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Size-dependent effective thermoelastic properties of nanocomposites with spherically anisotropic phases

H. Le Quang, Q.-C. He*

Laboratoire de Mécanique (LaM), Université de Marne-la-Vallée, 5 Boulevard Descartes, 77454 Marne-la-Vallée Cedex 2, France

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Abstract

Composites made of semi-crystalline polymers and nanoparticles have a spherulitic microstructure which can be reasonably represented by a spherically anisotropic volume element. Due to the high surface-to-volume ratio of a nanoparticle, the particle–matrix interface stress, usually neglected in determining the effective elastic moduli of particle-reinforced composites, may have a non-negligible effect. To account for the latter in estimating the effective thermoelastic properties of a composite consisting of nanoparticles embedded in a semi-crystalline polymeric matrix, this work adopts a coherent interface model for the nanoparticle–matrix interface and proposes an extended version of the classical generalized-self consistent method. In particular, Eshelby's formulae widely used to calculate the elastic energy change of a homogeneous medium due to the introduction of an inhomogeneity are extended to the thermoelastic case. The nanoparticle size effect on the effective thermoelastic moduli of the composite are theoretically shown and numerically illustrated.

Keywords: A. Voids and inclusions; B. Anisotropic material; B. Particulate reinforced material; B. Polymeric material; Spherical anisotropy

1. Introduction

Nanocomposites of semi-crystalline polymers are recently a subject of intense investigations (see, e.g., Kim et al., 2001; Liu et al., 2003; Nowacki et al., 2004; Causin

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*Corresponding author. Tel.: +33 160 957 786; fax: +33 160 957 799.
E-mail address: he@univ-mlv.fr (Q.-C. He).

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et al., 2006; Hadal et al., 2006). Semi-crystalline polymers, such as polyethylene and polypropylene, consist of spherulites which are formed of crystalline and amorphous regions arranged approximately in a spherically symmetric way (Bassett, 1981). Nanocomposites have been obtained by using semi-crystalline polymers as the matrix and nano-sized particles as the reinforcement. These composites often exhibit improved mechanical and physical properties compared to the conventional composites reinforced with micron-sized particles. In particular, clay is a preferred reinforcement mineral to synthesize nanocomposite because clay enhances mechanical and thermal properties, fire resistance and barrier characteristics of semi-crystalline polymers without significantly increasing the mass density nor altering the optical behavior. A nanocomposite made of a semi-crystalline polymer reinforced by nanoparticles has a microstructure which can be approximately represented by a spherically anisotropic volume element.

The problem of estimating the effective thermoelastic properties and conductivity of composites with spherically anisotropic microstructures was studied by Dryden (1988), Chen (1993), He and Cheng (1996), Milton (2002), and He and Benveniste (2004). In these studies, only the micron-sized particles were considered so that the effect of the matrix–particle interface energy (or stress) on the effective behavior of composites is small enough to be negligible. However, when nano-sized particles are involved as in the aforementioned semi-crystalline polymer nanocomposites, the matrix-particle interface energy can no longer be neglected in determining the effective moduli, because the interface-to-volume ratio is very high in a representative volume element of a composite with nanoparticles. This fact has been emphasized and exploited in recent investigations on nanomaterials and nano-sized structural elements (see, e.g., Miller and Shenoy, 2000; Sharma and Dasgupta, 2002; Dingreville et al., 2005; Duan et al., 2005a, b; Chen et al., 2007; Duan and Karihaloo, 2007). The objective of the present work is to estimate the effective thermoelastic properties of nanocomposites with spherically anisotropic microstructures, a semi-crystalline polymer reinforced with clay nanoparticles being taken as prototype.

To achieve our objective, a generalized-self consistent method is proposed in this work, extending the classical generalized-self consistent model (GSCM) of Kerner (1956), Van der Poel (1958), Smith (1974, 1975), Christensen and Lo (1979) (see also Christensen, 1990) in the following three directions:

- First, GSCM is broadened to thermoelasticity. In doing so, the energy self-consistency condition is formulated in the thermoelastic context by deriving an equation generalizing a formula of Eshelby (1956) largely invoked to calculate the elastic energy change of a homogeneous medium due to the introduction of an inhomogeneity.
- Second, the extended thermoelastic version of GSCM is implemented for phases of spherically transverse isotropy. This implementation hinges upon the solution of an auxiliary elastic problem in which a hollow sphere consisting of an elastic material of spherically transverse isotropy is subjected to uniform isotropic or simple shear loading on its inner and outer surfaces. When isotropic surface loading is concerned, the complete solution to this auxiliary problem is available (Dryden, 1988; Chen, 1993; He and Benveniste, 2004). However, when simple shear surface loading is considered, the existing solution given by Dryden (1988) and Chen (1993) to the auxiliary problem is in our opinion incomplete, since the positive definiteness of the elastic stiffness tensor has not fully been used to deal with the relevant fourth-order polynomial characteristic equation (31). The last point is remedied in the present work.