Mechanics of Materials 105 (2017) 16–28

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

Nonlinear effective properties of heterogeneous materials with ellipsoidal microstructure

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ARTICLE INFO

Article history:
Received 5 July 2016
Revised 21 October 2016
Available online 23 November 2016

Keywords:
Heterogeneous material
Nonlinear homogenization
Ellipsoidal microstructure
Ponte Castañeda–Willis estimate

ABSTRACT

The analysis and the synthesis of the nonlinear effective response of particulate composite materials are of great importance for developing new systems such as nonlinear elastic and electromagnetic metamaterials, nonlinear waveguides, nonlinear magnetoelectric devices and photonic or phononic crystals. Typically, classical homogenization schemes take into account the shape of the inhomogenieties but neglect the spatial correlation among them, a crucial feature for the above applications. In this paper we develop a nonlinear homogenization technique for dispersions of nonlinear particles in a linear matrix, which is able to take account of spatial correlation by means of the so-called ellipsoidal microstructure. While the linear result corresponds to the well known Ponte Castañeda–Willis estimate, we propose new formulae for the second and third order nonlinear behavior. We finally show applications to the nonlinear elastic Landau coefficients and to the nonlinear hypersusceptibility of transport processes.

1. Introduction

In recent times, a great number of investigations have been devoted to the elastic and electromagnetic nonlinear properties of particulate composite materials in view of their applications to modern nanotechnology. In fact, the physical nonlinearity of some elements composing a structured system allows for generating a tunable complex behavior, which may exploited to implement specific functions not existing in simple materials. For instance, efficient acoustic diodes have been designed by means of highly nonlinear elastic materials combined with one-dimensional phononic crystals (Liang et al., 2009, 2010) and they can be profitably exploited for thermal management at a microscopic scale (Li et al., 2012). The practical realization of these devices needs elastic materials with precisely tuned strong nonlinearities that can be obtained either through bubbly liquids with optimized concentration of gas (Liang et al., 2010) or soft materials (polymers) with pores (Brunet et al., 2013). Another emerging field is represented by the nonlinear acoustic metamaterials, which are able to control several features of propagating elastic waves (Herbold and Nesterenko, 2013; Manktelow et al., 2011; Kim et al., 2015). The elastic behavior can be coupled with the magnetic one, thus generating magnetoelastic metamaterials, where a new type of nonlinear response arises from this interaction (Lapine et al., 2012). One more example of nonlinear media is given by the granular crystals, which are capable of generating shock-absorbing materials, sound-focusing devices, acoustic switches, and other exotic devices (Porter et al., 2015; Lydon et al., 2015). Similar effects were studied in electrodynamics and optical diodes, transistors and other devices have been realized through non-linear electromagnetic components based on photonic crystals (Mingaleev and Kivshar, 2002; Soljacic and Joannopoulos, 2010). Also, the development of nonlinear electromagnetic metamaterials and plasmonic devices allowed to tune electromagnetic properties with the possibility of controlling the effect of specific nonlinearities (Mary et al., 2008; Kozyrev and van der, 2008; Xu et al., 2009; Lapine et al., 2014). Other largely investigated structures include nonlinear photonic crystals (Berger, 1998), nonlinear optical waveguides (Tsang and Liu, 2008) and nonlinear magnetoelectric devices Rose et al. (2012).

All these applications prove the need of designing heterogeneous materials with controlled elastic and electromagnetic nonlinearities. To do this, we require efficient models to predict the nonlinear behavior of composites as a function of their morphology. This task is usually performed by linear and nonlinear homogenization methods, which determine the effective physical properties of a given microstructure (Nemat-Nasser and Hori, 1993; Milton, 2002; Torquato, 2002; Kanaun and Levin, 2008). Most of the homogenization techniques consider parallel or random orientation of the inhomogeneities, without taking into

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http://dx.doi.org/10.1016/j.mechmat.2016.11.003

account their real spatial distribution. They have been developed for dealing with, e.g., ellipsoidal particles (Kachanov and Sevostianov, 2005; Giordano, 2003, 2005), cracks (Kachanov, 1994; Giordano and Colombo, 2007b, 2007a), and poroelastic materials (Berryman, 1997; Dormieux et al., 2002). The classical linear theory used for considering the spatial distribution of particles (i.e. their spatial correlation) is based on the Ponte Castañeda–Willis estimate, which takes into account the so-called ellipsoidal microstructure (Ponte Castañeda and Willis, 1995). This result has been derived by considering the Hashin-Shtrikman variational approach in the form developed by Willis (1977, 1978). While in its original form the inclusion shape and spatial distribution are considered jointly (Willis, 1977), in the second version these two features are introduced separately (Willis, 1978). This point is crucial to derive the Ponte Castañeda–Willis estimate, which considers arbitrary ellipsoidal particles and, independently, assumes the hypothesis of ellipsoidal symmetry for the spatial distribution of the particles. The result represents a generalization of the classical Mori and Tanaka's (1973) scheme, always giving tensors of effective moduli satisfying the necessary symmetry requirements (Ponte Castañeda and Willis, 1995). The relation between the Ponte Castañeda–Willis and Mori–Tanaka schemes has been thoroughly examined in the literature (Hu and Weng, 2000b, 2000a; Weng, 2010). From the point of view of the applications, the Ponte Castañeda–Willis estimate has been used to investigate the mechanical properties of multifractured materials (Dormieux and Kondo, 2016), nanocomposites (Cauvin et al., 2010), rocks (Wendt et al., 2003; Gruescu et al., 2007), and the response of magnetostrictive (Galipeau and Ponte Castañeda, 2012) or magneto-electro-elastic composites (Franciosi, 2013). It is important to remark that the variational principles have been also used for nonlinear composites with both nonlinear comparison solid (Talbot and Willis, 1985, 1987) and linear comparison solid (Ponte Castañeda, 1991, 1992; Suquet, 1993; Ponte Castañeda and Suquet, 1998).

In this paper, we approach the problem of determining the nonlinear effective properties of a composite materials described by the so-called ellipsoidal microstructure or, equivalently, by the ellipsoidal symmetry for the spatial distribution of particles. It means that the microstructure can be described by a population of arbitrary ellipsoidal particles exhibiting a specific nonlinearity, embedded in a linear matrix with a spatial distribution given by an arbitrary ellipsoidal correlation. By introducing a two-step multiscale procedure we can obtain the linear and nonlinear (second order and third order) physical properties of the heterogeneous material. We take into account ellipsoidal inhomogeneities of arbitrary shape and an arbitrary ellipsoidal correlation among particles. This allows to write the final linear and nonlinear effective properties in terms of two independent Eshelby tensors describing shape and distribution, respectively. The linear result coincides with the Ponte Castañeda–Willis estimate whereas the closed form expression for the nonlinear effective tensor represents a new achievement, which is explicit and well suited for the applications. We remark that all results can be also used in dynamic regime if we consider the wavelength of the propagating wave much larger than the particles size. In this case we are working in the so-called quasi-static regime and any inhomogeneity feels a nearly static applied field. Interestingly enough, although we show explicit examples analysing elastic and transport properties, the proposed scheme can be easily adopted to homogenize the fully coupled thermo-magneto-electro-elastic case as well.

The proposed methodology can be adopted for modeling novel composites behaviors but also for validating advanced numerical models and multiscale techniques largely used for the description of materials with random microstructure. Usually, these methodologies are based on boundary value problems defined on finite-size mesoscales (Ghosh, 2011; Salmi et al., 2012), sometimes generalized to consider non-classical materials such as, e.g., micropolar continua (Trovalusci et al., 2014, 2015). The central issue of these approaches, applied to random microstructures, concerns the proper definition of Representative Volume Element (RVE) (Ostoja-Starzewski, 2006). Since the proposed model, being entirely theoretical, does not require the RVE estimation, the comparison with numerical approaches can be useful to further validate the RVE selection process.

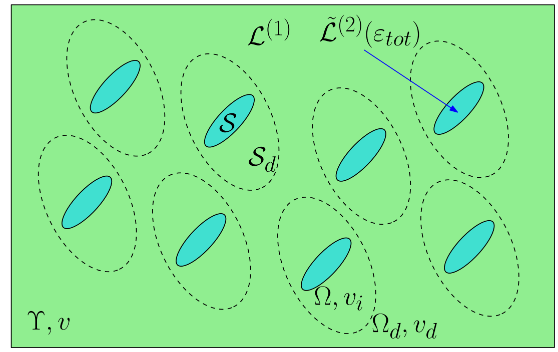

Fig. 1. Distribution of particles embedded in the matrix $\mathcal{L}^{(1)}$ showing the so-called ellipsoidal microstructure. Each nonlinear inhomogeneity (region Ω) has a volume $v_i = \text{mes}(\Omega)$, an Eshelby tensor $\mathcal{S}$ and a stiffness tensor $\tilde{\mathcal{L}}^{(2)}(\varepsilon_{tot})$. Moreover, all particles are surrounded by a security ellipsoidal surface Ω_d, having volume v_d and Eshelby tensor $\mathcal{S}_d$.

The structure of the paper follows. In Section 2, we introduce the problem statement, by defining the ellipsoidal microstructure and the related nonlinear homogenization issues. In Section 3, we review the Eshelby formalism for both linear and nonlinear inhomogeneities. In Section 4, we approach the first step of the multiscale procedure: we solve the homogenization problem for a nonlinear composite ellipsoid. In Section 5, we elaborate the second step of the homogenization: we determine the effective behavior of the dispersion of nonlinear inhomogeneities. In Section 6, we combine the two procedure in order to get the final results. Finally, in Sections 7 and 8 we show some applications to the second order nonlinear elastic Landau coefficients and to the third order nonlinear hypersusceptibility of transport processes.

2. Problem statement

We define here the microstructure and the methodology adopted in this work. The geometry of the system is represented in Fig. 1, where a population of inhomogeneities are dispersed in a linear matrix of stiffness $\mathcal{L}^{(1)}$. Each nonlinear inhomogeneity is characterized by an ellipsoidal region Ω, a volume $v_i = \text{mes}(\Omega)$, and an Eshelby tensor $\mathcal{S}$. Its nonlinear elastic response is characterized by a strain-dependent stiffness tensor $\tilde{\mathcal{L}}^{(2)}(\varepsilon_{tot})$. Moreover, every particle is surrounded by another ellipsoidal surface Ω_d, having internal volume v_d and Eshelby tensor $\mathcal{S}_d$. This is the so-called security surface and allows us to define the ellipsoidal symmetry for the spatial distribution of particles: the security regions of any couple of inhomogeneities cannot be overlapped. This principle imposes the spatial correlation among particles and may generate a form of anisotropy induced by the distribution of particles position. Indeed, even if we consider spherical inhomogenities, the overall behavior of the heterogeneous material will be anisotropic if the security surface are ellipsoidal.

It is important to remark that the (centres of the) inhomogeneities are uniformly randomly distributed within the material volume, provided that they are not overlapping (the composite is statistically homogeneous). It means that the probability density for finding an inclusion at a given position is a constant. However,