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FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Random field models and scaling laws of heterogenous media

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

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In many problems of solid mechanics (e.g., stochastic finite elements, statistical fracture mechanics) there is a need for resolution of dependent fields over scales not infinitely larger than the microscale. This task may be accomplished through a "meso-scale window" which becomes the classical Representative Volume Element (RVE) in the infinite limit relative to the microscale. It turns out that the material properties at such a mesoscale cannot be uniquely approximated by a random field of stiffness/compliance with locally isotropic realizations, but, rather, two random continuum fields with locally anisotropic realizations, corresponding respectively to Dirichlet and Neumann boundary conditions on the meso-scale, need to be introduced to bound the material response from above and from below. We discuss statistical characteristics of these two mesoscale random fields, including their spatial correlation structure, for anti-plane elastic response of random two-phase composites with Voronoi geometry at the percolation point. Particular attention is given to the scaling of effective responses obtained from both conditions, which sheds light on the minimum acceptable size of an RVE.

1. Does there exist a locally isotropic, inhomogeneous elastic continuum?

Every solid material possess a certain microstructure, whose complexity is very often characterized by a geometric and physical randomness of basic constituents – typical examples are polycrystals, composites, fibrous, cellular, and granular media. In studying mechanics of such materials one typically introduces an approximating continuum model which relies on a so-called Representative Volume Element (RVE). The constitutive properties – tensor $C^{\text{eff}}_{ijkl} \equiv \mathbf{C}^{\text{eff}}$ – of the RVE are usually being calculated either by a method of bounds (e.g., of Hashin–Shtrikman type) or by a less rigorous, but sometimes more convenient, effective medium theory (e.g., a self-consistent model); excellent reviews of these topics are provided in [1, 2, 3, 4]. The resulting constitutive response is deterministic, as it is tacitly assumed that the typical scales of variability of macroscopic stress, strain, and displacement fields are much larger than the RVE size.

Aside from this classical category of studies in micromechanics, there has been developed for the past two decades a subject area of Stochastic Finite Elements (SFE) [5, 6, 7], which aims at the inclusion of microscale material variability in the solution of boundary value problems set on scales much larger than the length

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scale d of the microstructure. In SFE the microstructural variability is accounted for by simply assuming perturbations C'_{ijkl} to be present in the Hooke's law

$$\begin{aligned} \sigma_{ij} &= C_{ijkl}(\mathbf{x},\omega)\varepsilon_{kl}, \qquad \mathbf{x}\in\mathbf{B}, \quad \omega\in\Omega, \\ C_{ijkl}(\mathbf{x},\omega) &= \langle C_{ijkl}\rangle + C'_{ijkl}(\mathbf{x},\omega). \end{aligned} \tag{1.1}$$

In other words, C_{ijkl} is taken as a random field over the material domain $\mathbf{B}$; here ω denotes a realization from a sample space Ω. In fact, typically a locally isotropic continuum is being assumed

$$C_{ijkl}(\mathbf{x},\omega) = \lambda(\mathbf{x},\omega)\delta_{ij}\delta_{kl} + \mu(\mathbf{x},\omega)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{1.2}$$

where λ and μ are the Lamé constants. Let us note here that the Statistical Fracture Mechanics [8] is another, yet related, area whose analyses often require random field models.

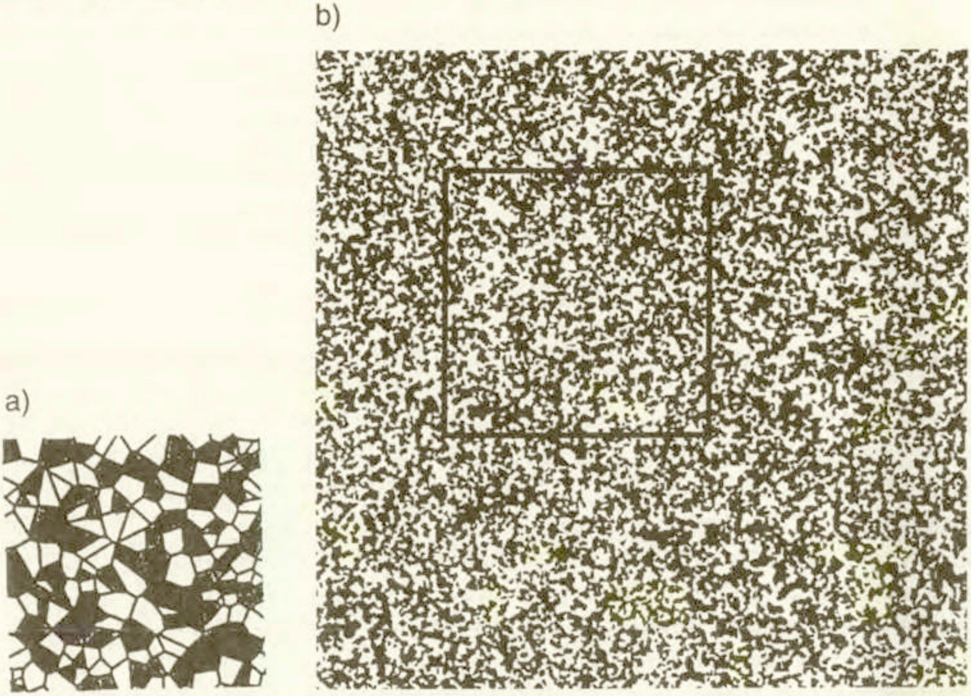

FIG. 1. A close-up of a two-phase material with a Voronoi mosaic microgeometry is shown in (a), and a larger sample with 250,000 grains at volume fraction 50% is depicted in (b), where an arbitrary window of length scale $L \times L$ is drawn. There are, on average, ten pixels per one Voronoi cell in (b).

The above considerations lead us to a basic issue of the dependence of effective Hookeś law on the size L of a so-called *window*, such as shown in Fig. 1. Here we

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introduce a nondimensional parameter, relative to the grain size d,

$$\sigma = \frac{L}{d} \tag{1.3}$$

to quantify this scale dependence.

It can easily be inferred from Fig. 1 that fluctuations are present for any finite window, but as its size tends to infinity, they die out to zero – this is the classical, deterministic, continuum limit $\delta \to \infty$, in which the RVE possesses a statistical representation of the microstructure with all the typical microheterogeneities. Below this limit we have a random field problem: $C_{ijkl}(\mathbf{x}, \omega, \delta)$ has to be described statistically. The question is: how do the statistics of effective moduli behave as a function of δ? Furthermore, as shown in our previous papers [9, 10, 11, 12] and discussed in Sec. 2 below, associated with the scale dependence of $C_{ijkl}(\mathbf{x}, \omega, \delta)$, there is an interesting issue of non-uniqueness of the effective constitutive response, and, in order to bound the latter rigorously, one can choose either essential or natural boundary conditions. In fact, according to the Hill's prescription [13] the relations between volume average stress and strain become the same in the $\delta \to \infty$ limit regardless of which of these two conditions have been used. Let us note that this is different from a methodology due to DRUGAN and WILLIS [14].

We note here that the problem of determination of the RVE received considerable attention in the field of porous materials [15]. In the terminology of that reference, our window would be called an Arbitrary Volume Element, the volume being equivalent to a window's area in two dimensions $(2-D)$. However, as shown in [12], connectivity of a soft phase versus a stiff one plays a very important role in the approach to the RVE: a matrix with rigid inclusions approaches the RVE limit quite rapidly ($\delta < 10$), while a matrix with very soft (hole-type) inclusions requires windows of the order of several hundred hole diameters to get there. This result motivates the setting of our present study in two-phase Voronoi mosaics, where, by varying the volume fraction of one phase versus another, we can go from a situation of a disconnected stiff phase embedded in a matrix of a soft one, through a system of percolation of both phases, up to a situation of a soft phase being disconnected in a matrix of a stiff one. In this paper we discuss scale dependence of effective moduli and their statistics in the most challenging regime: percolation point.

2. Scale-dependent hierarchies of bounds on effective moduli

In this section we focus on $2-D$, two-phase microstructures of linear elastic materials in antiplane shear. The microstructural geometry is specified by a Voronoi mosaic in which each cell is being occupied by either phase 1 or 2 according to a probability equal to the global volume fraction, which is chosen at

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50%, Fig. 1. This is the percolation point because the dual Delaunay network is six-coordinated on average (i.e., each Voronoi cell has a mean of six neighbors).

The Hooke's law of either phase (1 or 2) is given by

$$\sigma_i = C_{ij}\varepsilon_j, \quad i,j = 1,2, \qquad C_{ij} = C^{(1)}\delta_{ij} \quad \text{or} \quad C^{(2)}\delta_{ij}\,, \tag{2.1}$$

where, for simplicity of notation, we denote

$$\sigma_i \equiv \sigma_{i3}\,, \qquad \varepsilon_i \equiv \varepsilon_{i3}\,, \qquad i,j = 1,2. \tag{2.2}$$

On the microscale, the governing equation of this piecewise-constant material is

$$C\left(\frac{\partial^2 u}{\partial x_1} + \frac{\partial^2 u}{\partial x_2}\right) = 0, \qquad C = C^{(1)} \text{ or } C^{(2)}, \qquad u \equiv u_3\,. \tag{2.3}$$

The isotropy of both stiffness tensors $C^{(1)}$ and $C^{(2)}$ in (2.3) leads to a so-called *contrast* $\alpha \equiv C^{(2)}/C^{(1)}$, sometimes also called a *stiffness mismatch*; without loss of generality we assume $\alpha \geq 1$. Figure 1 depicts just one realization $\mathbf{B}(\omega)$ of a *random medium*, which, as is commonly done in mechanics of random media, is taken as a set $\mathbf{B} = \{\mathbf{B}(\omega);\ \omega \in \Omega\}$.

Let us note that there are several other physical problems equivalent to anti-plane shear by virtue of well known mathematical analogies – for example, in-plane conductivity. Also, the microstructure chosen here may be applied to model a range of different materials – examples are offered by duplex steels [16] for a finite α, or porous materials [15] for an extreme $\alpha = 0$ or ∞.

The effective moduli for a finite window domain of scale δ sampled in our material can be defined in several ways. Here we choose an approach based on an interpretation of a Hooke's law as one in which either a uniform strain ε_j^0 or a uniform stress σ_j^0 is prescribed. In the first case, we should choose essential (or displacement, Dirichlet) boundary conditions while in the second case, we should choose natural (or traction, Neumann) boundary conditions. The first setup is

$$\overline{\sigma}_i = C_{ij}^e \varepsilon_j^0 \qquad \text{under} \qquad u(\mathbf{x}) = \varepsilon_j^0 L_j \quad \forall\, \mathbf{x} \in \partial\mathbf{B}\,, \tag{2.4}$$

where $\overline{\sigma}_{ij}$ id the resulting mean (volume average) stress, and which leads to an effective stiffness $\mathbf{C}_\delta^e$. The second setup is

$$\overline{\varepsilon}_i = S_{ij}^n \sigma_j^0 \qquad \text{under} \qquad t(\mathbf{x}) = \sigma_j^0 n_j(\mathbf{x}) \quad \forall\, \mathbf{x} \in \partial\mathbf{B}\,, \tag{2.5}$$

where $\overline{\varepsilon}_{ij}$ is the resulting mean (volume average) strain, and leads to an effective compliance $\mathbf{S}_\delta^n$. Determination of either tensor, $\mathbf{C}_\delta^e$ or $\mathbf{S}_\delta^n$, requires three tests.

For any realization $\mathbf{B}(\omega)$, a window's response on the mesoscale (δ finite) is, under these definitions, nonunique – because $C_{ij}^e \neq (S_{ij}^n)^{-1}$ almost surely – and anisotropic. Thus, the answer to the question posed by the title of Sec. 1

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is negative. However, considering the ergodicity of the Poisson point process underlying our two-phase microstructure, it can be shown from the variational principles [11, 17, 18], that the ensemble averages of these two tensors provide, with the increasing scale δ, an ever tighter pair of bounds on $\mathbf{C}^{\text{eff}}$

$$\begin{aligned}(2.6)\qquad \mathbf{C}^R \equiv (\mathbf{S}^R)^{-1} \equiv \langle \mathbf{S}_1^n \rangle^{-1} \leq \langle \mathbf{S}_{\delta'}^n \rangle^{-1} \leq \langle \mathbf{S}_\delta^n \rangle^{-1} \\ \leq \mathbf{C}^{\text{eff}} \leq \langle \mathbf{C}_\delta^e \rangle \leq \langle \mathbf{C}_{\delta'}^e \rangle \leq \langle \mathbf{C}_1^e \rangle \equiv \mathbf{C}^V \qquad \forall\, \delta' < \delta.\end{aligned}$$

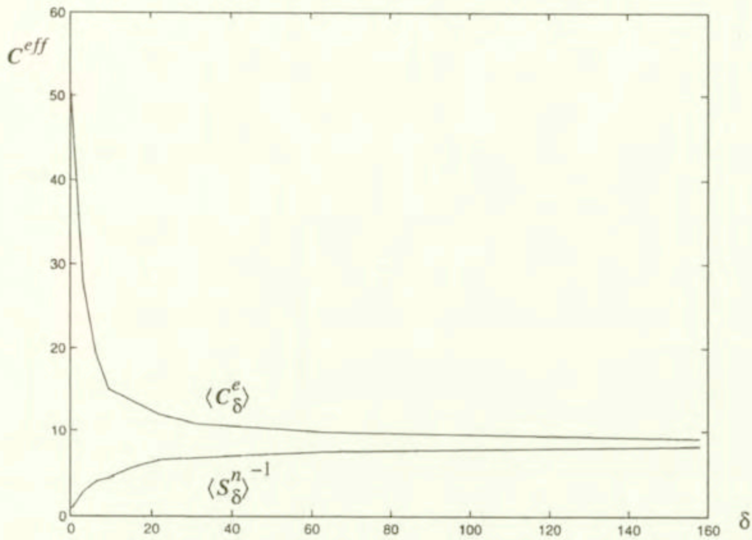

FIG. 2. Hierarchies of bounds on effective anti-plane moduli $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$ of the two-phase microstructure of Fig. 1 at $C^{(1)} = 1$ and contrast $\alpha = 100$.

In Fig. 2 we show this hierarchy for our two-phase Voronoi composite at contrast $\alpha = 100$ at 50% volume fraction of either phase. Although it is the percolation point for this system – the most challenging regime in random systems – the scale (i.e., δ) and contrast (i.e., α) dependence of both tensors follow, with very high accuracy, the laws first found for $2-D$ Bernoulli lattices [11], namely

$$(2.7)\qquad \langle \mathbf{C}_\delta^e \rangle = a_0 + a_1 \exp\left(a_2 \delta^{-a_3 \alpha}\right), \qquad \langle \mathbf{S}_\delta^n \rangle = b_0 + b_1 \exp\left(b_2 \delta^{-b_3 \alpha}\right).$$

Indeed, the contrast dependence in (2.7) has been verified for $\alpha = 10, 10^2, 10^3$, and 10^4.

The probability distributions of $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$ that are involved in the hierarchy (2.6) are now assessed in terms of the statistics of their traces and radii of the corresponding Mohr's circles; the radius is, of course, defined by $R \equiv C_{12,\max} = \sqrt{(C_{11} - C_{22})^2/4 + C_{12}^2}$. Figures 3 and 4 display, for five scales δ, these statistics for tensors $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$, respectively. They have been obtained by solving, through

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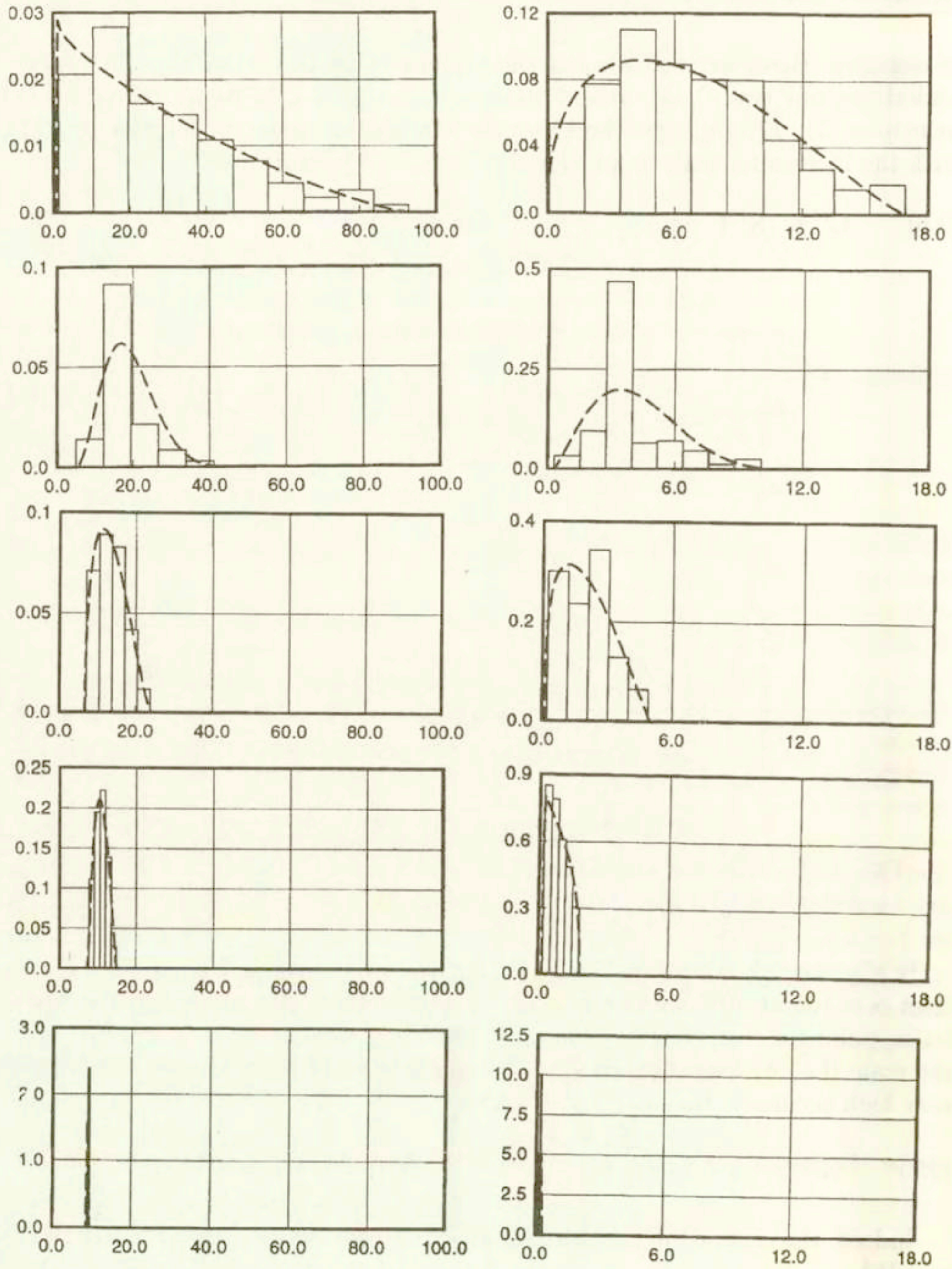

FIG. 3. The histograms and beta function probability fits to $\operatorname{tr} \mathbf{C}_\delta^e$ (left column) and R (right column) as functions of the window scale $\delta = 3.16,\ 6.32,\ 15.8,\ 31.6$, and 158 under displacement boundary condition of the two-phase microstructure of Fig. 1 at volume fraction 50%, $C^{(1)} = 1$, and contrast $\alpha = 100$.

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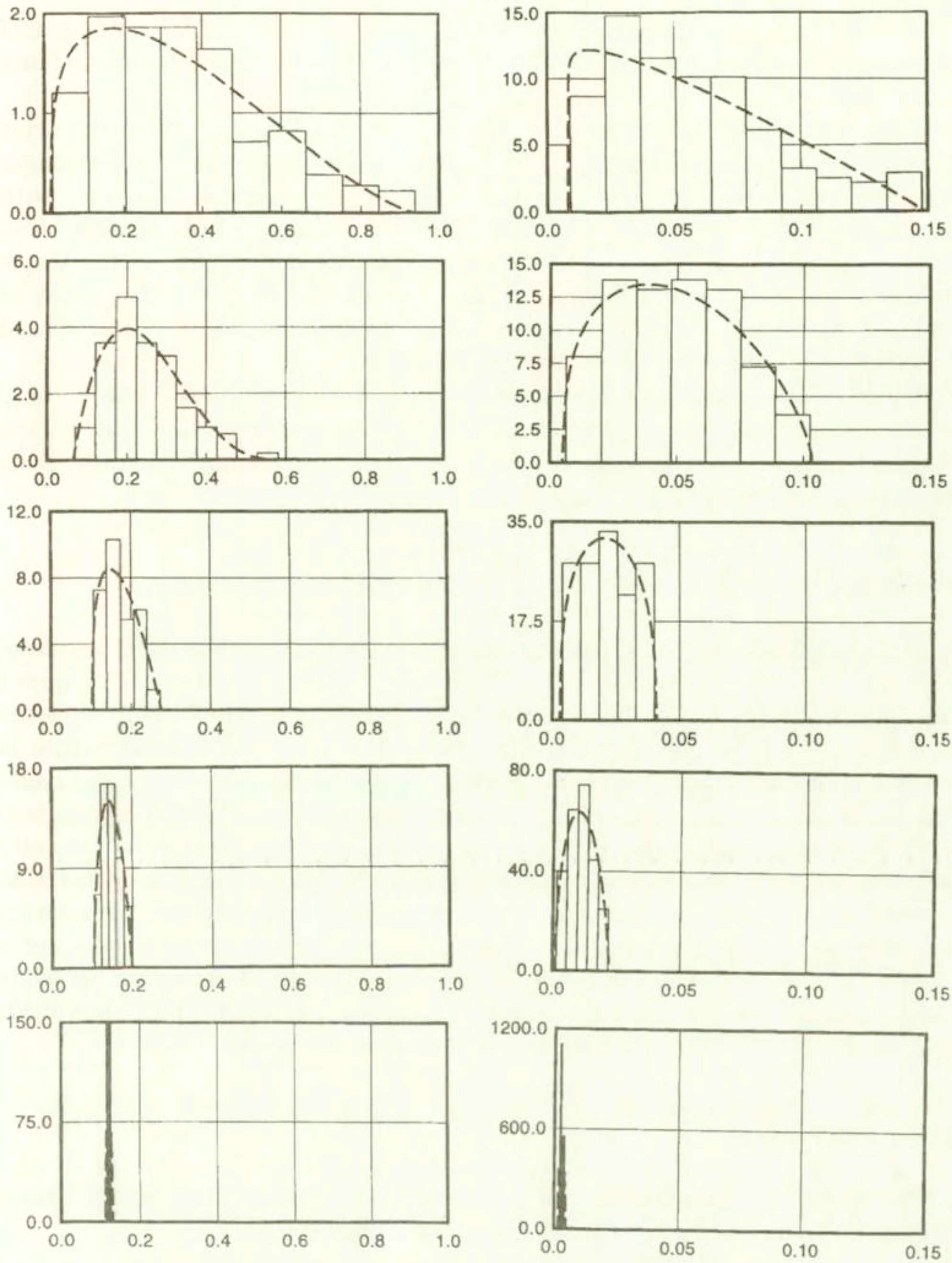

FIG. 4. The histograms and beta function probability fits to $\operatorname{tr}\mathbf{S}^{e}_{\delta}$ (left column) and R (right column) as functions of the window scale $\delta = 3.16,\ 6.32,\ 15.8,\ 31.6$, and 158 under traction boundary condition of the two-phase microstructure of Fig. 1 at volume fraction 50%, $C^{(1)} = 1$, and contrast $\alpha = 100$.

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a computational mechanics method, boundary value problems for a number of two-phase Voronoi composites $\mathbf{B}(\omega)$ of the set $\mathbf{B}$, all being generated in a Monte Carlo sense.

Note that while the traces have asymmetric distributions, their character is very similar for both tensors. The Mohr's circles' radii have even stronger skewness, and their coefficient of variation (COV) is practically constant with the changing scale: COV $\cong 0.5 \pm 0.05$; this holds again for both tensors. Also shown in Figs. 3 and 4 are Beta function probability density fits to the traces and radii, which, as discussed in [12], are very satisfactory for other types of composites as well. This latter reference also gives a discussion of the spatial correlation structure of random fields $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$.

These results provide a stepping stone for a stochastic finite element study of macroscopic response of a material with such a microstructure [19], where, following the approach developed earlier [20, 21], we recognize our meso-scale window to play the role of a single finite element.

3. Closure

It should finally be noted that there are other ways to define effective meso-scale responses. First of all, besides (2.4) and (2.5) one could consider mixed (displacement-traction) boundary conditions [22], which would result in some intermediate response. Next, by appropriately modifying the microstructure in the boundary zone through an introduction of a meso-scale periodicity, one could look at the displacement-periodic and traction-periodic conditions. A comparison of all the above cases, in the setting of matrix-inclusion composites, has recently been conducted in [23]. Other possible approaches include a homogenization formulation, and nonclassical (e.g., nonlocal) models. In particular, considering the presence of the grain-type microstructure, we face a question whether a classical or a micropolar continuum is more appropriate. A forthcoming study [24] outlines the determination of effective micropolar moduli, which thus sheds light on a heretofore enigmatic Cosserat characteristic length.

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