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Elastic property prediction by finite element analysis with random distribution of materials for tungsten/silver composite

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Abstract In the present numerical study, we introduce a finite element analysis for heterogeneous materials via a random distribution of materials to predict effective elastic properties. With this random distributing strategy, a large scale parametric analysis via finite element becomes feasible for the multi-phase heterogeneous solids. Taking a well-documented tungsten–silver bi-continuous material as an example, the numerical prediction provided here for the effective properties is checked by experimental testing data available in open publication. Discussions on the present finite element prediction and other approaches are also made by comparing with Hashin and Shtrikman (J Mech Phys Solids 11:127–140, 1963) bounds in the composite mechanics.

Introduction

The research of composites has been a field dominated by analytical modeling. There are a few monographs by Christensen [1], Mura [2], Taya and Arsenault [3], etc., covering most of the development and results before 1990s. It is noticed that these research results are mainly for the matrix-particulate type composites where the matrix and reinforcement particles/fibers are clearly identified. Numerical approaches, such as the finite element analysis (FEA), have been used traditionally in a supporting role in the research on matrix-particulate composites, mainly for verifications of the analytical models developed, though the latest development sees FEA being used for more exploring purpose on statistical features of the composites [4–6].

In the present article, we focus on another type of composites, the bi-continuous solids [7], in which the matrix and embedment cannot be clearly identified. This type of microstructure is widely observed in alloys, polymer blends, porous media, and cement-based materials such as concrete, to name a few. Prediction of this bi-continuous composite has been rarely seen in the open literature. It has been noticed that the analytical models developed for the matrix-particulate composites (e.g., Christensen and Lo [8]) cannot provide good predictions on the elastic properties of the bi-continuous composites (e.g., Roberts and Garboczi [9]) due to the requirement for a good definition of the morphological features of the composite. Meanwhile, it needs to point out that there also exist a number of bound theories (normally in pairs, i.e. upper and lower bounds under certain conditions) which were developed for gauging the elastic properties of composites predicated/estimated by various approaches. The most well-known and frequently cited one is that given by Hashin and Shtrikman [10], where the spatial distribution of each component of the composite is treated equally. Therefore, it is feasible for it to be used for both matrix-particulate composites and bi-continuous composites. Studies on bi-continuous composite recently have led to new development via the use of finite element analyses and statistical reconstructions (Garboczi and Day [11]). Roberts and Garboczi [9] made a reasonably accurate estimation on the elastic modulus for a silver–tungsten composite by using the

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statistic reconstruction technique. Their procedure is known for working on two "transparencies": one of the microscopic photo or statistically reconstructed "photo" of the micro morphology of the bi-continuous composite, and the other with very finely meshed elements with the elements' material properties yet to be specified. When the second transparency is put on top of the first, the material property of a specific element can be picked based on the morphology of the microstructure 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 for the situations where we do not have detailed statistical information about the microstructure of the composite. It is particularly true in the beginning stage of design of new composite materials, or when the micro morphology is difficult or impossible to obtain. In the following sections, we propose a simple scheme of assessing the elastic properties of the bi-continuous composite based on finite element meshing, where no microstructure information other than the volume fraction is needed as a prior.

Finite element analysis with random distribution of materials and analytical verification

Let us consider a unit cubic, which is called *specimen* here. The specimen is first discretetized into equal sized mesh called *domains* so that the volume fraction of the materials can be easily calculated. The domains are assigned randomly with different material properties for a given volume fraction of materials. This is done in a finite element modeling. First the mesh is generated, for instance, using a commercial package (e.g., ANSYS [12]) and material 1 of the bi-composite is assigned to all elements. The element file is opened. One then uses a numerical package (e.g., MATLAB [13]) to generate random numbers to select the elements in the file where material 2 is assigned to replace material 1. This modified element file is then put back to the finite element code with a random element assignment of materials 1 and 2 in the mesh.

The sudden change of properties in the neighboring elements may cause numerical errors so the mesh should generally be refined to have a few *smaller elements* in each domain. Alternatively, it might be possible to use higher order elements for each domain, where further division of domains into multiple smaller elements may become unnecessary, though this approach has not been followed here. Increasing the number of domains in the specimen will lead to a reduction in the statistical variation of the predicted effective modulus. Numerically, the increased number of elements inside each domain (and possibly the higher order elements for each domain) will lead to a "relaxation" of stresses in the domains surrounded by different material.

A schematic illustration of the domains and elements is shown in Fig. 1, using ANSYS. The figure represents one

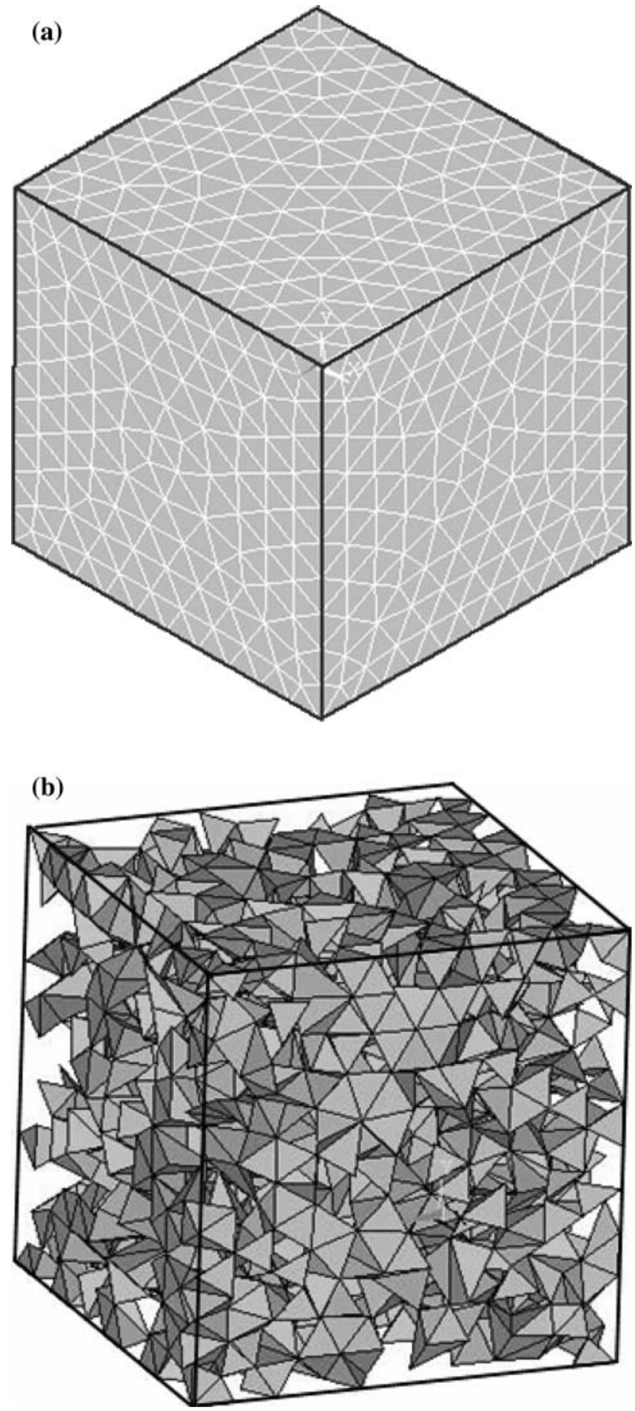

Fig. 1 (**a**) The model is discretized into 7660 domains (equal-size tetrahedron shaped). Each domain is further divided into eight Solid92 elements (10-node tetrahedron element). (**b**) Shaded elements show the domains selected randomly for material replacement by silver at volume fraction 20%. The numerical prediction of Young's modulus for this configuration is given in Fig. 3

eighth of a cubic sample under simple uniaxial tensile loading. Symmetric boundaries were assumed in all x, y, and z directions. Figure 1a shows the mesh generated with material 1 and Fig. 1b gives the randomly replaced mesh for material 2. The numerical calculation is carried out using a 10-node tetrahedron element Solid92 provided in ANSYS version 8.1. Each node has 6 degrees of freedom. The interfacial condition between domains remains perfect bonding as this is not affected by the change of material in the domains. No failure was defined for the interfacial properties since we are only interested in elastic deformation with a small deformation assumption. The boundary conditions are prescribed as follows.

As only one eighth of a cubic is modeled, in planes $x = 0$, $y = 0$, and $z = 0$, displacements u in the x, y, and z directions, respectively, are fixed as zero, representing symmetry. On plane $x = 1$, we apply a uniform stress in the x direction $\sigma_{xx} = S$.

The above loading and boundary conditions yield in the values of the elastic properties as

$$E = \frac{S}{\varepsilon_x} = \frac{S}{u_x(x=1)}, \tag{1a}$$

and

$$v = \left|\frac{\varepsilon_y}{\varepsilon_x}\right| = \left|\frac{u_y(y=1)}{u_x(x=1)}\right|, \tag{1b}$$

where the finite element results of the nodal displacement $u_x(x = 1)$ and $u_y(y = 1)$ are the nodal-averaged values on the corresponding planes. The normalized shear modulus predicted by the present finite element scheme is presented in Fig. 2, together with results available in publication for verification.

Here we recall the Hashin and Shtrikmen [10] bounds (HS bounds hereafter) which were derived without specifying the geometric shape or bias on any materials components in the composite. For an isotropic bi-composite, the upper and lower bounds are given by

$$\frac{c_1}{1+\frac{(1-c_1)(\mu_1-\mu_2)}{(\mu_2+\mu_{\text{lower}})}} \le \frac{\mu-\mu_2}{\mu_1-\mu_2} \le \frac{c_1}{1+\frac{(1-c_1)(\mu_1-\mu_2)}{(\mu_2+\mu_{\text{upper}})}} \tag{2}$$

where, for $(\mu_1-\mu_2)(k_1-k_2)\ge 0$,

$$\mu_{\text{lower}} = \frac{3}{2}\left(\frac{1}{\mu_2}+\frac{10}{9k_2+8\mu_2}\right)^{-1}$$

$$\mu_{\text{upper}} = \frac{3}{2}\left(\frac{1}{\mu_1}+\frac{10}{9k_1+8\mu_1}\right)^{-1}; \tag{3}$$

while for $(\mu_1-\mu_2)(k_1-k_2)<0$

$$\mu_{\text{lower}} = \frac{3}{2}\left(\frac{1}{\mu_2}+\frac{10}{9k_1+8\mu_2}\right)^{-1}$$

$$\mu_{\text{upper}} = \frac{3}{2}\left(\frac{1}{\mu_1}+\frac{10}{9k_2+8\mu_1}\right)^{-1} \tag{4}$$

Here μ and k are the shear and bulk modulus of the isotropic composite, the sub-indices indicate the two components of the bi-composite. c_1 is the volume fraction of the first material, and $c_2 = 1 - c_1$.

In Fig. 2, we also presented Budiansky [14] solution, a well-known self-consistent method (SCM) solution, to make comparison with our finite element numerical prediction. The self-consistent solution does not make bias on the components in the composite, but takes approximation on the interaction among the multiple phases and the shape of the phases (a spherical shape was used in Budiansky's original paper [14]). In terms of the shear modulus and bulk modulus, the self-consistent method gives the following non-linear equations.

$$\frac{c_1}{1+\beta^*\left(\frac{\mu_1}{\mu}-1\right)} + \frac{c_2}{1+\beta^*\left(\frac{\mu_2}{\mu}-1\right)} = 1 \tag{5}$$

$$\frac{c_1}{1+\alpha^*\left(\frac{k_1}{k}-1\right)} + \frac{c_2}{1+\alpha^*\left(\frac{k_2}{k}-1\right)} = 1 \tag{6}$$

where

$$\alpha^* = \frac{1+v^*}{3(1-v^*)} \quad \text{and} \quad \beta^* = \frac{2(4-5v^*)}{15(1-v^*)}, \tag{7}$$

with

$$v^* = \frac{3k-2\mu}{6k+2\mu}. \tag{8}$$

It is seen that the self-consistent approach has two important features: it poses no bias on any components in the composite; it also makes a perfect configuration for analytical modeling by putting a single inclusion inside the yet-to-be-determined composite. The first feature is used

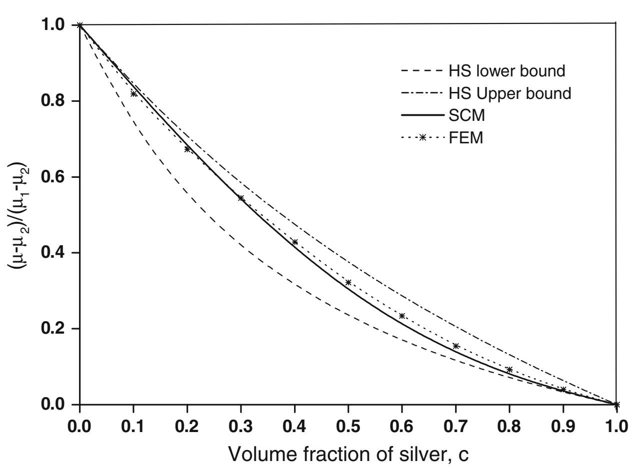

Fig. 2 Finite element prediction of the normalized shear modulus of the tungsten–silver composite compared with HS bounds and self-consistent method solutions

here for the bi-continuous composite. The interaction among the multiphase materials components, which is a weak point of the SCM, is taken care by the finite element approach. The second feature is modified for particulate-matrix type composites by introducing an inclusion-matrix-composite layout, which is sometimes called the generalized self-consistent model (GSCM) (Christensen and Lo [8]).

Experimental verification

In this section, we verify our FEA results on random distributions of materials with the experimental data (Table 1) obtained on tungsten–silver bi-continuous composite by Umekawa et al. [7] as shown in Fig. 3. The experimental test was conducted at a fixed volume composition, namely 20% silver and 80% tungsten. By elevating the temperature, the moduli of silver and tungsten changed, as shown in Table 1, leading to the corresponding change in the effective modulus of the composite.

For a comparison purpose, we also present solutions of GSCM in Fig. 3 based on the equations provided by Christensen and Lo [8] for two configurations, namely tungsten matrix with silver inclusions, and silver matrix with tungsten inclusions. Their model distinguishes the inclusion and matrix in the geometric layout. This is part of the reason their approach is sometimes called an "inclusion-matrix-composite" model. Their model guarantees that the inclusion material is enclosed by the matrix material in the composite. The numerical comparison in Fig. 3 shows that the elastic modulus predicted by the configuration of tungsten-inclusion in silver-matrix composite is close to the HS lower bound, while the modulus for configuration of the silver-inclusion in tungsten-matrix composite is closer to the HS upper bound. We may draw the conclusion that in general the Christensen and Lo [8]

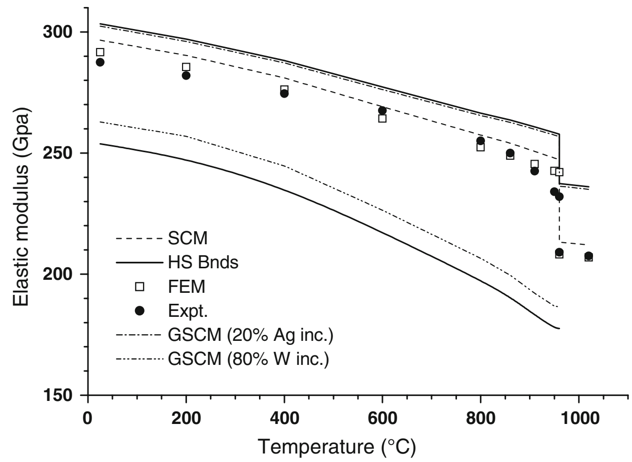

Fig. 3 The finite element prediction on elastic modulus of silver–tungsten composite compared with the experimental data obtained by Umekawa et al. [7]

model does not provide a good prediction for bi-continuous composite.

In Fig. 3, we also notice that the SCM solution fits well with the experimental data at temperatures less than the melting point of silver at 960 °C. However, for higher temperatures, the SCM prediction drifts away from the experimental data, while the finite element prediction remains very close to the experimental data. It was pointed out in Budiansky's original paper [14] that for some extreme cases, such as voids with zero elastic modulus, SCM leads to unrealistic results at certain volume fractions due to the fact that the interaction among the multiphase in the composite is taken into account in an approximated manner via the Eshelby ellipsoidal inclusion solution (e.g., Mura [2]). On the other hand, as the finite element analysis calculates the interaction among the multi-phases in a relatively accurate manner, the present finite element analysis with random material distribution scheme can be considered as a benchmark for the self-consistent method solution.

Table 1 Elastic material constants for silver and tungsten at various temperatures

Temperature, °C	E (silver), GPa	v (silver)	E (tungsten), GPa	v (tungsten)
25	70	0.36	400	0.28
200	69	0.36	392	0.28
400	63	0.36	383	0.28
600	54	0.36	373	0.28
800	45	0.37	363	0.28
860	42	0.37	361	0.28
910	39	0.37	359	0.28
950	37	0.37	357	0.28
960	37	0.37	356	0.28
960	0	0.5	356	0.28
1020	0	0.5	354	0.28

Concluding remarks

The present finite element simulation with randomly assigned material properties provides a simple, efficient and low-cost numerical procedure for prediction of elastic properties of bi-continuous composites. The present numerical procedure, which captures the characteristic feature of the composite, namely particulate/matrix versus bi-continuous types, may be the only choice for the macro properties of the material when the detailed information of a composite's microscopic morphology is not available. Efforts are undertaken to see whether this model can be improved to predict some of the microscopic information of the composite.

Another advantage of the present scheme is the structured procedure it provides. Firstly, the specimen is meshed into domains, and secondly, materials types are randomly assigned to the domains. Finally, mesh can be refined within the domains. All these can be performed using commercial software. In the present study, numerical calculations were carried out on a PC of 3 GHz speed and 1 GB RAM memory and completed within 1.5 h. As shown for each of the case in Figs. 2 and 3, the results are fairly accurate. Compared with Roberts and Garboczi's [9] prediction based upon their reconstruction scheme, the efforts and information needed via the current proposed approach are far less demanding. The accurate prediction by the present finite element method with the random material distribution scheme appears to indicate that an accurate description of the morphology might not be necessary. This posts a theoretical question: under what condition the exact micro-morphology is needed for the prediction of the materials' effective elastic properties? This remains to be verified.

Finally, it needs to be pointed out that although the present finite element analysis with a random material distribution is an effective approach for bi-continuous composites, it does not provide good prediction for particulate-matrix composites. Similarly, the analytical models, such as those reviewed by Christensen [15] which are well developed for particulate-matrix composites, are not able to make good prediction for bi-continuous composites. It appears that Roberts and Garboczi's [9] micro-morphology identification or reconstruction model is capable of handling both types of composites, namely the bi-continuous and particulate-matrix composites, although the "cost" and information needed for using this method are relatively higher.

References

1. Christensen R (1979) Mechanics of composite materials. Wiley, New York
2. Mura T (1982) Micromechanics of defects in solids. Martinus Nijhoff Publisher
3. Taya M, Arsenault RJ (1989) Metal matrix composites. Pergamon Press
4. Hu N, Wang B, Tan GW, Yao ZH, Yuan WF (2000) Comp Sci Technol 60:1811–1823. doi:10.1016/S0266-3538(00)00054-3
5. Iovane G, Nasedkin AV (2005) Comput Struc 84:19–24. doi:10.1016/j.compstruc.2005.09.002
6. Wang WX, Luo D, Takao Y, Kakimoto K (2006) Comput Struc 84:991–1001. doi:10.1016/j.compstruc.2006.02.013
7. Umekawa S, Kotfila R, Sherby OD (1965) J Mech Phys 13: 229–235. doi:10.1016/0022-5096(65)90012-8
8. Christensen R, Lo KH (1979) J Mech Phys Solids 27:315–330. doi:10.1016/0022-5096(79)90032-2
9. Roberts AP, Garboczi EJ (1999) J Mech Phys Solids 47: 2029–2055. doi:10.1016/S0022-5096(99)00016-2
10. Hashin Z, Shtrikman S (1963) J Mech Phys Solids 11:127–140. doi:10.1016/0022-5096(63)90060-7
11. Garboczi EJ, Day AR (1995) J Mech Phys Solid 43:1349–1362
12. MATLAB The MathWorks, Inc., Massachusetts (2005)
13. Version ANSYS 8.1, ANSYS, Inc., Southpointe (2005)
14. Budiansky B (1965) J Mech Phys Solids 13:223–227. doi:10.1016/0022-5096(65)90011-6
15. Christensen R (1990) J Mech Phys Solids 38:379–404. doi:10.1016/0022-5096(90)90005-O