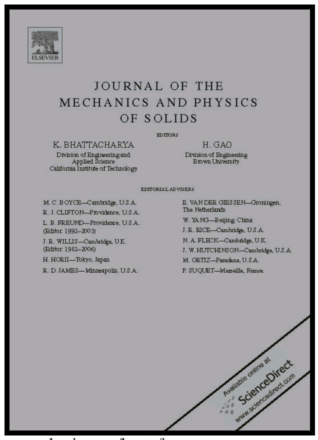
Author's Accepted Manuscript



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PII: S0022-5096(16)30300-3
DOI: http://dx.doi.org/10.1016/j.jmps.2016.05.002
Reference: MPS2889

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 25 June 2015
Revised date: 16 April 2016
Accepted date: 2 May 2016

Cite this article as: Zeliang Liu, John A. Moore and Wing Kam Liu, An extendec micromechanics method for probing interphase properties in polyme nanocomposites, *Journal of the Mechanics and Physics of Solids* http://dx.doi.org/10.1016/j.jmps.2016.05.002

An Extended Micromechanics Method for Probing Interphase Properties in Polymer Nanocomposites

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Abstract

Inclusions comprised on filler particles and interphase regions commonly form complex morphologies in polymer nanocomposites. Addressing these morphologies as systems of overlapping simple shapes allows for the study of dilute particles, clustered particles, and interacting interphases all in one general modeling framework. To account for the material properties in these overlapping geometries, *weighted-mean* and *additive* overlapping conditions are introduced and the corresponding inclusion-wise integral equations are formulated. An extended micromechanics method based on these overlapping conditions for linear elastic and viscoelastic heterogeneous material is then developed. An important feature of the proposed approach is that the effect of both the geometric overlapping (clustered particles) and physical overlapping (interacting interphases) on the effective properties can be distinguished. We apply the extended micromechanics method to a viscoelastic polymer nanocomposite with interphase regions, and estimate the properties and thickness of the interphase region based on experimental data for carbon-black filled styrene butadiene rubbers.

Keywords: Micromechanics, overlapping geometries, Boolean-Poisson model, polymer composite, viscoelasticity, interphase, inverse problem

1. Introduction

Nanoparticle-reinforced polymer composites have attracted intense attention in the research and industrial communities during the past decades. As the size of filler particles approaches the nano-scale, composite materials may exhibit advantageous thermal, electrical or mechanical properties, even with addition of a small amount of fillers [1, 2]. Because of these extraordinary behaviors, polymer nanocomposites also show promise as multi-functional materials in automotive and aerospace industries [3].

Many polymer fillers do not adhere to simple geometric shapes (i.e., spheres, diamonds, cylinders). Rather, fillers, such as carbon-black in tire applications, tend to have irregular geometries and to form networks of agglomerated filler particles [4]. Even, more pristine filler particle structures, such as nano-diamonds, will form larger aggregates unless explicitly processed to prevent such formation [5].

Both experiments and molecular dynamics (MD) simulations have suggested that there exists an interphase region in the vicinity of a nanoparticle, with dramatically different thermal-mechanical, mechanical and structural properties than observed in bulk polymer [6, 7, 8, 9]. For example, Cheng et al. measured the modulus of confined polymer films adjacent to a plane substrate through atomic force microscopy (AFM)-based indentation, and the thickness of the interphase is found to be around several tens of nanometers [9]. However, directly measuring mechanical properties (e.g., dynamic moduli) of the interphase in a nanoparticle-reinforced polymer composite can be challenging and/or time-consuming. In this paper, we are interested in using the overall mechanical properties of the polymer composite to inversely predict the

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