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Energy-based definition of equivalent inhomogeneity for various interphase models and analysis of effective properties of particulate composites

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ABSTRACT

A new concept of equivalent inhomogeneity is proposed to facilitate analysis of effective properties of composites with interphases using techniques devised for problems without interphases. The basic idea to replace the inhomogeneity and its interphase by a single equivalent inhomogeneity (combining properties of both) is akin to previously proposed developments but the criterion of equivalency is entirely different. It is based on Hill's energy equivalence principle, and is illustrated considering spherical inhomogeneity with Gurtin–Murdoch surface model and spring layer model of interphases. The validity of the suggested technique is documented by remarkably good agreement with the best available solutions for composites containing spherical inhomogeneities with spring layer model of interphase.

1. Introduction

Influence of interphases on the overall (effective) properties of composites may be significant and its analytical quantification has been an increasingly popular topic of research. Importance of such research stems from the fact that – as a result of changes in the interatomic interactions on the boundary between different materials, combined with specifics of manufacturing processes – interphases are present in all composite materials. Properties of those interphases vary, depending on the materials involved, and various models have been proposed to capture their influence on the overall behavior of composites e.g. Refs. [3,7,13,19]. Typically they are specified by formulas defining a difference (jump) in displacements and/or tractions across the interphase, whose thickness may be either finite or vanishingly small.

If the influence of interphases is anticipated to be small, they may be completely eliminated from analysis. This case is often referred to as *perfect interface (or perfect bonding)* and it is associated with continuity of both displacements and tractions. Analysis of composites with perfectly bonded constituents is easier than those with interphases, but even in this case the complexity is very high so that only approximate, e.g. Ref. [15], or numerical, e.g. Ref. [30], methods can be employed. They are described in many publications and most of them are summarized in a number of books [6,21,23,24,29,33], among others. Some of the approximate solutions are presented in closed-forms, which are their very attractive feature, and a feature exploited subsequently in this work. The numerical solutions, on the other hand, are often formally exact and provide results that are very useful as benchmarks when developing approximate approaches. Their main drawback is that they do not reveal any functional dependence of the results on the parameters describing the problem. A common disadvantage of the existing approximate and numerical approaches is that most of them need to be restricted to simple shapes of the composite's constituents – overwhelmingly to spheres in three-dimensional problems, very rarely spheroids or ellipsoids.

Presence of interphases makes the existing approaches used in analysis of composites more tedious than when the interphases are absent [1,2,4,5,7–10,12,18,19,26,27,31], among others. In addition, some of the existing methods are developed specifically for problems without interphases, and their extension to problems with existing interphase models is not presently available. With that in mind, the main task undertaken in this work is to present a general approach of converting problems with interphases to problems without interphases (or with perfect interfaces) that can be solved

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using any of the existing approaches, analytical or numerical. Specifically, the main topic here is to introduce a general energy-based approach (Hill's principle, cf. [20]), to find properties of the so-called equivalent inhomogeneity that would incorporate both the properties of the original inhomogeneity and of the interphase. So defined equivalent inhomogeneity is then perfectly bonded to the matrix and any method developed to analyze composites without interphases can be used to investigate influence of interphases.

There were number prior very different approaches to define equivalent inhomogeneities. Hashin [17,18], in application of his composite sphere assemblage to analysis of the effective bulk modulus, introduced a similar concept and discussed its possible extension to multi-layer systems. That idea has been subsequently followed within the so-called differential scheme [31,32]. In this approach layers of infinitesimal thickness were successively added to the original spherical inhomogeneity to form an interphase with properties varying across its thickness. With addition of each layer the properties of the system were defined either by the Mori–Tanaka scheme or Hashin – Strickmann upper bound estimate [16]. Equivalent inhomogeneities have also been presented in the contributions of Duan [9,10] and Gu [12] in which two different models of interphases were considered: the Gurtin–Murdoch material surface model and the spring layer model. Their definitions were identical and based on equality of the energy changes (introduced in Ref. [11]) caused by insertion of a spherical inhomogeneity together with its interphase and the changes caused by insertion of the equivalent inhomogeneity. While the bulk modulus of the equivalent inhomogeneity obtained that way was identical as that of Hashin [18] and depended only on the properties of the original inhomogeneity and of the interphase, its shear modulus, however, turned out to also include the moduli of the matrix. The formula defining equivalent shear modulus expectedly reflects the properties of the entire system, not just those of the inhomogeneity and its interphase that it is supposed to replace. Thus, for a specific inhomogeneity and its specific interphase, the criterion adopted by Duan [9,10] and Gu [12] leads to infinite number of “equivalent inhomogeneities” which seems non-physical, and it is unlike any of the previously presented equivalent inhomogeneities [18,31].

It is finally noted that all of the previous definitions of equivalent inhomogeneity very fundamentally rely on the spherical shape of the inhomogeneities. That is also true about the recent contribution of the present authors [28], in which equivalent inhomogeneity for the spring layer model has been defined using exact Lurie's solution for sphere, [22]. None of those approaches can be reformulated to cover shapes other than spheres and various models of interphases. As a result such practically important materials as short fiber composites, or composites with carbon nanotubes reinforcement in which interphases have a very pronounced influence, cannot be analyzed.

The notion of the energy-equivalent inhomogeneity presented here is conceptually akin to that recently presented in Ref. [27], and leads to the equivalent properties which do not include properties of the matrix and which result in remarkable effective properties of composites. While the approach pursued there was theoretically applicable to inhomogeneities of arbitrary shapes, it was restricted only to Gurtin–Murdoch model of interphases. In the original version the approach is not flexible enough to account for other models of interphases, such as the spring layer model. Its generalization presented here is capable to cover not only arbitrary shapes of inhomogeneities but also a number of different interphase models. Its outline is presented in Section 2. In Section 3 specifics related to two illustrative cases are discussed, one, for completeness, summarizes the existing results involving Gurtin–Murdoch material surface model of the interphase and the second represents a new application of the proposed approach for the spring layer model. Some details pertinent to Section 3 are moved to the Appendices A and B. While the approach presented here can be used in conjunction with any approach applicable to analyze materials without interphases, the Method of Conditional Moments (MCM) [21,25] is used in this work and it is outlined in Section 4. The MCM is chosen in view of the fact that random composites are considered in this work and that it is a method whose original development did not allow for presence of interphases. Numerical results and their discussion are presented in Section 5, and conclusions are included in Section 6.

2. General formulation of the problem

The main idea of the Energy Equivalent Inhomogeneity (EEI) consists in using the energy approach to replace the system consisting of the original inhomogeneity and surrounding interphase of thickness h (with $h=0$ as a special case) by a single uniform inhomogeneity. Various types of interphases may be considered, but both the interphase and the inhomogeneity are assumed elastic with their own distinct properties.

To find the properties of the EEI the well-established homogenization approach is followed. It is assumed that the displacements at the matrix/interphase boundary result from an arbitrary constant overall strain $\boldsymbol{\varepsilon}_{eq}$. At equilibrium these displacements cause the attendant strain fields (or displacement jumps) within the original inhomogeneity and the interphase, both of which depend on $\boldsymbol{\varepsilon}_{eq}$. The strain energy associated with the equilibrium state of such system, being the sum of the energies of the original inhomogeneity and its interphase, is then a quadratic function of $\boldsymbol{\varepsilon}_{eq}$. Equating this energy of the inhomogeneity-interphase system to the energy of equivalent inhomogeneity [20], whose homogeneous deformation is *arbitrary* $\boldsymbol{\varepsilon}_{eq}$, yields properties of the equivalent inhomogeneity in terms of the mechanical and geometrical data describing the original inhomogeneity and the interphase.

The exact solution of the problem just described is possible only under very rare circumstances; in many cases it is, however, possible to analytically obtain an accurate approximate solution. Given that the interphase is typically thin and that the matrix/interphase displacements correspond to a constant $\boldsymbol{\varepsilon}_{eq}$, it is plausible to assume that the strain field within the original inhomogeneity will be nearly uniform $\boldsymbol{\varepsilon} \neq \boldsymbol{\varepsilon}_{eq}$. Thus, it is assumed here that the original inhomogeneity (of arbitrary shape) undergoes rigid body motion, described by the unknown displacement vector $\mathbf{u}$ (of an arbitrary reference point O, Fig. 1) and small rotation tensor $\boldsymbol{\omega}$ (about that reference point), as well as deformation described by a constant small strain tensor $\boldsymbol{\varepsilon}$.[1] Consequently, the energy equivalence takes the following form

$$E = \frac{1}{2} V_{eq} \boldsymbol{\varepsilon}_{eq} : \mathbf{C}_{eq} : \boldsymbol{\varepsilon}_{eq} = E_{\mathrm{i}}\left(\boldsymbol{\varepsilon}_{eq}, \boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}_{eq}), \boldsymbol{\omega}(\boldsymbol{\varepsilon}_{eq}), u(\boldsymbol{\varepsilon}_{eq})\right) + \frac{1}{2} \int_{V_1} \boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}_{eq}) : \mathbf{C}_1 : \boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}_{eq}) dV_1, \tag{2.1}$$

where V_{eq} is the sum of the volumes of the original inhomogeneity V_1 and of the interphase V_{i} (i.e. volume of equivalent inhomogeneity), E_{i} is the strain energy of the interphase, $\mathbf{C}_1$ and $\mathbf{C}_{eq}$

[1] Further simplifications are possible in specific situations, for instance for inhomogeneities with sufficient degree of symmetry $\mathbf{u}$, or even both $\mathbf{u}$ and $\boldsymbol{\omega}$ are equal to zero.