Effective thermoelastic properties of nanocomposites with prescribed random orientation of nanofibers

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Summary. Nanocomposites (NC) are modeled as a linearly elastic composite medium, which consists of a homogeneous matrix containing a statistically homogeneous random field of spheroid nanofibers with prescribed random orientation. Estimation of symmetric effective thermoelastic properties of NC was performed by the effective field method taking into account the random orientation of nanofibers as well as justified selection of spatial correlations of fiber location.

Experimental research and molecular dynamic simulation indicated that nanofibers can be effectively considered in the framework of continuum mechanics as the homogeneous prolate spheroidal anisotropic homogeneous inclusions (see [1]) with a large aspect ratio ($\alpha\approx1000$). In this paper, a nanocomposite is modeled as a linearly elastic composite medium, which consists of a homogeneous matrix containing a statistically homogeneous random field of nanofibers v_i with prescribed random orientation described by the orientation distribution function (ODF). Estimation of effective elastic moduli of nanocomposites was performed by means of the effective field method (MEF, see for references and details [2]) based on effective field hypothesis: each fiber is embedded in the homogeneous effective field that is dependant on prescribed random orientation of this fiber [contrary to the Mori-Tanaka method (MTM) where the effective field coincides with the average stresses in the matrix]. It may be noted the certain drawbacks of the extension of Mori-Tanaka method to multiphase composites: Mori-Tanaka moduli may violate the Hashin-Shtrikman bounds and are nonsymmetric for the general diphase composites. In the authors' knowledge, no models exist that satisfy all of theoretical criteria mentioned above for arbitrary phase anisotropy and fiber-orientation distributions, and a micromechanical approximation devoid of the mentioned contradictions is highly desirable.

MEF was used in the framework of quasicrystalline approximation when the spatial correlations of inclusion location called "correlation hole" take particular ellipsoidal forms. This "correlation hole" v_i^0**,** enclosing the representative fiber v_i, does not occupy the centers of surrounding fibers (since they cannot overlap) and are compatible with mutual orientations of fibers. The independent justified choice of shapes of inclusions and correlation holes provides the formulae of effective moduli which are completely explicit and easy to use. If the shapes of fibers v_i and the correlation holes v_i^0 coincide, then the estimations of the effective moduli $\boldsymbol{L}^*$ are symmetric and coincide for both the MEF and MTM for both the arbitrary random field of isotropic fibers and aligned anisotropic fibers. However, the main advantage of the proposed approach is that it is free from some drawbacks of other approximations such as the Mori-Tanaka scheme, which can generate tensors of effective moduli which fails to satisfy a necessary symmetry requirement. Most significantly, the MEF's estimations are found to be in disagreement with corresponding estimations by the MTM in the case of the randomly oriented anisotropic inclusions in the composites. The current approach takes into account both the anisotropic moduli of fibers and specific shape of the correlation holes v_i^0 reflecting the anisotropy of ODF that was not considered in the past (see, e.g., [3]). In the parametric analysis we considered both isotropic (see [4]) and anisotropic fibers (see [1]) in the Epon 862 matrix (see [5]). Three random orientations of fibers were considered: aligned fibers parallel to the axis Ox_1 (1-D uniform random orientation), uniform plane random orientation of fiber parallel to the plane Ox_1x_2 (2-D uniform random orientation), and 3-D uniform random orientation. The effective elastic Young's moduli E^* and UDRI's experimental data [6] vs. the fiber volume concentrations c of the isotropic and anisotropic fibers with 3-D uniform random orientation are presented in Fig. 1. In the case of 3D uniform random orientation of nanofibers, the tensors of the effective elastic moduli $\boldsymbol{L}^*$ obtained by the MTM and MEF are symmetric and coincide in cases with the same domain shapes v_i and v_i^0 for both the isotropic and anisotropic fibers. It can be seen that Young's modulus E^* estimated for anisotropic fibers is 1.5 times stiffer than E^* for the isotropic fibers, although the transversal Young modulus E_3 of anisotropic fibers is 30 times softer than E_3 for the isotropic fibers. However, for 2D uniform random orientation of fibers, the MTM generates the tensors of effective moduli which fail to satisfy a necessary symmetry requirement (see Fig. 2). To avoid the deficiency in the case of 2D uniform random orientation of nanofibers, the MEF was applied with the reasonable shape of "correlation hole" v_i^0 in the form of oblate spheroid (with aspect ratio $1/\alpha$) with big semiaxes parallel to the plane Ox_1x_2. In comparison, the estimations of the effective elastic moduli by the MEF and by MTM are different for any nonzero components of the tensor L^*_{ijkl}. The matrix of effective moduli estimated by the MEF is symmetric ($L^*_{ijkl}= L^*_{klij}$) in all the range of a fiber concentration c stadied, and their elastic moduli. The diagonal elements of the matrices L^*_{ijkl} estimated by the MEF and by the MTM agree well at $c<0.5$ (for example, the Young's moduli E^*_1 and E^*_3 estimated by both the MEF and MTM are agree well, see Fig. 3, however,

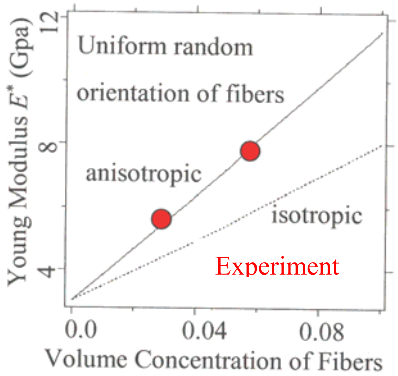

Fig. 1. Modulus E^* (GPa) vs c

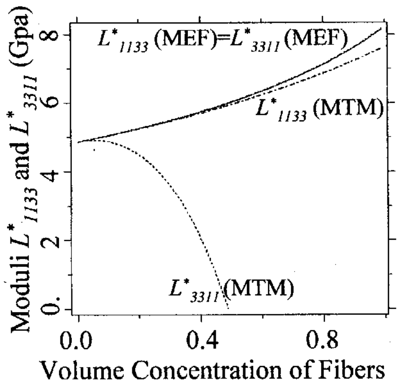

Fig. 2. L^*_{1133} and L^*_{3311} (GPa) vs c

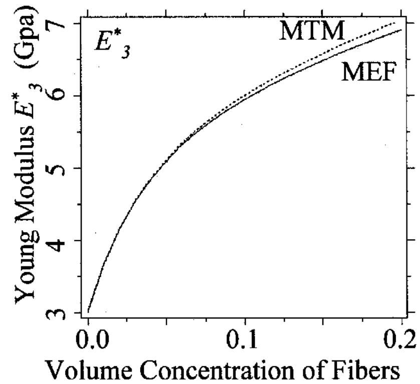

Fig. 3. E^*_3 (GPa) vs c

the nondiagonal elements can differ to a great extent for $c>0.2$. Thus, the matrix L^*_{ijkl} estimated by the MTM is not symmetric ($L^*_{ijkl} \neq L^*_{klij}$, see Fig. 2).

The same approach was used for the estimation of effective coefficient of thermal expansion (CTE). As expected, CTEs estimated by both MTM and by MEF coincide for both 1-D and 3-D uniform random orientation for both the anisotropic and isotropic fibers. However, for 2-D uniform random orientation, the estimations carried by the MTM and by MEF are differ from one another. Further, the prediction of the behavior of composite materials by the use of mechanical properties of the constituents and their microstructure ultimately lead to the estimation of statistical averages of stress fields in the constituents and at the interface fiber-matrix. These stress concentrators depend on the orientation of the fiber being considered as well as on the justified choice of the shape of correlation holes, concentration and ODF of nanofibers. Additional significant impact of CNT on the effective properties of nanocomposites is based on the fact that CNTs provide very high interfacial area if embedded in the matrix. The interface fiber-matrix was modeled as a thick coating with cylindrically anisotropic varying thermoelastic properties distinguishing from the properties of the fiber and matrix. The MEF prescribed above for homogeneous spheroidal fibers was generalized in the light of the model [7] for the coated fibers based on the notion of fictitious homogeneous spheroidal fibers. The parametric analyses indicate essential dependence of effective properties on the parameters of interface coating.

In conclusion, the results of the parametric analyses can be summarized as following (see [8]):

1) Effective stiffness of NC is defined by the axial stiffness of fibers rather than their transversal stiffness.

2) The variation of fiber orientation is critical and can lead to the variation of the effective stiffness of nanocomposites as much as 6 times for the fiber volume concentration $c<0.1$.

3) The estimation method of the effective stiffness of nanocomposites is critical. For the plane uniform orientation of anisotropic fibers, the use of the MTM is inappropriate as revealed by the MEF prediction.

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