Towards scaling laws in random polycrystals

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ARTICLE INFO

Article history:
Available online xxxx

Keywords:
Random media
Scaling
Scale effect
Homogenization
Mesoscale
Effective response

ABSTRACT

We propose a methodology to set up unifying scaling laws describing the response of multifarious random polycrystals. The methodology employed falls in the realm of stochastic micro-mechanics and is consistent with the Hill condition. Within this framework, we introduce the concept of a scaling function that describes "finite size scaling" of both elastic and inelastic crystalline aggregates. While the finite size is represented by the mesoscale, the scaling function depends on an appropriate measure quantifying the single crystal anisotropy. Based on the scaling function, we construct a material scaling diagram, from which one can assess the approach to a representative volume element (RVE) for many different polycrystals. We demonstrate these concepts on the scaling of the fourth-rank elasticity and the second-rank thermal conductivity tensors.

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1. Introduction

Determining the effective material properties of polycrystalline aggregates has been a topic of great interest over the past few decades. The simplest response of an aggregate is the isotropic response, obtained by orienting a large number (strictly infinite) of single crystals uniformly in the rotation space. Although the effective aggregate response is isotropic, the response of single crystals that make up the aggregate is rarely isotropic. Most single crystal material properties are tensors of various ranks such as the second-rank conductivity tensor, third-rank piezoelectric modulus tensor and the fourth-rank elasticity tensor to name a few [9]. Although the number of independent material constants for an elastic single crystal can be up to twenty-one, one needs just two material constants to characterize the isotropic aggregate response completely. Along similar lines, the single crystal conductivity tensor can have up to six independent material constants, whereas the isotropic aggregate conductivity needs just one constant. At this stage, one can clearly visualize the reduction in the number of material constants in going from the length scale of a single crystal (microscale) to that of a polycrystal (macroscale). The latter corresponds to a so-called representative volume element (RVE). The following questions arise naturally: "How do polycrystal properties scale with increasing length scales?", "What will the aggregate response at mesoscales (intermediate scale of observation relative to grain size) be?", "At what scales does one recover the effective aggregate response (i.e., the RVE)?" and finally: "Can we set up universal scaling laws for a variety of different polycrystal?"

In the following, we employ the framework of stochastic (micro-) mechanics to seek answers to the above questions [10]; previous applications included linear and finite (thermo)elastic, inelastic and even permeable materials. In this approach, we set up and solve stochastic Dirichlet and Neumann boundary value problems consistent with the Hill condition. In doing so, we obtain scale-dependant bounds on the aggregate response at all length scales. Furthermore, within the above framework, the concept of a scaling function is introduced to establish unifying scaling laws for a variety of materials in linear elasticity

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and Fourier-type heat conductivity. It turns out that the scaling function depends upon the mesoscale and a universal anisotropy measure quantifying the single crystal anisotropy. Finally, the scaling function is used to construct the material scaling diagram that clearly defines the mesoscale separating the realization dependent microscale from the macroscale for a variety of materials. In the subsequent sections, we formulate the above methodology to establish scaling laws for the second-rank conductivity and the fourth-rank elasticity tensor. Generalizations to other tensorial properties are relatively straight forward using the proposed methodology.

2. Scaling of second-rank tensors

2.1. A note on the Hill condition

Consider a specific realization, $\mathbf{B}_\delta(\omega)$ of a random medium $\mathbf{B}_\delta$. Here, ω ($\in \Omega$) indicates a specific realization of the polycrystal taken from the sample space Ω, while the subscript δ, defined as

$$\delta = \frac{l}{d} = (N_G)^{\frac{1}{3}}, \tag{2.1}$$

is the dimensionless parameter specifying the mesoscale of the polycrystalline aggregate comprising N_G grains, where d is some characteristic length scale (like the crystal size), and l is the length scale of observation, or window size.

Remark 1. Our δ is the reciprocal of the Knudsen number, Kn, in fluid mechanics, which is defined as the ratio of the mean free path length of the molecules to a characteristic length. As is well known, for low-density gases (such as the exosphere) Kn is high, and the continuum assumption of fluid mechanics is not applicable. Our study will actually quantify the approach to a uniform continuum in conductivity and elasticity of polycrystals as δ increases.

Focusing on Fourier-type conductivity, we have the following governing equation within the pth crystal of a polycrystal

$$C_{ij}^{(p)}(\mathbf{R}^{(p)}, \omega)\nabla^2 T = 0, \quad \omega \in \Omega, \quad 1 \leqslant p \leqslant N_G \tag{2.2}$$

where T stands for the temperature, $\mathbf{R}^{(p)}$ represents the rotation tensor for the pth crystal, $C_{ij}^{(p)}(\mathbf{R}^{(p)}, \omega) = R_{ip}R_{jq}C_{pq}^{\text{ref}}$ is the piecewise-constant thermal conductivity tensor. The key issue being addressed here concerns the passage from Eq. (2.2) to the following equation applicable for the polycrystal as a whole

$$C_{ij}^{\text{eff}}\nabla^2 T = 0, \tag{2.3}$$

where C_{ij}^{eff} represents the effective conductivity tensor of the polycrystal. We approach this problem by using an approach that is consistent with the Hill condition for conductivity

$$\overline{\mathbf{q} \cdot \nabla T} = \bar{\mathbf{q}} \cdot \overline{\nabla T} \Longleftrightarrow \int_{\partial B_\delta} (\mathbf{q} \cdot \mathbf{n} - \bar{\mathbf{q}} \cdot \mathbf{n})(T - \overline{\nabla T} \cdot \mathbf{x}) dS = 0 \ \forall x \in \partial B_\delta \tag{2.4}$$

where, we employ $\mathbf{q}$ ($=q_i$) for the heat flux, ∇T ($T_{,i}$) for the temperature gradient, $\mathbf{x}$ (x_i) for the position vector and $\mathbf{n}$ (n_i) for the surface normal and the overbar indicates the volume average. If we include $1/2$ in front of $\overline{\mathbf{q} \cdot \nabla T}$, we recognize it as a volume average of entropy production density at constant temperature. Similarly, by including $1/2$ in front of $\bar{\mathbf{q}} \cdot \overline{\nabla \mathbf{T}}$, we interpret the resulting quantity as the entropy production density (again at constant temperature) computed from volume averages of heat flux and temperature gradient. Thus, by analogy to mechanical problems (see Section 3.1), the Hill condition establishes the equivalence between the energetic-type and mechanical-type approaches for setting up constitutive equations [11,10,13]. The Eq. (2.4) suggests three types of uniform boundary conditions:

(i) essential (Dirichlet):

$$T = \nabla T^0 \cdot \mathbf{x}, \tag{2.5a}$$

(ii) natural (Neumann):

$$\mathbf{q} \cdot \mathbf{n} = \mathbf{q}^0 \cdot \mathbf{n}, \tag{2.5b}$$

(ii) mixed-orthogonal:

$$(\mathbf{q} \cdot \mathbf{n} - \mathbf{q}^0 \cdot \mathbf{n})(T - \nabla T^0 \cdot \mathbf{x}) = 0. \tag{2.5c}$$

By increasing the mesoscale δ (effectively, the number of grains in $\mathbf{B}_\delta$) and by setting up stochastic boundary value problems with the above boundary conditions and upon ensemble averaging, one obtains rigorous bounds on the constitutive response of the aggregate.

The methodology outlined here works, provided the hypotheses of spatial homogeneity and ergodicity hold for the random field $\boldsymbol{\Theta}(\mathbf{x}, \omega)$ of material parameters involved. In particular, we assume $\boldsymbol{\Theta}(\mathbf{x}, \omega)$ to be a wide-sense stationary (WSS) random field with a constant mean and finite-valued autocorrelation [10].

$$\langle \Theta(x_1) \rangle = \mu,$$
$$\langle \Theta(x_1) \langle \Theta(x_1) \Theta(x_1 + h) \rangle \rangle = R_\Theta(h) < \infty. \tag{2.6}$$

The random field $\Theta(\mathbf{x}, \omega)$ is mean-ergodic if its spatial average equals the ensemble average [10]

$$\frac{1}{V} \int_v \Theta(\mathbf{x}, \omega) dV = \overline{\Theta(\omega)} = \langle \Theta(\mathbf{x}) \rangle = \int_\Omega \Theta(\mathbf{x}, \omega) dP. \tag{2.7}$$

The proposed homogenization methodology is illustrated in Fig. 1. The single crystal has a reference conductivity tensor C_{pq}^{ref} with only three independent constants in its principal direction c_1, c_2 and c_3. By using a set of uniformly generated rotation tensors (Fig. 1), the reference tensor is rotated to assign the material property for each individual crystal in the polycrystal. Using (2.5a) and (2.5b), the boundary value problems are solved and, upon ensemble averaging, one obtains bounds on the aggregate conductivity.

2.2. Bounds on the conductivity

At this point, we recall that the ergodicity and WSS properties of the microstructure, and obtain the hierarchy of scale-dependent bounds as follows:

$$\langle \mathbf{S}_1^n \rangle^{-1} \leqslant \ldots \leqslant \langle \mathbf{S}_{\delta'}^n \rangle^{-1} \leqslant \langle \mathbf{S}_\delta^n \rangle^{-1} \leqslant \ldots \leqslant \mathbf{C}_\infty^{eff} \ldots \leqslant \langle \mathbf{C}_\delta^e \rangle \leqslant \langle \mathbf{C}_{\delta'}^e \rangle \ldots \leqslant \langle \mathbf{C}_1^e \rangle \quad \text{for } \forall \delta' \leqslant \delta. \tag{2.8}$$

Such bounds date back to [11,5]. Using (2.8) along with the definition of isotropic conductivity tensor, we obtain the following hierarchy of bounds on the isotropic conductivity measure

$$c^R \leqslant \ldots \leqslant \langle c_{\delta'}^n \rangle \leqslant \langle c_\delta^n \rangle \leqslant \ldots \leqslant c_\infty^{eff} \ldots \leqslant \langle c_\delta^e \rangle \leqslant \langle c_{\delta'}^e \rangle \ldots \leqslant c^V \quad \text{for } \forall \delta' \leqslant \delta, \tag{2.9}$$

where c^V and c^R are the Voigt (arithmetic mean estimate of the conductivity) and Reuss (harmonic mean estimate of the conductivity) estimates of the conductivity.

2.3. Scaling function in heat conduction

Consider a given realization of the polycrystal at some mesoscale δ. The application of Eq. (2.5a) yields a mesoscale random conductivity tensor $\mathbf{C}_\delta^e(\omega)$ such that

$$\overline{\mathbf{q}}_\delta(\omega) = \mathbf{C}_\delta^e(\omega) \cdot \nabla T^0. \tag{2.10}$$

Similarly, (2.5b) yields a mesoscale random resistivity tensor $\mathbf{S}_\delta^n(\omega)$ such that

$$\overline{\nabla T_\delta}(\omega) = \mathbf{S}_\delta^n(\omega) \cdot \mathbf{q}^0. \tag{2.11}$$

In general, for any given realization $\omega (\in \Omega)$, $\mathbf{C}_\delta^e(\omega)$ and $\mathbf{S}_\delta^n(\omega)$ are anisotropic. We obtain an isotropic response only by assigning the crystal orientations uniformly (distributed uniformly on a unit sphere; also see Shoemake [16]) and upon ensemble
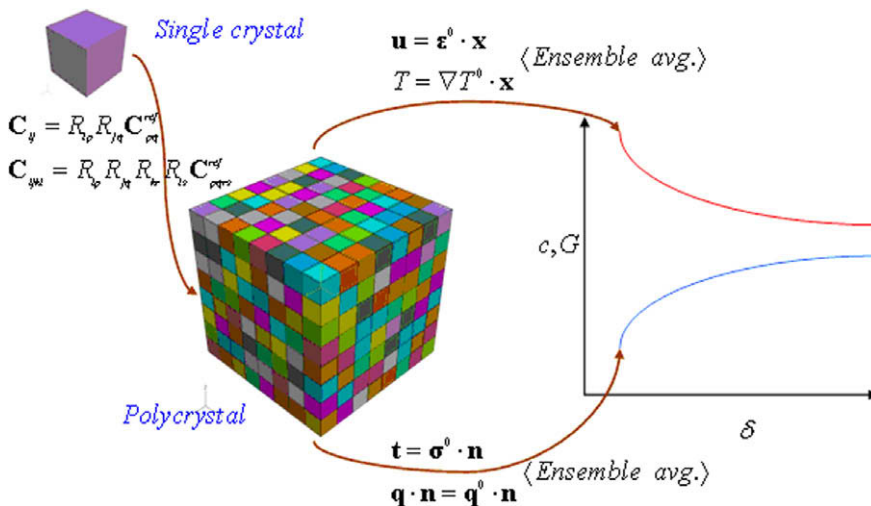

Fig. 1. Homogenization methodology for second- and fourth-rank tensors. In general, **C** (**S**) represents the conductivity (resistivity) tensor or the elastic modulus (compliance) tensor depending upon the context (heat conduction or elasticity).

averaging over the realization space. Thus, the ensemble averaged isotropic conductivity and resistivity tensors can be expressed as follows

$$\langle \mathbf{C}_\delta^e \rangle = \langle c_\delta^e \rangle \mathbf{I},$$ (2.12)

$$\langle \mathbf{S}_\delta^n \rangle = \frac{1}{\langle c_\delta^n \rangle} \mathbf{I}.$$ (2.13)

In the above, $\mathbf{I}$ represents the second-rank identity tensor, $\langle c_\delta^e \rangle$ and $\langle c_\delta^n \rangle$ are ensemble averaged isotropic conductivity measures under essential and natural boundary conditions respectively. By contracting (2.12) and (2.13), we obtain the following scalar equation

$$\langle \mathbf{C}_\delta^e \rangle : \langle \mathbf{S}_\delta^n \rangle = 3 \frac{\langle c_\delta^e \rangle}{\langle c_\delta^n \rangle}.$$ (2.14)

In the limit $\delta \to \infty$ the conductivity tensor must be the exact inverse of the resistivity tensor, and so we obtain

$$\lim_{\delta \to \infty} \langle \mathbf{C}_\delta^e \rangle : \langle \mathbf{S}_\delta^n \rangle = 3.$$ (2.15)

Now, we postulate the following relationship between the left hand side of (2.14) and (2.15)

$$\langle \mathbf{C}_\delta^e \rangle : \langle \mathbf{S}_\delta^n \rangle = lim_{\delta \to \infty} \langle \mathbf{C}_\delta^e \rangle : \langle \mathbf{S}_\delta^n \rangle + g(c_1, c_2, c_3, \delta),$$ (2.16)

Where $g(c_1, c_2, c_3, \delta)$ defines the *scaling function*. Substituting (2.16) and (2.15) into (2.14), we obtain

$$g(c_1, c_2, c_3, \delta) = 3 \left(\frac{\langle c_\delta^e \rangle}{\langle c_\delta^n \rangle} - 1 \right).$$ (2.17)

Notice that the right hand side of (2.17) is dimensionless. Thus, the scaling function $g(c_1, c_2, c_3, \delta)$ must also take a non-dimensional form in c_1, c_2 and c_3. The Eq. (2.16) extends the concept introduced earlier in permeability of random porous media when setting up of an effective Darcy law [1].

The scaling function $g(c_1, c_2, c_3, \delta)$ introduced in (2.17) has the following properties (see also [13]

$$g(c_1, c_2, c_3, \delta = \infty) = 0.$$ (2.18)

Again, the scaling function becomes null if the crystals are locally isotropic

$$g(c_1 = c_2 = c_3, \delta) = 0.$$ (2.19)

One can further establish the following bounds on the scaling function:

$$g(c_1, c_2, c_3, \infty) \leqslant g(c_1, c_2, c_3, \delta) \leqslant g(c_1, c_2, c_3, 1) \ \forall 1 \leqslant \delta \leqslant \infty.$$ (2.20)

Using (2.18) and (2.17) in (2.20), we obtain

$$0 \leqslant g(c_1, c_2, c_3, \delta) \leqslant A_2^U(1) = 3 \left(\frac{c^V}{c^R} - 1 \right) \ \forall 1 \leqslant \delta \leqslant \infty,$$ (2.21)

where $A_2^U(1) = 3 \left(\frac{c^V}{c^R} - 1 \right)$ may be interpreted as a measure quantifying the single crystal anisotropy (see also, Ranganathan and Ostoja-Starzewski [14]) of the second-rank conductivity tensor.

Based on (2.21), one can interpret the scaling function as the evolution of anisotropy with δ in the mesoscale domain, thus

$$g(c_1, c_2, c_3, \delta) = A_2^U(\delta)$$ (2.22)

The simplest form for (2.22), the decoupled form

$$g(c_1, c_2, c_3, \delta) = A_2^U(\delta) = A_2^U(1) h_2(\delta)$$ (2.23)

is a very good approximation for single-phase aggregates made of single crystals of trigonal, hexagonal, and tetragonal type with $c_1 = c_2 \neq c_3$. It takes the following form based on numerical simulations (see also [13])

$$g(c_1, c_2, c_3, \delta) = A_2^U(\delta) = A_2^U(1) h_2(\delta) \simeq A_2^U(1) \exp \left[-0.9135(\delta - 1)^{0.5} \right]$$ (2.24)

Notice that, for all practical purposes, one may determine the size of RVE to within any accuracy by choosing a preferred value for the scaling function g: as g decreases, the size of RVE increases. Thus, based on (2.24), we plot the contours of g in the $\left(A_2^U(1), \delta \right)$ space as illustrated in Fig. 2. It is evident from the plot that for a fixed value of g, the mesoscale size increases with increase in single crystal anisotropy. In other words, higher the single crystal anisotropy, more the number of grains necessary to homogenize the aggregate response. This fact is again confirmed in Fig. 3a–c (plotted by choosing $g(c_1, c_2, c_3, \delta) = 0.01$ which corresponds to an error of 0.3 % in the estimates of conductivity obtained under the uniform essential and the uniform natural boundary conditions) for aggregates made of tetragonal, trigonal and hexagonal crystals, respectively. The following distinct regions can be readily identified in these plots:
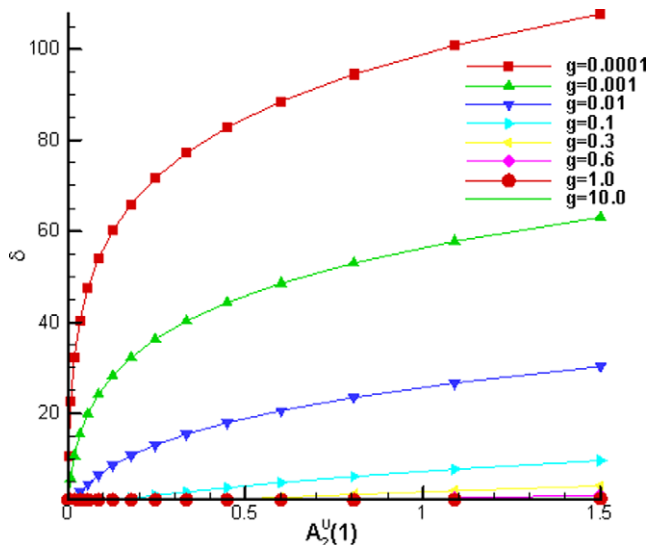
Fig. 2. Contours of scaling function in the $\left(A_2^U(1), \delta\right)$ space.

(i) *Microscale:* In this region, the aggregate response is realization dependent. This is because, the scaling function for any combination of the single crystal anisotropy and the number of grains will turn out to be greater than 0.01. Also, for any given realization, the response is in general anisotropic.

(ii) *Limiting mesoscale:* Fig. 3a–c, have been plotted for $g(c_1, c_2, c_3, \delta) = 0.01$. The limiting mesoscale separates the microscale region from the macroscale region. One can determine the approximate size of RVE from these plots at this scale.

(iii) *Macroscale:* In this region, the aggregate response is isotropic and realization independent. The aggregate response is virtually independent of the boundary conditions that stem from the Hill condition (Eqs. 2.3a,b,c).

3. Scaling of fourth-rank tensors

3.1. Hill condition

In this section, we focus on the scaling of the fourth-rank elasticity tensor. For the elasticity problem, the governing equation within the pth crystal of a polycrystal is

$$C_{ijkl}^{(p)}(\mathbf{R}^{(p)}, \omega)u_{k,lj} = 0_i, \quad \omega \in \Omega, \quad 1 \leqslant p \leqslant N_G \tag{3.1}$$

where $C_{ijkl}^{(p)}(\mathbf{R}^{(p)}, \omega) = R_{ip}R_{jq}R_{kr}R_{ls}C_{pqrs}^{\text{ref}}$ is the piecewise-constant elastic modulus tensor, $\mathbf{u}(=u_i)$ represents the displacement vector. Analogous to Section 2.1, the key question that is being addressed here is to understand the passage from Eq. (3.1) to the following equation applicable for the polycrystal as a whole using the Hill condition

$$C_{ijkl}^{\text{eff}}u_{k,lj} = 0_i, \tag{3.2}$$

Where C_{ijkl}^{eff} represents the effective elastic modulus tensor of the polycrystal. Now, the Hill condition stems from the following condition [7,4,2,3]

$$\overline{\sigma_{ij} : \varepsilon_{ij}} = \overline{\sigma_{ij}} : \overline{\varepsilon_{ij}} \iff \int_{\partial B_\delta} \left(t_i - \overline{\sigma_{ij}} \cdot n_j\right) \cdot \left(u_i - \overline{\varepsilon_{ij}} \cdot x_j\right) dS = 0 \ \forall x \in \partial B_\delta. \tag{3.3}$$

where $\boldsymbol{\sigma}(\sigma_{ij})$ represents the Cauchy stress tensor and $\boldsymbol{\varepsilon}(\varepsilon_{ij})$ being the small strain tensor. Notice that the term $\overline{\sigma_{ij} : \varepsilon_{ij}}$ represents an energetic approach while $\overline{\sigma_{ij}} : \overline{\varepsilon_{ij}}$ represents the mechanistic approach. The three uniform boundary conditions stem from Eq. (3.3)

(i) displacement (Dirichlet):

$$u_i = \varepsilon_{ij}^0 x_j, \tag{3.4a}$$

(ii) traction (Neumann):
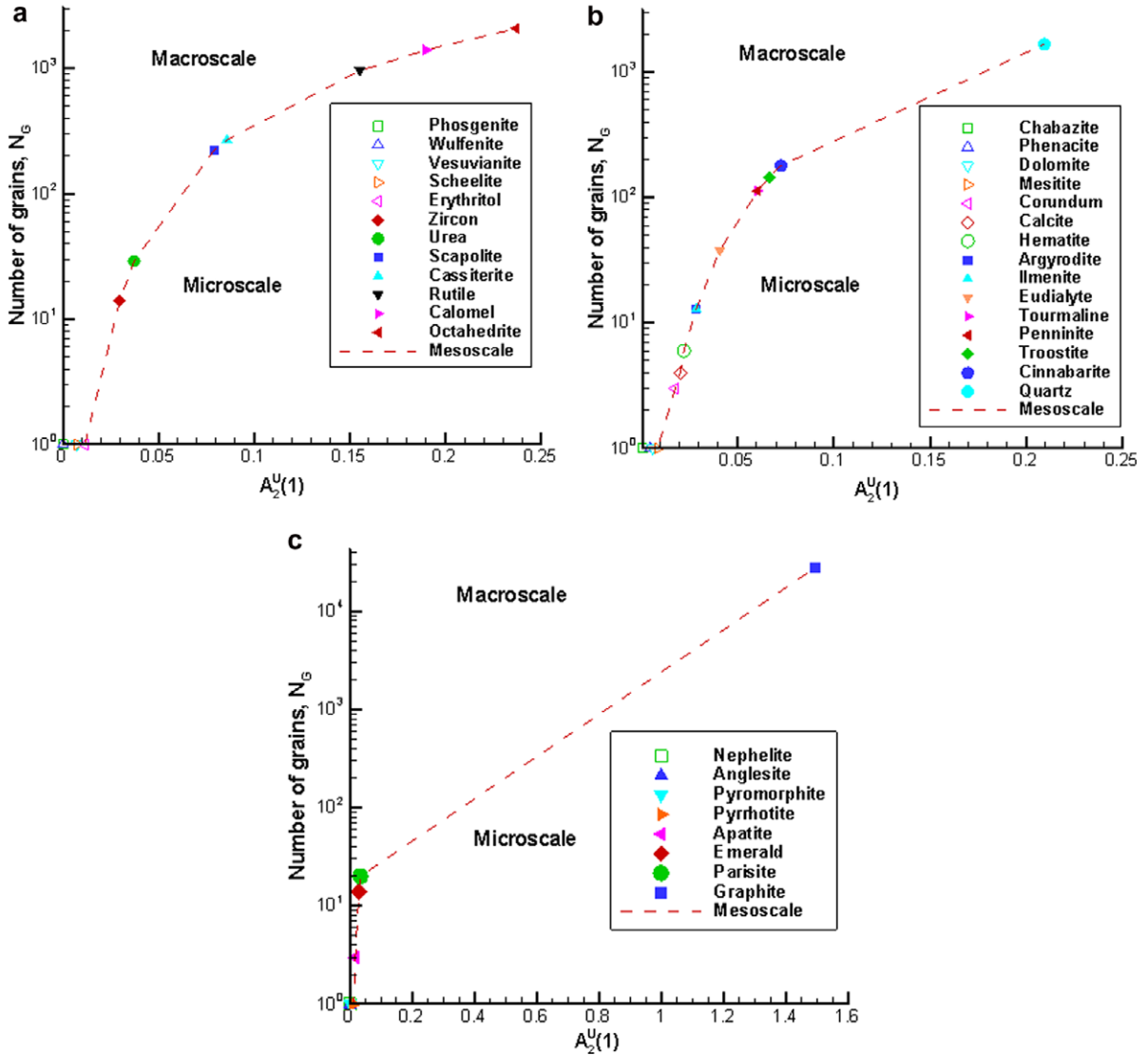
$$t_i = \sigma_{ij}^0 n_j, \tag{3.4b}$$

Fig. 3. (a) Material scaling diagram at $g = 0.01$ (tetragonal crystals). (b) Material scaling diagram at $g = 0.01$ (trigonal crystals). (c) Material scaling diagram at $g = 0.01$ (hexagonal crystals).

(iii) mixed-orthogonal:

$$\left(t_i - \sigma_{ij}^0 n_j\right)\left(u_i - \varepsilon_{ij}^0 x_j\right) = 0. \tag{3.4c}$$

With increasing mesoscale δ, we obtain scale-dependent bounds (Fig. 1) on the elastic response of the aggregate by setting up and solving stochastic boundary value problems consistent with the above boundary conditions. As discussed in Section 2.1, we assume the microstructure to exhibit the wide-sense stationary and mean-ergodic properties.

3.2. Bounds on elastic response

At this point we recall that the ergodicity and WSS properties of the microstructure, together with the variational principles of elasticity theory, imply a hierarchy of scale-dependent bounds on the elastic response

$$\left\langle \mathbf{S}_1^t \right\rangle^{-1} \leqslant \ldots \leqslant \left\langle \mathbf{S}_{\delta'}^t \right\rangle^{-1} \leqslant \left\langle \mathbf{S}_\delta^t \right\rangle^{-1} \leqslant \ldots \leqslant \mathbf{C}_\infty^{\text{eff}} \ldots \leqslant \left\langle \mathbf{C}_\delta^d \right\rangle \leqslant \left\langle \mathbf{C}_{\delta'}^d \right\rangle \ldots \leqslant \left\langle \mathbf{C}_1^d \right\rangle \quad \text{for } \forall \delta' \leqslant \delta. \tag{3.5}$$

Such bounds date back to [4,15], and have recently been applied to microstructures with very complex geometries [6]; see the review in Ostoja-Starzewski [10]. Using (3.5) along with the definition of isotropic elasticity tensor, we obtain the following hierarchy of bounds on the shear and bulk modulus

$$G^R \leqslant \ldots \leqslant \langle G_{\delta'}^t \rangle \leqslant \langle G_{\delta}^t \rangle \leqslant \ldots \leqslant G_{\infty}^{eff} \ldots \leqslant \langle G_{\delta}^d \rangle \leqslant \langle G_{\delta'}^d \rangle \ldots \leqslant G^V, \tag{3.6a}$$

$$K^R \leqslant \ldots \leqslant \langle K_{\delta'}^t \rangle \leqslant \langle K_{\delta}^t \rangle \leqslant \ldots \leqslant K_{\infty}^{eff} \ldots \leqslant \langle K_{\delta}^d \rangle \leqslant \langle K_{\delta'}^d \rangle \ldots \leqslant K^V \quad \text{for } \forall \delta' \leqslant \delta, \tag{3.6b}$$

where G^R, G^V, K^R and K^V represent, respectively, the Reuss and the Voigt estimates of the shear and bulk modulus.

3.3. Elastic scaling function

The application of (3.4a) on a particular realization of a polycrystal yields a mesoscale random stiffness tensor $\mathbf{C}_{\delta}^d(\omega)$ such that

$$\bar{\boldsymbol{\sigma}}_{\delta}(\omega) = \mathbf{C}_{\delta}^d(\omega) : \boldsymbol{\varepsilon}^0. \tag{3.7}$$

Similarly, (3.4b) yields a mesoscale random compliance tensor $\mathbf{S}_{\delta}^t(\omega)$ such that

$$\bar{\boldsymbol{\varepsilon}}_{\delta}(\omega) = \mathbf{S}_{\delta}^t(\omega) : \boldsymbol{\sigma}^0. \tag{3.8}$$

By uniformly distributing the crystal orientations and upon ensemble averaging, we recover the isotropic aggregate response. In such a case, the averaged stiffness and compliance tensors can be expressed in terms of the shear modulus, G, and the bulk modulus, K, as follows

$$\langle \mathbf{C}_{\delta}^d \rangle = 2 \langle G_{\delta}^d \rangle \mathbf{K} + 3 \langle K_{\delta}^d \rangle \mathbf{J}, \tag{3.9a}$$

$$\langle \mathbf{S}_{\delta}^t \rangle = \frac{1}{2 \langle G_{\delta}^t \rangle} \mathbf{K} + \frac{1}{3 \langle K_{\delta}^t \rangle} \mathbf{J}. \tag{3.9b}$$

In the above, $\mathbf{J}$ and $\mathbf{K}$ represent the spherical and the deviatoric parts of the unit fourth order tensor, $\mathbf{I}$. By contracting (3.6a) and (3.6b), we obtain the following scalar equation

$$\langle \mathbf{C}_{\delta}^d \rangle : \langle \mathbf{S}_{\delta}^t \rangle = 5 \frac{\langle G_{\delta}^d \rangle}{\langle G_{\delta}^t \rangle} + \frac{\langle K_{\delta}^d \rangle}{\langle K_{\delta}^t \rangle}. \tag{3.10}$$

In the limit $\delta \to \infty$ the stiffness tensor must be the exact inverse of the compliance tensor, and so we obtain

$$\lim_{\delta \to \infty} \langle \mathbf{C}_{\delta}^d \rangle : \langle \mathbf{S}_{\delta}^t \rangle = 6. \tag{3.11}$$

Now, we postulate the following relationship between the left hand side of (3.10) and (3.11), that is

$$\langle \mathbf{C}_{\delta}^d \rangle : \langle \mathbf{S}_{\delta}^t \rangle = lim_{\delta \to \infty} \langle \mathbf{C}_{\delta}^d \rangle : \langle \mathbf{S}_{\delta}^t \rangle + f(C_{ij}, \delta), \tag{3.12}$$

where $f(C_{ij}, \delta)$ defines the *elastic scaling function*. The parameter C_{ij} represents all the single crystal elastic constants depending on the crystal type. For aggregates made up of cubic single crystals, $C_{ij} \equiv (C_{11}, C_{12}, C_{44})$ and for triclinic systems, C_{ij} will include all the 21 independent single crystal constants. Substituting (3.12) and (3.11) in (3.10), we obtain

$$f(C_{ij}, \delta) = 5 \frac{\langle G_{\delta}^d \rangle}{\langle G_{\delta}^t \rangle} + \frac{\langle K_{\delta}^d \rangle}{\langle K_{\delta}^t \rangle} - 6. \tag{3.13}$$

For the specific case of cubic crystals, the bulk modulus is scale independent [12,8] and (3.13) can be re-written as

$$f(C_{11}, C_{12}, C_{44}, \delta) = 5 \left(\frac{\langle G_{\delta}^d \rangle}{\langle G_{\delta}^t \rangle} - 1 \right). \tag{3.14}$$

The scaling function $f(C_{ij}, \delta)$ introduced in (3.13) has the following properties (see also [12])

$$f(C_{ij}, \delta = \infty) = 0. \tag{3.15}$$

(3.15) states that the scaling function is identically zero at infinite mesoscales. Again, the scaling function becomes null if the crystals are locally isotropic, that is

$$f(iso(C_{ij}), \delta) = 0. \tag{3.16}$$

The term $iso(C_{ij})$ accounts for all the possible combinations of the single crystal elastic constants that will ensure an isotropic single crystal response. One can further establish the following bounds on the scaling function

$$f(C_{ij}, \infty) \leqslant f(C_{ij}, \delta) \leqslant f(C_{ij}, 1) \ \forall 1 \leqslant \delta \leqslant \infty. \tag{3.17}$$

Using (3.15) and (3.13) in (3.17), we obtain

$$0 \leqslant f(C_{ij}, \delta) \leqslant A_4^U(1) = 5\frac{G^V}{G^R} + \frac{K^V}{K^R} - 6 \; \forall 1 \leqslant \delta \leqslant \infty, \tag{3.18}$$

where the quantity $A_4^U(1) = 5\frac{G^V}{G^R} + \frac{K^V}{K^R} - 6$ represents the universal anisotropy index quantifying the single crystal anisotropy (see also [14]) of the fourth-rank elasticity tensor.

Based on (3.18), one can interpret the elastic scaling function as the evolution of the universal elastic anisotropy index in the mesoscale domain, thus

$$f(C_{ij}, \delta) = A_4^U(\delta). \tag{3.19}$$

The simplest form for (3.19), having a separable structure

$$f(C_{ij}, \delta) = A_4^U(\delta) = A_4^U(1)h_4(\delta), \tag{3.20}$$

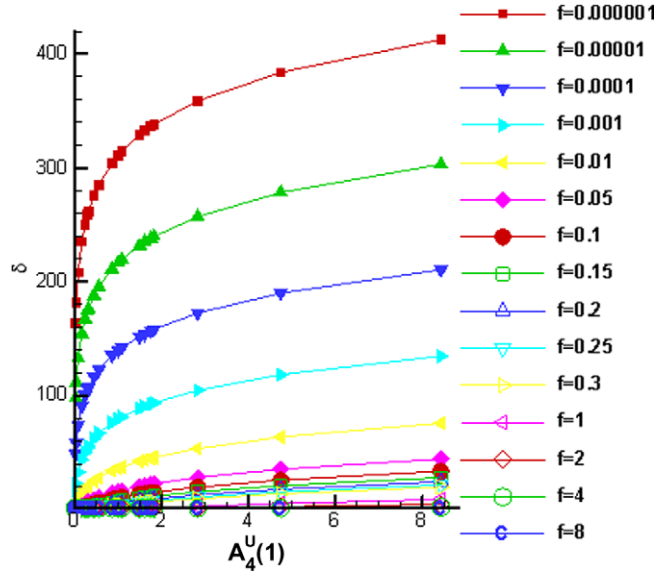
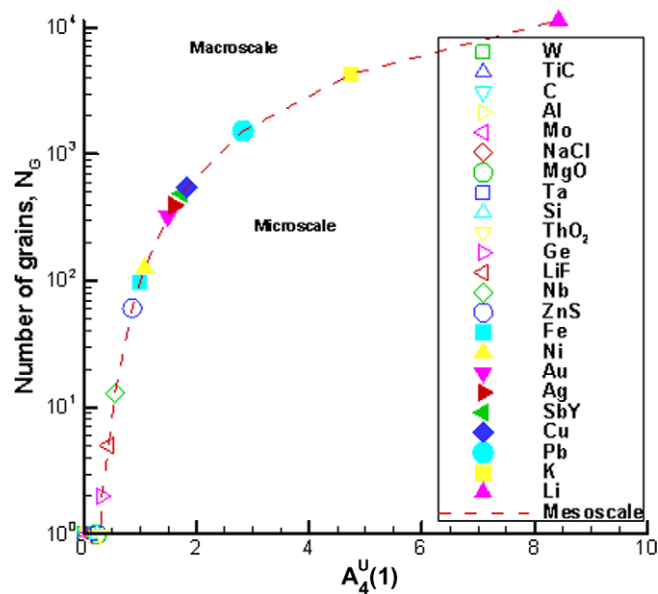**Fig. 4.** Contours of scaling function in the $\left(A_4^U(1), \delta\right)$ space.

Fig. 5. Material scaling diagram at $f = 0.23$ for cubic crystals.

is a very good approximation for single-phase aggregates made up of single crystals of cubic type. It takes the following form based on numerical simulations (see also [12])

$$f(C_{ij}, \delta) = A_4^U(\delta) = A_4^U(1) h_4(\delta) \simeq A_4^U(1) \exp\left[-0.767(\delta - 1)^{0.5}\right]. \tag{3.21}$$

If we recall that for cubic crystals the conductivity tensor is automatically isotropic but the elasticity tensor is not, we are led to the following.

Remark 2. For aggregates made up of cubic single crystals, the scaling function is identically zero in the heat conduction problem whereas it is generally non-zero and is governed by (3.21) in the elasticity problem.

Similar to what was done for conductivity in Section 2, one may determine the size of RVE within any desired precision by choosing a convenient (preferred) value for the scaling function. Based on (3.21), in Fig. 4 we plot the contours of the scaling function in the $\left(A_4^U(1), \delta\right)$ space. It is evident that for a fixed value of the scaling function, the mesoscale size increases with increase in single crystal anisotropy. In other words, the higher the single crystal anisotropy, the greater is the number of grains necessary to homogenize the aggregate response. This fact is again confirmed in Fig. 5 (plotted for $f = 0.23$) for a variety of aggregates made up of cubic single crystals. Again, notice the distinct regions (microscale, limiting mesoscale and macroscale) in these plots.

4. Conclusions

We have proposed a general methodology to establish scaling laws in tensorial materials properties. The concept of a scaling function was introduced and its specific form was derived for a variety of single-phase aggregates. We interpreted the scaling function as the evolution of an appropriate anisotropy measure in the mesoscale domain. Although in this article, we have discussed the scaling behavior of second- and fourth-rank tensors, it is relatively straightforward to extend the formulation to tensors of other ranks. One might also extend the proposed methodology to multi-phase aggregates (or alloys). In such problems, it would be of interest to determine whether the decoupling of the scaling function in terms of an anisotropy index and the mesoscale (i.e. a separable structure) would still be valid.

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