debonding to the crack resistance of the composites was provided by integration over the particle size distribution and

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* Corresponding author at: Department of Applied Mechanics, Aalto University, Espoo, Finland. Tel.: +358 465244943.
E-mail address: jairan.nafardastgerdi@aalto.fi (J. Nafar Dastgerdi).

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Nomenclature

f_p, f_d	the volume fractions of the intact and damaged reinforcements respectively
f_{p0}	the initial reinforcement volume fraction
df_p	the volume fraction of the particles debonded during the incremental deformation
$d\sigma^p$	The incremental stress in the intact particle
$d\sigma$, $d\bar{\sigma}$	the incremental overall composite stress and the incremental average stress
L_1, L_0	tangential moduli tensor for the particle and matrix, respectively
$d\varepsilon_0$, $d\bar{\varepsilon}$	the incremental overall composite strain and the incremental average strain
$d\sigma^{pt}_{1,2}, \sigma^{pt}_3$	the perturbed parts of stress
$d\varepsilon^{pt}_{1,2}, \varepsilon^{pt}_3$	the perturbed parts of strain
$d\varepsilon^*_{1,2}, \varepsilon^*_3$	Eshelby's equivalent transformation strain
I	the fourth-rank identity tensor
S	Eshelby's tensor for the spherical inclusion
σ^p	stress in the intact particle
L	the effective material matrix
$d\varepsilon^m$	incremental average strain of the matrix
$d\varepsilon^p$	incremental average strain of the intact particle
$d\varepsilon^d$	incremental average strain of the damaged particle
$d\sigma^m$	incremental average stress of the matrix
δ_{ij}	the Kronecker delta
$d\sigma_{ij}$, $d\varepsilon_{ij}$	incremental stress and strain respectively
$d\sigma_{kk}$, $d\varepsilon_{kk}$	the hydrostatic part of incremental stress and strain
$d\sigma'_{ij}$, $d\varepsilon'_{ij}$	the deviatoric part of incremental stress and strain
κ_0, μ_0	the bulk modulus and the shear modulus of the matrix
κ_1, μ_1	the bulk modulus and the shear modulus of particles
σ_e	the von Mises equivalent stress
$d\varepsilon^p_e$	the incremental equivalent plastic strain
$d\varepsilon^{pl}_{ij}$	the incremental plastic strain
ν_0	Poisson's ratio of the matrix
ν'_0	the equivalent Poisson's ratio of the matrix in elastic–plastic deformation
μ'_0	the equivalent shear modulus in elastic–plastic deformation
H'	the work-hardening ratio of the matrix
σ_0	the yield stress of the matrix
E_0	The initial Young's modulus of the matrix
σ	the normal stress at the interface
σ_{cr}	the threshold bond strength between the particle and matrix
γ	the specific interface adhesive energy
a	the radius of particle
P	the probability of debonding at the interface
S_0, m	material parameters

dissipation zone size. One of the open problems is an accurate mechanical modeling of multi-phase nanostructured materials that can account for nonlinear phenomena such as the cumulative debonding between the matrix and the nanofillers up to the ultimate state of failure. Thus, study on the criterion for the interfacial debonding is necessary for the design of nanocomposites [7,8]. Interfacial debonding in polymer/nanoparticle composites was studied in [9] by means of Eshelby's equivalent inclusion method combined with an energy-derived debonding criterion stating a relationship between the interfacial adhesion strength and the work of adhesion of the components. Boutaleb et al. [10] proposed a micromechanical analytical model, in order to address the problem of stiffness and yield stress prediction in the case of nanocomposites consisting of silica nanoparticles embedded in a polymer matrix. This model takes into account an interphase corresponding to a perturbed region of the polymer matrix around the nanoparticles. Odegard et al. [11] developed a continuum-based elastic micromechanics model for silica nanoparticle/polyimide composites with various nanoparticle/polyimide interfacial treatments. The model incorporated the molecular structures of the nanoparticle, polyimide, and interfacial regions, which were determined using a molecular modeling method that involved coarse-grained and reverse-mapping techniques. Zappalorto et al. [12] developed a closed form expression for the critical debonding stress accounting for the existence of an interphase zone of different properties between the nanoparticle and the matrix.

For debonding damage of particulate-reinforced composites, Tohgo and Chou [13] and Tohgo and Weng [14] developed an incremental damage theory based on the Eshelby's equivalent inclusion method [15] and Mori–Tanaka's mean field concept [16]. They showed that the influence of the debonding damage on the stress–strain response of the composites is very drastic. The effective elastic–plastic behavior of a particle-reinforced composite including debonding damage was also discussed by Zhao and Weng [17]. In [18], the macroscopic constitutive relationship of particulate-reinforced viscoelastic composite materials was investigated. It was ascertained that the macroscopic strain rate, the particle-size dispersity, the relaxation time of the matrix, and the interface adhesive strength are key mechanical factors for this kind of particulate-reinforced composites where the microvoids nucleation and growth are the driving damage process. With regard to averaging the elastic moduli by a modification of the Mori–Tanaka method, Iwakuam and Koyama [19] introduced a so-called virtual matrix to evaluate the elastoplastic behavior of composites and polycrystals with interfacial debonding.

In nanocomposites, a variety of damage modes such as fracture of reinforcements, interfacial debonding between reinforcements and matrix, cracking in matrix, plastic yielding of nanovoids (created by debonded nanoparticles) and matrix shear banding develop from the early stage of deformation under monotonic or cyclic loads. These damage modes mainly affect the mechanical performance of the nanocomposites. Therefore to extend the application of the nanocomposites and to develop even a new composite, thorough understanding of the micromechanics of damage process is essential. Lauke [20] and Williams [21] analysed the energy dissipation phenomena by considering, besides particle debonding, voiding and subsequent yielding of the polymer. Salviot et al. [22] developed a hierarchical multi-scale model to assess the fracture toughness improvements due to the debonding of nanoparticles and the plastic yielding of nanovoids. The same authors have recently proposed a multiscale analytical model to quantify the toughness improvement due to the shear banding around nanoparticles [23]. They also proved that nanocomposite toughening is strongly affected by the size of nanoparticles and by surface treatments. Hsieh et al. [24] experimentally observed two dominant mechanisms responsible of toughening improvements: localized shear banding of the polymer and particle debonding followed by subsequent plastic void growth.

In this investigation, an elasto-plastic incremental constitutive equation of particulate reinforced nanocomposite considering the debonding of the reinforcement and as well as the elastoplasticity using micromechanics principles is presented. This model is valid