MATERIALICA+ Research Group
Computational Design & Structural Analysis

Politechnika Krakowska im. Tadeusza Kościuszki

SCHWARZ'S METHOD AND ITS APPLICATIONS TO EFFECTIVE PROPERTIES OF DISPERSED COMPOSITES

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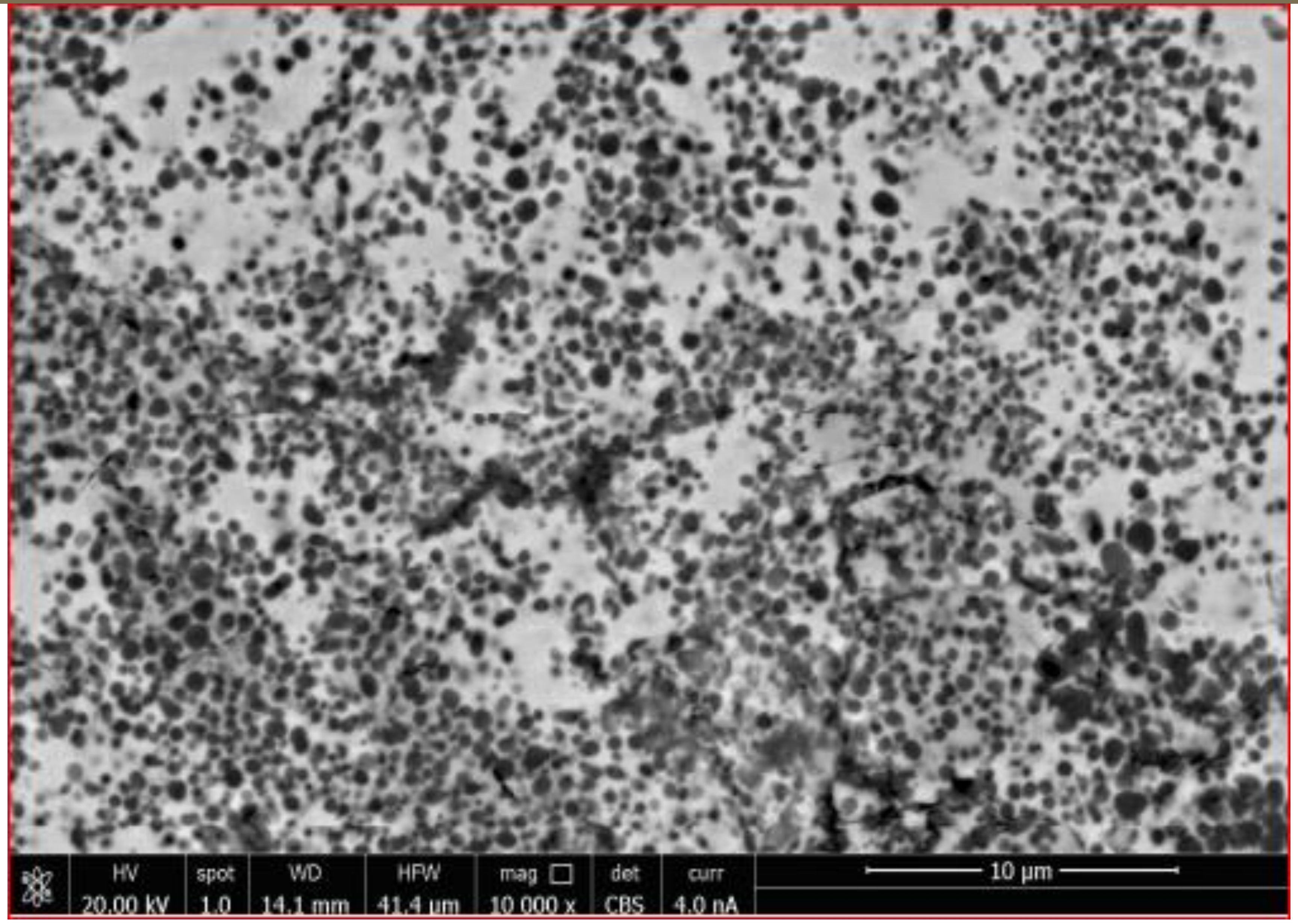
ABSTRACT

The study of **structurally disordered** dispersed patterns and the hidden relationships between the geometric random characteristics of composites and their physical properties is a common focus in various branches of mechanics, mathematics, and physics. Our objective is to address the challenge of providing a constructive quantitative description of the chaos/regularity, e.g., dislocations, exhibited by composites. The mathematical results are based on the generalized alternating **method of Schwarz** and the Riemann-Hilbert problem for a multiply connected domain.

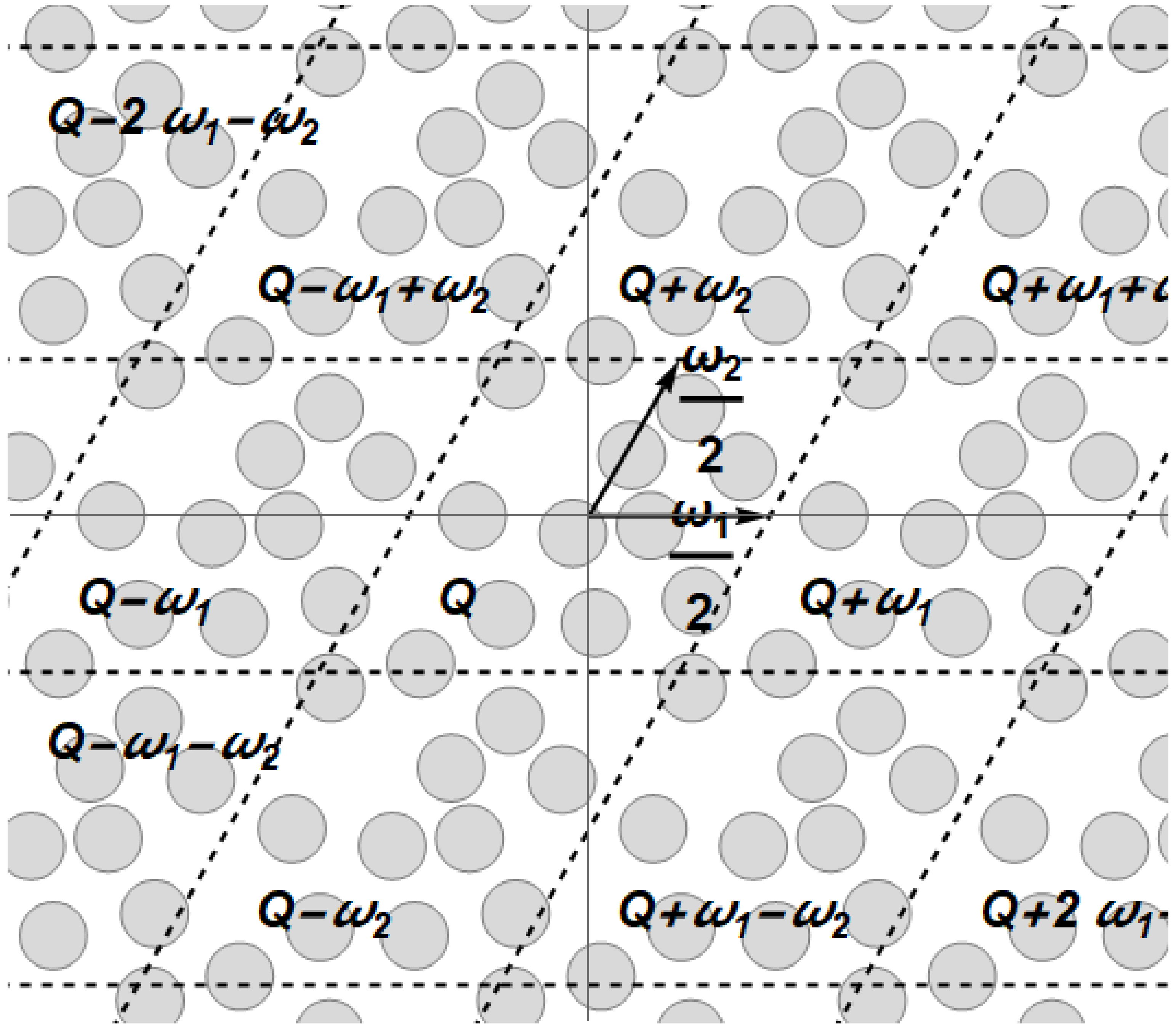
The current state of the art of the theory of composites is outlined. We discuss the notions of ***model* and *empirical method*** used in the framework of material sciences, highlighting the discrepancies when various engineering approaches overlook asymptotic precision and conditionally convergent series.

We propose the **computationally effective method of structural sums** coinciding with the lattice sums for regular composites. In particular, the results yield new **high-order analytical exact and asymptotic justified formulas for the effective conductivity and elasticity tensors** of dispersed composites with isotropic phases. We specifically investigate the macroscopic properties of dispersed regular and random composites with a qualitative analysis of the degree of randomness, anisotropy, and clustering.

2D STATIONARY PROBLEM



Microstructure of TiC–FeCr composite

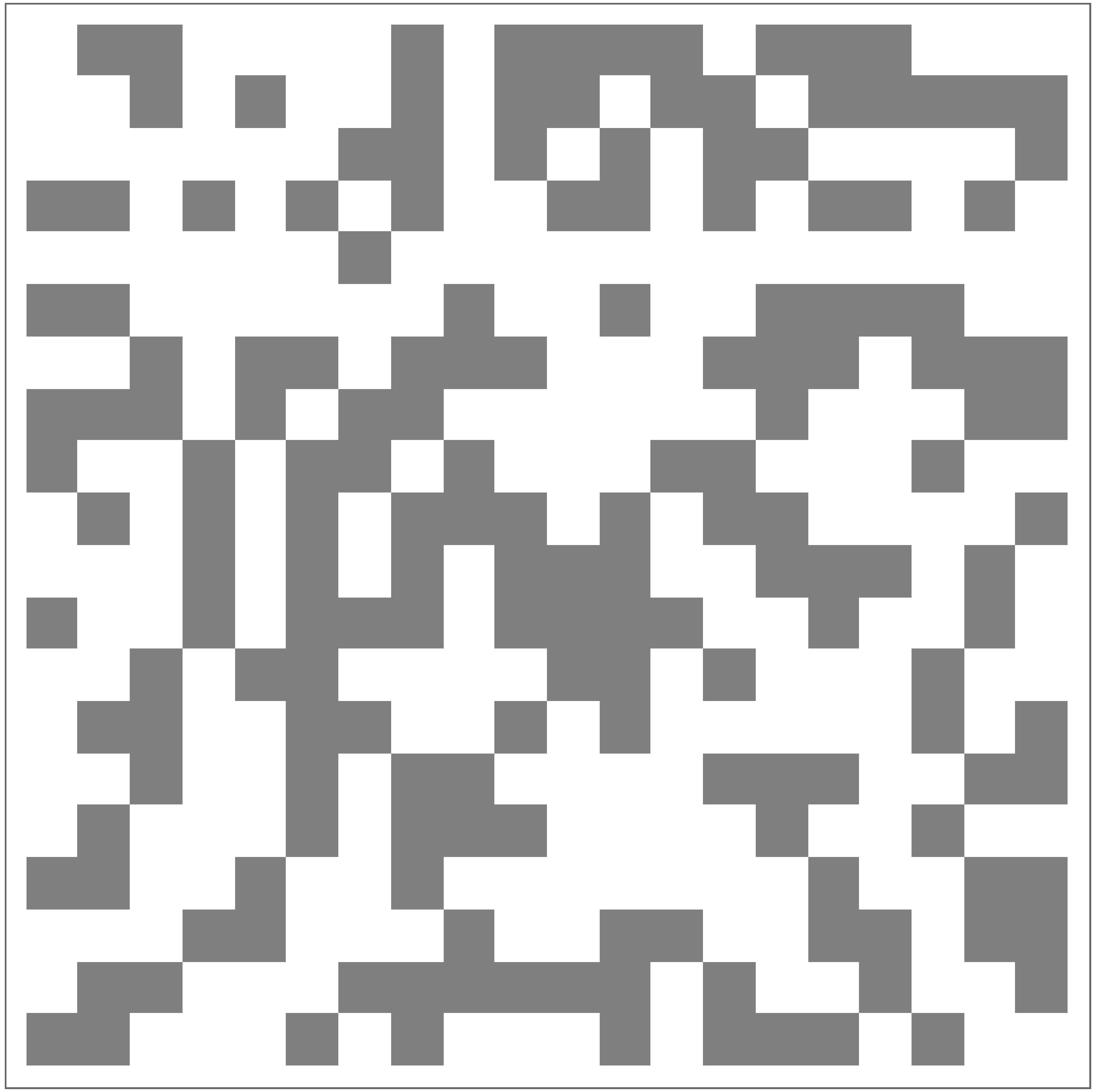


The conception of homogenization:

a) Physical: we have two-phase material with different properties of components. To determine averaged properties.

b) Mathematical: we have PDE with highly oscillating coefficients. To determine PDE (its coefficients) when the periodicity cell shrinks to a point ($\varepsilon \to 0$) $\Leftrightarrow$ the domain is extended to infinity . (Bakhvalov, Lions, (1972) …)

NUMERICAL APPROACH (FEM ETC.)



20x20 discretization cells (pixels) of two-phase composites with a random assignment to each cell.

The number of variants 2^{400}

The number of atoms in observable Universe 10^{80}

The ratio $2^{400}/10^{80} \approx 10^{40}$.

Dykhne's formula for a random isotropic checkerboard $\sigma_e = \sqrt{\sigma_1 \sigma_2}$

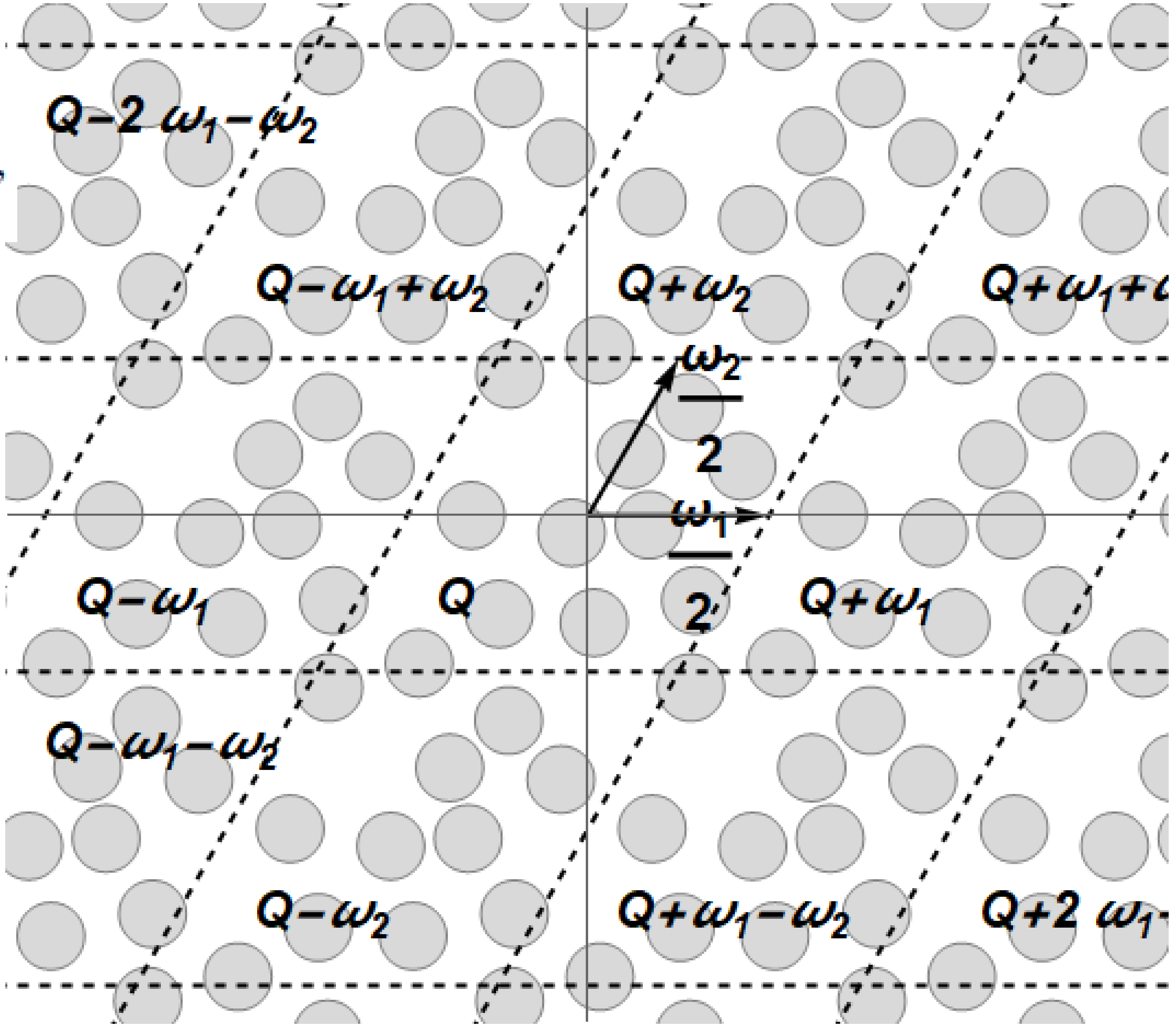
$\mathbb{R}$ -LINEAR PROBLEMS FOR DOUBLY PERIODIC DOMAIN; ANTI-PLANE SHEAR (CONDUCTIVITY)

$$u = u_k, \quad \frac{\partial u}{\partial \mathbf{n}} = \sigma \frac{\partial u_k}{\partial \mathbf{n}} \quad \text{on } L_k, \quad k = 1, 2, \ldots, N,$$

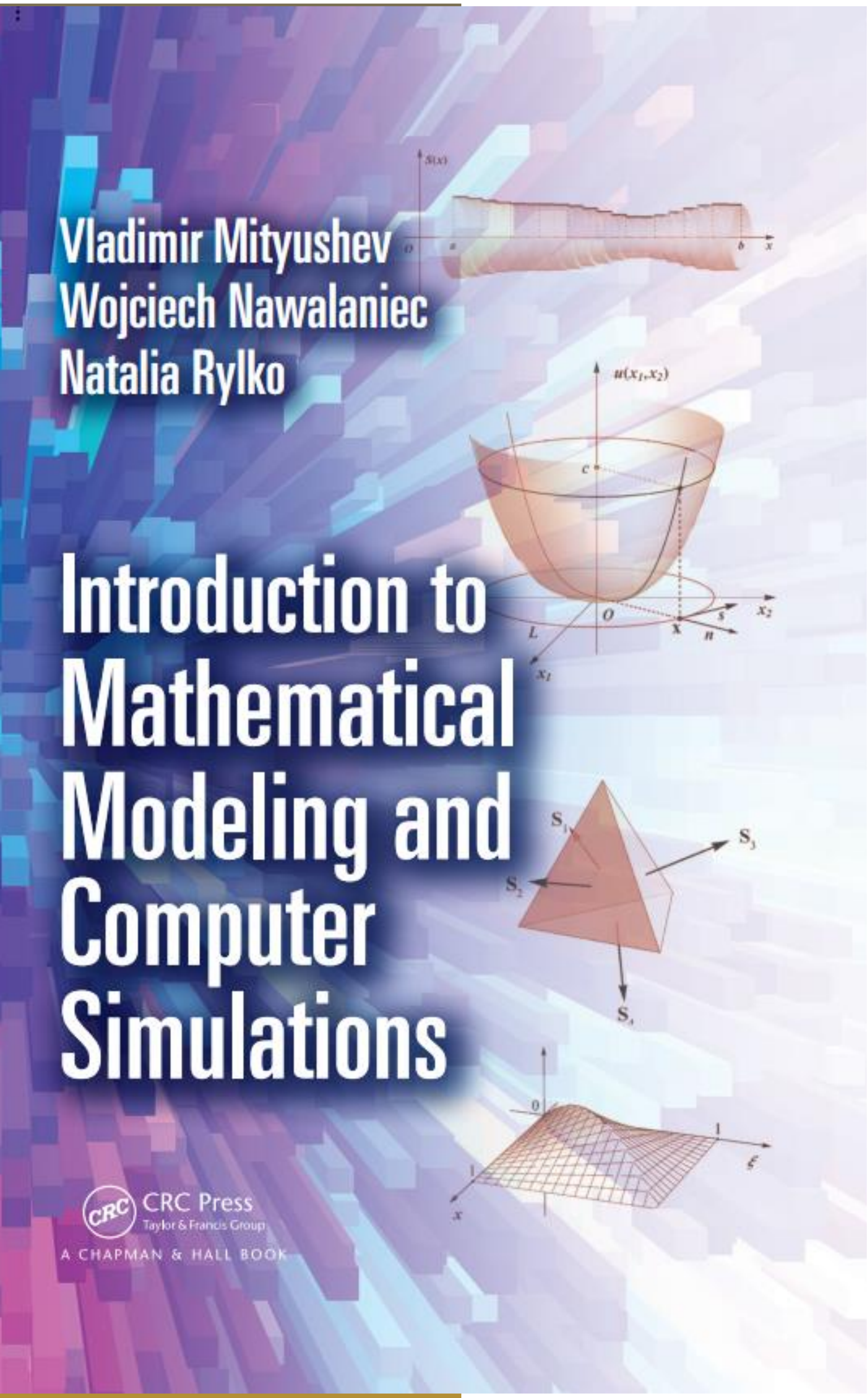
$$u(z + \omega_1) = u(z) + \xi_1, \; u(z + \omega_2) = u(z) + \xi_2$$

with given constants ξ_1 and ξ_2

The main mathematical result is an extension of the Poisson's formula for a disk to a multiply connected domain.



ABOUT MATHEMATICAL MODELING



This textbook is intended for readers who want to understand the main principles of Modeling and Simulations in settings that are important for the applications without using profound mathematical tools required by most advanced texts. It can be useful for beginning applied mathematicians and engineers who use Mathematical Modeling. Our goal is to outline Mathematical Modeling using simple mathematical description that make it accessible for first- and second-year students.

2018 open access Chapter 1 (in preparation the secon edition 2024)

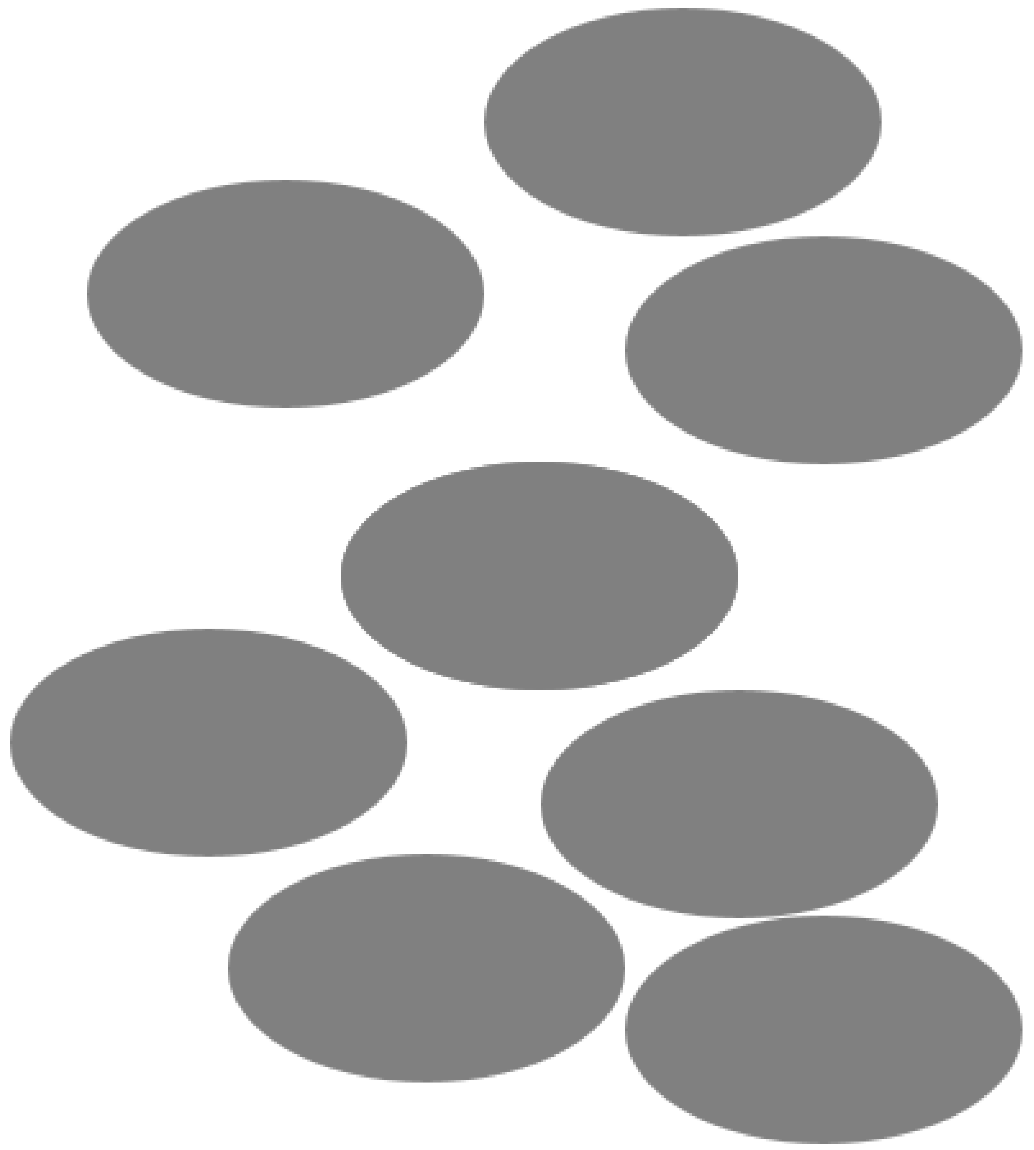
Mathematical models related to ODE are perfectly developed [J. Banasiak, 2013; J. Banasiak, M., Lachowicz 2014, …].

Mathematical modeling in modern engineering theory of composites frequently presented in a different way.

VARIOUS „MODELS” OF COMPOSITES

Let $r(1 \pm \alpha)$ denote the semi-axes of ellipses ($0 \leq \alpha < 1$ and $r > 0$) of conductivity λ embedded in the host of the normalized unit conductivity. Introduce the contrast parameter $\rho = (\lambda - 1) / (\lambda + 1)$ and the concentration v of ellipses. The components of the effective conductivity tensor

$$\boldsymbol{\lambda} = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{12} & \lambda_{22} \end{pmatrix}$$



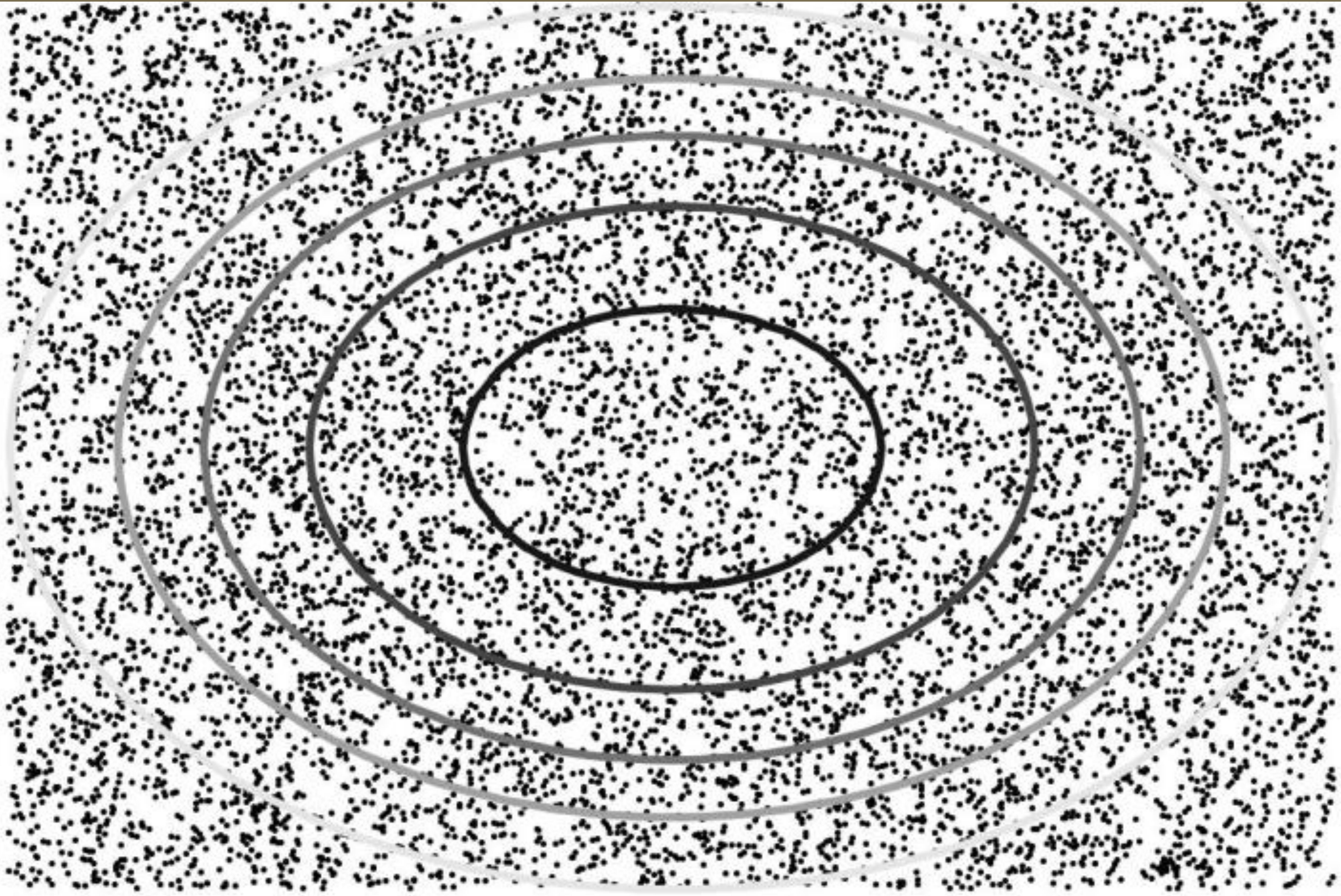
aligned with the coordinate axes ellipses were estimated by Galeener

$$\lambda_{11} \approx 1 + \frac{2\varrho\nu}{1 - \varrho(\nu + \alpha)}, \quad \lambda_{22} \approx 1 + \frac{2\varrho\nu}{1 - \varrho(\nu - \alpha)}$$

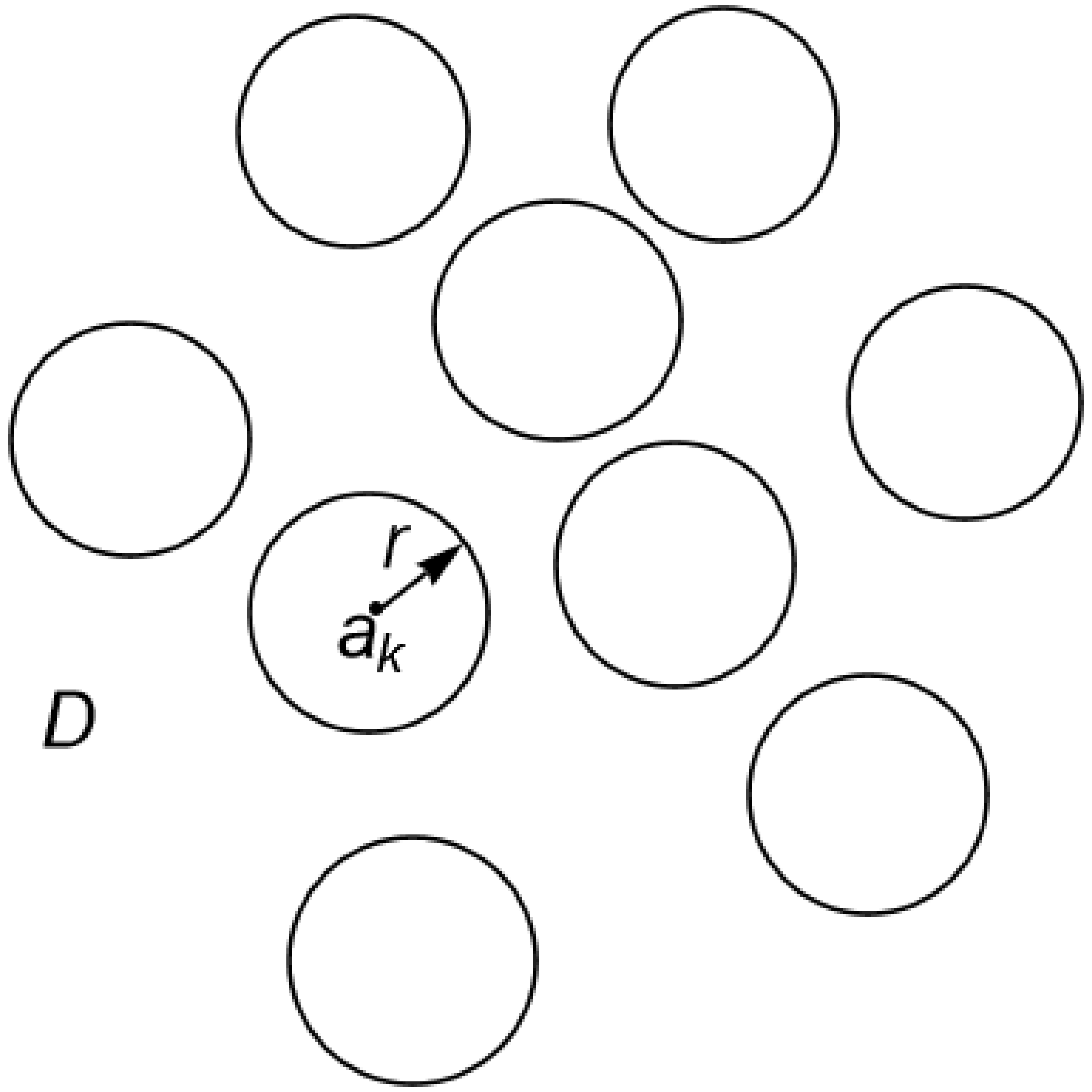
and by Cohen

$$\lambda_{11} \approx 1 + \frac{2\varrho\nu}{1 - \varrho(\alpha + \nu(1 - \alpha))}, \quad \lambda_{22} \approx 1 + \frac{2\varrho\nu}{1 + \varrho(\alpha - \nu(1 + \alpha))}$$

EXTENDING CLUSTER OF INCLUSIONS



MAXWELL'S APPROACH



Consider the boundary value problem with a finite number of circular of radius *r* inclusions on plane

$$u = u_k, \quad \frac{\partial u}{\partial \mathbf{n}} = \sigma \frac{\partial u_k}{\partial \mathbf{n}} \quad \text{on } L_k, \quad k = 1, 2, \ldots, n,$$

equivalent to the $\mathbb{R}$-linear problem

$$\phi^+(t) = a(t)\,\phi^-(t) + b(t)\,\overline{\phi^-(t)} + c(t), \quad t \in L. \qquad (\mathbb{R})$$

$$a(t) = \frac{\sigma_k + 1}{2},\ b(t) = \frac{\sigma_k - 1}{2},\ c(t) = t.$$

The dipole moment (capacity) of the cluster is the coefficient c_{-1} in the expansion of the complex potential at infinity *n*

$$\phi(z) = c_0 + c_{-1} z^{-1} + c_{-2} z^{-2} + \ldots$$

MAXWELL'S APPROACH

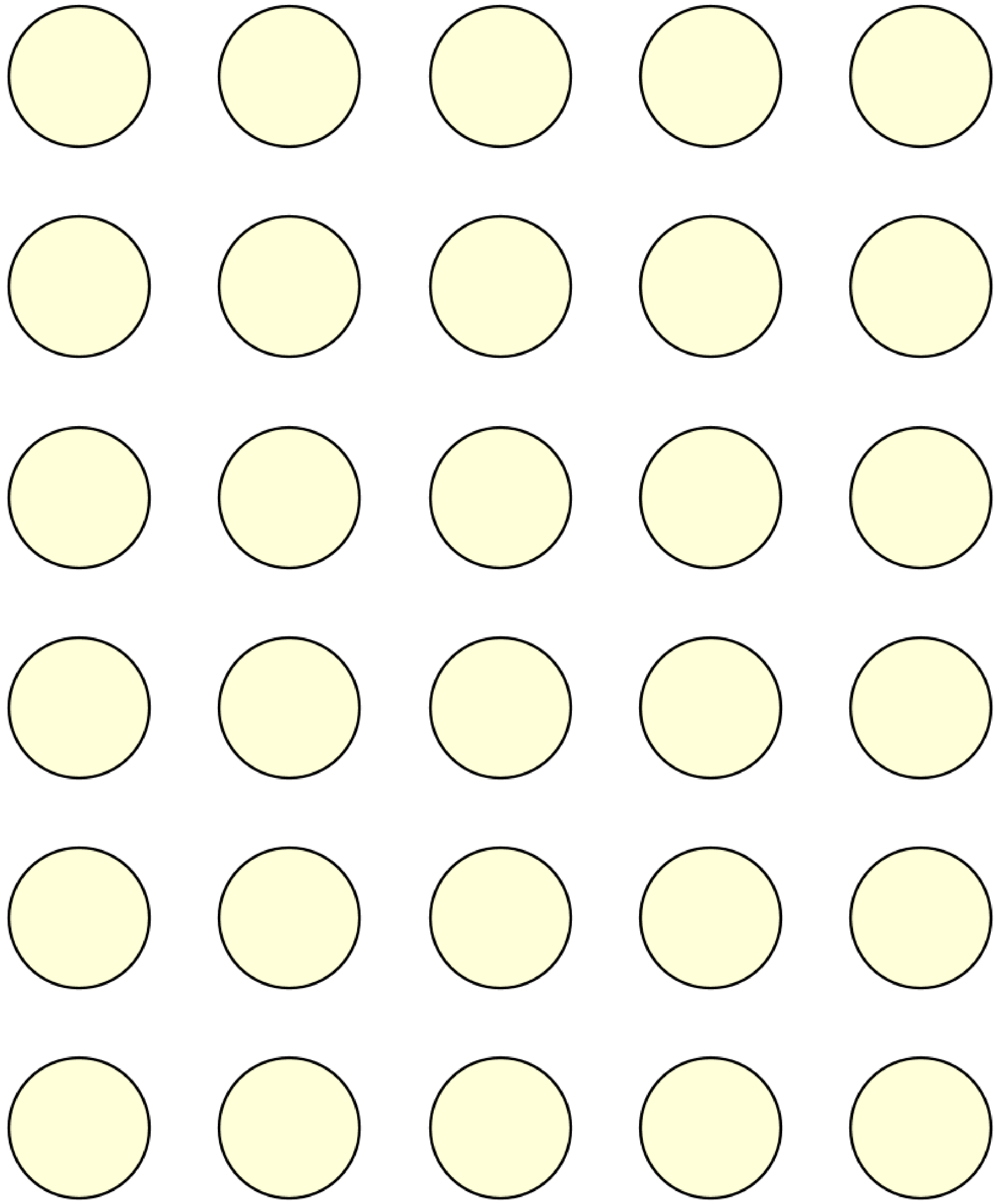
Calculation of the dipole moment

$$\mathcal{M}^{(n)} = \varrho\left(1 + \varrho r^2 e_2^{(n)}\right) + O(r^4) \quad \text{where} \quad e_2^{(n)} = \sum_{k=1}^{n} \sum_{m \neq k} \frac{1}{(a_k - a_m)^2}.$$

Maxwell's homogenization suggests that the dipole moment of the cluster is equal to the dipole moment of the homogenized medium, where *f* is the concentration of clusters.

$$f\mathcal{M}^{(n)} = \frac{\sigma_e^{(n)} - \sigma}{\sigma_e^{(n)} + \sigma}. \quad \Rightarrow \quad \sigma_e \approx \sigma \frac{1 + \varrho f}{1 - \varrho f}$$

SQUARE ARRAY OF DISKS



The sum $e_2^{(n)}$ in the limit case $n \to \infty$ becomes the lattice sum

$S_2 = \sum_{m_1, m_2} \frac{1}{(m_1 + i\, m_2)^2}$, where m_1, m_2 run over integers except $m_1 = m_2 = 0$.

This series is conditionally convergent.

The same holds for $e_2^{(n)}$, as $n \to \infty$.

This is the source of various „models” in the theory of composites, e.g., Mori-Tanaka method (about 10 000 citations).

SELF-CONSISTENT CONCEPT

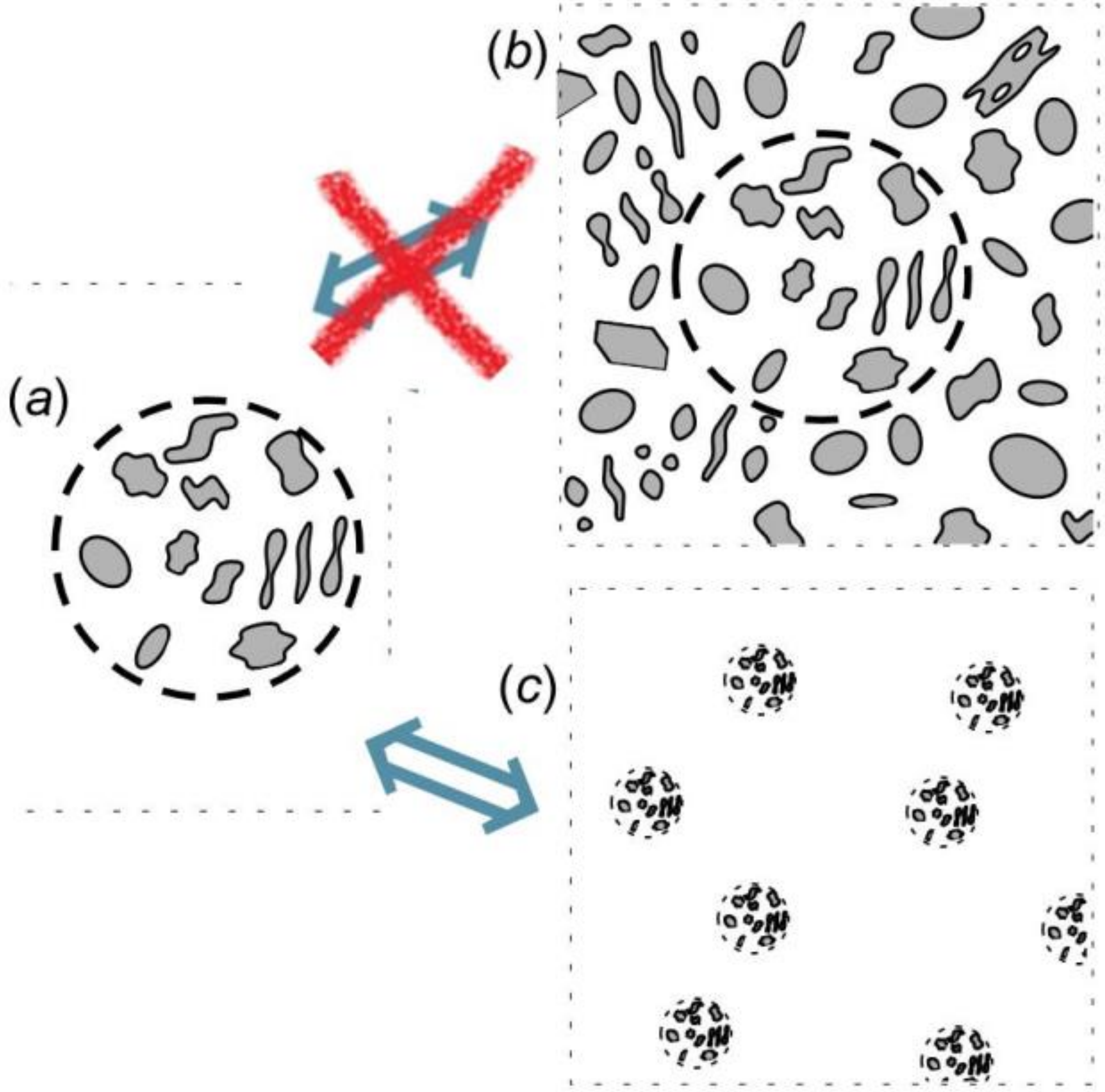
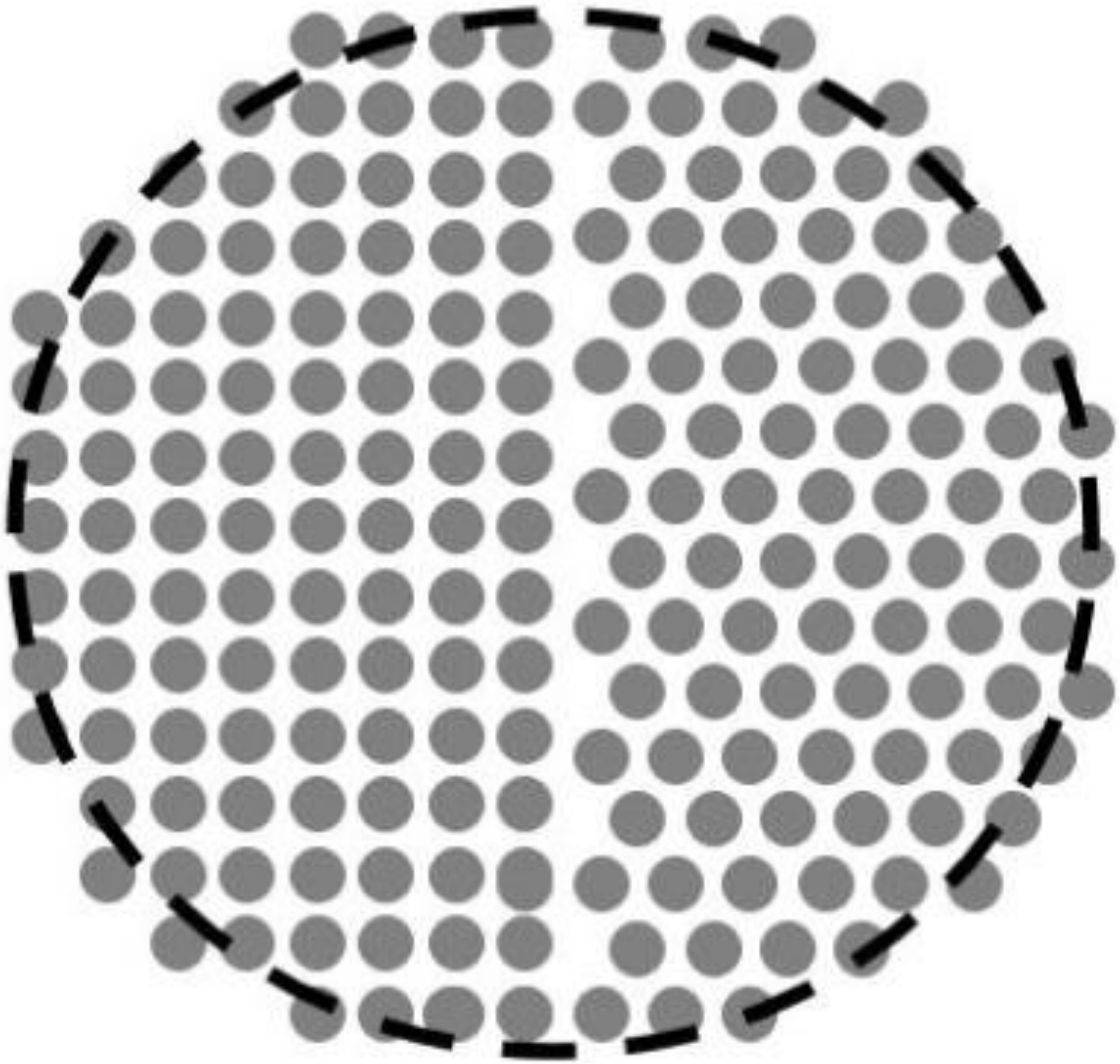


Illustration of the methodologically wrong and correct self-consistent concepts: a finite collection (a) embedded in the infinite medium and bounded by the dashed circle does not represent a composite (b) and does represent dilute clusters (c).

SQUARE AND HEXAGONAL ARRAYS ENCLOSED TO A CIRCLE



LATTICE SUMS

$$S_m = \sum_{m_1,m_2}{}' (m_1\omega_1 + im_2\omega_2)^{-m}, \quad m = 2,3,\ldots,$$

Eisenstein summation method:

$$\sum_{m_1,m_2}{}^e := \lim_{M_2\to+\infty} \lim_{M_1\to+\infty} \sum_{m_2=-M_2}^{M_2} \sum_{m_1=-M_1}^{M_1}$$

$$\Rightarrow \quad S_2 = \frac{2}{\omega_1}\zeta\left(\frac{\omega_1}{2}\right)$$

Rayleigh (1892) calculated $S_2 = \pi$ for the square array by the Eisenstein summation method (1847) but referred only to Weierstrass (1856-1864).

EISENSTEIN FUNCTION

$$\wp(z) = \frac{1}{z^2} + \sum_{\omega \in \mathscr{Q}}' \left[\frac{1}{(z-\omega)^2} - \frac{1}{\omega^2} \right];$$

$$\zeta(z) = \frac{1}{z} + \sum_{\omega \in \mathscr{Q}}' \left[\frac{1}{z-\omega} + \frac{1}{\omega} + \frac{z}{\omega^2} \right]$$

Weierstrass' functions (1864)

Eisenstein's functions (1847):

$$E_1(z) = \zeta(z) - S_2 z, \quad E_2(z) = \wp(z) + S_2.$$

$$E_l(z) = \frac{(-1)^l}{(l-1)!} \frac{d^{l-2}\wp(z)}{dz^{l-2}}, \quad l = 3, 4, \ldots.$$

SOCHOCKI'S FORMULAS ON TORUS

Sochocki's formulas:

$$\Phi^{+}(t) = \tfrac{1}{2}h(t) + \tfrac{1}{2\pi i}\int_L h(\tau)E_1(\tau - t)\mathrm{d}\tau,$$

$$\Phi^{-}(t) = -\tfrac{1}{2}h(t) + \tfrac{1}{2\pi i}\int_L h(\tau)E_1(\tau - t)\mathrm{d}\tau, \; t \in L_k.$$

Cauchy-type integral:

$$\Phi(z) = \frac{1}{2\pi i}\int_L h(t)E_1(t - z)\,\mathrm{d}t, \; z \in D^{+} \cup D$$

$\mathbb{R}$ -LINEAR PROBLEMS FOR DOUBLY PERIODIC DOMAIN; ANTI-PLANE SHEAR (CONDUCTIVITY)

$$\varphi(t) = \varphi_k(t) - \rho_k \overline{\varphi_k(t)}, \quad t \in L_k \quad (k = 1, 2, \ldots, N)$$

Let the contrast parameter $\rho = \frac{\sigma - 1}{\sigma + 1}$ be the same for all inclusions (two-phase composite).

Apply Cauchy-type integral over *L* to the boundary value problem. Obtain the system of integral equations:

$$\varphi_k(z) = \sum_{m=1}^{N} \frac{\varrho}{2\pi i} \int_{L_m} \overline{\varphi_m(t)} E_1(t - z)\, \mathrm{d}t + z + c_k, \; z \in D_k \; (k = 1, 2, \ldots, N)$$

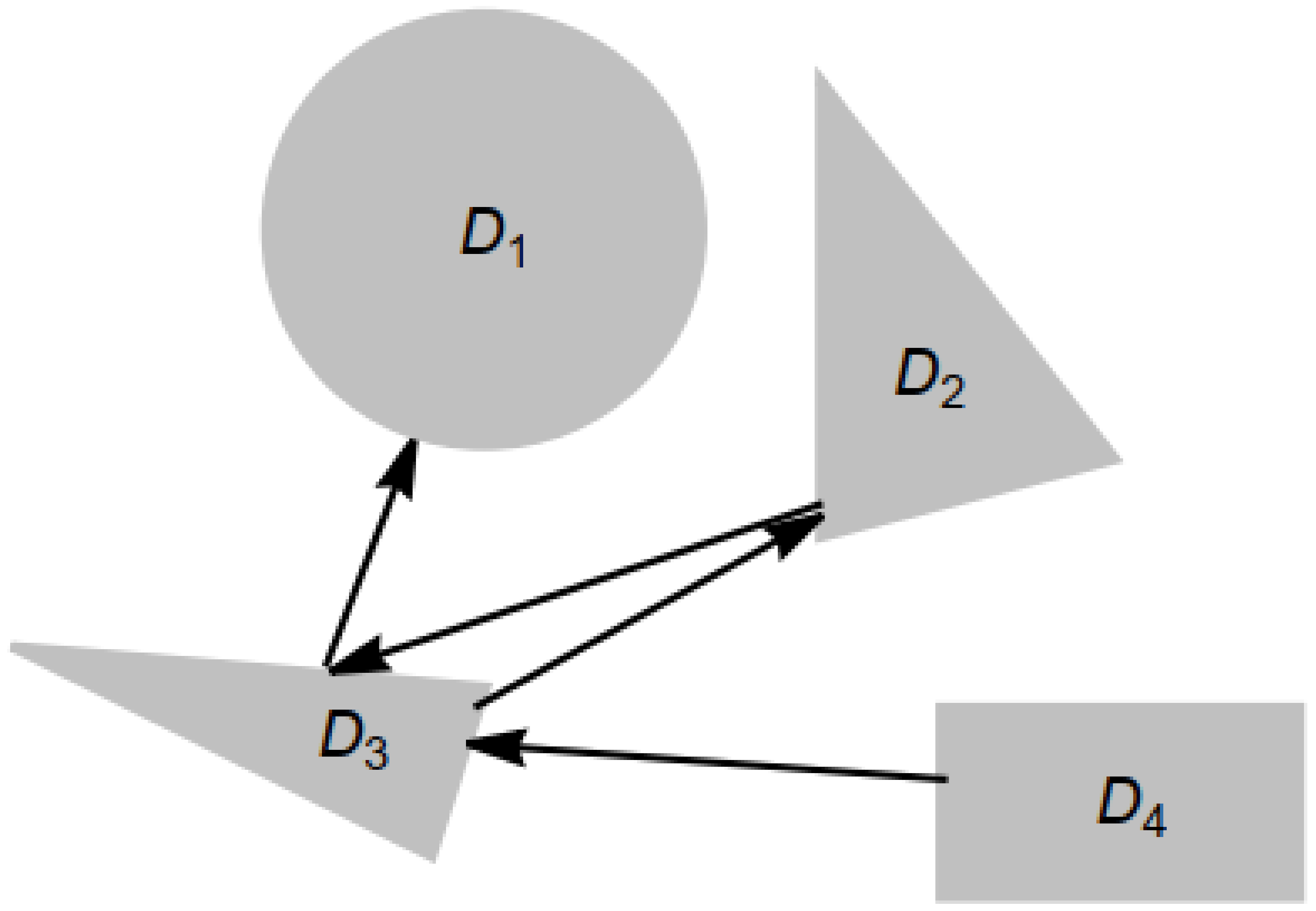
GENERAL SCHWARZ'S SCHEME FOR DISPERSED COMPOSITES

$$u_k = \rho A_k u_k + \rho \sum_{m \neq k} A_m u_m + u_0, \quad \text{in } D_k, \quad k = 1, 2, \ldots, N$$

The method of successive approximations leads to the contrast expansion

$$u_k = u_0 + \rho \sum_{k_1} A_{k_1} u_0 + \rho^2 \sum_{k_1,k_2} A_{k_1} A_{k_2} u_0 + \rho^3 \sum_{k_1,k_2} A_{k_1} A_{k_2} A_{k_3} u_0 + \ldots$$

The term 4-3-2-3-1:



STRUCTURAL SUMS

Definition

$$e_{m_1,\ldots,m_q} = \frac{1}{N^{1+\frac{1}{2}(m_1+\cdots+m_q)}} \times$$

$$\sum_{k_0,k_1,\ldots,k_n} E_{m_1}(a_{k_0}-a_{k_1})\mathbf{C}E_{m_2}(a_{k_1}-a_{k_2})\ldots\mathbf{C}^{q+1}E_{m_q}(a_{k_{q-1}}-a_{k_q})$$

Examples

$$e_2 = \frac{1}{N^2}\sum_{k_0=1}^{N}\sum_{k_1=1}^{N} E_2(a_{k_0}-a_{k_1}),$$

$$e_{22} = \frac{1}{N^3}\sum_{k_0=1}^{N}\sum_{k_1=1}^{N}\sum_{k_2=1}^{N} E_2(a_{k_0}-a_{k_1})\overline{E_2(a_{k_1}-a_{k_2})}$$

The set of complex values completely determines a composite

$$\mathscr{E}_1 = \{e_2\},\ \mathscr{E}_2 = \{e_{22}\},\ \mathscr{E}_3 = \{e_{33}, e_{222}\},\ \mathscr{E}_4 = \{e_{44}, e_{332}, e_{233}, e_{2222}\}, \ldots.$$

2-point correlation

3-point correlation

STRUCTURAL SUMS (E-SUMS)

Decomposition series for the effective permittivity (may be complex value) / conductivity / shear modulus (physical constants, geometry, concentration):

$$\boldsymbol{\varepsilon}_{\perp} = I + 2\varrho f\left(I + A_1 f + A_2 f^2 + \cdots\right),$$

$$A_1 = \frac{\varrho}{\pi}\mathbf{e}_2, \quad A_2 = \frac{\varrho^2}{\pi^2}\mathbf{e}_{22}, \quad A_3 = \frac{1}{\pi^3}\left[-2\varrho^2\mathbf{e}_{33} + \varrho^3\mathbf{e}_{222}\right],$$

$$A_4 = \frac{1}{\pi^4}\left[3\varrho^2\mathbf{e}_{44} - 2\varrho^3(\mathbf{e}_{332} + \mathbf{e}_{233}) + \varrho^4\mathbf{e}_{2222}\right],$$

$$A_5 = \frac{1}{\pi^5}\left[-4\varrho^2\mathbf{e}_{55} + 2\varrho^3(\mathbf{e}_{442} + 2\mathbf{e}_{343} + \mathbf{e}_{244}) - \right.$$
$$\left. -2\varrho^4(\mathbf{e}_{3322} + \mathbf{e}_{2332} + \mathbf{e}_{2233}) + \varrho^5\mathbf{e}_{22222}\right],$$

$$A_6 = \frac{1}{\pi^6}\left[5\varrho^2\mathbf{e}_{66} - 8\varrho^3(\mathbf{e}_{255} + 3\mathbf{e}_{354}) + \right.$$
$$+\varrho^4(6\mathrm{Re}\,\mathbf{e}_{2244} + 12\mathrm{Re}\,\mathbf{e}_{2343} + 4\mathbf{e}_{3333} + 3\mathbf{e}_{2442}) -$$
$$\left. -4\varrho^5(\mathbf{e}_{22233} + \mathbf{e}_{22332}) + \varrho^6\mathbf{e}_{222222}\right],$$

STRUCTURAL SUMS (E-SUMS)

$$
\begin{aligned}
A_7 = \frac{1}{\pi^7} [& -6\varrho^2 \mathbf{e}_{77} + 10\varrho^3 (\mathbf{e}_{266} + 4\mathbf{e}_{365} + 3\mathbf{e}_{464}) \\
& -2\varrho^4 (2\mathbf{e}_{2255} + 6\mathbf{e}_{2354} + 6\mathbf{e}_{2453} + 2\mathbf{e}_{2552} + 3\mathbf{e}_{3344} + 9\mathbf{e}_{3443} \\
& +6\mathbf{e}_{3542} + 3\mathbf{e}_{4433} + 6\mathbf{e}_{4532} + 2\mathbf{e}_{5522}) \\
& +2\varrho^5 (3\mathrm{Re}\, \mathbf{e}_{22244} + 6\mathrm{Re}\, \mathbf{e}_{22343} + 3\mathrm{Re}\, \mathbf{e}_{22442} + 4\mathrm{Re}\, \mathbf{e}_{23333} + 3\mathbf{e}_{23432} \\
& +2\mathbf{e}_{33233}) - 2\varrho^6 (2\mathbf{e}_{222233} + 2\mathbf{e}_{222332} + \mathbf{e}_{223322}) + \varrho^7 \mathbf{e}_{2222222}] .
\end{aligned}
$$

$$
\begin{aligned}
A_8 = \frac{\varrho^2}{\pi^8} [& 7\mathbf{e}_{88} + \varrho^4 \mathrm{Re}\, (6\mathbf{e}_{244222} + 8\mathbf{e}_{333322} + 6\mathbf{e}_{442222}) + 16\varrho^2 \mathrm{Re}\, \mathbf{e}_{5533} \\
& -2\varrho^5 (\mathbf{e}_{2223322} + 2\mathbf{e}_{2233222} + 4\mathbf{e}_{2332222} + 4\mathbf{e}_{3322222}) + \varrho^4 (6\mathbf{e}_{222343} \\
& +6\mathbf{e}_{223432} + 3\mathbf{e}_{224422} + 4\mathbf{e}_{233233} + 4\mathbf{e}_{233332} + 6\mathbf{e}_{234322} + 4\mathbf{e}_{332233} \\
& +4\mathbf{e}_{332332} + 6\mathbf{e}_{343222}) - \varrho^3 (12\mathbf{e}_{22354} + 12\mathbf{e}_{22453} + 6\varrho^3 \mathbf{e}_{23344} + 18\mathbf{e}_{23443} \\
& +12\mathbf{e}_{23542} + 6\mathbf{e}_{24433} + 12\mathbf{e}_{24532} + 8\mathbf{e}_{25522} + 12\mathbf{e}_{33343} + 6\mathbf{e}_{33442} + 12\mathbf{e}_{34333} \\
& +18\mathbf{e}_{34432} + 12\mathbf{e}_{35422} + 12\mathbf{e}_{44233} + 6\mathbf{e}_{44332} + 12\mathbf{e}_{45322} + 8\mathbf{e}_{55222}) \\
& +\varrho^2 (20\mathbf{e}_{2365} + 30\mathbf{e}_{2464} + 20\mathbf{e}_{2563} + 5\mathbf{e}_{2662} + 36\mathbf{e}_{3454} + 48\mathbf{e}_{3553} + 20\mathbf{e}_{3652} \\
& +9\mathbf{e}_{4444} + 36\mathbf{e}_{4543} + 30\mathbf{e}_{4642} + 20\mathbf{e}_{5632} + 10\mathbf{e}_{6622}) \\
& -\varrho (30\mathbf{e}_{376} + 60\varrho \mathbf{e}_{475} + 60\varrho \mathbf{e}_{574} + 30\varrho \mathbf{e}_{673} + 12\varrho \mathbf{e}_{772}) + \varrho^6 \mathbf{e}_{22222222}] .
\end{aligned}
$$

SHEAR MODULUS OF MACROSCOPICALLY ISOTROPIC EASTIC COMPOSITES (P.DRYGAŚ)

$$\frac{G_e}{G} = \frac{1 + \operatorname{Re} A}{1 - \kappa \operatorname{Re} A}, \qquad A = \sum_{s=1}^{\infty} A^{(s)} f^s,$$

$$A^{(1)} = \varrho_3, \quad A^{(2)} = -\frac{2}{\pi}\varrho_3^2 e_3^{(1)(1)} = 0,$$

$$A^{(3)} = \frac{1}{\pi^2}\varrho_3\left[4\varrho_3^2 e_{3,3}^{(1,1)(1,0)} + 6\varrho_3 e_4^{(0)(1)} + \frac{\varrho_1 - \varrho_3}{1+\varrho_1}\left(e_{2,2}^{(0,0)(1,0)} - e_{2,2}^{(0,0)(1,1)}\right)\right]$$

$$A^{(4)} = \frac{1}{\pi^3}\left[-2\varrho_1\varrho_2\varrho_3 e_{3,3}^{(0,0)(1,0)} - 12\varrho_3^3 e_{4,3}^{(0,1)(1,0)} - 12\varrho_3^3 e_{3,4}^{(1,0)(1,0)} - 18\varrho_3^3 e_{4,4}^{(1,1)(1,0)} - 8\varrho_3^4 e_{3,3,3}^{(1,1,1)(1,0,1)} - 2\varrho_3^2\frac{\varrho_3 - \varrho_1}{1+\varrho_1}\left(e_{2,2,3}^{(0,0,1)(0,0,1)} + e_{2,2,3}^{(0,0,1)(1,1,0)} + 2e_{2,2,3}^{(0,0,1)(1,0,1)}\right)\right]$$

$$A^{(5)} = \frac{1}{\pi^4}\left[3\varrho_3(\varrho_1\varrho_2 + 12\varrho_3^2)e_{4,4}^{(0,0)(1,0)} + 24\varrho_3^3\left(5\operatorname{Re}\left(e_{5,4}^{(0,1)(1,0)}\right) + 2e_{5,5}^{(1,1)(1,0)}\right) + 8\varrho_1\varrho_2\varrho_3^2 e_{3,3,3}^{(0,0,1)(1,0,1)} + 16\varrho_3^5 e_{3,3,3,3}^{(1,1,1,1)(1,0,1,0)} + 24\varrho_3^4\left(2e_{4,3,3}^{(0,1,1)(1,0,1)} + e_{3,4,3}^{(1,0,1)(1,0,1)} + 3e_{4,4,3}^{(1,1,1)(1,0,1)}\right)\right.$$

HASHIN-SHTRIKMAN BOUNDS

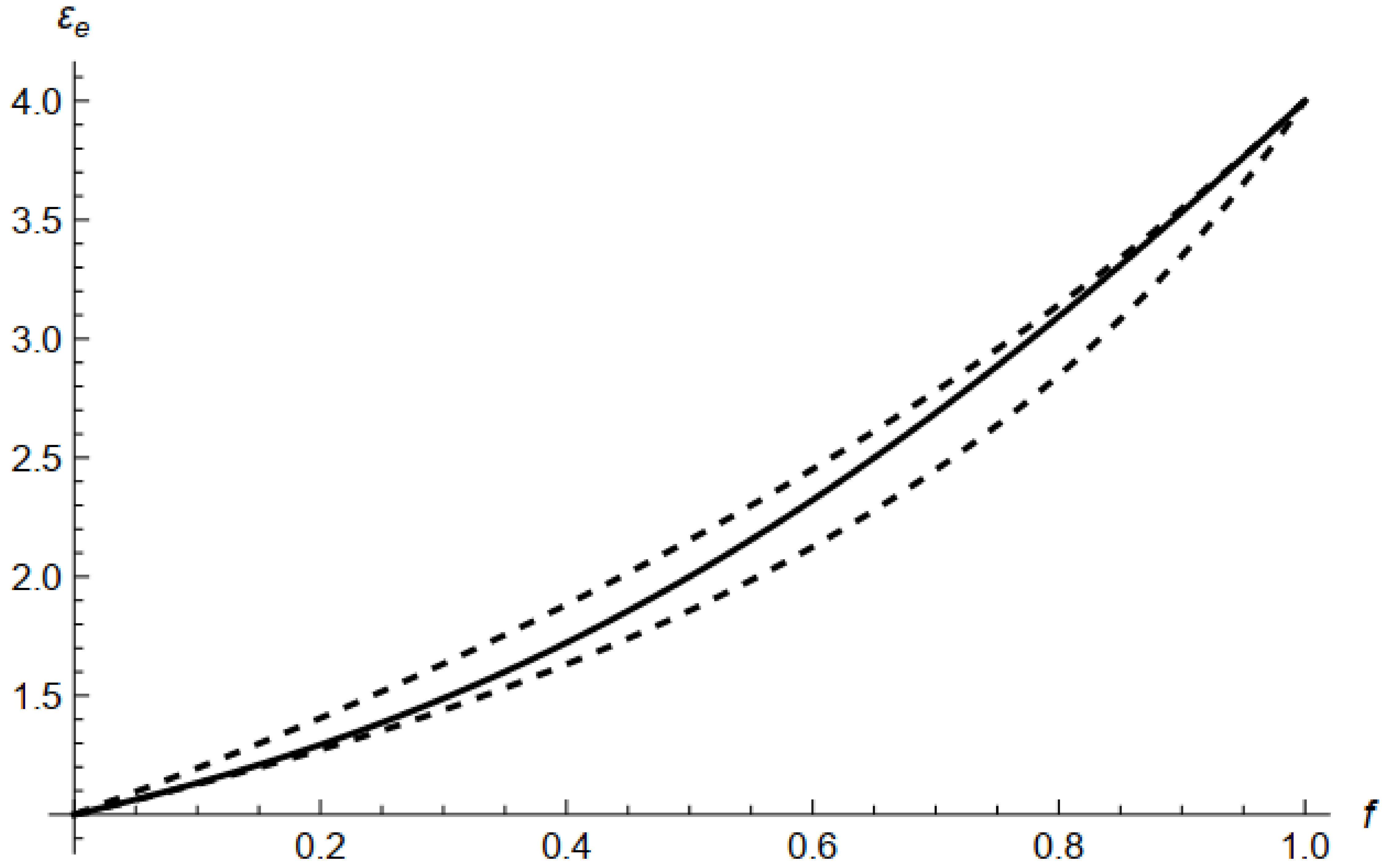
Hashin-Shtrikman bounds for two-phase composites with the permittivity $\varepsilon_1 > \varepsilon_2$. The bounds are based on the 2-point corellation functions.

$$\varepsilon_2^L = \varepsilon_2 \frac{\varepsilon_1(1+f)+\varepsilon_2(1-f)}{\varepsilon_1(1-f)+\varepsilon_2(1+f)}, \quad \varepsilon_2^U = \varepsilon_1 \frac{\varepsilon_1 f+\varepsilon_2(2-f)}{\varepsilon_1(2-f)+\varepsilon_2 f}.$$

BRUGGEMAN’S EQUATION (10 000 CITATIONS)

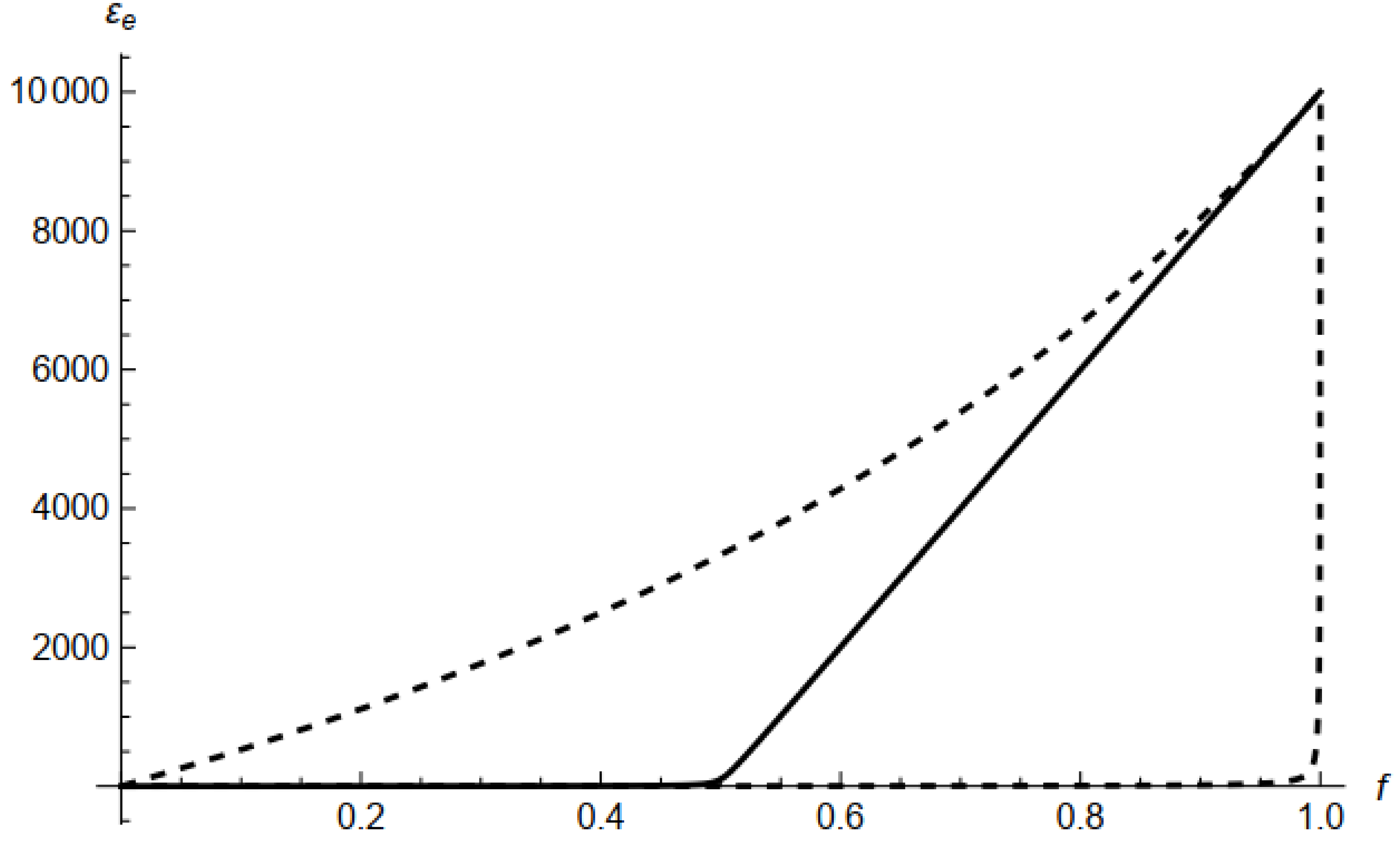
$$f\,\frac{\varepsilon_1-\varepsilon_e}{\varepsilon_1+\varepsilon_e}+(1-f)\,\frac{1-\varepsilon_e}{1+\varepsilon_e}=0$$

Hashin-Shtrikman bounds (dashed) and Bruggeman’s formula (solid) for $\varepsilon_1 = 4$



BRUGGEMAN'S EQUATION (10 000 CITATIONS)

Hashin-Shtrikman bounds (dashed) and Bruggeman's formula (solid) for $\varepsilon_1 = 10\ 000$



STRUCTURAL SUMS

"Theorem":

RVE (representative volume element) and the macroscopic constants are determined by means of the geometry. The e-sums completely describe the geometry.

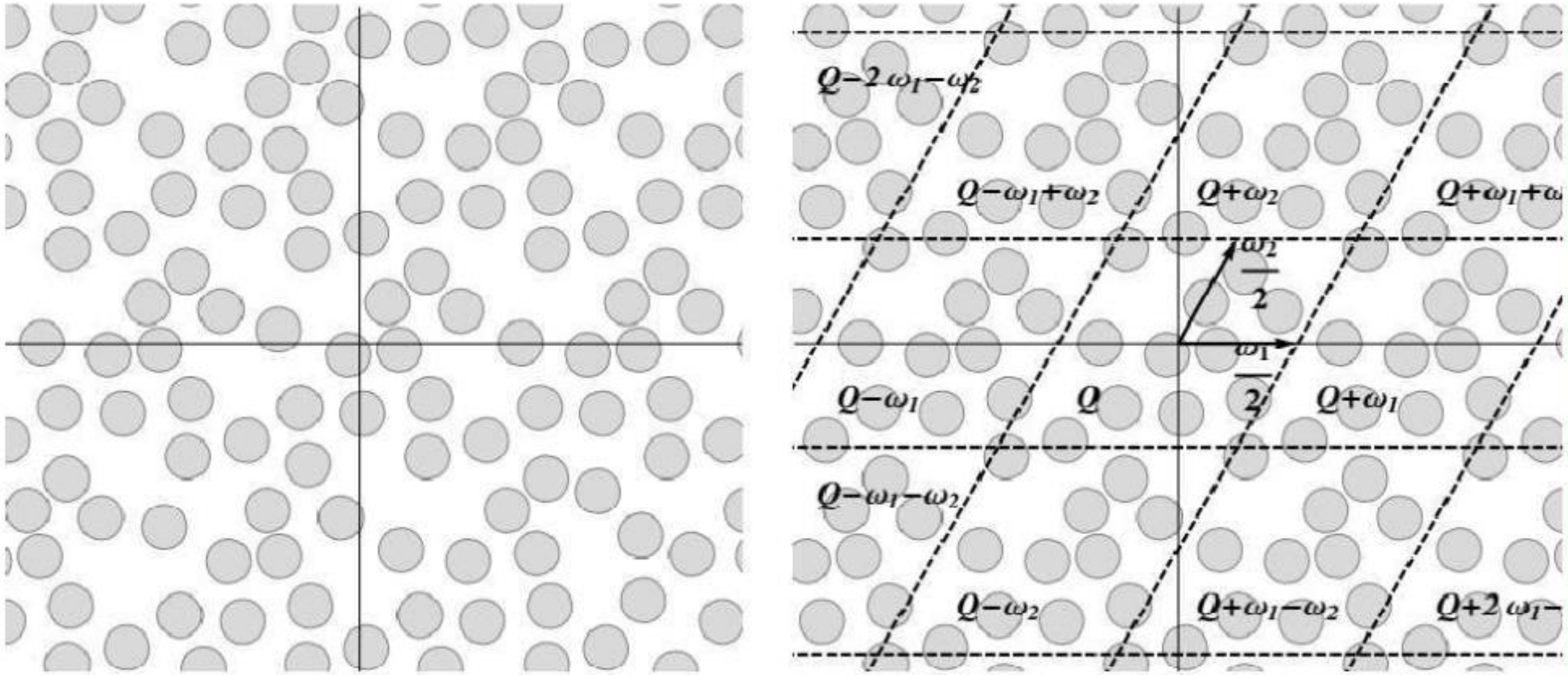
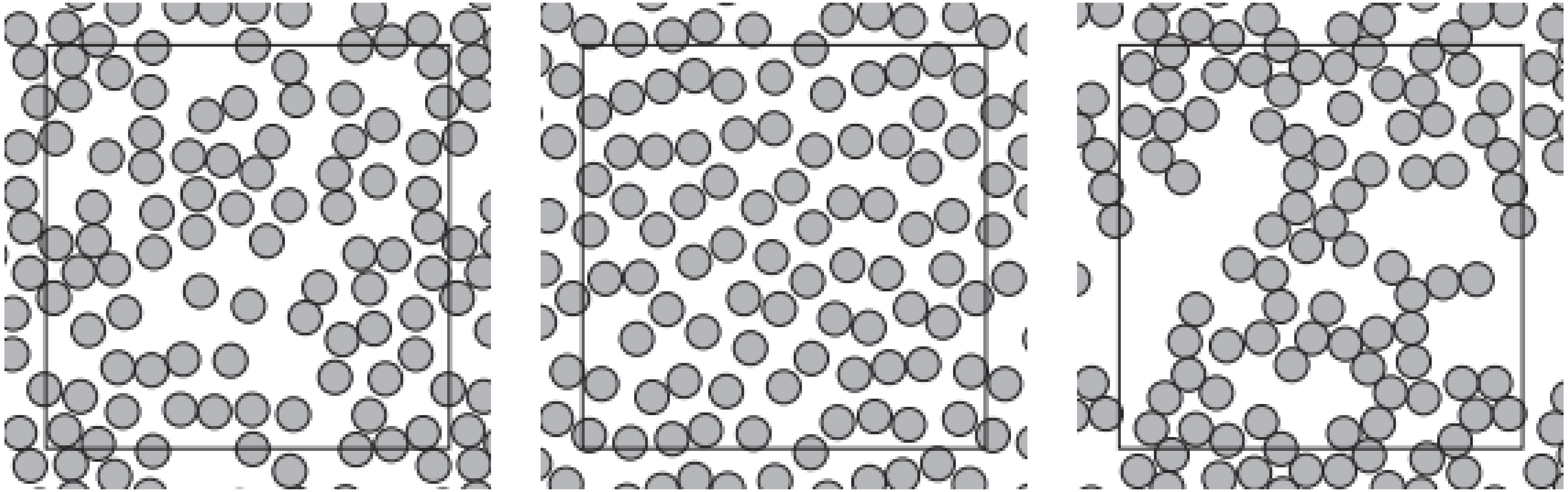


Figure 4.4 From 100 inclusions in large cell to 12 inclusions per representative cell by instant computer computations.

STRUCTURAL SUMS

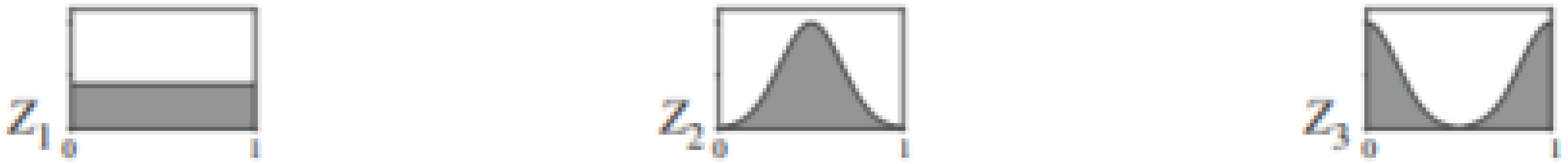


Try to guess which structure is isotropic.

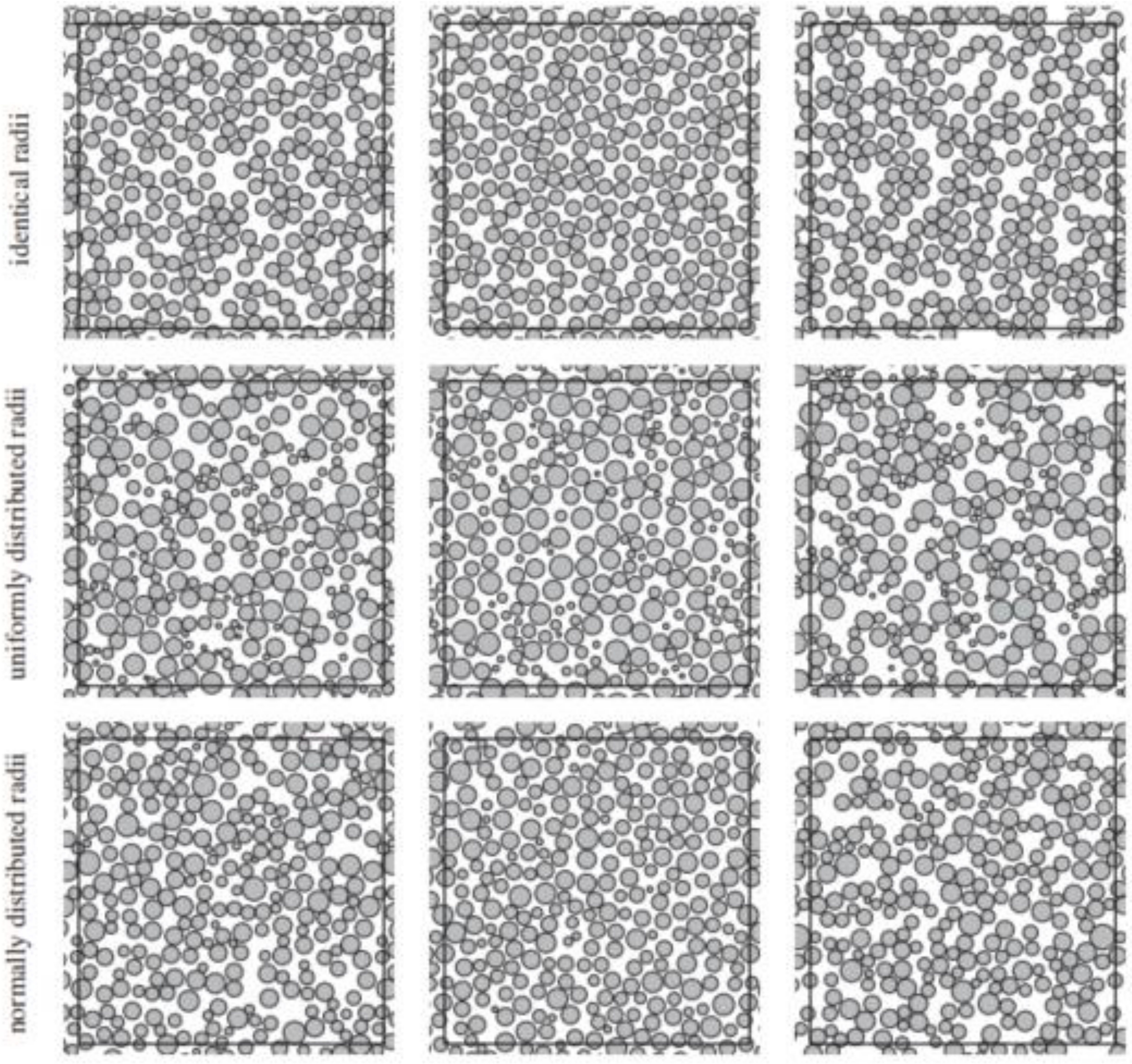
$e_2 = \pi,$ isotropy up to O(f^3)

$e_{222} = 2\pi e_{22} - \pi^3$ isotropy up to O(f^4)

STRUCTURAL SUMS



Sample configurations from each class of distributions of disks used in classification problems. Rows correspond to considered radii distributions; columns specify distributions related to the distance of the circle’s displacement.



THEORETICAL SIMULATIONS BY MACHINE LEARNING

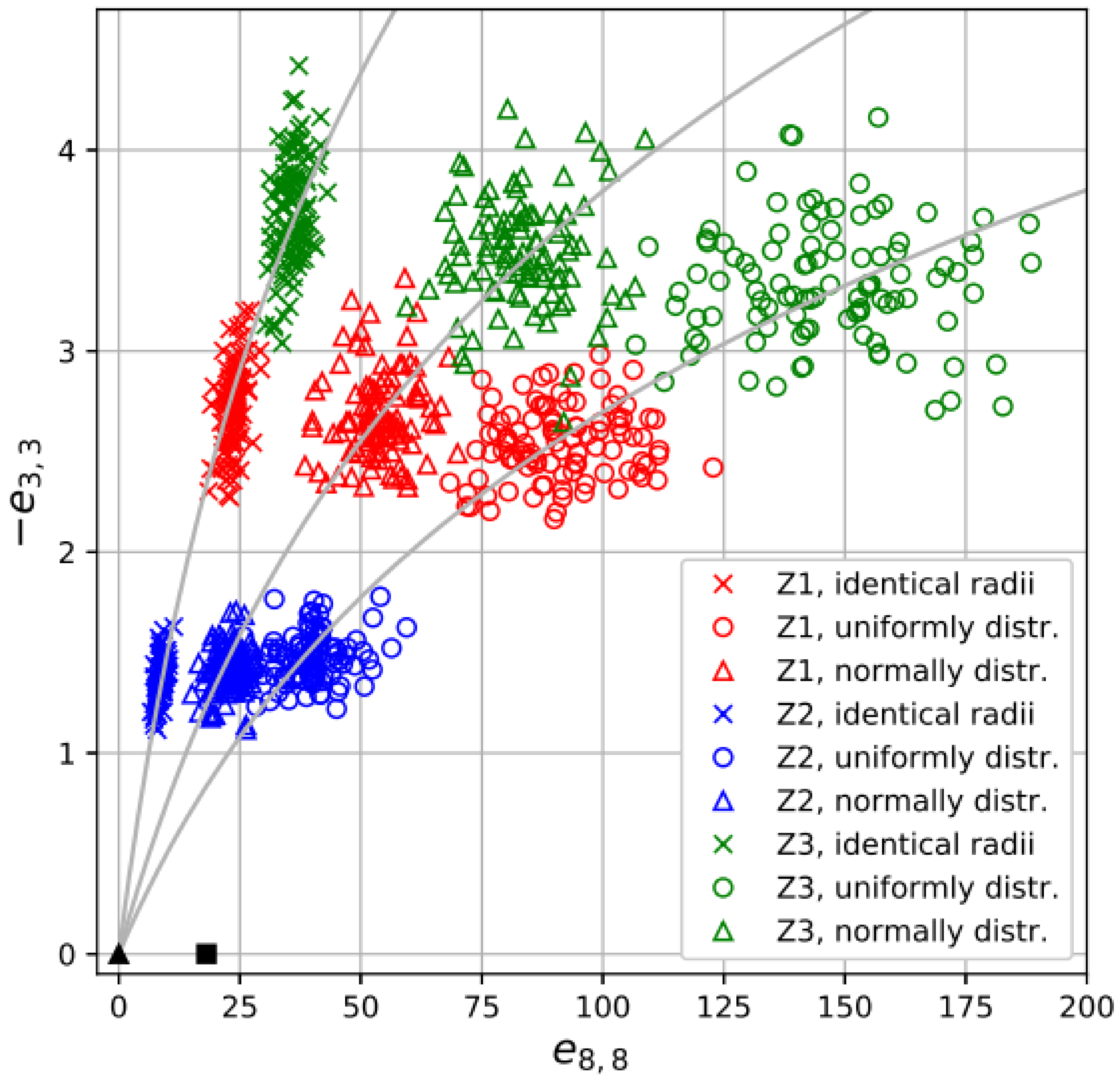


Figure 5.2: Values of $-e_{3,3}$ against $e_{8,8}$ for samples from considered distributions. The fitted curves are $3.118 \log(0.061x + 1)$ (identical radii, crosses), $2.526 \log(0.034x + 1)$ (normally distributed radii, triangles), $1.987 \log(0.028x + 1)$ (uniformly distributed radii, disks).

ANALYTICAL REPRESENTATIVE VOLUME ELEMENT

- New aRVE theory is proposed to classify composites. Hill’s theory can be considered rather as conditions to an RVE

- This aRVE theory is based on the high order approximation formulas for the effective properties of composites

- Fast formulae and algorithms are used not reached by standard computations. The number of treated inclusions per cell can be 1000000 while up to 100 is used in standard approaches.

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Thank you very much

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