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Multi-scale approach for modeling the transversely isotropic elastic properties of shale considering multi-inclusions and interfacial transition zone

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ABSTRACT

Multiscale approach based explicit analytic predictions are obtained for the transversely isotropic properties of shale rock considering the multi-inclusion and *interfacial transition zone* (ITZ) effects. Representative volume elements (RVEs) are utilized to describe the material's hierarchical microstructures from the nanoscale to the macroscale. A new multilevel micromechanical homogenization scheme is presented to quantitatively estimate the material's transversely isotropic properties with the multi-inclusion and ITZ effects. The ITZ is characterized by the interphase material, whose effects are calculated by modifying the generalized self-consistent model. Furthermore, the explicit form solutions for the transversely isotropic properties are obtained by utilizing the Hill polarization tensor without numerical integration and the standard tensorial basis with the analytic inversions of fourth-rank tensors. To verify the proposed multiscale framework, predictions obtained via the proposed model are compared with experimental data and results estimated by the previous work, which show that the proposed multi-scaling approaches are capable of predicting the macroscopic behaviors of shale rocks with the multi-inclusion and ITZ effects. Finally, the influences of ITZ and inclusion properties on the material's macroscopic properties are discussed based on the proposed multiscale framework.

1. Introduction

Shale rock is especially critical for success of many fields of petroleum engineering and may also be important for the development of sustainable nuclear waste storage solutions.[1,2] Owing to the direct economic importance of shale rock, many efforts have been dedicated to model the material's mechanical properties, which can be mainly classified into two categories. The first category focuses on the empirical formulations to evaluate the properties of shale rock.[3–8] For examples, Dewhurst et al. presented the empirical strength prediction for preserved shales[3]; Farrokhrouz et al. proposed the empirical estimation of uniaxial compressive strength of shale formations[4]; Sayers used the clay-particle orientation distribution function to characterize shale elastic-anisotropy in dynamic measurements.[5] These formulations are obtained by means of laboratory or site tests, which is the phenomenological way to formulate the behavior of shale rock. The main limitation of such traditional approach is that it requires the extensive and costly experimental programs to characterize the material's properties. An attractive alternative to handle this kind of problem is provided by the framework of micromechanics, which reduces the laboratory expenses, meanwhile helps us throw light on the relations between the material's complicated microstructures and the macroscopic properties of shale rock.[9–14] Hornby et al. proposed a theoretical framework to predict the effective elastic properties of shale rocks based on the effective-medium method and found that the anisotropy of shale macroscopic elasticity was attributed to shape, orientation, and connection of the solid and fluid phase.[9] Giraud et al. used the Hill tensor to estimate the effective poroelastic properties of transversely isotropic rock-like composites.[10] Bobko et al. employed a strength homogenization approach to interpret the nanoindentation results and developed scaling relationships for indentation hardness with clay packing density.[12] Guo et al. presented a shale rock physics model for analysis of the brittleness index, mineralogy and porosity in Barnett shale.[13]

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Despite many attempts, progress in developing consistent micromechanics models that link mineralogy at the nanoscale to macroscopic properties of shale rock has been limited, due to the lack of experimental data on the fundamental elastic properties of shale elementary building blocks, and links between those properties, morphology and macroscopic properties.[15] Recently, Ortega et al. proposed a multiscale framework to predict the transversely properties of shale rock with the self-consistent method and only the quartz inclusion is considered.[15] Actually there are many types of inclusions, such as quartz, calcite and dolomite, in the shale rock.[9–14] And the inclusions are not perfectly bonded to the matrix phase of shale rock, which implies that there are *interfacial transition zones* (ITZs).[16–19] To address these issues, in this extension we propose a multiscale (from nanoscale to macroscale) predicting framework for the shale rock's transversely isotropic properties considering the multi-inclusion and ITZ effects with a new multilevel micromechanical homogenization scheme. Furthermore, in contrast with the composites containing isotropic phases, very few explicit analytical results can be found in literatures related to three-dimensional matrix composites with anisotropic components due to the significant mathematical difficulties appearing in such problems.[20] In our work, the standard tensorial basis[20] and the Hill polarization tensor without numerical integration[10] are modified to get the explicit form solutions for the transversely isotropic properties of the shale rock with multi-inclusion and ITZ effects.

2. Fundamentals of continuum micromechanics

2.1. The effective properties of the composite

One goal of continuum micromechanics is to estimate the effective elastic properties of the material defined over the representative volume element (RVE). The RVE is based on a 'mesoscopic' length scale, which is considerably larger than the characteristic length scale of particles (inhomogeneities) but smaller than the characteristic length scale of a macroscopic specimen.[21] Take a two-phase composite as an example, the effective elastic stiffness tensor C^* of the composite is defined through

$$\bar{\boldsymbol{\sigma}} = \mathbf{C}^*: \bar{\boldsymbol{\varepsilon}} \tag{1}$$

with

$$\bar{\boldsymbol{\sigma}} \equiv \frac{1}{V}\int_V \boldsymbol{\sigma}(\mathbf{x})d\mathbf{x} = \frac{1}{V}\left[\int_{V_0} \boldsymbol{\sigma}(\mathbf{x})d\mathbf{x} + \int_{V_1} \boldsymbol{\sigma}(\mathbf{x})d\mathbf{x}\right] \tag{2}$$

$$\bar{\boldsymbol{\varepsilon}} \equiv \frac{1}{V}\int_V \boldsymbol{\varepsilon}(\mathbf{x})d\mathbf{x} = \frac{1}{V}\left[\int_{V_0} \boldsymbol{\varepsilon}(\mathbf{x})d\mathbf{x} + \int_{V_1} \boldsymbol{\varepsilon}(\mathbf{x})d\mathbf{x}\right] \tag{3}$$

where V is the volume of an RVE, V_0 is the volume of the matrix, and V_1 is the volume of the inhomogeneity.

The effective elastic properties depend on the corresponding elastic moduli, the volume fraction of each constitute component, and the microstructures (e.g. the spatial distribution of the components) of the specific composite.[22] Due to the complex microstructures, many approximations instead of the exact solutions for these effective properties are developed in accordance with Eshelby's work.[23–25]

2.2. The Eshelby solution and the polarization tensor

Eshelby derived the elastic field inside and outside an ellipsoidal inclusion in an infinite medium, and proposed the celebrated *equivalent inclusion principle* to relate the elastic inclusions and inhomogeneities.[23–25] The main theory behind the idea can be summarized as below. Consider an ellipsoid inhomogeneity (particle with properties different from those of the homogeneous matrix) embedded in an infinite matrix. According to Eshelby's equivalence principle, the perturbed strain field $\boldsymbol{\epsilon}'(\mathbf{x})$ induced by inhomogeneity can be related to specified eigenstrain $\boldsymbol{\varepsilon}^*(\mathbf{x})$ by replacing the inhomogeneity with the matrix material (or vice versa). That is, for the domain of the inhomogeneity with elastic stiffness tensor $\mathbf{C}_1$, we have

$$\mathbf{C}_1: \left[\boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}'(\mathbf{x})\right] = \mathbf{C}_0: \left[\boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}'(\mathbf{x}) - \boldsymbol{\epsilon}^*(\mathbf{x})\right] \tag{4}$$

with

$$\boldsymbol{\epsilon}'(\mathbf{x}) = \mathbf{S}: \boldsymbol{\epsilon}^*(\mathbf{x}) \tag{5}$$

where $\boldsymbol{\varepsilon}^0$ is the uniform strain field induced by far-field loads for a homogeneous matrix material only. $\mathbf{S}$ is the Eshelby tensor associated with the inhomogeneity, which can be represented by the Hill polarization tensor $\mathbf{P}$ as $\mathbf{S}=\mathbf{P}:C_0$, and $\mathbf{C}_0$ and $\mathbf{C}^1$ are the stiffness tensors of the matrix and the inhomogeneity. For details see Ref. 26.

For a real material, there are usually many different inhomogeneities in the RVE. Therefore, it is difficult to obtain the exact perturbed strain field due to so many randomly distributed inhomogeneities that influence each other. Through making a set of assumptions, different micromechanical methods such as the Mori–Tanaka method,[27,28] the self-consistent method[29] and Ju's method[21,34–38] have been derived based on the Eshelby solutions to estimate the effective properties of heterogeneous materials.

3. Multiscale representation of hierarchical structures of shale rock

3.1. Hierarchical structures of shale rock

Shale rocks are heterogeneous in nature and generally consist of different constituents or phases, such as clay material, quartz and calcite. Further, the constituents of materials can be treated as homogeneous at a certain length scale, but when observed at a smaller length scale, the constituents themselves may become heterogeneous, i.e. a multiscale phenomenon for heterogeneous shale rock materials.[9–15] According to Ref. 13, the components of shale rocks should include clays, kerogen, cracks, pores, quartz, calcite and dolomite. The rock properties are dependent on the microstructure parameters such as the orientation of clay platelets and cracks, pore/crack connectivity and shale mineralogical composition, including quartz, calcite and dolomite.[11] There are many other researches that characterize the microstructures and properties of shale rock at different length scales.[30–33]

3.2. Multiscale models of shale materials

Due to these heterogeneous and multiscale natures, it is usually impractical and often impossible to describe all the precise characters of the microstructure of shale rocks. To characterize the material's heterogeneous and multiscale features, a new multiscale model is proposed based on Ref. 2 to represent the hierarchical and heterogeneous structures of shale rock by taking multi-inclusions, such as quartz, calcite and dolomite, and the ITZs into considerations, as exhibited in Fig. 1.

Similar with Ref. 2, the fundamental scale of shale materials is assumed to be the scale of elementary clay particles, which can be defined by scale '0'; at scale 'I', the material can be seen as porous clay composite. The characteristic size of scale 'II' is in the submillimeter and millimeter range, and the material is composed of