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Effective Elastic Property Estimation for Bi-continuous Heterogeneous Solids

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Abstract: In the present study we performed finite element simulation for bi-continuous heterogeneous solids via a random distribution of materials to predict effective elastic properties. With a random distributing scheme, a statistical analysis via finite element becomes feasible for the multiphase heterogeneous solids. Using a two-phase bi-continuous material as example, the numerical prediction of the effective properties is obtained in terms of a mean value and standard deviation with a sample size of 30 for each of given volume fraction. The finite element simulation results fall within the analytical bounds proposed by Hashin and Shtrikman (1963) based on the principle of variation. Comparison between the effective modulus based on the present bio-continuous morphology with the matrix-fiber configuration shows big difference.

Keyword: Finite element analysis, effective modulus, bi-continuous solids, statistics.

1 Introduction

Heterogeneous solids are of great engineering interests. Prediction and estimation of the macroscopic effective properties of the heterogeneous solids has been an active research field for solid mechanics and materials science researchers. We may classify the heterogeneous solids in terms of the micro-morphological feature into two basic groups. The first group of heterogeneous solids is the so-called the particulate composite where matrix and reinforcement particles/fibers are clearly identified. Modeling this type of composite has been mainly via analytical approaches (see the review article by Christensen (1990)). There are a few books by Christensen (1979), Mura (1982), Taya and Arsenault (1989) covered most development and results before 1990s. Some of the recent development, such as, Gao et al (2006) and Gornet et al (2006), indicate that failure predication is of great concern. The second group of the heterogeneous solids is called bi-continuous solids, in which matrix and particles cannot be clearly identified. This type of micro-structure is widely observed in polycrystalline, polymer blends, porous media and cement-based materials such as concrete (Haecker *et al*, 2005), to name a few. Research on this bi-continuous solid has been lagged behind its counterpart, the matrix-particulate composites. It has also been noticed that the analytical models developed for the matrix-particulate composite (for example, Christensen and Lo, 1979) are not able to make good prediction/estimation on the elastic properties of bi-continuous composite (for example, Roberts and Garboczi (1999)). Fortunately, people developed a few bounds (normally in pairs, i.e. upper and lower bound under certain conditions) for gauging the effective elastic properties of the heterogeneous solids predicated/estimated by the various approaches. The most well-known and frequently-used pair of such bounds is by Hashin and Shtrikman (1963), where the spatial distribution of each component of the composite is treated equally. Therefore, it can be used for both matrix-particulate composites and bi-continuous composites. In the present paper, our interest is on the bi-continuous composites.

An existing analytical model for the bi-continuous configuration is the self-consistent scheme (Bu-

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diansky, 1965). However, it is an approximate model as the interaction among phases was roughly counted. Studies on bi-continuous composite recently had a new development via finite element and statistical reconstruction (Garboczi and Day, (1995)). With years of accumulation of the knowledge and finite element program, Roberts and Garboczi (1999) made very accurate estimation on elastic modulus for silver-tungsten composite by using the statistic reconstruction technique. Recently, Sundararaghavan and Zabaras (2005) further developed this scheme. Their procedure is working on two "transparencies". On the first transparency, they copied the microscopic photo or statistic reconstructed "photo" of the micro morphology of the bi-continuous composite. The second transparency copied with very fine meshed elements, while the elements' material properties are yet to be specified. When the second transparency is put on the top of the first transparency, one can pick up the material property of a specific element based on the morphology of the micro-structure of the composite recorded on the first transparency. Apparently, the accuracy of this approach depends on the information of the micro-morphology of the composite. Hereby, we are concerned that the situations when we do not have detailed statistical information about the micro-structure of the composite. It is particularly true in the beginning stage of designing new materials, or when the morphology is difficult to obtain. Therefore, in the following sections we propose a simple scheme of assigning properties based on the finite element mesh for the bi-continuous composite, where no other micro-structure information than the volume fraction is needed a prior.

Mechanics issue is the main concern of the present paper. Therefore, we make the presentation with non–interrupted stream for the mechanics related topics in Section 2 and 3. The secondary issues regarding the statistics due to the random distribution of the materials and numerical accuracy in refining the domains are discussed in Section 4 after we have the whole picture of the mechanics issues.

2 Finite element analysis with randomly distributed material components

Let us consider a two-dimensional plane strain configuration. The present scheme shows no difficulties for the 3-dimensioal configuration, although memory and computational time demands are larger. The ***specimen*** is firstly discretetized into equal sized ***domains*** so that volume fraction of the materials can be easily calculated. The domains are assigned with different materials properties randomly for a given volume fractions of components via a MATLAB program. The detailed procedure is described as follows. Firstly, we use the commercial ANSYS 8.1 finite element package to mesh the specimen into multiple domains. Secondly, we copy the element file of ANSYS, which contains the material column, into an Excel spreadsheet. A random selection program is written in MATLAB for randomly picking up "1" and "2". The random selection of "1" and "2", which represent Material 1 and 2, is then replacing the material column in Excel. Thirdly, this file is re-input into ANSYS as the element file where we have defined Material 1 and 2 (Epoxy and Glass listed in Table 1). In order to minimize the numerical error due to the sudden change of material properties from one domain to other domain, each domain is further refined into a few ***elements***. Increasing the number of domains in the specimen can reduce the statistical variation of the predicted effective modulus. Physically, the increasing number of elements inside of each domain leads a "relaxation" of the stressed domain which may be surrounded by domains with different material properties It is seen that there is not difficult to extend this random selection process to include more than two component materials.

The schematic illustration of the domains and elements are shown in Fig.1. The numerical calculation is carried out by using the eight-node plane strain element PLANE82 in ANSYS. The boundary conditions are prescribed as follows:
along $x = 0$, $u_x = 0$,
along $y = 0$, $u_y = 0$,
along $x = 1$. $\sigma_{xx} = S$, uniform stress.

The above deformation provides us the value

Table 1: Elastic properties of the material components used in finite element calculation

Material component	Elastic modulus	Poisson's ratio
Glass (material 1)	73.1 GPa	0.22
Epoxy (material 2)	3.41 GPa	0.35

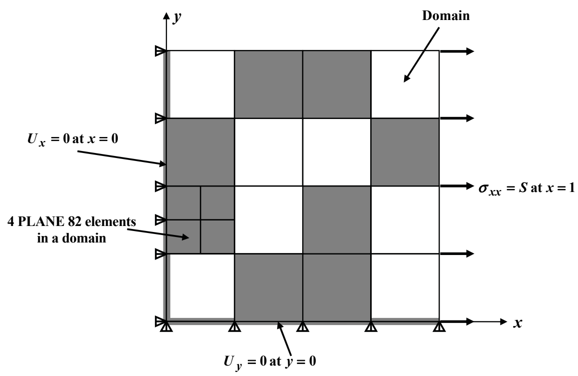


Figure 1: Squared domains and elements in a bi-continuous material.

of in-plane shear modulus for later comparison with various analytical results. It is noted that the aforementioned configuration implies a transversely isotropic material under in-plane ($x-y$ plane) deformation. Thus, we have,

$$\varepsilon_x = \frac{\sigma_x}{E_{11}} - \frac{\nu_{12}\sigma_y}{E_{11}} - \frac{\nu_{13}}{E_{11}}\sigma_z \tag{1a}$$

$$\varepsilon_y = -\frac{\nu_{12}\sigma_x}{E_{11}} + \frac{\sigma_y}{E_{11}} - \frac{\nu_{13}}{E_{11}}\sigma_z \tag{1b}$$

$$\varepsilon_z = -\frac{\nu_{31}\sigma_x}{E_{33}} - \frac{\nu_{31}\sigma_y}{E_{33}} + \frac{\sigma_z}{E_{33}} = 0 \tag{1c}$$

It is seen that $\sigma_y = 0$ and $\sigma_z \neq 0$. From Eq.(1a) and Eq.(1b), we have

$$\varepsilon_x - \varepsilon_y = \frac{(1+\nu_{12})\sigma_x}{E_{11}} \tag{2a}$$

or

$$\mu_{12} = \frac{E_{11}}{2(1+\nu_{12})} = \frac{S}{2[\varepsilon_x - \varepsilon_y]} = \frac{S}{2[u_x(x=1) - u_y(y=1)]} \tag{2b}$$

The finite element numerical result of the nodal displacement $u_x(x=1) - u_y(y=1)$ is averaged along the lines for the calculation of effective modulus of the composite. An alternative loading configuration is given in Appendix. The in-plane shear modulus deducted from Eq.(2b) is presented in Fig.2 as the finite element prediction.

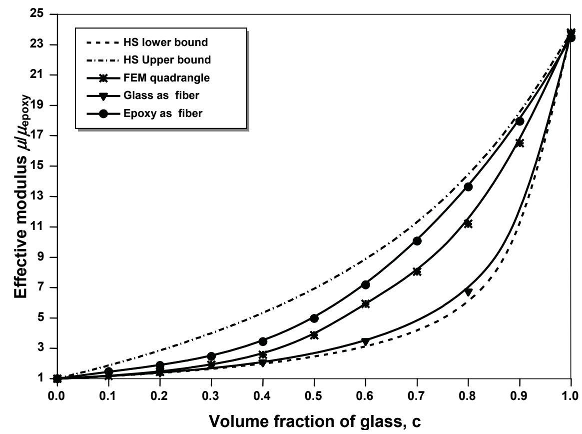


Figure 2: Effective modulus of the composite normalized by epoxy modulus vs. the volume fraction of glass. Christensen and Lo (1979) model was applied for both hard fiber and soft fiber, which gave two predictions. The hard fiber (glass as fiber) model prediction is close the lower Hashin and Shtrikmen (HS) (1963) bound and the soft fiber (epoxy as fiber) model prediction is close to the HS upper bounds. The present finite element bi-continuous model prediction is located between them.

The numerical simulation is carried out with sample size of $n = 30$. For a given volume fractions of Material 1 and Material 2, the materials of two phases are randomly distributed for$n = 30$ specimens. Each of the specimens provides an effective modulus. The mean value ($\overline{\mu}$) and standard deviation (s) of the sample are obtained. According to Central Limit Theorem in statistics (e.g. Mendenhall *et al* (2006)), we have a 95%-confidence interval for the effective modulus of the population as

$$\overline{\mu} \pm 1.96 \times \frac{s}{\sqrt{n}}. \tag{3}$$

This interval can be narrowed by increasing the sample size or reducing the sample standard deviation. These statistic matters will be discussed later in Section 4. The finite element results presented in Fig. 2 are the mean value of the sample ($n = 30$). Detailed data are presented in Table 2. We will elaborate more numerical accuracy in Section 4, after we clear the physical significance in the following section.

3 Related analytical solutions and comparison

For verification, we recalled the Hashin and Shtrikmen (1963) bounds which were derived without specifying the geometric shape or bias on any materials components in the composite. For the in-plane shear modulus of a transversely-isotropic composite, the bounds are given by (Christensen, 1979)

$$\mu_{lower} = \mu_2 + \frac{c_1}{1/(\mu_1 - \mu_2) + c_2(K_2 + 2\mu_2)/[2\mu_2(K_2 + \mu_2)]} \tag{4}$$

$$\mu_{upper} = \mu_1 + \frac{c_2}{1/(\mu_1 - \mu_2) + c_1(K_1 + 2\mu_1)/[2\mu_1(K_1 + \mu_1)]} \tag{5}$$

$$\mu_{lower} \leq \mu_{12} \leq \mu_{upper} \tag{6}$$

where c_1 and c_2 are the volume fractions of the Material 1 and 2, respectively. In the equations, $K = k + \mu/3$ is the plane strain bulk modulus for an isotropic material, and μ and k are the shear and bulk modulus of isotropic components. In applying this bound calculation, one has to take $\mu_1 > \mu_2$. It is seen when the properties of two phases are not too dissimilar, the Hashin and Shtrikman (1963) bounds are very restrictive and can be used for predictive purpose. Hereby, in order to demonstrate our model, we adopted the two material components as glass and epoxy. The shear modulus difference between these two materials is as high as 23. The materials properties are given in Table 1.

For a comparison purpose, we also made calculation based on the equations provided by Christensen and Lo (1979) for two configurations, namely, epoxy matrix with glass fibers, and glass matrix with epoxy fibers. Their model distinguished the fiber and matrix in the geometric layout. That is why sometimes their model is called "fiber-matrix-composite" model. The name of model stated exactly the sequence of the layout of the materials. Their model required that each fiber is fully enclosed by the matrix in the composite. The numerical comparison in Fig.2 shows that the shear modulus of the glass-fiber-epoxy-matrix composite is closer to the HS lower bound, while the modulus of the epoxy-fiber-glass-matrix composite is closer to the HS upper bound. Our finite element prediction is in between the modules of two composites. We may draw the conclusion that Christensen and Lo (1979) model does not gives a good prediction for the bi-continuous composite in general, which is also noticed by Roberts and Garboczi (1999).

As the most accurate estimation for the effective modulus of the composite materials, Roberts and Garboczi's (1999) scheme covers both the bi-continuous and the matrix-inclusion configurations. The present finite element statistical simulation, although were not made based on the exact micro-morphology, captured the most important feature of the bi-continuous composite. It should give a better prediction than the Budiansky (1965) analytical solution where the interactions among the different phases of materials were roughly approximated by Eshelby inclusion solution (1957). In our finite element statistical simulation, the interaction among different phases is calculated exactly.

4 Statistical matters and element type

For the aforementioned meshing with square domain and 8-node square elements, after the random program assigned the material properties for all the domains, the morphology of the microstructures of the composite for the various volume fractions is shown in Fig. 3. Readers can have visual feeling about the term "bi-continuous", where no particulate or matrix can be identified.

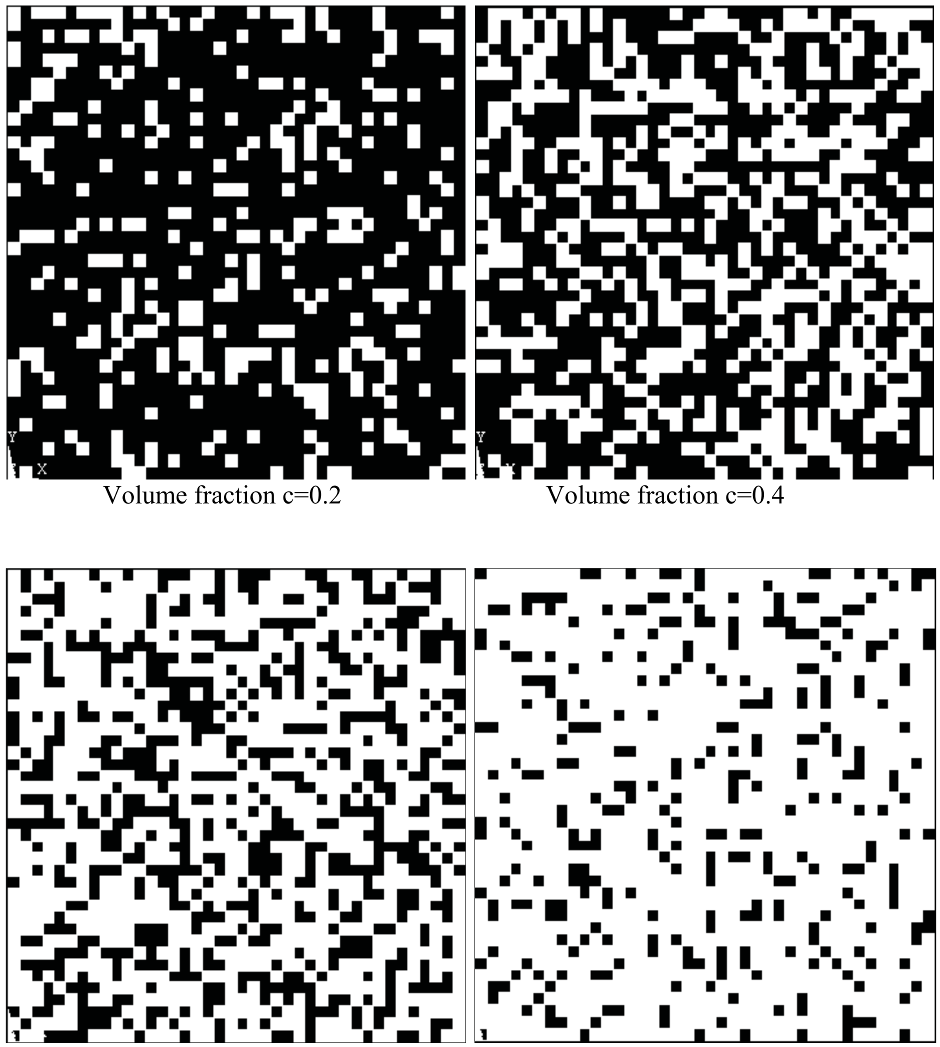
Table 2: Finite element simulation with sample $n = 30$ are carried out for 40 by 40 squared domains and 3 by 3 PLANE82 elements in each of the domains. The sample ($n = 30$) mean value of the shear modulus, standard deviation and relative variance are listed for various volume fraction of glass.

Volume fraction of glass	**shear modulus** (Gpa) ($\overline{\mu}$)	**standard deviation (s)** (Gpa)	$s/\overline{\mu}$
0	1.26		
10	1.53	0.00386	0.252%
20	1.93	0.0101	0.522%
30	2.51	0.0277	1.11%
40	3.42	0.0590	1.72%
50	4.84	0.0887	1.83%
60	7.16	0.204	2.86%
70	10.60	0.234	2.21%
80	15.62	0.366	2.34%
90	22.16	0.261	1.18%
100	29.96		

According to Roberts and Garboczi (1999), information on micro-structural morphology is ranked from low level to high level. The most basic and lowest level information is the volume fraction, then, is followed by surface/volume ratio, and directional information. In our meshing scheme, we only identified the volume fraction of each phase material. We are not able to capture the exact surface/volume ratio and micro-morphology and higher order information. Nevertheless, we may use different type of element to change surface/volume ratio to see its effect on the macroscopic effective properties. Since the present study is carried out by using commercial software ANSYS, we only demonstrate this aspect by using different element type available in ANSYS. In Section 2, the micro-structural morphology is formed by using PLAN82 with geometric aspect ratio 1 to 1. It is straightforward to change the element aspect ratio to have a micro-structure which produces anisotropic effective properties in the macro scale. In the present study, we only focus on the isotropic composite (or transversely isotropic composite to be exact). The effect of different element ratio will be studied elsewhere.

As the second type of element, we used 6-node triangle element to have some insight that the micro-morphology changes affect and macro-scale effective modulus. The microscopic morphology and detailed numbers of nodes, element and domains are given in Fig. 4 and Fig.5. We will elaborate the statistical procedure and argument by using the volume fraction of 50% (glass) -50%(epoxy). The numerical simulations (sample size of $n = 30$) carried out for the six-node triangle element are summarized in Table 3, 4 and 5 with different number of domains and refinement in each of the domains. It is seen that by increasing the number of domains the sample standard deviation decreases, and by increasing the number of elements in each of the domain, the mean value of the effective shear modulus (Eq. (3)) decrease. The former is consistent with statistical expectation; while the latter is in consistent with mechanics expectation.

Apparently, high accuracy and narrow statistical interval (Eq. (3)) needs large number of domains and larger number elements inside of each of the domains. We will choose an acceptable level of accuracy based on the consideration of engineering knowledge and limitation of our computation power. From an engineering measurement point of view, 10% scattering in measured data for the elastic modulus is commonly encountered in the real world. Based on this fact, we could accept the standard deviation of 1600-domain configuration, where sample standard deviation ($s/\overline{\mu}$) is about 1.85% (for example, row 3, Table 3) Assuming the sample data for the effective modulus follow a normal distribution, we have 99% of the



Volume fraction c=0.2 Volume fraction c=0.4

Volume fraction c=0.6 Volume fraction c=0.8

Figure 3: The specimen is divided into 40 by 40 domains. Each domain consists of 3 by 3 PLANE82 elements. Microscopic morphologies for various volume fractions are illustrated for qualitative impression.

Table 3: Effective shear modulus (50% epoxy and 50% glass) obtained for 1600 triangle domains with different level of refinement in the domains.

Number of elements in a domain	Mean value of shear modulus (Gpa)	Standard deviation (Gpa)	$s/\overline{\mu}$
1 (n =30)	5.47	0.14	2.55%
4 (n =30)	4.92	0.098	1.99%
16 (n =30)	4.76	0.088	1.85%
64 (n =30)	4.67	0.086	1.83%

data fall within

$$\overline{\mu}\left(1 \pm 2.58 \times \frac{s}{\overline{\mu}}\right) = \overline{\mu}(1 \pm 4.8\%). \qquad (7)$$

Regarding to the refinement within each of the domains, ideally, we would like to have more elements so that the mean value of the shear modulus is closer to the real value as the smaller number of elements tends to keep the effective material "stiff". However, this objective is constrained by

Table 4: Effective shear modulus (50% epoxy and 50% glass) obtained for 3600 triangle domains with different level of refinement in the domains.

Number of elements in a domain	Mean value of shear modulus (Gpa)	Standard deviation (Gpa)	$s/\overline{\mu}$
1 (n =30)	5.51	0.086	1.56%
4 (n =30)	4.96	0.066	1.33%
16 (n =30)	4.79	0.060	1.26%

Table 5: Effective shear modulus (50% epoxy and 50% glass) obtained for 6400 triangle domains with different level of refinement in the domains.

Number of elements in a domain	Mean value of shear modulus (Gpa)	Standard deviation (Gpa)	$s/\overline{\mu}$
1 (n =30)	5.55	0.054	0.96%
4 (n =30)	4.99	0.044	0.88%
16 (n =30)	4.82	0.041	0.86%

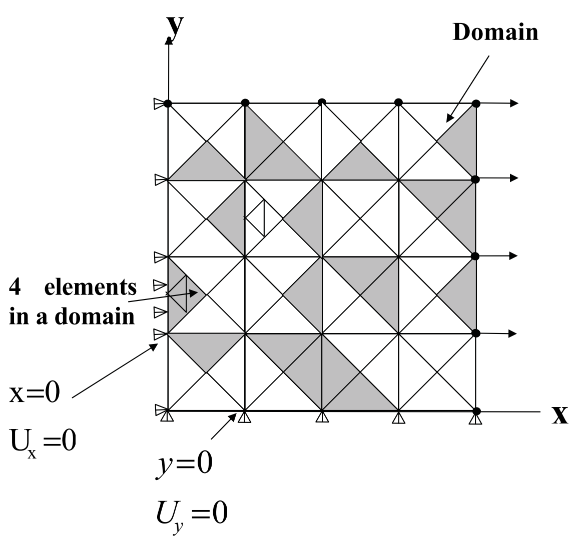


Figure 4: Triangle domain with two phases.

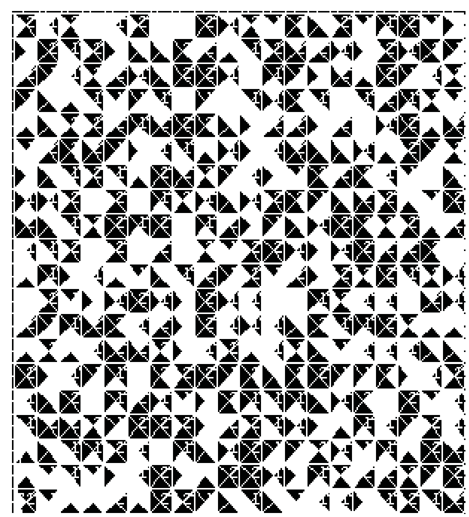


Figure 5: Micro-morphological patter of 1600 triangle domains with 50% of epoxy and 50% of glass.

our computation power and cost (time). For our present computational power (an ordinary personal computer), we can only have around a dozen of elements in each of the domains. We carried out our numerical simulation by using 9 elements in the squared domain and 16 elements in the triangle domains. The statistical features of these two configurations are about the same in terms of mean value and standard deviation, as shown in Table 2 and Table 3 (the row of 50% volume fraction). Therefore, we may conclude that the element type has almost no effect on the prediction of the effective modulus for the bi-continuous solids for our cases. The real mean value (the population mean in the statistical terminology) of the shear modulus with more elements in the domain is expected to be a couple of percents lower than the data presented in Table 2 and Fig. 3. The trend can be seen in Table 3, where a higher level refinement was carried out for 64 elements in the domain.

5 Concluding Remarks

The statistical finite element simulation with random assigning material properties provides a simple and low cost numerical procedure for predicting the elastic properties of the bi-continuous composite. The present numerical procedure includes ((i) meshing the specimen into domains, (ii) randomly assigning the materials type to the domains, (iii) refining the mesh within domains). They are all done by commercial software (ANSYS and MATLAB).

There are two key issues in the above presentation, namely, the mechanics issues and statistical numerical matters. We present the mechanical issue first as we would like to clarify that the bi-continuous solids are different from the particulate/matrix composites. The bi-continuous solids deserve our attention (solid mechanics researchers) as it has certain features that particulate/matrix composites do not have. For example, in the heat conduction and electric conductivity problems, only the bi-continuous solids show the percolation phenomenon; while the particulate/matrix composites never show the percolation. For the second issue, i.e. the statistical and numerical matters, due to the constraint of our computational power and cost, we selected lower accuracy configuration as discussed in Section 4, which does not affect our methodology and conceptual presentation.

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Appendix: An alternative of loading configuration

If we prescribe the boundary conditions as follows,
(1) along $x = 0$, $u_x = 0$,
(2) along $y = 0$, $u_y = 0$,
(3) along $x = 1$. $\sigma_x = S$, uniform tensile stress,
(4) along $y = 1, \sigma_y = -S$, uniform compression stress,
we have a pure shear deformation in$x - y$ plane. The normal stress in the $z-$direction vanishes. Thus, we have

$$\varepsilon_x = \frac{\sigma_x}{E_{11}} - \frac{\nu_{12}\sigma_y}{E_{11}} - \frac{\nu_{13}}{E_{11}}\sigma_z \tag{A1a}$$

$$\varepsilon_y = -\frac{\nu_{12}\sigma_x}{E_{11}} + \frac{\sigma_y}{E_{11}} - \frac{\nu_{13}}{E_{11}}\sigma_z \tag{A1b}$$

$$\varepsilon_z = -\frac{\nu_{31}\sigma_x}{E_{33}} - \frac{\nu_{31}\sigma_y}{E_{33}} + \frac{\sigma_z}{E_{33}} = 0 \tag{A1c}$$

It is seen from Eq. (A1c) that $\sigma_z = 0$. The strain energy is given by

$$U = \frac{1}{2}(\sigma_x\varepsilon_x + \sigma_y\varepsilon_y) = \frac{(1+\nu_{12})S^2}{E_{11}} \tag{A2a}$$

By collecting the strain energy of all the elements from ANSYY, we haveU_{total}. The in-plane shear modulus is calculated as

$$\mu_{12} = \frac{S^2}{2U_{total}} \tag{A2b}$$

Alternatively, we can use the displacement data

$$\varepsilon_x = \frac{(1+\nu_{12})\sigma_x}{E_{11}}, \tag{A3a}$$

and

$$\mu_{12} = \frac{E_{11}}{2(1+\nu_{12})} = \frac{S}{2u_x(x=1)}. \tag{A3b}$$

We have tried both schemes and have consistent number of effective shear modulus.