The effect of inclusions on macroscopic composite elasticity: A systematic finite-element analysis of constituent and bulk elastic properties

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Abstract. The bulk physical properties of composite systems are difficult to predict – even when the properties of the constituent materials in the system are well known. We conducted a finite-element method simulation to examine the inclusion effect by substituting an inclusion phase (second phase) into a host phase (first phase). We have organized the simulation results as a function of the elasticity of host and inclusion phases. In this procedure, special attention was paid to the initial change of elastic constants as the inclusion volume ratio was varied. To accomplish this, we introduced a new parameter \( D_{ij} \) defined as the derivatives of the normalized stiffness elastic constant over the inclusion volume ratio. We succeeded in obtaining useful systematic formulations for \( D_{ij} \). These formulations are expected to be applicable to the study of composite systems in many disciplines, such as geophysics, mechanics, material engineering, and biology. The present results provide much more effective constraints on the physical properties of composite systems, like rocks, than traditional methods, such as the Voigt-Reuss bounds.

1. Introduction

Composite systems are found universally. Natural rock, in particular, is the composite system that this paper focuses on. However, they are also found in a diverse range of technological fields, including some biological tissues, and in many industrial composite goods, such as fiber reinforced plastic, metallic alloys, and concrete. Therefore, the evaluation of the macroscopic physical properties of composite objects is intensively studied not only in the earth sciences but also in other disciplines, such as material engineering.

Among the various physical rock properties, macroscopic elasticity, or composite elasticity, has attracted special interest in the context of geophysical exploration for natural resources. Furthermore, the macroscopic elasticity of composite material is itself of fundamental interest because of nontrivial interactions among inclusions. Therefore, the inclusion effect on composite elasticity has been investigated by various means including finite element methods (FEMs) (e.g., [1, 2]).

Although a single spherical inclusion in an isotropic elastic body can be analyzed explicitly by means of exact analytical solutions, interactions among multiple inclusions cannot be solved analytically. Therefore, many practical approaches, including average or bound approaches and self-consistent approaches, have been proposed and applied intensively and extensively [1, 2]. The Voigt–Reuss bound [3] has generally been used as a first choice for constraining composite elasticity because of the relatively simple expressions involved.
Owing to the recent rapid progress, the FEM has enabled us to fully evaluate the macroscopic elasticity of composite material numerically – without introducing any specific assumptions or simplifications. This superiority in the method inspired us to conduct the present FEM analysis of the inclusion effect in composite materials. We start the study with a 2-D analysis, for simplicity, before moving on to a full 3-D simulation.

2. Geometry and procedures

Here, we explain the basics of the geometry and method of the finite-element analysis applied in this work. Figure 1 shows an example of aligned inclusions in an isotropic elastic body that can be used to study the inclusion effect. The example is referred to as a $7 \times 7$ buffered layer FEM model, in which uniform displacements were applied to the outermost edges as a boundary condition. Note that only a quarter of the geometry of the model is shown (Figure 1), because the FEM analysis can be conducted assuming symmetric and antisymmetric conditions. We can recognize excellent homogeneity inside the geometric bounds of the model; inhomogeneity caused by the boundary is rapidly relaxed in peripheral layers. In other words, the peripheral layer is an extremely effective buffer for homogenizing the stress-strain state in the interior of the model.

Plane strain and plane stress are two typical conditions that can be readily modeled in a 2-D analysis. In plane-strain analysis, strains $\varepsilon_3, \varepsilon_4,$ and $\varepsilon_5,$ involving displacement in the z direction, are commonly assumed to be zero, whereas in plane-stress analysis, stresses $\sigma_3, \sigma_4,$ and $\sigma_5$ are commonly assumed to be zero. The strains and stresses are considered to occur in thick and thin 2-D plates, respectively. The results for the 3-D problem lie between those for the 2-D plain stress and plain strain analyses. Therefore, the present 2-D results are helpful in constraining the inclusion problem in 3-D.

Let $u$ and $v$ be defined as displacement in the x and y directions, respectively. In the 2-D analysis, we can classify three types of forced displacement on the outermost edges: (1) uniform forced displacement in the x direction, e.g., $u = -1 \times 10^{-6}$ on the x edge, while free in the y direction, or no constraint on the y edge; (2) uniform forced displacement in the y direction, e.g., $v = -1 \times 10^{-6}$ on the y edge, while free in the x direction, or no constraint on the x edge; (3) coupled uniform forced displacement in the y and x directions, e.g., $v = 1 \times 10^{-6}$ on the y edge, and $u = 1 \times 10^{-6}$ on the x edge.

We can easily obtain the average strain along a line from the resulting displacement. We then formulate simultaneous equations between the averaged stress over the observed line and the averaged strain. Note that we follow orthodox notations for elasticity: stress $\sigma$, strain $\varepsilon$, and stiffness elastic constant $C$. For plane-strain analysis, we have

\[
\begin{align*}
\sigma_1 &= C_{11} \varepsilon_1 + C_{12} \varepsilon_2, \\
\sigma_2 &= C_{12} \varepsilon_1 + C_{22} \varepsilon_2.
\end{align*}
\]

Note that we can make two sets of simultaneous equations corresponding to uniaxial compressions in the x and y directions. Consequently, we have four redundant equations for three unknown parameters, $C_{11}, C_{12},$ and $C_{22}$. For shear deformation, we have a single equation for $C_{66}$:

\[
\sigma_6 = C_{66} \varepsilon_6.
\]

The host and the inclusion phases are specified with subscripts “1” and “2”, respectively. We systematically changed the elasticity of the inclusion phase of the second phase and surveyed the area of $0.0<\nu_1, \nu_2<0.45$ and $0.0001<R_E=E_2/E_1<10000$.

We considered the normalized elastic constant $C^* = (C/C_0)$, where $C_0$ is the original elastic constant of the first host phase. We introduce a new parameter $D$ as the derivative of $C^*$ over the volume ratio of the inclusion phase, $\phi$:

\[
D_{\phi}(R_E, \nu_1, \nu_2) = \lim_{\phi \to 0} \frac{\partial C^*_\phi(R_E, \nu_1, \nu_2)}{\partial \phi}.
\]

This parameter is important for the evaluation of the effect of dilute inclusions on macroscopic elasticity.
Figure 1. Example of a multi-buffer layer model at $N = 7$; a quarter-part $7 \times 7$ model representation. The left bottom corner in each plot is the actual center of the $7 \times 7$ model. The left and lower edges have symmetric or antisymmetric boundary conditions applied. The short vertical and horizontal edges at the left bottom corner are the observation lines for mean stress and displacement. In this case, circles are the second inclusion phases, and the remaining part is the first host phases. Although the area ratio of circles is shown to be relatively large, actual ratios for deriving $D$ were much smaller ($\sim 10^{-3}$). (a) Initial geometry and mesh plot. Note that $x$ and $y$ directions are horizontal and vertical, respectively, as shown in this plot. Small black open circles are due to the FEM software (COMSOL®) function to specify the boundary of edges in the model geometry. (b) Stress distribution in the compression test in the $y$ direction. (c) Same as (b) but in the $x$ direction. (d) Shear deformation.
Figure 2. The initial slope of elastic constants, $D_{11}$ (blue solid line) and $D_{66}$ (red dotted line) vs. $R_E (=E_2/E_1)$ at $\nu_1=\nu_2=0.25$ calculated by the present FEM analysis.

Figure 3. The left hand limit of $D_1$ or $D_1^-$ vs. Poisson ratio of matrix $\nu_1$. Blue and red lines correspond to $D_{11}$ and $D_{66}$ based on Eqs. (4) and (5). The symbol ‘*’ corresponds to results obtained by the FEM analysis. Note that some inconsistency between Eq. (4) and the FEM results may be caused by inaccuracy of FEM results at larger Poisson ratios ($\nu_1>0.4$).
**3. Results and discussion**

Figure 2 shows the results for ν₁=ν₂=0.25. This is a typical example that is homogeneous regarding the Poisson ratio between the two phases. The trends of D were investigated by changing Rₑ (=E₂/E₁). For an isotropic elastic material, C₁₁ and C₆₆ are expressed by Lame’s elastic constants, as C₁₁=λ+2μ and C₆₆=μ. Note that D₁₁ and D₆₆ are consistent each other at ν=0.25 or λ=μ. From the plot, we can see that the right and left bound limits, D⁺ and D⁻, are 1.5 and -3, respectively.

Figure 3 shows D⁻ as a function of ν₁. We can see that the results are expressed quite well by the following equations.

\[
D_{11}^{-}(ν₁) = D_{22}^{-}(ν₁) = -3 + \frac{8 ν₁(0.25 - ν₁)}{(1 - 2 ν₁)}, \quad (4)
\]

\[
D_{66}^{-}(ν₁) = -4(1 - ν₁) \quad (5)
\]

Figure 4 shows D⁺ as a function of ν₁. We found that the trends fit quite well with a simple functional form:

\[
D_{11}^{+} = \frac{5}{3} + \frac{2 ν₁(1+ν₁)}{5(1-ν₁)}, \quad (6)
\]

\[
D_{66}^{+} = \frac{4}{3} + \frac{2 ν₁(1+ν₁)}{5(1-ν₁)}, \quad (7)
\]

Note that these extreme D values are commonly irrespective of ν₂; this is a reasonable outcome.
Figure 5. Variations of $D$ versus $x = \log_{10}(R_E)$ for various Poisson’s ratio values as shown on each plot. Red symbols and dark blue line for $D_{11}$ are FEM results and Eq. (8), respectively. Light blue symbols and green line for $D_{66}$ are FEM results and Eq. (9), respectively.
Finally, we successfully produced the following simple functional forms.

\[
D_{11}(x) = \left( \frac{D_{11}^+ - D_{11}^-}{2} \right) \tanh \left( \frac{1}{2} \left( x + 4.6 \nu_1 \nu_2 - 0.8 \nu_1 + 0.7 \nu_2 + 0.7 \right) \right) + \left( \frac{D_{11}^- + D_{11}^+}{2} \right) \tag{8}
\]

\[
D_{66}(x) = \left( \frac{D_{66}^+ - D_{66}^-}{2} \right) \tanh \left( \frac{1}{2} \left( x - \nu_1 - \nu_2 + 1 \right) \right) + \left( \frac{D_{66}^- + D_{66}^+}{2} \right) \tag{9}
\]

where \( x = \log_{10}(R_E) \).

The performance of the formulas is shown in Figure 5. We can see that Eqs. (8) and (9) are consistent with the FEM results throughout for both \( \nu_1 \) and \( \nu_2 \). However, for \( \nu_1 = \nu_2 = 0.25 \), we can recognize a small difference between Eqs. (8) and (9), even though the FEM results for \( D_{11} \) and \( D_{66} \) are identical for the condition of \( \nu_1 = \nu_2 = 0.25 \). This indicates a limitation in the accuracy of the Eqs. (8) and (9). Although we can readily derive such functional forms that are close to the FEM results, we need to emphasize that Eqs. (8) and (9) are practical compromises. Introducing more complicated functional forms does not significantly benefit the practical outcomes.

It is useful to compare the present results with the Voigt-Reuss bounds. Here \( C_1 \) and \( C_2 \) are original elastic constants for the first and the second phases. Define the normalized elastic constants \( C_1^* \) and \( C_2^* \) as \( C_i/C_1 \) and \( C_2/C_1 \), respectively. Obviously, \( C_1^* \) equals 1 from its definition. It is noted that the Voigt-Reuss bound is reduced to be same results for both \( D_{11} \) and \( D_{66} \) for the condition where \( \nu_1 = \nu_2 = 0.25 \). Therefore, we simply specify the Voigt and Reuss bounds by \( D_V \) and \( D_R \), respectively. They are expressed as

\[
D_V = \frac{\partial C^*_V}{\partial \phi} = \frac{\partial \left( 1 - \phi \right)}{\partial \phi} + \phi C^*_2 = C^*_2 - 1 \tag{10}
\]
Figure 6 shows a comparison between the present results and the calculated Voigt-Reuss bounds. We can see that the Voigt-Reuss bounds fail to constrain the macroscopic elasticity of composite material when the contrast in elastic constants between the two phases is significantly large. Furthermore, note that the present $D$ value falls outside the Voigt-Reuss bounds near $R_e \sim 1$. This difference may be caused by geometric effects. The present result depends on a specific circular geometry for the inclusions, whereas the Voigt-Reuss bounds depend simply on volume ratio between the two phases. This inconsistency clearly supports the utility and necessity of our FEM method for evaluating the bulk properties of mixed-media with specific constituent geometries.

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