Effective Constitutive Properties of Linear Elastic Cellular Solids With Randomly Oriented Cells

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A new methodology to derive the linear effective constitutive law for a group of composites with random microstructure of a special kind is described as an extension of the methodology proposed in Warren and Kraynik (1988) and of the methodology used in polycrystal theory. The results are expressed in the form of specific bounds on effective elastic constants. Practical importance is in the specific bounds when the methodology is applied to cellular solids. Several examples are shown and compared with other published results. The new contribution of this paper lies in the presentation of the methodology, derivation of new specific bounds in two dimensions, and comments related to already published works on cellular solids.

1 Introduction

Proper description of the macroscopic behavior of composites has been the subject of considerable research for many years; thus several methodologies and techniques have been developed in this area. This paper starts with a short outline of homogenization techniques for composite materials and some remarks related to cellular solids.

In many types of statistically homogeneous composites the ratio of the characteristic size of heterogeneities to the size of the full medium, δ, is very small, making numerical solutions that account completely for these heterogeneities (for instance, by finite elements) almost impossible. Thus homogenization techniques are often used. When solving mechanical problems, one replaces the original problem by a problem defined on a fictitious homogeneous medium with certain effective properties. These properties depend on the mechanical properties of the phases, their volume fractions, and the particular microstructure. The fictitious homogeneous medium is the limit (as δ tends to zero) of a sequence of heterogeneous media. Actual composites correspond to very small but nonzero δ, and thus the effective properties must be understood in an approximate sense.

There are two limit cases of actual composites that require different modeling in order to determine the effective properties: composites with a random microstructure (random composites) and composites with a periodic microstructure (periodic composites). In deterministic theories, the first type allows the introduction of a representative volume element (RVE), which is, roughly speaking, the smallest possible region of the composite with the same effective properties as the original one (Hashin, 1970; 1983; Nemat-Nasser and Hori, 1993; Ostoja-Starzewski, 1998). In the case of a periodic microstructure, a basic cell, defined as the (smallest possible) region which can construct the full medium by periodic repetition, can be introduced (Duvaut, 1976; Bensoussan, Lions, and Papanicolau, 1978; Suquet, 1985a, b; Bakhvalov and Panasenko, 1989; Guedes, 1990; Nemat-Nasser and Hori, 1993). In both cases two levels are involved: the macrolevel, which is the level of the fictitious medium, and the microlevel, i.e., the level of the (rescaled) RVE or basic cell. If the microscale is defined such that the basic cell has a unit volume, the term unit cell is often used instead.

For periodic composites, effective properties related to some particular microstructure are obtainable in an exact form, at least numerically. However, due to the complexity of the random microstructure, effective properties of random composites can only be expressed either in the form of representative functions (usually semiempirical) or in the form of bounds. For effectively isotropic two-phase composites (with perfectly bonded phases) the well-known Voigt and Reuss bounds were improved using the Hashin-Shtrikman variational principle (Hashin and Shtrikman, 1962a, 1963) in Hashin and Shtrikman (1963), giving the Hashin-Shtrikman bounds. They are optimal if, besides the phase properties, only the information about the phase volume fractions is available.

In stochastic theories, additional quantitative characterization of the microstructure can be expressed by n-point correlation functions (Torquato and Stell, 1982) permitting the determination of improved bounds for specific models of microstructures: spherical inclusion models (Torquato, 1991, 1994, 1998), cell models (Lu and Torquato, 1990), etc. In addition, a local effective property may be defined for a mesoscale window (statistical volume element corresponding to a lower scale than a RVE). This approach forms the base of stochastic finite elements (Ostoja-Starzewski, 1993, 1994, 1998), permitting a numerical calculation of effective properties again in the form of bounds.

Along this line, the polycrystal theory was developed. The first Voigt and Reuss bounds on their effective constitutive properties were improved using the already mentioned Hashin-Shtrikman variational principle for polycrystals with various types of single-crystal symmetry in Hashin and Shtrikman (1962b), Peselnick and Meister (1965), Meister and Peselnick (1966), Watt (1979, 1980), and Watt and Peselnick (1980). More recent work on polycrystals has been devoted to the optimality of the Voigt and Reuss bounds (Avellaneda and Milton, 1989).

Cellular solids can be either found in the nature (cork, coral, stalk and leaves of plants, some biomaterials, etc.) or manufactured by foaming of polymers, metals, and ceramics or by other technologies. They can be used for absorption of the kinetic energy, for thermal insulation, etc. The importance of cellular materials as well as the necessity of suitable methodologies allowing a detailed description of their properties increases.

A cellular solid (foam) is composed of an interconnected network of solid struts and shell parts, which can be assigned to cells that are (usually with some modifications) repeated in the medium, not necessarily in a periodic manner. Cellular solids can be classified as open-cell foams, consisting only of solid struts, and

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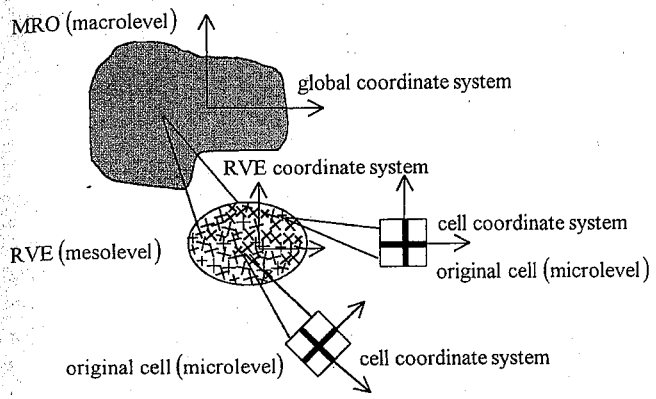

Fig. 1 Medium consisting of randomly oriented cells

closed-cell foams, containing mainly shell parts; see the main monograph on cellular solids by Gibson and Ashby (1988). Actual foams can be partly open and partly closed. Cellular solids can be viewed as composites with void and solid (generally nonhomogeneous) phases.

One of the main parameters that characterize a particular foam is the relative density, s (the ratio of the foam density to the solid phase density), which is low, usually limited by $s = 0.3$ (Gibson and Ashby, 1988). Due to this fact at least one dimension of the solid phase (thickness) at the cell level is small compared to the characteristic cell size. This condition provides motivation for the application of structural theories in homogenization calculations, as shown in Dimitrovová (1997) for periodic foams and in Dimitrovová (1997) and Dimitrovová and Faria (1999), where bounds on the effective properties of open-cell foams were derived. Since they are strictly lower than the bounds for foams (including closed-cell ones), they cannot be obtained by adapting, e.g., the two-phase composite Hashin-Shtrikman bounds. Characterization of random foams by representative functions, fitting some experimental data, can be found in Gibson and Ashby (1988) or Christensen (1994). Effective property calculation for some open-cell foams is presented in Warren and Kraynik (1988).

This paper provides a generalization of Warren and Kraynik's methodology, which is also an extension of the polycrystal methodology, allowing a determination of the effective constitutive properties of some random composites by terms closely related to their particular microstructure.

2 Composites With Randomly Oriented Cells

Two-phase composites with linear homogeneous isotropic phases (and the related foams) are only considered in this paper. The proposed methodology relates to composites with random microstructure of a special kind, named media consisting of randomly oriented cells (MRO). Before their definition, some auxiliary terms are introduced. Let a periodic composite and its possible basic cell be given and defined as the original periodic medium (OPM) and the original cell, respectively. Let us fix the local coordinate system in the basic cell and call it the cell coordinate system. Then MRO (Fig. 1) are defined as random media satisfying the following requirements: (i) particular original cells appear in a RVE with all possible rotations of the cell coordinate system; (ii) all rotational angles of the cell coordinate system are present in a RVE with the same probability. Consequently, the effective isotropy of MRO is ensured.

In order to calculate MRO (effective) properties, in addition to the micro and macrolevel used in homogenization techniques, it is necessary to introduce the mesolevel (Fig. 1). Thus, the original cells correspond to meso-points forming the RVE. Each meso-point is characterized by the same OPM (effective) properties and the nonhomogeneity in MRO is caused by the different rotations of

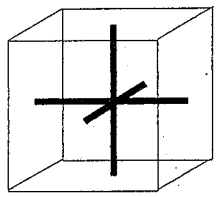

Fig. 2 A basic cell of the regular cubic lattice

the meso-points. This description is similar to the polycrystal model (Hashin and Shtrikman, 1962b), if single crystals are considered as the original cells. However, as in (Warren and Kraynik, 1988), we assume that the original cell size does not vary, otherwise relative volumes of equally oriented original cells would have to be considered (Hashin and Shtrikman, 1962b), (Ferrari and Johnson, 1988).

The partition of the RVE into original cells requires an approximation, but the error (smaller for foams due to the large volume fraction of the void phase) introduced in this way is not important due to the different scales. The reasons why OPM was introduced are: (a) MRO phase volume fractions can be easily kept and (b) OPM permits a unique characterization of the meso-point effective properties (meso-properties). MRO model was already used in Warren and Kraynik (1988) with OPM as the cubic lattice (Fig. 2).

In the polycrystal theory, the boundary of the single crystals need not be considered, thus no assumption about the single-crystal shapes is required. However, for specific purposes, the polycrystal microstructure may be idealized, e.g., by Voronoi cells (Werner, Siegmund, Weinhandl, and Fischer, 1994; Ostoja-Starzewski, 1993, 1994) or by spheres or layered models (Schulgasser, 1983; Avellaneda and Milton, 1989).

In some cases, it may be preferable to define MRO by repeated elements fulfilling the requirements (i) and (ii) in a RVE, but to which no OPM can be related as, e.g., in the example of the tetrahedral lattice (Fig. 3) in (Warren and Kraynik, 1988). In order to calculate effective properties of a repeated element or, in other words, to characterize the meso-properties, boundary conditions like uniform strain, uniform stress or others can be imposed on the boundary. Meso-properties are not uniquely stated, but usually it is possible to determine whether the calculated properties correspond to an upper or a lower estimate of the actual properties.

The following condition holds for the tensor of MRO elastic stiffnesses in matrix representation, $\mathbf{C}^{\mathrm{MRO}}$, which is to be determined:

$$\boldsymbol{\Sigma}^{\mathrm{MRO}} = \mathbf{C}^{\mathrm{MRO}} \cdot \mathbf{E}^{\mathrm{MRO}}, \tag{1}$$

where $\cdot$ stands for the matrix multiplication and $\boldsymbol{\Sigma}^{\mathrm{MRO}}$ and $\mathbf{E}^{\mathrm{MRO}}$ for the macro-stress and macro-strain tensor in vector representation, respectively. The macro-stress (macro-strain) is defined as the volume average of the micro-stress (micro-strain) over a RVE. In MRO model averaging can be divided into two steps. In the first step the microlevel fields are averaged with respect to the cell coordinate system in each original cell separately, giving OPM stress $\boldsymbol{\Sigma}^{\mathrm{OPM}}$ and strain $\mathbf{E}^{\mathrm{OPM}}$. In the second step $\boldsymbol{\Sigma}^{\mathrm{OPM}}$ and $\mathbf{E}^{\mathrm{OPM}}$ are rotated in each original cell (meso-point) to the RVE coordinate

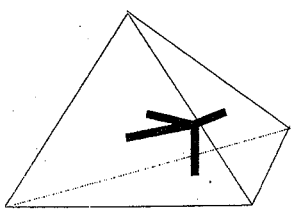

Fig. 3 A repeated element in the tetrahedral lattice

system and then the averaging operator is applied. The second step is equivalently given by the orientational average of OPM values, which is expressed by the invariant integral (Lagzdins, Tamuzs, Teters and Kregers, 1992). We use the notation $\mathbf{\Sigma}^{MRO} = [\mathbf{\Sigma}^{OPM}]$ and $\mathbf{E}^{MRO} = [\mathbf{E}^{OPM}]$ in this case.

Due to the complexity of the MRO microstructure it is obvious that $\mathbf{C}^{MRO}$ cannot be generally available in an exact form, but only in the form of specific MRO bounds. We state them in Section 3 under the assumption of uniform meso-strain or meso-stress, justifying the usage of the names specific MRO Voigt and Reuss bounds. They are expressed in terms of OPM properties and thus are closely related to the particular microstructure. The distance between them depends on the level of the OPM anisotropy. Specific MRO Voigt (Reuss) bound must not be confused with the two-phase composite Voigt (Reuss) bound resulting from the assumption of uniform micro-strain (micro-stress).

The above bounds can be improved using the Hashin-Shtrikman variational principle (Hashin and Shtrikman, 1962a, 1963) in cases, where the related OPM has some kind of effective symmetry, yielding the specific MRO Hashin-Shtrikman bounds. In Section 4 the case when the related OPM possesses a cubic (square in two dimensions) symmetry is treated. Let k and K be bulk moduli in two and three dimensions, respectively, ${}^1G$ and ${}^2G$ be two shear moduli (the isotropy condition is ${}^1G = {}^2G = G$), then in two dimensions under plane stress (superscript σ) ${}^{\sigma}\mathbf{C}^{OPM}$ reads as

$$\begin{bmatrix} {}^{\sigma}k^{OPM} + {}^{\sigma,1}G^{OPM} & {}^{\sigma}k^{OPM} - {}^{\sigma,1}G^{OPM} & 0 \\ {}^{\sigma}k^{OPM} - {}^{\sigma,1}G^{OPM} & {}^{\sigma}k^{OPM} + {}^{\sigma,1}G^{OPM} & 0 \\ 0 & 0 & {}^{\sigma,2}G^{OPM} \end{bmatrix}. \quad (2)$$

If the generalized plane-strain assumption is adopted, (2) is extended in a usual way, the "in-plane" part is formally the same, but the moduli correspond to the plane-strain assumption (superscript ϵ). $\mathbf{C}^{OPM}$ in three dimensions is given by

$$\begin{bmatrix} K^{OPM} + 4\,{}^1G^{OPM}/3 & K^{OPM} - 2\,{}^1G^{OPM}/3 & K^{OPM} - 2\,{}^1G^{OPM}/3 & 0 & 0 & 0 \\ K^{OPM} - 2\,{}^1G^{OPM}/3 & K^{OPM} + 4\,{}^1G^{OPM}/3 & K^{OPM} - 2\,{}^1G^{OPM}/3 & 0 & 0 & 0 \\ K^{OPM} - 2\,{}^1G^{OPM}/3 & K^{OPM} - 2\,{}^1G^{OPM}/3 & K^{OPM} + 4\,{}^1G^{OPM}/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & {}^2G^{OPM} & 0 & 0 \\ 0 & 0 & 0 & 0 & {}^2G^{OPM} & 0 \\ 0 & 0 & 0 & 0 & 0 & {}^2G^{OPM} \end{bmatrix}. \quad (3)$$

In Section 5 the four specific bounds are applied to cellular solids, explicit analytical results are presented, compared with results published in Warren and Kraynik (1988), Gibson and Ashby (1988), and Christensen (1994), and some conclusions are stated.

The first contribution of this paper is in the extension of the polycrystal methodology to MRO and the key issue in the proposed methodology is the proper characterization of the meso-properties. Furthermore, the specific MRO Hashin-Shtrikman bounds derived in Section 4 for two-dimensional media have not been previously published (analogous bounds for three-dimensional media can be adapted from polycrystal bounds by replacing the single-crystal properties by the OPM properties).

The second contribution of this paper is in the generalization of the methodology proposed in Warren and Kraynik (1988). The calculation of effective properties is shown there only for foams consisting of straight equilateral struts and it is not presented in a general way. The final result corresponds to the specific MRO Voigt bound, thus here a correct interpretation of this result is provided, along with the establishment of a link between the methodology in Warren and Kraynik (1988) and the methodology for polycrystals.

3 Specific MRO Voigt and Reuss Bounds

It holds (based on the polycrystal theory) that the specific MRO Voigt (Reuss) bound on $\mathbf{C}^{MRO}$ can be obtained by orientational average (orientational average and inverse) of the OPM elastic stiffnesses $\mathbf{C}^{OPM}$ (compliances $\mathbf{D}^{OPM}$). The statement can be justified as follows: let a MRO and its RVE be taken. Let us assume that (in the vector representation) $(\mathbf{E}^{MRO})_1 = E_{11}^{MRO} = \alpha = [\mathbf{E}^{OPM}]_1$, while the other components are zero. Then

$$\mathbf{\Sigma}^{MRO} = [\mathbf{\Sigma}^{OPM}] = [\mathbf{C}^{OPM} \cdot \mathbf{E}^{OPM}] = \alpha[\mathbf{C}^{OPM}]_1, \quad (4)$$

where $[\mathbf{C}^{OPM}]_1$ denotes the first column of $[\mathbf{C}^{OPM}]$. Consequently, taking into account the assumption about uniform meso-strain, $[\mathbf{C}^{OPM}] \geq \mathbf{C}^{MRO}$ and $[\mathbf{C}^{OPM}]$ is the specific MRO Voigt (upper) bound on $\mathbf{C}^{MRO}$. Inequalities between matrices are taken in the sense that the corresponding difference is positive (negative) semi-definite.

Analogously, when the only nonzero component is $\Sigma_{11}^{MRO} = \beta = [\mathbf{\Sigma}^{OPM}]_1$, one gets

$$\mathbf{E}^{MRO} = [\mathbf{E}^{OPM}] = [\mathbf{D}^{OPM} \cdot \mathbf{\Sigma}^{OPM}] = \beta[\mathbf{D}^{OPM}]_1, \quad (5)$$

where $[\mathbf{D}^{OPM}]_1$ denotes the first column of $[\mathbf{D}^{OPM}]$, consequently $[\mathbf{D}^{OPM}]^{-1} \leq \mathbf{C}^{MRO}$ and $[\mathbf{D}^{OPM}]^{-1}$ is the specific MRO Reuss (lower) bound on $\mathbf{C}^{MRO}$.

Summing up,

$$[\mathbf{D}^{OPM}]^{-1} \leq \mathbf{C}^{MRO} \leq [\mathbf{C}^{OPM}]. \quad (6)$$

$[\mathbf{C}^{OPM}]$ and $[\mathbf{D}^{OPM}]$ are not mutually inverse and equalities in (6) are saturated only for $\mathbf{C}^{OPM} = [\mathbf{C}^{OPM}]$ (equivalently $\mathbf{D}^{OPM} = [\mathbf{D}^{OPM}]$) holding, e.g., for an effectively isotropic OPM.

Let us determine $[\mathbf{C}^{OPM}]$ and $[\mathbf{D}^{OPM}]$. An arbitrary rotation of the cell coordinates in three dimensions is described by three independent parameters. Direction cosines are not convenient (they give nine parameters with six additional constraints of orthonormality), thus it is usual to use Eulerian angles. The choice is not unique; we adopt the one from (Warren and Kraynik, 1988), zxz with the link to φ, θ, ψ. The invariant integral for a fourth-order tensor $\mathbf{R}$ is defined as

$$[\mathbf{R}]_{ijkr} = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} R_{mnpq} T_{im} T_{jn} T_{kp} T_{rq} \sin\theta d\varphi d\theta d\psi. \quad (7)$$

In (7), the summation convention was adopted, all subscripts take values 1, 2, 3, and the transformation matrix $\mathbf{T}$ is

$$\mathbf{T} = \begin{bmatrix} \cos\varphi\cos\psi - \sin\varphi\cos\theta\sin\psi & \sin\varphi\cos\psi + \cos\varphi\cos\theta\sin\psi & \sin\theta\sin\psi \\ -(\cos\varphi\sin\psi + \sin\varphi\cos\theta\cos\psi) & -(\sin\varphi\sin\psi - \cos\varphi\cos\theta\cos\psi) & \sin\theta\cos\psi \\ \sin\varphi\sin\theta & -\cos\varphi\sin\theta & \cos\theta \end{bmatrix}. \tag{8}$$

When expressing $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$ we used an adjustment of (7) to the matrix representation of fourth-order constitutive tensors according to (Lekhnitskii, 1981). $[\mathbf{C}^{\mathrm{OPM}}]$ or $[\mathbf{D}^{\mathrm{OPM}}]$ can be given in the form of single contributions of $\mathbf{C}^{\mathrm{OPM}}$ or $\mathbf{D}^{\mathrm{OPM}}$ components, which is summarized in Table 1. Only components ij with $i, j = 1, 2, 3$ and components 44, 55, and 66 of $\mathbf{C}^{\mathrm{OPM}}$ or $\mathbf{D}^{\mathrm{OPM}}$ contribute to $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$. One can conclude from Table 1 that $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$ are isotropic and that the specific bounds on K^{MRO} and G^{MRO} are (subscripts V and R stand for Voigt and Reuss bounds, respectively)

$$K_V^{\mathrm{MRO}} = \frac{C_{11}^{\mathrm{OPM}} + C_{22}^{\mathrm{OPM}} + C_{33}^{\mathrm{OPM}} + 2(C_{23}^{\mathrm{OPM}} + C_{31}^{\mathrm{OPM}} + C_{12}^{\mathrm{OPM}})}{9},$$

$$K_R^{\mathrm{MRO}} = \frac{1}{D_{11}^{\mathrm{OPM}} + D_{22}^{\mathrm{OPM}} + D_{33}^{\mathrm{OPM}} + 2(D_{23}^{\mathrm{OPM}} + D_{31}^{\mathrm{OPM}} + D_{12}^{\mathrm{OPM}})},$$

$$G_V^{\mathrm{MRO}} = \frac{C_{11}^{\mathrm{OPM}} + C_{22}^{\mathrm{OPM}} + C_{33}^{\mathrm{OPM}} - (C_{23}^{\mathrm{OPM}} + C_{31}^{\mathrm{OPM}} + C_{12}^{\mathrm{OPM}}) + 3(C_{44}^{\mathrm{OPM}} + C_{55}^{\mathrm{OPM}} + C_{66}^{\mathrm{OPM}})}{15},$$

$$G_R^{\mathrm{MRO}} = \frac{15}{4(D_{11}^{\mathrm{OPM}} + D_{22}^{\mathrm{OPM}} + D_{33}^{\mathrm{OPM}}) - 4(D_{23}^{\mathrm{OPM}} + D_{31}^{\mathrm{OPM}} + D_{12}^{\mathrm{OPM}}) + 3(D_{44}^{\mathrm{OPM}} + D_{55}^{\mathrm{OPM}} + D_{66}^{\mathrm{OPM}})}. \tag{9}$$

Let the generalized plane-strain assumption be adopted and the independence of the MRO microstructure on coordinate 1 be assumed in the two-dimensional case. The invariant integral is

$$[\mathbf{R}]_{ijkr} = \frac{1}{2\pi}\int_0^{2\pi} R_{mnpq} T_{im} T_{jn} T_{kp} T_{rq}\, d\varphi, \tag{10}$$

where

$$\mathbf{T} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{bmatrix}. \tag{11}$$

Table 2 summarizes the results in the same way as Table 1; if contributions of $\mathbf{D}^{\mathrm{OPM}}$ are different from those of $\mathbf{C}^{\mathrm{OPM}}$, they are written in brackets. Components 24, 34, 56 and 42, 43, 65 should be included in Table 2, but due to the symmetry of $\mathbf{C}^{\mathrm{OPM}}$ and $\mathbf{D}^{\mathrm{OPM}}$, their contributions to $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$ cancel. One can conclude from Table 2 that MRO are transversely isotropic and that the specific bounds on in-plane constants can be written as (for the sake of simplicity superscripts ϵ or σ in $\mathbf{C}^{\mathrm{OPM}}$ and $\mathbf{D}^{\mathrm{OPM}}$ components are omitted):

$${}^{\epsilon}k_V^{\mathrm{MRO}} = \frac{C_{22}^{\mathrm{OPM}} + C_{33}^{\mathrm{OPM}} + 2C_{23}^{\mathrm{OPM}}}{4},$$

$${}^{\epsilon}k_R^{\mathrm{MRO}} = \frac{D_{11}^{\mathrm{OPM}}}{D_{11}^{\mathrm{OPM}}(D_{22}^{\mathrm{OPM}} + D_{33}^{\mathrm{OPM}} + 2D_{23}^{\mathrm{OPM}}) - (D_{12}^{\mathrm{OPM}} + D_{13}^{\mathrm{OPM}})^2},$$

$${}^{\epsilon}G_V^{\mathrm{MRO}} = \frac{C_{22}^{\mathrm{OPM}} + C_{33}^{\mathrm{OPM}} - 2C_{23}^{\mathrm{OPM}} + 4C_{44}^{\mathrm{OPM}}}{8},$$

$${}^{\epsilon}G_R^{\mathrm{MRO}} = \frac{2}{D_{22}^{\mathrm{OPM}} + D_{33}^{\mathrm{OPM}} - 2D_{23}^{\mathrm{OPM}} + D_{44}^{\mathrm{OPM}}}. \tag{12}$$

In the case of plane stress the only formal difference is in k_R^{MRO}:

$${}^{\sigma}k_R^{\mathrm{MRO}} = \frac{1}{D_{22}^{\mathrm{OPM}} + D_{33}^{\mathrm{OPM}} + 2D_{23}^{\mathrm{OPM}}}, \tag{13}$$

Table 1 Contributions of $\mathbf{C}^{\mathrm{OPM}}$ and $\mathbf{D}^{\mathrm{OPM}}$ components to $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$, respectively, in the three-dimensional case

Contributions to $[\mathbf{C}^{\mathrm{OPM}}]$ or $[\mathbf{D}^{\mathrm{OPM}}]$ components	Components from $\mathbf{C}^{\mathrm{OPM}}$				Components from $\mathbf{D}^{\mathrm{OPM}}$			
	ii for i=1,2,3	ij for i≠j, i,j=1,2,3	ii for i=4,5,6	rest	ii for i=1,2,3	ij for i≠j, i,j=1,2,3	ii for i=4,5,6	rest
ii for i=1,2,3	1/5	1/15	4/15	0	1/5	1/15	1/15	0
ij for i≠j, i,j=1,2,3	1/15	2/15	-2/15	0	1/15	2/15	-1/30	0
ii for i=4,5,6	1/15	-1/30	1/5	0	4/15	-2/15	1/5	0
rest	0	0	0	0	0	0	0	0

Table 2 Contributions of $\mathbf{C}^{\mathrm{OPM}}$ and $\mathbf{D}^{\mathrm{OPM}}$ components to $[\mathbf{C}^{\mathrm{OPM}}]$ and $[\mathbf{D}^{\mathrm{OPM}}]$, respectively, in the two-dimensional case

Contributions to $[\mathbf{C}^{\mathrm{OPM}}]$ ($[\mathbf{D}^{\mathrm{OPM}}]$) components	Components from $\mathbf{C}^{\mathrm{OPM}}$ ($\mathbf{D}^{\mathrm{OPM}}$)						
	11	12,13	21,31	55,66	22,33	23,32	44
11	1	0	0	0	0	0	0
12,13	0	1/2	0	0	0	0	0
21,31	0	0	1/2	0	0	0	0
55,66	0	0	0	1/2	0	0	0
22,33	0	0	0	0	3/8	1/8	1/2 (1/8)
23,32	0	0	0	0	1/8	3/8	-1/2 (-1/8)
44	0	0	0	0	1/8 (1/2)	-1/8 (-1/2)	1/2

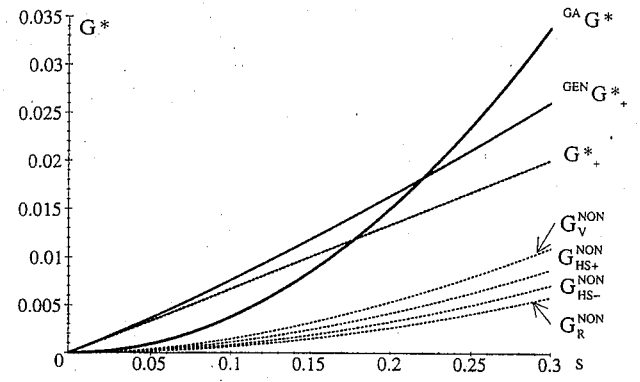

Fig. 4 Comparison of the proposed curve ${}^{GA}G^*$ with the upper bound (linearized form, G_+^*; with nonlinear effect included, ${}^{GEN}G_+^*$) and with the specific MRO bounds if OPM is the nonaligned lattice (G_V^{NON}, G_R^{NON}, G_{HS+}^{NON} and G_{HS-}^{NON})

but, in fact, all bounds differ since the $\mathbf{C}^{OPM}$ and $\mathbf{D}^{OPM}$ components must be also taken in accordance with the assumption of plane stress.

If only some estimate of meso-properties is available (either it is difficult to express OPM properties using the periodicity boundary conditions or only repeated elements are introduced in MRO characterization) it can be easily verified that introducing $\mathbf{C}_{est}^{OPM}$ and $(\mathbf{C}_{est}^{OPM})^{-1}$ with $\mathbf{C}_{est}^{OPM} \geq \mathbf{C}^{OPM}$, specific upper and lower bounds from (9) and (12)–(13) are still upper and lower bounds. This does not hold for $\mathbf{C}_{est}^{OPM} < \mathbf{C}^{OPM}$.

If the related OPM possesses effective cubic or square symmetry, its bulk modulus is invariant under rotation, so $K^{OPM} = K_V^{OPM} = K_R^{OPM} = K^{MRO}$ or $k^{OPM} = k_V^{OPM} = k_R^{OPM} = k^{MRO}$ (in two dimensions this holds for plane stress as well as generalized plane strain). Then in three dimensions,

$$G_V^{MRO} = \frac{2\,{}^1G^{OPM} + 3\,{}^2G^{OPM}}{5}, \quad G_R^{MRO} = \frac{5}{\frac{2}{{}^1G^{OPM}} + \frac{3}{{}^2G^{OPM}}}, \tag{14}$$

and in two dimensions (with the corresponding superscript),

$$G_V^{MRO} = \frac{{}^1G^{OPM} + {}^2G^{OPM}}{2}, \quad G_R^{MRO} = \frac{2}{\frac{1}{{}^1G^{OPM}} + \frac{1}{{}^2G^{OPM}}}. \tag{15}$$

We stated in Section 2 that the distance between the specific bounds depends on the level of OPM anisotropy, which is now expressible as the ratio between ${}^1G^{OPM}$ and ${}^2G^{OPM}$.

4 Specific MRO Hashin-Shtrikman Bounds

In this section the specific MRO Hashin-Shtrikman bounds, as improvements of (15), are derived for two-dimensional media, if the related OPM is effectively square symmetric. Three-dimensional analogs of these bounds, i.e., improvements of (14), can be taken from Hashin and Shtrikman (1962b), provided that single-crystal properties are replaced by OPM properties.

The improvement of (15), based on the Hashin-Shtrikman variational principle, follows the basic steps from Hashin and Shtrikman (1962b). Let us adopt the generalized plane-strain assumption and let U^{MRO} stand for the strain energy density in the given MRO. It is proved in Hashin and Shtrikman (1962a) that U^{MRO} is the stationary value of some functional U^P. In addition to terms related to the MRO, the functional U^P contains characteristics of a reference medium, which is geometrically identical to the MRO. The reference medium is assumed to be homogeneous, transversely isotropic (at the mesolevel in our case). Its properties are unknown and chosen in a way to optimize the bounds, derived later on. The most important term in U^P is the stress polarization tensor $\mathbf{P}$ given by $\mathbf{P} = \boldsymbol{\Sigma}^{MRO} - \mathbf{C}^0 \cdot \mathbf{E}^{MRO}$, where $\mathbf{C}^0$ are effective elastic stiffnesses of the reference medium.

If $\mathbf{C}^{MRO} - \mathbf{C}^0$ is positive (negative) definite, U^{MRO} is the absolute maximum (minimum) of U^P. In the derivation of the bounds a special kind of the stress polarization field $\mathbf{P}$ is chosen, and then, $\mathbf{P}$ can be taken as the only variable in U^P. Consequently, the extreme condition is obtained by taking the variation of U^P with respect to $\mathbf{P}$. Let us denote the polarization field that satisfies this extreme condition by $\mathbf{P}^S$. The stationary value $U^{P,S}$ is

$$U^{P,S} = U^0 + \tfrac{1}{2}[\mathbf{P}^S] \cdot \mathbf{E}^0, \tag{16}$$

where $\mathbf{E}^0$ is the macro-strain in the reference medium. Since the orientational average $[\mathbf{P}^S]$ has to be introduced into (16), not $\mathbf{P}^S$ but $[\mathbf{P}^S]$ can be solved from the extreme condition. Using the same notation B_2 and β as in (Hashin and Shtrikman, 1962b), one obtains

$$[\mathbf{P}^S] = \frac{2B_2}{1 + 2\beta B_2}\,\mathbf{E}^0. \tag{17}$$

The constant β is determined in (Hashin, 1965) in terms of the (not yet specified) moduli ${}^\epsilon k^0$ and ${}^\epsilon G^0$, but obviously ${}^\epsilon k^0 = {}^\epsilon k^{OPM}$. Thus

$$\beta({}^\epsilon k^{OPM}, {}^\epsilon G^0) = -\frac{{}^\epsilon k^{OPM} + 2\,{}^\epsilon G^0}{4\,{}^\epsilon G^0({}^\epsilon k^{OPM} + {}^\epsilon G^0)}. \tag{18}$$

B_2 is a component with subscript 44 of the orientational average of matrix representation of a tensor $((\mathbf{C}^{OPM} - \mathbf{C}^0)^{-1} - \beta\mathbf{I})^{-1}$, where $\mathbf{I}$ is the identity tensor. It is given by

$$B_2 = \frac{1}{\frac{2}{{}^{\epsilon,1}G^{OPM} - {}^\epsilon G^0} - 4\beta({}^\epsilon k^{OPM}, {}^\epsilon G^0)} + \frac{1}{\frac{2}{{}^{\epsilon,2}G^{OPM} - {}^\epsilon G^0} - 4\beta({}^\epsilon k^{OPM}, {}^\epsilon G^0)}. \tag{19}$$

The specific bounds on ${}^\epsilon G^{MRO}$ can then be expressed from the following expression:

$${}^\epsilon G^0 + \frac{B_2}{1 + 2B_2\beta({}^\epsilon k^{OPM}, {}^\epsilon G^0)}. \tag{20}$$

If $\mathbf{C}^{OPM} - \mathbf{C}^0$ is positive definite (${}^{\epsilon,1}G^{OPM} > {}^\epsilon G^0$ and ${}^{\epsilon,2}G^{OPM} > {}^\epsilon G^0$), (20) yields the lower bound; the upper bound is obtained when $\mathbf{C}^{OPM} - \mathbf{C}^0$ is negative definite (${}^{\epsilon,1}G^{OPM} < {}^\epsilon G^0$ and ${}^{\epsilon,2}G^{OPM} < {}^\epsilon G^0$). Since (20) is a monotonically increasing function of ${}^\epsilon G^0$, the best lower (upper) bound is obtained for the highest (lowest) possible ${}^\epsilon G^0$ ensuring that $\mathbf{C}^{OPM} - \mathbf{C}^0$ is still positive definite (negative definite). Let, e.g., ${}^{\epsilon,1}G^{OPM} > {}^{\epsilon,2}G^{OPM}$. Consequently (+ and − stand for the upper and the lower bounds, respectively, HS refers to Hashin-Shtrikman bounds):

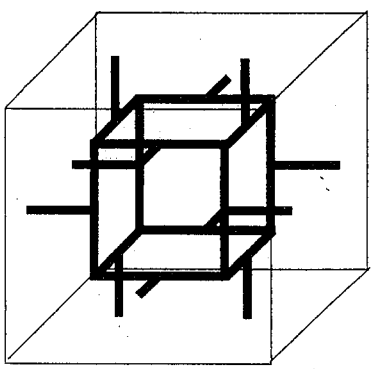

Fig. 5 A basic cell of the nonaligned lattice

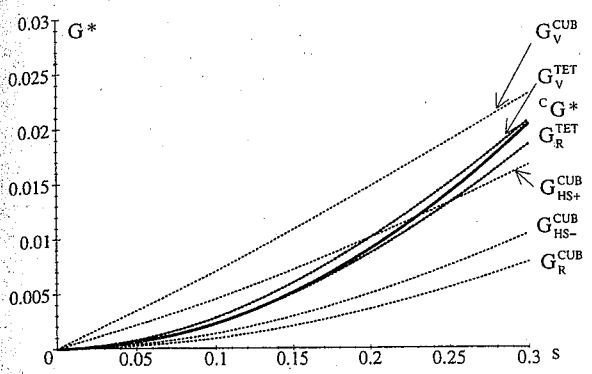

Fig. 6 Comparison of the specific MRO bounds of the tetrahedral lattice (G_V^{TET} and G_R^{TET}) and the specific MRO bounds if OPM is the regular cubic lattice (G_V^{CUB}, G_R^{CUB}, G_{HS+}^{CUB}, and G_{HS-}^{CUB}) with the proposed curve $^cG^*$ (full line)

$$ {}^{\epsilon}G_{HS+}^{MRO} = {}^{\epsilon,1}G^{OPM} + \frac{1}{2\left(\frac{1}{{}^{\epsilon,2}G^{OPM} - {}^{\epsilon,1}G^{OPM}} - \beta({}^{\epsilon}k^{OPM}, {}^{\epsilon,1}G^{OPM})\right)} \quad \text{and} $$

$$ {}^{\epsilon}G_{HS-}^{MRO} = {}^{\epsilon,2}G^{OPM} + \frac{1}{2\left(\frac{1}{{}^{\epsilon,1}G^{OPM} - {}^{\epsilon,2}G^{OPM}} - \beta({}^{\epsilon}k^{OPM}, {}^{\epsilon,2}G^{OPM})\right)}. \quad (21) $$

The case when ${}^{\epsilon,1}G^{OPM} < {}^{\epsilon,2}G^{OPM}$ can be treated similarly, yielding the same results, only + and − have to be exchanged. The bounds under the plane-stress assumption are formally equal, only the plane-strain shear and bulk moduli are replaced by the plane-stress ones.

In the three-dimensional case when, e.g., ${}^1G^{OPM} > {}^2G^{OPM}$, it holds

$$ G_{HS+}^{MRO} = {}^1G^{OPM} + \frac{3}{\frac{5}{{}^2G^{OPM} - {}^1G^{OPM}} - 4\beta(K^{OPM}, {}^1G^{OPM})} \quad \text{and} $$

$$ G_{HS-}^{MRO} = {}^2G^{OPM} + \frac{2}{\frac{5}{{}^1G^{OPM} - {}^2G^{OPM}} - 6\beta(K^{OPM}, {}^2G^{OPM})}, \quad (22) $$

where $\beta(K^{OPM}, G^0)$ is given by

$$ \beta(K^{OPM}, G^0) = -\frac{3(K^{OPM} + 2G^0)}{5G^0(3K^{OPM} + 4G^0)}. \quad (23) $$

5 Examples and Comparisons

Let us apply the above theory to foams. We restrict ourselves to open-cell foams, since then explicit analytical results of OPM properties can be simply obtained, see (Dimitrovová, 1997).

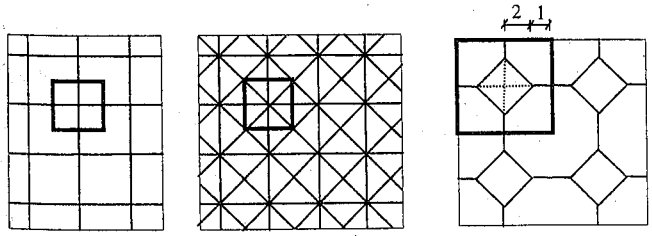

Fig. 7 The regular square, the square with two obliques, and the diamond lattices

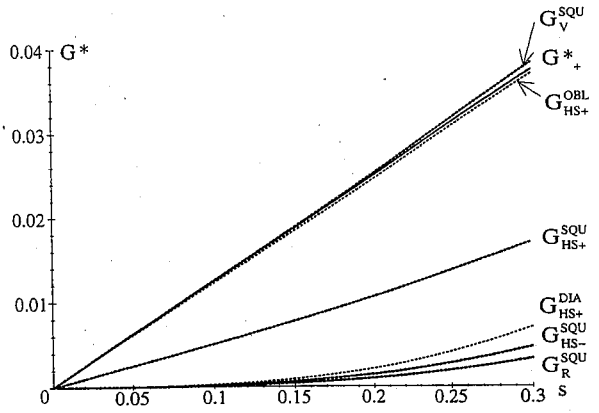

Fig. 8 Comparison of the specific MRO bounds related to the regular square lattice (G_V^{SQU}, G_R^{SQU}, G_{HS+}^{SQU}, and G_{HS-}^{SQU}), the square lattice with two obliques (G_{HS+}^{OBL}) and the diamond lattice (G_{HS+}^{DIA}) with the linearized upper bound G_+^* (full line)

Mainly OPM with cubic (square in two dimensions) effective symmetry are assumed and the struts composing the foams are taken with constant square cross-sectional areas. In two-dimensional cases the plane stress assumption is adopted. All curves in the graphs are plotted as functions of the relative density s and in a dimensionless form (divided by the Young's modulus of the solid phase), however, for the sake of simplicity the notation from the previous sections is not altered.

The first comments are related to the proposed function for dimensionless effective shear modulus G^* of isotropic open-cell foams from (Gibson and Ashby, 1988), ${}^{GA}G^* = 3s^2/8$. This function is compared in Fig. 4 with the linearized upper bound $G_+^* = s/15$ of open-cell foams derived in (Dimitrovová, 1997) and with four specific bounds (superscript NON) related to MRO with OPM as the nonaligned lattice (Fig. 5). The choice of the basic cell was inspired by Gibson and Ashby (1988), who did not use it as a periodic cell but rather as a conceptual cell expressing the bending response of open-cell foams. The specific bounds G_{HS+}^{NON} and G_{HS-}^{NON} are quite close, allowing a good estimate of an actual MRO response. The response is soft and so this particular MRO could be used as a model for very soft open-cell foams. It is seen that, although ${}^{GA}G^*$ is fitted to the experimental data, it is above G_+^* for higher s (69 percent for $s = 0.3$). To explain this fact: first, it should be pointed out that G_+^* does not include the bending contribution (it was shown in (Dimitrovová, 1997) that it is small and it is not well defined since it varies for different optimal media) and that s in G_+^* is expressed from a simplified relation. For the optimal medium derived in (Dimitrovová, 1997) and for $s = 0.3$ the increase in G_+^* due to the bending contribution is five percent (it is little different for another cross-sectional shape) and the increase due to the higher-order terms in s is 22 percent; the curve with both nonlinear effects, ${}^{GEN}G_+^*$, is also included in Fig. 4. Second, recent experimental data for G^* in (Gibson and Ashby, 1988) are available only for $s \in [0.01, 0.03]$. The extension of ${}^{GA}G^*$ from low values of s (where it reflects only the bending response) to high values of s neglects the axial contribution, which now becomes more important. It would make the curve representing G^* more straight and lower, see (Dimitrovová, 1997). Moreover, for high values of s, ${}^{GA}G^*$ coincides with the data for closed-cell foams, which are generally stiffer. As regards the other data presented in (Gibson and Ashby, 1988) as data of open-cell foams, G^* could be calculated from the data of Young's modulus and Poisson's ratio obtained by Gent and Thomas (1959). Such values follow the curve ${}^{GA}G^*$. Gent and Thomas' data are for $s \in [0.1, 1]$. Close to $s = 1$, when the specimens are not any more cellular, the significance of the data is questionable in our context. Also, no photographs are shown in Gent and Thomas (1959), the specimens for s close to 0.3 may be partly closed-cell foams, since the data basically coincide with other data of closed-cell foams.

Other comments are related to the paper by Warren and Kraynik (1988). The first example there, the tetrahedral lattice (superscript TET), is MRO composed of repeated elements (Fig. 3). Meso-properties are calculated (for an arbitrarily rotated element) under uniform boundary strain applied at the center of the strut cross sections and under no restriction on cross-sectional rotations. Repeated elements are self-equilibrated, but it is difficult to justify the equilibrium between neighboring ones. Meso-properties thus correspond to some upper estimate. The final result in (Warren and Kraynik, 1988) is in fact G_V^{TET}, which should not be presented as the actual response. Also the calculation could be reduced by calculating the meso-properties with respect to some fixed coordinates and then introducing them into (9). $\mathbf{C}^{\mathrm{TET}}$ does not possess cubic symmetry, thus specific bounds from (22) are not applicable, but $K_V^{\mathrm{TET}} = K_R^{\mathrm{TET}}$. Two specific bounds G_V^{TET} and G_R^{TET} are compared in Fig. 6 with a function for open-cell foams with mainly bending response proposed in (Christensen, 1994), ${}^{c}G^* = 9s^2/40$, and with four specific bounds (superscript CUB) related to the second example in (Warren and Kraynik, 1988), where OPM is the regular cubic lattice (Fig. 2). Boundary conditions of the kind described above incidentally coincide with the periodicity boundary conditions, however, again only G_V^{CUB} (its linearization coincides with G_+^*) is presented in (Warren and Kraynik, 1988). It is seen from Fig. 6 that G_V^{TET} and G_R^{TET} are quite close and that ${}^{c}G^*$ (which was also fitted to experimental data) shows an excellent agreement with them. It can be thus concluded that the tetrahedral lattice is a very good model for an open-cell foam representation. The distance between the other four specific bounds is very large ($G_{\mathrm{HS}+}^{\mathrm{CUB}}$ and $G_{\mathrm{HS}-}^{\mathrm{CUB}}$ provide a significant improvement of G_V^{CUB} and G_R^{CUB}), since ${}^{1}G^{\mathrm{OPM}}$ expresses only axial response, while ${}^{2}G^{\mathrm{OPM}}$ expresses only bending response. In the specific bounds the axial response becomes the essential one, since the curves are almost straight. It is seen that in this case the estimate of the actual response by G_V^{CUB} could lead to a significant discrepancy. Thus a proper understanding of the results is very important.

To conclude the comparative remarks, we also show some two-dimensional examples in order to justify the specific bounds (21) proved in Section 4. Related OPM are the following: the regular square, the square with two obliques and the diamond lattices (Fig. 7; basic cells are marked by bold lines). In Fig. 8 the specific bounds (superscripts SQU, OBL, and DIA) are compared with the linearized upper bound $G_+^* = s/8$ (Dimitrovová and Faria, 1999). Since the square with two obliques (strong medium) and the diamond lattice (soft medium) are "almost" effectively isotropic, the specific bounds practically coincide and in Fig. 8 only $G_{\mathrm{HS}+}^{\mathrm{OBL}}$ and $G_{\mathrm{HS}+}^{\mathrm{DIA}}$ are plotted. The regular square lattice possesses a high level of anisotropy, which justifies the distances between the four specific bounds (Fig. 8). As was found for the three-dimensional analog of this medium, G_V^{SQU} in its linearized form coincides with G_+^*.

6 Conclusions

In this paper a simple and practical way of expressing effective elastic constants of MRO in the form of specific bounds is proposed. The distances between the specific bounds depend on the level of the OPM anisotropy. Several examples of open-cell foams where the specific bounds can be expressed in an explicit analytical form were shown. From the three-dimensional examples we conclude that: (i) the proposed function in Gibson and Ashby (1988) should reflect the axial response of open-cell foams for higher relative densities and should be slightly lower there; (ii) the basic cell of the nonaligned lattice taken as an original cell forms a very soft MRO medium, which is not convenient to use as a general characterization; (iii) the tetrahedral lattice, with very close specific bounds (permitting a good estimate of the actual response) provides a very good model for open-cell foam characterization; (iv) MRO with OPM with a high level of anisotropy cannot be characterized by the specific Voigt bound. This is also the reason why we provided improvements of specific Voigt and Reuss bounds in two-dimensional case, for MRO with effectively square symmetric OPM, which is a common property of many two-dimensional media. As an additional result, related to Dimitrovová (1997) and Dimitrovová and Faria (1999), we found two more G^*-optimal media, namely, MRO with OPM as the regular cubic or square lattice.

The simplifying assumptions stated in the beginning of Section 2 are not inevitable for the proposed methodology; thus an extension of the methodology to more general composites can be developed.

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