

MICROMECHANICS AND HOMOGENIZATION

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**Materials Containing Coated and Uncoated  
Spherical Inhomogeneities**

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Václav Nežerka, 2012

## **Acknowledgement**

I would like to thank my supervisor, Jan Zeman, who supported me, introduced me to the issues of micromechanics and explained me patiently everything I needed.

# Contents

<b>I</b>	<b>Theoretical Background</b>	<b>1</b>
<b>1</b>	<b>Elasticity Equations</b>	<b>2</b>
1.1	Strain-to-Displacement Relations . . . . .	2
1.2	Equilibrium Equations . . . . .	4
1.3	Constitutive Relations . . . . .	5
<b>2</b>	<b>Volumetric and Deviatoric Components</b>	<b>8</b>
2.1	Hydrostatic and Deviatoric Stresses . . . . .	8
2.2	Volumetric and Deviatoric Strains . . . . .	9
2.3	Constitutive Relations . . . . .	9
2.3.1	Lamé’s Constants . . . . .	10
2.3.2	Tensorial Notation . . . . .	12
2.3.3	Engineering Notation . . . . .	13
<b>3</b>	<b>Stiffness Homogenization</b>	<b>14</b>
3.1	Basic Assumptions . . . . .	14
3.1.1	Representative Volume Element . . . . .	14
3.1.2	Inhomogeneities . . . . .	14
3.1.3	Averaging . . . . .	15
3.2	Energy methods . . . . .	16
3.2.1	Voigt and Reuss Bounds . . . . .	16
3.3	Eigenstrain . . . . .	18
3.4	Dilute (Non-Interacting) Defect Distribution . . . . .	19
3.5	Mori-Tanaka Model . . . . .	20
<b>4</b>	<b>Homogenization with Coated Particles</b>	<b>22</b>
4.1	Dilute Concentration Factors by Herve-Zaoui Scheme . . . . .	22
4.1.1	Volumetric Part . . . . .	22

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4.1.2	Deviatoric Part . . . . .	23
4.2	Modification of Mori-Tanaka Model . . . . .	23
<b>5</b>	<b>Strength Estimation</b>	<b>24</b>
5.1	Quadratic Strain Averages . . . . .	24
<b>II</b>	<b>Appendix</b>	<b>26</b>
<b>A</b>	<b>Herve-Zaoui Solution</b>	<b>27</b>
A.1	Volumetric Part . . . . .	27
A.2	Deviatoric Part . . . . .	27

# Introduction

In this work the basic homogenization techniques and micromechanical modeling strategies are discussed with an emphasis on a practical (engineering) application without any comprehensive theoretical background. In particular, the work is aimed at the homogenization of cementitious materials and mortars, where the microstructure on the micro- and meso-level can be approximated by spherical inhomogeneities with coating (those that chemically react and create various hydration products) and without coating (inert materials, e.g. sand, and voids). Several works proved that the discussed homogenization techniques can be used for concretes and mortars.

Several works, [1], [2] and [3], provided an inspiration for the development of micromechanical models. These works exploit the Mori-Tanaka method ([4] and [5]) to estimate the effective stiffness of a composite. Pichler et al. [1] estimated the mortar strength assuming that only the deviatoric stress is responsible for a failure of the material, therefore the quadratic average of the deviatoric stress in the lime matrix was chosen as an adequate indicator for the determination of mortar strength. Even though there are a few simplifications in these models, the results in [1], [2] and [3] quite well correspond to the available experimental data.

# **Part I**

## **THEORETICAL BACKGROUND**

# Chapter 1

## Elasticity Equations

The governing equations of elasticity involve displacement, strain and stress fields, and they are valid if the structure undergoes only small deformations and the material behaves in a linearly elastic manner. Scheme of the overall system appears summarized in Fig. 1.1.

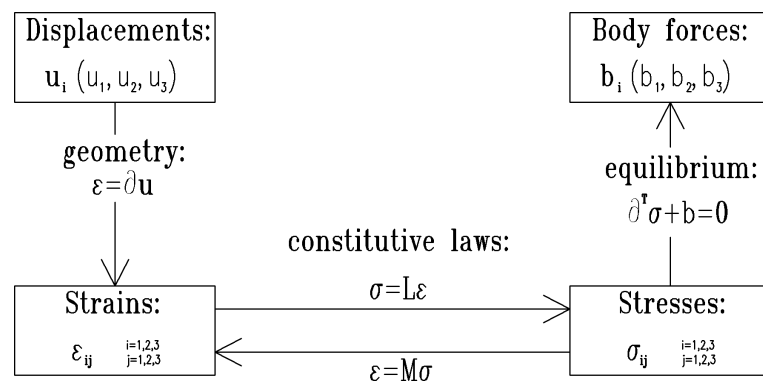


Figure 1.1: Diagram describing relationship between displacements, strains, stresses and body forces

### 1.1 Strain-to-Displacement Relations

The displacements of the points within an elastic body are described by three components  $(u, v, w)$  or  $(u_1, u_2, u_3)$ , all of them dependent on the position in the Cartesian coordinate system  $(x, y, z)$  or  $(x_1, x_2, x_3)$ . In a matrix notation, the displacements are arranged in a vector as follows:

$$\mathbf{u}(\mathbf{x}) = \begin{pmatrix} u_1(x_1, x_2, x_3) \\ u_2(x_1, x_2, x_3) \\ u_3(x_1, x_2, x_3) \end{pmatrix} \quad (1.1)$$

while in the index notation, the field of displacements can be described as  $u_i(x_j)$ , where  $i = 1, 2, 3$  and  $j = 1, 2, 3$ .

Strains describe the deformation of the body and here only infinitesimal strains are dealt with. At a point, the stretching, e.g. in the  $x$ -direction, can be seen as the differential displacement per unit

length. The  $x$ -component of strain is then

$$\varepsilon_x = \lim_{\Delta x \rightarrow 0} \frac{\Delta u(x, y, z)}{\Delta x} = \frac{\partial u}{\partial x} \quad (1.2)$$

and therefore, the normal strain can be understood as a displacement gradient. The distortion of the material, which can be described as the change in originally right angles, is the sum of tilts imparted to vertical and horizontal lines (also called engineering strain):

$$\gamma_{xy} = \gamma_1 + \gamma_2 \approx \tan \gamma_1 + \tan \gamma_2 = \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \quad (1.3)$$

For other displacement gradients  $\varepsilon_y$ ,  $\varepsilon_z$  and distortions  $\gamma_{yz}$ ,  $\gamma_{zx}$  the same reasoning can be applied with cyclic change of coordinates  $x \rightarrow y \rightarrow z \rightarrow x$  and displacements  $u \rightarrow v \rightarrow w \rightarrow u$ .

The strain is a second order tensor and therefore the components can be arranged in a matrix form as

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x & 1/2 \gamma_{xy} & 1/2 \gamma_{xz} \\ 1/2 \gamma_{yx} & \varepsilon_y & 1/2 \gamma_{yz} \\ 1/2 \gamma_{zx} & 1/2 \gamma_{zy} & \varepsilon_z \end{pmatrix} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix} \quad (1.4)$$

where, in the tensorial notation, shear strains (distortions) are halves of the engineering strains (e.g.  $\gamma_{12} = 1/2 \gamma_{xy}$ ).

The index notation provides a compact description of all the components of three-dimensional states of strain:

$$\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (1.5)$$

where the comma denotes differentiation with respect to the following spatial variable (partial derivative). This double-subscript index notation leads naturally to a matrix arrangement of the strain components, in which the  $i$ - $j$  component of the strain becomes the matrix element in the  $i^{\text{th}}$  row and the  $j^{\text{th}}$  column. Since the strain tensor is symmetric, i.e.  $\varepsilon_{ij} = \varepsilon_{ji}$ , there are six rather than nine independent strains. In the symbolic notation the strain-displacement relationship can be expressed as  $\boldsymbol{\varepsilon} = \nabla_s \mathbf{u}$ .

Sometimes it is convenient to arrange the strain components in a vector, or rather pseudovector. Because strain is actually a 2<sup>nd</sup> order tensor, like stress or moment of inertia, it has mathematical properties very different from those of vectors. That must be taken into account while transforming or calculating the norm of strain. The ordering of the elements in the pseudovector is arbitrary, but it is conventional to list them in order (1, 1), (2, 2), (3, 3), (2, 3), (1, 3), (1, 2) [6]. This arrangement yields so-called Voigt notation.

Following the rules of a matrix multiplication, the strain pseudovector can also be written in terms of the displacement vector and a proper operator. The strain-displacement relationship can be



expressed as  $\boldsymbol{\varepsilon} = \boldsymbol{\partial}\mathbf{u}$ :

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} \quad (1.6)$$

In so-called Mandel notation, the components of strain are arranged in the pseudovector and the shear components of strain tensor are multiplied by  $\sqrt{2}$  as follows:

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2} \varepsilon_{23} \\ \sqrt{2} \varepsilon_{13} \\ \sqrt{2} \varepsilon_{12} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ 0 & \frac{\sqrt{2}}{2} \frac{\partial}{\partial z} & \frac{\sqrt{2}}{2} \frac{\partial}{\partial y} \\ \frac{\sqrt{2}}{2} \frac{\partial}{\partial z} & 0 & \frac{\sqrt{2}}{2} \frac{\partial}{\partial x} \\ \frac{\sqrt{2}}{2} \frac{\partial}{\partial y} & \frac{\sqrt{2}}{2} \frac{\partial}{\partial x} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} \quad (1.7)$$

Such arrangement brings simplifications to many operations.

## 1.2 Equilibrium Equations

The force equilibrium on an infinitesimal cube results in the following equations (Cauchy's equations):

$$\begin{aligned} \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + b_x &= 0 \\ \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + b_y &= 0 \\ \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \sigma_z}{\partial z} + b_z &= 0 \end{aligned} \quad (1.8)$$

where  $b_i$  are body forces, such as gravity. By a closer observation it can be seen that the previous equation can be expressed in compact a matrix-pseudovector form as  $\partial^T \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}$ . The Cauchy's equation can be also written using the index notation as

$$\sigma_{ij,j} + b_i = 0 \quad (1.9)$$

and in the symbolic notation as  $\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}$ , where the stress tensor can be visualized by a matrix as

$$\boldsymbol{\sigma} = \sigma_{ij} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \quad (1.10)$$

and is also symmetric (because of a moment equilibrium on the infinitesimal cube). The element in the  $i^{\text{th}}$  row and the  $j^{\text{th}}$  column of this matrix is the stress on the  $i^{\text{th}}$  face in the  $j^{\text{th}}$  direction.

On the body surface the equilibrium of internal stress and surface traction acting on the boundary can be expressed by the Cauchy's formula. The traction  $\mathbf{t}$  is associated with any plane characterized by its normal  $\mathbf{n}$  and can be understood as a stress on the surface of the body. Therefore the static boundary conditions can be written as  $\mathbf{n} \cdot \boldsymbol{\sigma} = \bar{\mathbf{t}}$  where  $\bar{\mathbf{t}}$  is the prescribed traction (applied stress) at the boundary  $\Gamma_t$  and  $\mathbf{n}$  contains the multiples of the cosine angles between the investigated plane and coordinate system (it is a projection onto the coordinate axes).

### 1.3 Constitutive Relations

The previous sections deal only with the kinematics (geometry) and the static equilibrium of the body; however, they do not provide insight on the role of the material itself. The kinematic equations relate strains to displacement gradients, and the equilibrium equations relate stress to the applied tractions on loaded boundaries and also provide the relations among stress gradients within the material. More equations, relating the stresses to strains are needed, and these are provided by the material's constitutive relations [6]. In this section, only isotropic elastic materials are dealt with.

In the general case of a linear relation between components of the strain and stress tensors, we might propose a statement of the form:

$$\sigma_{ij} = L_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^t) \quad (1.11)$$

where  $L_{ijkl}$  is a 4<sup>th</sup> order tensor and  $\varepsilon_{kl}^t$  is the initial (or eigen / stress-free) strain. Because the indices  $kl$  do not appear in the equation after summation, they are called "dummy indices". Previous expression constitutes a sequence of nine equations, since each component of  $\sigma_{ij}$  is a linear combination of all the components of  $\varepsilon_{kl}$ . For instance

$$\sigma_{23} = L_{2311}\varepsilon_{11} + L_{2312}\varepsilon_{12} + \dots + L_{2333}\varepsilon_{33} \quad (1.12)$$

Based on each of the indices of  $L_{ijkl}$  taking on values from 1 to 3, we might expect 81 independent components in  $\mathbf{L}$ . However, both the stress tensor and the strain tensor are symmetric ( $\sigma_{ij} = \sigma_{ji}$  and  $\varepsilon_{ij} = \varepsilon_{ji}$ ), we must also have  $L_{ijkl} = L_{ijlk}$  and  $L_{ijkl} = L_{jikl}$ . These relations are called minor symmetries. The major symmetry of the stiffness tensor is expressed as  $L_{ijkl} = L_{klij}$ . This reduces

the number of components in  $\mathbf{L}$  to 36, as can be seen from a linear relation between the pseudovector forms of the strain and stress [6]:

$$\begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{yz} \\ \tau_{xz} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} & \cdots & L_{16} \\ L_{21} & L_{22} & \cdots & L_{26} \\ \vdots & \vdots & \ddots & \vdots \\ L_{61} & L_{62} & \cdots & L_6 \end{pmatrix} \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{pmatrix} \quad (1.13)$$

or, using the Mandel notation:

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{12} \end{pmatrix} = \begin{pmatrix} L_{1111} & L_{1122} & L_{1133} & \sqrt{2}L_{1123} & \sqrt{2}L_{1113} & \sqrt{2}L_{1112} \\ L_{2211} & L_{2222} & L_{2233} & \sqrt{2}L_{2223} & \sqrt{2}L_{2213} & \sqrt{2}L_{2212} \\ L_{3311} & L_{3322} & L_{3333} & \sqrt{2}L_{3323} & \sqrt{2}L_{3313} & \sqrt{2}L_{3312} \\ \sqrt{2}L_{2311} & \sqrt{2}L_{2322} & \sqrt{2}L_{2333} & 2L_{2323} & 2L_{2313} & 2L_{2312} \\ \sqrt{2}L_{1311} & \sqrt{2}L_{1322} & \sqrt{2}L_{1333} & 2L_{1323} & 2L_{1313} & 2L_{1312} \\ \sqrt{2}L_{1211} & \sqrt{2}L_{1222} & \sqrt{2}L_{1233} & 2L_{1223} & 2L_{1213} & 2L_{1212} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{13} \\ \sqrt{2}\varepsilon_{12} \end{pmatrix} \quad (1.14)$$

It can be shown that the  $\mathbf{L}$  matrix in this form is also symmetric and therefore it contains only 21 independent elements. If the material exhibits symmetry in its elastic response, the number of independent elements in the  $\mathbf{L}$  matrix can be further reduced. In the simplest case of an isotropic material, having the same stiffness in all directions, only two elements are independent - for example Young's modulus ( $E$ ) and Poisson's ratio ( $\nu$ ). From these, so-called shear modulus can be calculated:

$$G = \frac{E}{2(1 + \nu)} \quad (1.15)$$

If a body is loaded by the stress  $\sigma_x$ , the resulting deformation in  $x$ -direction is  $\varepsilon_x = \sigma_x/E$  and the other normal components of strain are  $\varepsilon_y = \varepsilon_z = -\nu\varepsilon_x = -\nu\sigma_x/E$ . In the general stress-state, the other normal strain components are derived analogically (but the material must be isotropic):

$$\varepsilon_x = \frac{1}{E}(\sigma_x - \nu\sigma_y - \nu\sigma_z) \quad (1.16a)$$

$$\varepsilon_y = \frac{1}{E}(-\nu\sigma_x + \sigma_y - \nu\sigma_z) \quad (1.16b)$$

$$\varepsilon_z = \frac{1}{E}(-\nu\sigma_x - \nu\sigma_y + \sigma_z) \quad (1.16c)$$

In case of isotropic material, each shear deformation is proportional to the corresponding shear stress with the constant of proportionality  $1/G$ :

$$\gamma_{xy} = \frac{\tau_{xy}}{G} = \frac{2(1 + \nu)}{E}\tau_{xy} \quad (1.17a)$$

$$\gamma_{xz} = \frac{\tau_{xz}}{G} = \frac{2(1 + \nu)}{E}\tau_{xz} \quad (1.17b)$$

$$\gamma_{yz} = \frac{\tau_{yz}}{G} = \frac{2(1 + \nu)}{E}\tau_{yz} \quad (1.17c)$$

The six above equations can be written in the matrix form as

$$\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{13} \\ \varepsilon_{12} \end{pmatrix} = \frac{1}{E} \begin{pmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1+\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1+\nu \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} \quad (1.18)$$

which can be written in a compact form as

$$\boldsymbol{\varepsilon} = \mathbf{M}\boldsymbol{\sigma} \quad (1.19)$$

where  $\mathbf{M}$  is the elastic compliance matrix. However, if the Mandel notation is used (which is necessary in some applications) the last 3 diagonal terms in the compliance matrix must be divided by 2. By inversion of  $\mathbf{M}$ , we get the generalized Hook's law:

$$\boldsymbol{\sigma} = \mathbf{M}^{-1}\boldsymbol{\varepsilon} = \mathbf{L}\boldsymbol{\varepsilon} \quad (1.20)$$

where

$$\mathbf{L} = \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-2\nu \end{pmatrix} \quad (1.21)$$

is the elastic stiffness matrix of an isotropic material. In the Mandel notation the last 3 diagonal terms must be multiplied by 2 (see equation (1.14)).

Table 1.1: Summary of basic elasticity equations

equations	tensorial form		engineering form	domain
	index notation	symbolic notation		
kinematic	$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$	$\boldsymbol{\varepsilon} = \nabla_s \mathbf{u}$	$\boldsymbol{\varepsilon} = \boldsymbol{\partial} \mathbf{u}$	volume $\Omega$
constitutive	$\sigma_{ij} = L_{ijkl} \varepsilon_{kl}$	$\boldsymbol{\sigma} = \mathbf{L} : \boldsymbol{\varepsilon}$	$\boldsymbol{\varepsilon} = \mathbf{L} \boldsymbol{\varepsilon}$	volume $\Omega$
static	$\sigma_{ij,j} + \bar{b}_i = 0$	$\nabla \cdot \boldsymbol{\sigma} + \bar{\mathbf{b}} = \mathbf{0}$	$\boldsymbol{\partial}^T \boldsymbol{\sigma} + \bar{\mathbf{b}} = \mathbf{0}$	volume $\Omega$
kinematic b.c.	$u_i = \bar{u}_i$	$\mathbf{u} = \bar{\mathbf{u}}$	$\mathbf{u} = \bar{\mathbf{u}}$	surface $\Gamma_u$
static b.c.	$\sigma_{ij} n_j = \bar{t}_i$	$\mathbf{n} \cdot \boldsymbol{\sigma} = \bar{\mathbf{t}}$	$\mathbf{n} \boldsymbol{\sigma} = \bar{\mathbf{t}}$	surface $\Gamma_t$

## Chapter 2

# Volumetric and Deviatoric Components

### 2.1 Hydrostatic and Deviatoric Stresses

A state of hydrostatic compression is the one in which no shear stresses exist and where all the normal stresses are equal. For this stress state it is obviously true that

$$\sigma_m = \frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3} = \frac{1}{3}\sigma_{kk} \quad (2.1)$$

This quantity (so called mean stress) is one third of invariant  $I_1$  (so called hydrostatic or volumetric stress), which is a reflection of hydrostatic pressure being the same in all directions, not varying with axis rotations. Then the volumetric stress-state is in matrix representation of the tensor  $\sigma_{ij}$  defined as follows:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_m & 0 & 0 \\ 0 & \sigma_m & 0 \\ 0 & 0 & \sigma_m \end{pmatrix} \quad (2.2)$$

The stress tensor is then composed of the volumetric part and the deviatoric part:

$$\sigma_{ij} = \frac{1}{3}\sigma_{kk}\delta_{ij} + s_{ij} \quad (2.3)$$

where the symbol  $\delta_{ij}$  is the Kronecker delta, which is defined as

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (2.4)$$

The hydrostatic stress state can be then represented by

$$\mathbf{s} = \begin{pmatrix} \sigma_{11} - \sigma_m & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} - \sigma_m & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} - \sigma_m \end{pmatrix} \quad (2.5)$$

The hydrostatic (volumetric) stress is related to the change of volume of a material during deformation, while the deviatoric part is responsible for the distortion. This concept is also convenient because the material responds to these stress components in very different ways. For instance, plastic and viscous behavior is caused dominantly by the distortional components, with the volumetric component causing only an elastic deformation [6].

The graphical representation of the stress tensor decomposition is shown in the following figure:

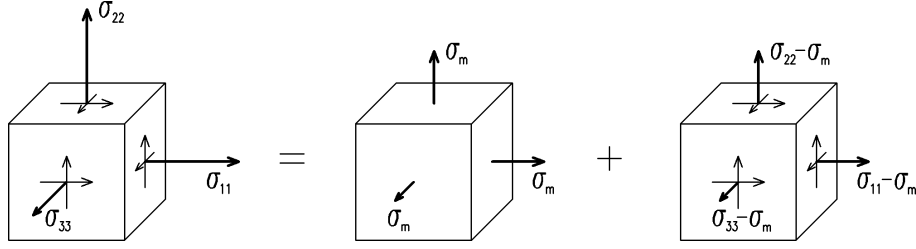


Figure 2.1: Decomposition of stress in volumetric and deviatoric parts

## 2.2 Volumetric and Deviatoric Strains

In a cubical element, originally of volume  $V = abc$ , subjected to normal strains in all three directions, the change in the element's volume is

$$\begin{aligned} \frac{\Delta V}{V} &= \frac{a'b'c' - abc}{abc} = \frac{a(1 + \varepsilon_x)b(1 + \varepsilon_y)c(1 + \varepsilon_z) - abc}{abc} = \\ &= (1 + \varepsilon_x)(1 + \varepsilon_y)(1 + \varepsilon_z) - 1 \approx \varepsilon_x + \varepsilon_y + \varepsilon_z \end{aligned} \quad (2.6)$$

where products of strains are neglected. The volumetric strain is therefore the sum of the diagonal elements in the strain tensor (also called trace of the matrix, or  $\text{Tr}(\varepsilon)$ ). In the index notation, this can be written simply as

$$\varepsilon_V = \frac{\Delta V}{V} = \varepsilon_{kk} \quad (2.7)$$

Similarly to the mean stress  $\sigma_m$ , the mean strain is calculated as

$$\varepsilon_m = \frac{\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}}{3} = \frac{1}{3}\varepsilon_{kk} \quad (2.8)$$

and the strain tensor can be then composed of the volumetric and deviatoric part:

$$\varepsilon_{ij} = \frac{1}{3}\varepsilon_{kk}\delta_{ij} + e_{ij} \quad (2.9)$$

The volumetric and deviatoric strain states can be represented by a matrix in a similar fashion as volumetric and deviatoric stress states, see. equations 2.2 and 2.5.

## 2.3 Constitutive Relations

Since  $\varepsilon_V$  is a relative change of volume, it must be independent of the coordinate system (therefore, it is so called invariant). The relation between volumetric strain and mean stress can be derived as follows:

$$\begin{aligned} \varepsilon_V &= \frac{1}{E}(\sigma_x - \nu\sigma_y - \nu\sigma_z) + \frac{1}{E}(-\nu\sigma_x + \sigma_y - \nu\sigma_z) + \frac{1}{E}(-\nu\sigma_x + \sigma_y - \nu\sigma_z) = \\ &= \frac{1 - 2\nu}{E}(\sigma_x + \sigma_y + \sigma_z) = \frac{3(1 - 2\nu)}{E} \frac{(\sigma_x + \sigma_y + \sigma_z)}{3} = \frac{\sigma_m}{K} \end{aligned} \quad (2.10)$$

where

$$K = \frac{E}{3(1 - 2\nu)} \quad (2.11)$$

is so called bulk modulus connecting the mean volumetric stress  $\sigma_m$  with the volumetric strain  $\varepsilon_V$ . However, the volumetric change is proportional to the mean stress only in case of an isotropic material. Note that as  $\nu \rightarrow 0.5$ ,  $K \rightarrow \infty$ , which means that the material becomes infinitely stiff as the Poisson's ratio approaches 0.5. Values of the Poisson's ratio greater than 0.5 are not possible since such values imply that a tensile hydrostatic stress would cause a volumetric contraction.

The normal component of the deviatoric deformation  $e_x$  can be expressed as

$$\begin{aligned} e_x &= e_x - \varepsilon_m = \frac{1}{E}(\sigma_x - \nu\sigma_y - \nu\sigma_z) - \frac{1}{3K}\sigma_m = \\ &= \frac{1}{E}[(s_x + \sigma_m - \nu(s_y + \sigma_m) - \nu(s_z + \sigma_m))] - \frac{1 - 2\nu}{E}\sigma_m = \\ &= \frac{1}{E}(s_x - \nu s_y - \nu s_z) \end{aligned} \quad (2.12)$$

and since the sum of the deviatoric normal components is equal to zero:

$$\begin{aligned} s_x + s_y + s_z &= (\sigma_x - \sigma_m) + (\sigma_y - \sigma_m) + (\sigma_z - \sigma_m) = \sigma_x + \sigma_y + \sigma_z - 3\sigma_m = \\ &= 3\sigma_m - 3\sigma_m = 0 \end{aligned} \quad (2.13)$$

the following equality holds:

$$\nu s_x = -\nu s_y - \nu s_z \quad (2.14)$$

Therefore the relationship between the first components of the deviatoric stress and strain tensors can be express as

$$\nu e_x = \frac{1}{E}(s_x + \nu s_x) = \frac{1 + \nu}{E}s_x = \frac{s_x}{2G} \quad (2.15)$$

The same relation holds for the other normal components of the deviatoric strain tensor as well.

### 2.3.1 Lamé's Constants

For the diagonal terms in the strain tensor, for instance the strain  $\varepsilon_{11}$ , the strain-stress relationship can be expressed as

$$\varepsilon_{11} = \frac{1}{E}\sigma_{11} - \frac{1}{E}\nu(\sigma_{22} + \sigma_{33}) = \frac{1 + \nu}{E}\sigma_{11} - \frac{1}{E}\nu(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad (2.16)$$

which can be, using the index notation, for all normal strains expressed as

$$\varepsilon_{ij} = \frac{1 + \nu}{E}\sigma_{ij} - \frac{\nu}{E}\sigma_{kk} \quad \text{if } i = j \quad (2.17)$$

The shear components of the stress tensor, for instance the strain

$$\varepsilon_{12} = \frac{1 + \nu}{E} \sigma_{12} \quad (2.18)$$

can be, using the index notation, expressed generally as

$$\varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} \quad \text{if } i \neq j \quad (2.19)$$

The equations (2.17) and (2.19) can be written in a single expression by making use of the Kronecker delta, defined in equation (2.4):

$$\varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \frac{\nu}{E} \delta_{ij} \sigma_{kk} \quad (2.20)$$

The isotropic elasticity law can be decomposed into its volumetric and deviatoric parts,  $\sigma_{kk} = 3K\varepsilon_{kk}$  and  $s_{ij} = 2\mu e_{ij}$ . The required form of the stress-strain relationship (dependence of stress on strains), using so-called Lamé's constants  $\mu$  and  $\lambda$  has a form

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\delta_{ij}\varepsilon_{kk} \quad (2.21)$$

In order to establish the relationship between Lamé's constants, Young's modulus and Poisson's ratio, it is necessary to compare the two forms of the constitutive equations for an isotropic elastic material with equation (2.21). However, in order to make that comparison, the equations for strain-stress relationship must be inverted, because the previous equation expresses the stress components in terms of the strain components.

By simple arrangement, the following equation can be obtained:

$$\sigma_{kk} = \frac{E}{1 - 2\nu} \varepsilon_{kk} \quad (2.22)$$

and the whole equation (2.20) can be inverted:

$$\sigma_{ij} = \frac{E}{1 + \nu} \varepsilon_{ij} + \frac{E\nu}{(1 + \nu)(1 - 2\nu)} \delta_{ij} \varepsilon_{kk} \quad (2.23)$$

Therefore by comparison with equation (2.21), the Lamé's constants can be expressed as

$$\mu = G = \frac{E}{1 + \nu} \quad (2.24)$$

and

$$\lambda = \frac{E\nu}{(1 + \nu)(1 - 2\nu)} = K - \frac{2}{3}G \quad (2.25)$$

in terms of  $E$ ,  $\nu$ ,  $K$  and  $G$ .



Table 2.1: Relations between elastic constants

	basic pair of elastic constants			
	$\lambda, \mu$	$\mu, K$	$E, G$	$E, \nu$
$\lambda$	$\lambda$	$K - \frac{2}{3}\nu$	$\frac{G(E - 2G)}{3G - E}$	$\frac{E\nu}{(1 + \nu)(1 - 2\nu)}$
$\mu$	$\mu$	$\mu$	$G$	$\frac{E}{2(1 + \nu)}$
$K$	$\lambda + \frac{2}{3}G$	$K$	$\frac{GE}{3(3G - E)}$	$\frac{E}{3(1 - 2\nu)}$
$E$	$\frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}$	$\frac{9K\mu}{3K + \mu}$	$E$	$E$
$\nu$	$\frac{\lambda}{2(\lambda + \mu)}$	$\frac{3K - 2\mu}{2(3K + \mu)}$	$\frac{E}{2G} - 1$	$\nu$

### 2.3.2 Tensorial Notation

In the tensorial notation, there is needed the use of the unit fourth-order tensor,  $I_{ijkl}$ , having the components  $I_{ijkl} = \delta_{ik}\delta_{jl}$ , with Kronecker delta being called the unit second-order tensor. This tensor exhibits the major symmetry but not the minor symmetry, and it has the important property that  $\mathbf{I} : \boldsymbol{\epsilon} = \boldsymbol{\epsilon} : \mathbf{I} = \boldsymbol{\epsilon}$  for any second order tensor  $\boldsymbol{\epsilon}$  [7].

Sometimes it is useful to work with the symmetrized unit fourth-order tensor,  $\mathbf{I}_S$ , with components

$$I_{ijkl}^S = \frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} \quad (2.26)$$

This tensor exhibits the minor and major symmetries, but the identity  $\mathbf{I} : \boldsymbol{\epsilon} = \boldsymbol{\epsilon} : \mathbf{I} = \boldsymbol{\epsilon}$  holds only if the second-order tensor  $\boldsymbol{\epsilon}$  is symmetric [7].

Using the Lamé's constants, the stiffness tensor in linear isotropic elasticity can be expressed as

$$L_{ijkl}^e = \lambda\delta_{ik}\delta_{jl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad (2.27)$$

or in a symbolic notation as  $\mathbf{L}_e = \lambda\boldsymbol{\delta} \otimes \boldsymbol{\delta} + 2\mu\mathbf{I}_S$ . The generalized Hooke's law can be then presented as

$$\boldsymbol{\sigma} = \mathbf{L}_e : \boldsymbol{\epsilon} = \lambda\boldsymbol{\delta} \otimes \boldsymbol{\delta} : \boldsymbol{\epsilon} + 2\mu\mathbf{I}_S : \boldsymbol{\epsilon} = 3\lambda\boldsymbol{\delta}\varepsilon_m + 2\mu\mathbf{e} \quad (2.28)$$

where  $\varepsilon_m = 1/3 \boldsymbol{\delta} : \boldsymbol{\epsilon}$  is one third of the trace of the strain tensor, representing the relative change of volume as defined in Section 2.2. The volumetric part of the strain tensor is then  $\varepsilon_m\boldsymbol{\delta}$ , and when it is subtracted from the strain tensor, we obtain the deviatoric strain tensor:

$$\mathbf{e} = \boldsymbol{\epsilon} - \boldsymbol{\delta}\varepsilon_m = \boldsymbol{\epsilon} - \frac{1}{3}\boldsymbol{\delta} \otimes \boldsymbol{\delta} : \boldsymbol{\epsilon} = \left( \mathbf{I}_S - \frac{1}{3}\boldsymbol{\delta} \otimes \boldsymbol{\delta} \right) : \boldsymbol{\epsilon} = \mathbf{I}_D : \boldsymbol{\epsilon} \quad (2.29)$$

Therefore the deviatoric projection tensor is defined as

$$\mathbf{I}_D = \mathbf{I}_S - \frac{1}{3}\boldsymbol{\delta} \otimes \boldsymbol{\delta} \quad (2.30)$$

and the volumetric projection tensor as

$$\mathbf{I}_V = \frac{1}{3}\boldsymbol{\delta} \otimes \boldsymbol{\delta} \quad (2.31)$$

Then the volumetric-deviatoric decomposition of the strain tensor can be done as follows:

$$\boldsymbol{\varepsilon} = \mathbf{I}_S : \boldsymbol{\varepsilon} = (\mathbf{I}_V + \mathbf{I}_D) : \boldsymbol{\varepsilon} = \mathbf{I}_V : \boldsymbol{\varepsilon} + \mathbf{I}_D : \boldsymbol{\varepsilon} = \varepsilon_m \boldsymbol{\delta} + \mathbf{e} \quad (2.32)$$

and the stress tensor can be decomposed in the same way:

$$\boldsymbol{\sigma} = \mathbf{I}_S : \boldsymbol{\sigma} = (\mathbf{I}_V + \mathbf{I}_D) : \boldsymbol{\sigma} = \mathbf{I}_V : \boldsymbol{\sigma} + \mathbf{I}_D : \boldsymbol{\sigma} = \sigma_m \boldsymbol{\delta} + \mathbf{s} \quad (2.33)$$

The elastic stiffness tensor can be also decomposed into its volumetric and deviatoric part. Realizing that  $\boldsymbol{\delta} \otimes \boldsymbol{\delta} = 3\mathbf{I}_V$ , we can rewrite the stiffness tensor in the linear isotropic elasticity as

$$\begin{aligned} \mathbf{L}_e &= \lambda \boldsymbol{\delta} \otimes \boldsymbol{\delta} + 2\mu \mathbf{I}_S = 3\lambda \mathbf{I}_V + 2\mu(\mathbf{I}_V + \mathbf{I}_D) = (3\lambda + 2\mu)\mathbf{I}_V + 2\mu \mathbf{I}_D = \\ &= 3K \mathbf{I}_V + 2G \mathbf{I}_D \end{aligned} \quad (2.34)$$

because the coefficient  $(3\lambda + 2\mu)$  is recognized as three times bulk modulus  $K$  and  $\mu = G$  is the shear modulus (see Table 2.1). The generalized Hooke's law

$$\boldsymbol{\sigma} = \mathbf{L}_e : \boldsymbol{\varepsilon} = (3K \mathbf{I}_V + 2G \mathbf{I}_D) : \boldsymbol{\varepsilon} = 3K \mathbf{I}_V : \boldsymbol{\varepsilon} + 2G \mathbf{I}_D : \boldsymbol{\varepsilon} = 3K \varepsilon_m \boldsymbol{\delta} + 2G \mathbf{e} \quad (2.35)$$

can be split into the volumetric and deviatoric part:

$$\sigma_m = 3K \varepsilon_m \quad \text{and} \quad \mathbf{s} = 2G \mathbf{e} \quad (2.36)$$

### 2.3.3 Engineering Notation

While the tensorial notation is useful in theoretical derivations, for developing a numerical algorithm that should be implemented into a computer code, it is more convenient to store the stress and strain components in one-dimensional arrays (pseudovectors) and stiffness moduli in matrices [7]. However, the double contraction of stress tensor  $\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}$  used for calculation of norm or strain energy density is equal to the pseudovector multiplication  $\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}$  only if the shear components in the pseudovector are multiplied by the factor of  $\sqrt{2}$ , i.e. using the Mandel notation (see section 1.14). The same holds for the norm of stress tensor. For the purpose of the volumetric-deviatoric decomposition, the engineering counterpart of the unit second-order tensor (Kronecker delta) is established as  $\boldsymbol{\delta} = (1 \ 1 \ 1 \ 0 \ 0 \ 0)^T$ . Then the volumetric-deviatoric decomposition is in the engineering notation based on projection matrices

$$\mathbf{I}_V = \frac{1}{3}\boldsymbol{\delta}\boldsymbol{\delta}^T \quad \text{and} \quad \mathbf{I}_D = \mathbf{I} - \frac{1}{3}\boldsymbol{\delta}\boldsymbol{\delta}^T \quad (2.37)$$

with  $\mathbf{I}$  representing the identity matrix. Using the Mandel notation, the elastic stiffness matrix can be simply expressed by means of the volumetric and deviatoric projection matrices as  $\mathbf{L}_e = 3K \mathbf{I}_V + 2G \mathbf{I}_D$ .

## Chapter 3

# Stiffness Homogenization

Many materials are inhomogeneous, i.e., they consist of dissimilar constituents (phases) that are distinguishable at some small length scale. The behavior of inhomogeneous materials is determined, on the one hand, by the relevant material properties of the constituents and, on the other hand, by their geometry and topology (phase arrangement) [8].

A macroscopically homogeneous material may have a heterogeneous microstructure at the microscopic level. Under certain conditions, the material can be described at the macroscopic level as homogeneous with spatially constant effective properties. This means that the microstructure is averaged; this micro-to-macro transition is called homogenization

### 3.1 Basic Assumptions

Defects in an elastic material give rise to inhomogeneous stress and strain fields by which the defects can be characterized. Equivalence between an inhomogeneous material and some homogeneous material with a certain eigenstrain or eigenstress distribution can be established [8].

Instead of modeling a material with its microstructure (texture) it is much more efficient to consider the material as homogenous, having some effective (macroscopic) properties. In this case the modeled body has to be large enough to include all inhomogeneities and avoid influence of local fields by their averaging.

#### 3.1.1 Representative Volume Element

The suitable volume for homogenization is called "representative volume element" (RVE). The representative volume element must be big enough to include enough inhomogeneities (statistically homogeneous distribution of the defects or heterogeneities), but small enough to have the stresses and strains within the RVE uniform (size with respect to the analyzed detail of a structure).

#### 3.1.2 Inhomogeneities

The term inhomogeneity is understood as an inclusion of a material embedded in a matrix, having different material properties from those of the matrix. Inhomogeneities are instead of eigenstrains in

a homogeneous material characterized by inhomogeneous, i.e., spatially varying, material properties are called inhomogeneities.

In analytical (mean-field) methods we first describe these defects by an equivalent eigenstrain in some homogeneous comparison material in order to then apply again Eshelby's result [9] (see Section 3.3). This strategy involves replacing an actual perfectly bounded inhomogeneity (superscript  $(r)$ ), subjected to the eigenstrain  $\varepsilon^t$ , with an equivalent (fictitious) homogeneous inclusion subjected to the equivalent eigenstrain. This equivalent eigenstrain must be chosen in such a way, that the inhomogeneity and the equivalent homogeneous inclusion attain the same stress state  $\sigma^{(r)}$  and the same constrained strain [10].

### 3.1.3 Averaging

The macro-stresses and macro-strains, which characterize the mechanical state of the macroscopic material point, are defined as the volumetric averages of the microscopic fields, e.g.

$$\langle \sigma_{ij} \rangle = \Sigma_{ij} = \frac{1}{|\Omega|} \int_{\Omega} \sigma_{ij} \, d\mathbf{x} \quad (3.1)$$

In case of the effective (average) stress in the volume  $\Omega$ . The macro-strains are calculated then in a similar fashion as

$$\langle \varepsilon_{ij} \rangle = E_{ij} = \frac{1}{|\Omega|} \int_{\Omega} \varepsilon_{ij} \, d\mathbf{x} \quad (3.2)$$

Often a volume  $\Omega$  of a heterogeneous material consists of  $n$  subdomains and a matrix with volume fractions

$$c^{(r)} = \frac{|\Omega^{(r)}|}{|\Omega|} \quad (3.3)$$

where  $r = 0, \dots, n$ , with  $r = 0$  representing the matrix itself. Obviously then

$$\sum_{r=0}^n c^{(r)} = 1 \quad (3.4)$$

if the inclusion (inhomogeneity) properties are piecewise constant. In case of such microstructure, consisting of discrete phases, we have

$$\Sigma_{ij} = \sum_{r=0}^n c^{(r)} \Sigma_{ij}^{(r)} \quad (3.5)$$

since

$$\begin{aligned} \Sigma_{ij} &= \frac{1}{|\Omega|} \int_{\Omega} \sigma_{ij} \, d\mathbf{x} = \frac{1}{|\Omega|} \left( \sum_{r=0}^n \int_{\Omega^{(r)}} \sigma_{ij} \, d\mathbf{x} \right) = \frac{1}{|\Omega|} \left( \frac{|\Omega^{(r)}|}{|\Omega^{(r)}|} \sum_{r=0}^n \int_{\Omega^{(r)}} \sigma_{ij} \, d\mathbf{x} \right) = \\ &= \sum_{r=0}^n c^{(r)} \Sigma_{ij}^{(r)} \end{aligned} \quad (3.6)$$

and analogously for the strains it hold that

$$E_{ij} = \sum_{r=0}^n c^{(r)} E_{ij}^{(r)} \quad (3.7)$$

which means that the total stress (or strain) is the sum of phase stress (or strain) with the weight  $c^{(r)}$ .

## 3.2 Energy methods

Unlike in case of analytical solutions, the energy methods are used for the determination of an exact range within which the effective properties of a heterogeneous material are located. The derivation is based on extremum principles of the elasticity theory which allow to derive strict upper and lower bounds for the effective properties from energetic expressions [9].

### 3.2.1 Voigt and Reuss Bounds

The advantage of Voigt and Reuss bounds is that they are easy to calculate and can be considered as the upper and lower bounds for the effective elastic properties of a heterogeneous material. This can be shown from the principle of minimum potential energy, stating that among all kinematically admissible strain fields the true strains attain the one having the minimum potential energy [9].

In a homogeneous material, the boundary conditions lead to homogeneous (spatially constant) stress and strain fields. The simplest approximation is to assume the micro-fields to be constant, in accordance with the boundary conditions [9]. The first possibility is to prescribe linear displacements at the boundary  $\mathbf{u}|_{\Gamma} = \mathbf{E} \cdot \mathbf{x}$  and therefore  $\mathbf{E} = \text{const.} = \langle \boldsymbol{\varepsilon} \rangle$ . The second possibility is loading by uniform tractions at the boundary  $\mathbf{t}|_{\Gamma} = \boldsymbol{\Sigma} \cdot \mathbf{n}$  where  $\boldsymbol{\Sigma} = \text{const.} = \langle \boldsymbol{\sigma} \rangle$ .

These approximations are exact only in one-dimensional special cases of different materials arranged "in parallel" (Voigt) or "in series" (Reuss). Despite obvious deficiencies, the simple approximations by Voigt and Reuss bear the advantage that they yield exact bounds for the true effective elastic constants of a heterogeneous material.

If the displacements are prescribed along the entire boundary of a volume  $\Omega$ , the potential of the boundary loads vanishes (the body does not move) and the total potential energy (or internal energy) of a kinematically admissible strain field  $\hat{\boldsymbol{\varepsilon}}$  can be expressed as

$$\hat{\Pi}(\hat{\boldsymbol{\varepsilon}}) = \frac{1}{2} \int_{\Omega} \hat{\boldsymbol{\varepsilon}} : \mathbf{L} : \hat{\boldsymbol{\varepsilon}} \, d\Omega = \frac{\Omega}{2} \langle \hat{\boldsymbol{\varepsilon}} : \mathbf{L} : \hat{\boldsymbol{\varepsilon}} \rangle \quad (3.8)$$

In case of prescribed displacement on the boundary, the strain energy according to the Hill's lemma, expressing the equality between the average strain energy density  $\langle W_e \rangle$  in the RVE by means of the microscopic or macroscopic quantities [9]:

$$\langle W_e \rangle = \frac{1}{2} \langle \boldsymbol{\varepsilon} : \mathbf{L} : \boldsymbol{\varepsilon} \rangle = \frac{1}{2} \langle \boldsymbol{\varepsilon} \rangle : \mathbf{L}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle = \frac{1}{2} \mathbf{E} : \mathbf{L}^{\text{eff}} : \mathbf{E} \quad (3.9)$$

is  $\Pi(\boldsymbol{\varepsilon}) = \frac{\Omega}{2} \langle \boldsymbol{\varepsilon} \rangle : \mathbf{L}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle$ . From the extremum principle (we seek for the minimum) stating that  $\hat{\Pi}(\hat{\boldsymbol{\varepsilon}}) \geq \Pi(\boldsymbol{\varepsilon})$  it follows that

$$\langle \hat{\boldsymbol{\varepsilon}} : \mathbf{L} : \hat{\boldsymbol{\varepsilon}} \rangle \geq \langle \boldsymbol{\varepsilon} \rangle : \mathbf{L}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle \quad (3.10)$$

for all strain fields  $\hat{\boldsymbol{\varepsilon}}$  that satisfy the boundary condition (prescribed displacements). In the Voigt approximation the strain field is given by  $\mathbf{E} = \text{const.} = \langle \boldsymbol{\varepsilon} \rangle$  and insertion into equation (3.10) yields

$$\langle \boldsymbol{\varepsilon} \rangle : \langle \mathbf{L} \rangle : \langle \boldsymbol{\varepsilon} \rangle \geq \langle \boldsymbol{\varepsilon} \rangle : \mathbf{L}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle \quad (3.11)$$

or

$$\langle \boldsymbol{\varepsilon} \rangle : (\langle \mathbf{L} \rangle - \mathbf{L}^{\text{eff}}) : \langle \boldsymbol{\varepsilon} \rangle \geq 0 \quad (3.12)$$

Because of the quadratic form of  $\langle \varepsilon \rangle$ , the average elasticity tensor  $\langle \mathbf{L} \rangle$  is larger than  $\mathbf{L}^{\text{eff}}$  and therefore presents an upper bound for the effective elasticity tensor.

Analogously, from the principle of minimum complementary energy, where stress fields  $\hat{\boldsymbol{\sigma}}$  have to satisfy equilibrium with prescribed tractions,  $\mathbf{t}$ , a lower bound can be found. In this case the complementary energy is given by

$$\hat{\Pi}^c(\hat{\boldsymbol{\sigma}}) = \frac{\Omega}{2} \langle \hat{\boldsymbol{\sigma}} : \mathbf{M}^{\text{eff}} : \hat{\boldsymbol{\sigma}} \rangle \quad (3.13)$$

If the boundary tractions are uniform,  $\mathbf{t}|_{\partial\Omega} = \boldsymbol{\Sigma} \cdot \mathbf{n}$  where  $\boldsymbol{\Sigma} = \text{const.} = \langle \boldsymbol{\sigma} \rangle$ , the complementary energy according to the Hill's lemma is  $\Pi^c(\boldsymbol{\sigma}) = \frac{\Omega}{2} \langle \boldsymbol{\sigma} \rangle : \mathbf{M}^{\text{eff}} : \langle \boldsymbol{\sigma} \rangle$ . From the condition  $\hat{\Pi}^c(\hat{\boldsymbol{\sigma}}) \geq \Pi^c(\boldsymbol{\sigma})$  it follows that

$$\langle \hat{\boldsymbol{\sigma}} : \mathbf{M} : \hat{\boldsymbol{\sigma}} \rangle \geq \langle \boldsymbol{\sigma} \rangle : \mathbf{M}^{\text{eff}} : \langle \boldsymbol{\sigma} \rangle \quad (3.14)$$

for all admissible fields  $\hat{\boldsymbol{\sigma}}$ . Such field is used in the Reuss approximation, yielding

$$\langle \boldsymbol{\sigma} \rangle : (\langle \mathbf{M} \rangle - \mathbf{M}^{\text{eff}}) : \langle \boldsymbol{\sigma} \rangle \geq 0 \quad (3.15)$$

Because of the quadratic form of  $\langle \boldsymbol{\sigma} \rangle$ , the average elasticity tensor  $\langle \mathbf{M} \rangle$  is larger than  $\mathbf{M}^{\text{eff}}$  and therefore presents an upper bound for the effective compliance tensor.

When these two results (Voigt and Reuss approximation) are combined, the effective elasticity tensor always lies between these two bounds:

$$\mathbf{L}_{\text{Voigt}}^{\text{eff}} = \langle \mathbf{L} \rangle \geq \mathbf{L}^{\text{eff}} \geq \langle \mathbf{M} \rangle^{-1} = \mathbf{L}_{\text{Reuss}}^{\text{eff}} \quad (3.16)$$

In case of materials with discrete isotropic phases that are isotropically distributed, the effective material properties are also isotropic. Obviously from equation (3.16) the upper (Voigt) bound for effective elastic stiffness tensor can be found simply as

$$\mathbf{L}_{\text{Voigt}}^{\text{eff}} = \langle \mathbf{L} \rangle = \sum_{r=0}^n c^{(r)} \mathbf{L}^{(r)} \quad (3.17)$$

and since the isotropic elasticity tensor can be decomposed into volumetric and deviatoric parts,  $\mathbf{L} = 3K\mathbf{I}_V + 2G\mathbf{I}_D$ , the upper bound for the effective bulk and shear moduli can be found as

$$K_{\text{Voigt}}^{\text{eff}} = \sum_{r=0}^n c^{(r)} K^{(r)} \quad \text{and} \quad G_{\text{Voigt}}^{\text{eff}} = \sum_{r=0}^n c^{(r)} G^{(r)} \quad (3.18)$$

However, if one of the phases is rigid (e.g.,  $\mathbf{L}^{(1)} \rightarrow \infty$ ) one obtains  $\mathbf{L}^{\text{eff}} \rightarrow \infty$  from the Voigt approximation.

The lower bound for the elastic constants can be found in a similar fashion. It is clear that from equation (3.16) the lower (Reuss) bound for effective elastic stiffness tensor can be found as

$$\mathbf{M}_{\text{Reuss}}^{\text{eff}} = \langle \mathbf{M} \rangle = \sum_{r=0}^n c^{(r)} \mathbf{M}^{(r)} \quad (3.19)$$

After projection into volumetric and deviatoric part we obtain the formula for bulk and shear moduli:

$$\frac{1}{K_{\text{Reuss}}^{\text{eff}}} = \sum_{r=0}^n \frac{c^{(r)}}{K^{(r)}} \quad \text{and} \quad \frac{1}{G_{\text{Reuss}}^{\text{eff}}} = \sum_{r=0}^n \frac{c^{(r)}}{G^{(r)}} \quad (3.20)$$

However, in case of a matrix containing cavities or cracks having vanishing stiffness (e.g.,  $\mathbf{L}^{(1)} \rightarrow 0$ ), the Reuss approximation leads to  $\mathbf{L}^{\text{eff}} \rightarrow 0$ .

### 3.3 Eigenstrain

Since the eigenstrain is not caused by stress, eigenstrains are also referred to as stress-free transformation strains (superscript  $t$ ). Formally, all kinds of strain that may prevail in a material in the absence of stress, can be interpreted as eigenstrains; typical examples are thermal or plastic strains. In the framework of infinitesimal deformations the total strains  $\varepsilon_{ij}$  are sum of elastic strains,  $\varepsilon_{ij}^e = M_{ijkl}\sigma_{kl}$ , and the eigenstrains:  $\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^t$ . The stress-strain relationship is then [9]

$$\sigma_{ij} = L_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^t) \quad (3.21)$$

The phase transformation in solids, where atomic rearrangements change the geometry of the lattice, gives rise to spatial distribution of eigenstrain  $\varepsilon_{ij}^t(\mathbf{x})$ . If non-vanishing eigenstrains prevail, only in some bounded subregion  $\Omega$  of the homogeneous material, this region is called an inclusion and the surrounding material is called a matrix. It has to be emphasized that the elastic properties of an inclusion and the matrix are the same; otherwise the region  $\Omega$  would be called an inhomogeneity [9].

Probably J.D. Eshelby (1916-1981) has found the most important analytical solution of micromechanics [10]. It is valid for an unbounded domain which contains an ellipsoidal inclusion  $\Omega^{(r)}$  with principal axes  $a_i$ . If the eigenstrains in the inclusion are constant ( $\varepsilon_{kl}^t = \text{const.}$ ) then the remarkable result holds that the total strains  $\varepsilon_{kl}$  inside the inclusion are constant as well. Via fourth-order Eshelby's tensor  $S_{ijkl}$  they depend linearly on the eigenstrains [9]

$$\varepsilon_{ij} = S_{ijkl}\varepsilon_{kl}^t \quad \text{in} \quad \Omega^{(r)} \quad (3.22)$$

The Eshelby's tensor is symmetric in the first and second pair of indices, but in general it is not symmetric with regard to an exchange of these pairs (exhibits the minor but not the major symmetry) [9]:

$$S_{ijkl} = S_{jikl} = S_{ijlk} \quad \text{but} \quad S_{ijkl} \neq S_{klij} \quad (3.23)$$

In case of an isotropic material, its components depend only on Poisson's ratio  $\nu$ , the ratios of the principal axes  $a_i$ , and their orientation with respect to some Cartesian coordinate system. The respective expressions are very long and can be found in literature, e.g. in [11]. Only in case of an isotropic material there exists a closed-form representation of the tensor  $S_{ijkl}$ , and the fields outside the inclusion. The Eshelby solution for ellipsoidal inclusions is of fundamental importance for analytical homogenization techniques (e.g. Mori-Tanaka).

Starting from the general ellipsoid various special cases can be derived. For instance, the two-dimensional solution for an infinitely long cylinder of elliptic cross section in plane strain is obtained from the limit process  $a_3 \rightarrow \infty$  [9].

For a spherical inclusion ( $a_i = a$ ) in an isotropic material the dependence on the principal axes and their orientation vanishes (geometric isotropy) and the Eshelby tensor reduces to

$$S_{ijkl} = \alpha^{(0)}\frac{1}{3}\delta_{ij}\delta_{kl} + \beta^{(0)}\left(I_{ijkl}^S - \frac{1}{3}\delta_{ij}\delta_{kl}\right) = \alpha^{(0)}\mathbf{I}_V + \beta^{(0)}\mathbf{I}_D \quad (3.24)$$

where

$$\alpha^{(0)} = \frac{1 + \nu^{(0)}}{3(1 + \nu^{(0)})} = \frac{3K^{(0)}}{3K^{(0)} + 4G^{(0)}} \quad \text{and} \quad \beta^{(0)} = \frac{2(4 - 5\nu^{(0)})}{15(1 - \nu^{(0)})} = \frac{6(K^{(0)} + 2G^{(0)})}{5(3K^{(0)} + 4G^{(0)})} \quad (3.25)$$

are scalar parameters. The superscript (0) stands for the matrix. The entire (i.e., elastic and geometric) isotropy of the problem then allows the decomposition into volumetric and deviatoric strain, which highlights the meaning of the parameters  $\alpha$  and  $\beta$  [9]:

$$\varepsilon_{kk} = \alpha \varepsilon_{kk}^t \quad \text{and} \quad \varepsilon_{ij} = \beta \varepsilon_{ij}^t \quad \text{in} \quad \Omega^{(r)} \quad (3.26)$$

Therefore the fourth rank Eshelby tensor turns out to be isotropic when the shape of the inclusion is spherical and can be characterized by the constraint constants  $\alpha$  and  $\beta$  (representing the volumetric and the deviatoric parts of the constraint, respectively).

### 3.4 Dilute (Non-Interacting) Defect Distribution

The simplest situation for modeling is when the inhomogeneities or defects are so dilutely distributed in the homogeneous matrix that their interaction among each other and with the boundary of the RVE can be neglected ("dilute distribution"), see Figure 3.1.

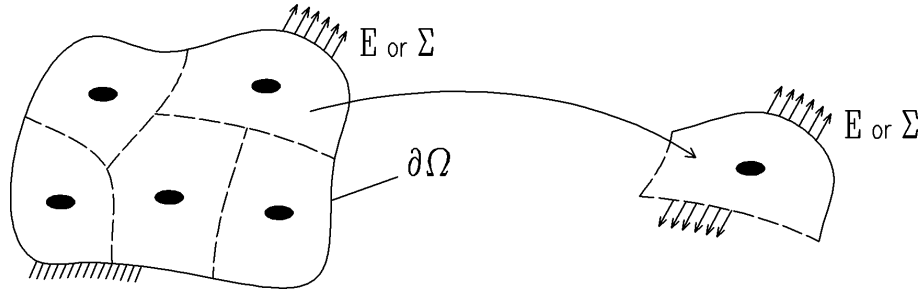


Figure 3.1: Model of dilute phase distribution [9]

If a sample of an inhomogeneous material is subjected to the external load  $\mathbf{E}$ , then the average strain in individual phases can be calculated as  $\mathbf{E}^{(r)} = \mathbf{A}^{(r)} : \mathbf{E}$ , where  $\mathbf{A}^{(r)}$  represents a strain concentration factor for a phase  $r$ . The superscript  $r$  attains the values from 1 (possibly even 0 if the matrix is included) to the number of phases  $n$ . The strain concentration factor can be calculated as follows (for details and derivation see e.g. [8]):

$$\mathbf{A}_{\text{dil}}^{(r)} = [\mathbf{I} + \mathbf{S} : \mathbf{M}^{(0)} : (\mathbf{L}^{(r)} - \mathbf{L}^{(0)})]^{-1} \quad \text{where} \quad r = 1, \dots, n \quad (3.27)$$

where  $\mathbf{I}$  represents the fourth order unity tensor with components  $I_{ijkl} = 1/2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ , where  $\delta_{ij}$  is a Kronecker delta defined in equation (2.4);  $\mathbf{S}$  is the Eshelby tensor,  $\mathbf{M}^{(0)}$  is a compliance tensor representing the matrix, the  $\mathbf{L}^{(r)}$  and  $\mathbf{L}^{(0)}$  are stiffness tensors, representing the individual phases and the matrix, respectively.

The subscript "dil" in equation (3.27) stands for a "dilute distribution", because equation (3.27) is valid under the assumption that the inhomogeneity is embedded in an infinite matrix. The assumption of dilutely distributed non-interacting inhomogeneities is a starting point for a refinement of the model accounting for a mutual interaction of inhomogeneities, such as the Mori-Tanaka scheme introduced next.



### 3.5 Mori-Tanaka Model

The Mori-Tanaka model, [4] and [5], formally equals to that of a dilute distribution. However, the strain in individual inhomogeneities is not directly dependent on the externally applied load (macroscopic strain), but rather on a strain in the matrix (see Figure 3.2), which is approximated by a constant field  $\mathbf{E}^{(0)}$ :

$$\mathbf{E}^{(r)} = \mathbf{A}_{\text{dil}}^{(r)} : \mathbf{E}^{(0)} \quad (3.28)$$

The relationship between the macroscopic strain and strain in the matrix can be found using a simple reasoning:

$$\begin{aligned} \mathbf{E} &= c^{(0)} \mathbf{E}^{(0)} + \sum_{r=1}^n c^{(r)} \mathbf{E}^{(r)} = c^{(0)} \mathbf{E}^{(0)} + \sum_{r=1}^n c^{(r)} \mathbf{A}_{\text{dil}}^{(r)} : \mathbf{E}^{(0)} = \\ &= \left( c^{(0)} \mathbf{I} + \sum_{r=1}^n c^{(r)} \mathbf{A}_{\text{dil}}^{(r)} \right) : \mathbf{E}^{(0)} \end{aligned} \quad (3.29)$$

where  $c$ , having a superscript  $(0)$  and  $(r)$ , stands for a volume fraction of the matrix and inhomogeneities, respectively. The relationship between the average matrix strain and the macroscopic strain can be described simply as  $\mathbf{E}^{(0)} = \mathbf{A}_{\text{MT}}^{(0)} : \mathbf{E}$ , where

$$\mathbf{A}_{\text{MT}}^{(0)} = \left( c^{(0)} \mathbf{I} + \sum_{r=1}^n c^{(r)} \mathbf{A}_{\text{dil}}^{(r)} \right)^{-1} \quad (3.30)$$

is the Mori-Tanaka strain concentration factor. The strain in the individual inhomogeneities is then provided by

$$\mathbf{E}^{(r)} = \mathbf{A}_{\text{dil}}^{(r)} : \mathbf{E}^{(0)} = \mathbf{A}_{\text{dil}}^{(r)} : \mathbf{A}_{\text{MT}}^{(0)} : \mathbf{E} \quad (3.31)$$

The relationship between the macroscopic stress  $\Sigma$  and strain  $\mathbf{E}$  can be obtained as follows:

$$\Sigma = \sum_{r=0}^n c^{(r)} \Sigma^{(r)} = \sum_{r=0}^n c^{(r)} \mathbf{L}^{(r)} : \mathbf{E}^{(r)} = \sum_{r=0}^n c^{(r)} \mathbf{L}^{(r)} : \mathbf{A}^{(r)} : \mathbf{E} = \mathbf{L}^{\text{eff}} : \mathbf{E} \quad (3.32)$$

where  $\mathbf{L}^{\text{eff}}$  is the effective stiffness tensor, and in case of the Mori-Tanaka scheme it can be obtained as

$$\mathbf{L}^{\text{eff}} = \left( c^{(0)} \mathbf{L}^{(0)} + \sum_{r=1}^n c^{(r)} \mathbf{L}^{(r)} : \mathbf{A}_{\text{dil}}^{(r)} \right) : \mathbf{A}_{\text{MT}}^{(0)} \quad (3.33)$$

In the special case of an isotropic matrix containing isotropic spherical inhomogeneities, the Mori-Tanaka model yields also an isotropic overall behavior, irrespective of the spatial arrangement of the phases. Using the equations (3.31), (3.25) and knowing that the elastic stiffness tensor can be decomposed into volumetric and deviatoric parts,  $\mathbf{L} = 3K\mathbf{I}_V + 2G\mathbf{I}_D$ , all the terms in equation (3.33) can be decomposed into their volumetric and deviatoric parts. Since the volumetric and deviatoric components are independent of each other, the dilute concentration factors defined in equation (3.27) can be represented separately by their volumetric and deviatoric part as

$$A_{\text{dil},K}^{(r)} = \frac{K^{(0)}}{K^{(0)} + \alpha^{(0)}(K^{(r)} - K^{(0)})} \quad \text{and} \quad A_{\text{dil},G}^{(r)} = \frac{G^{(0)}}{G^{(0)} + \beta^{(0)}(G^{(r)} - G^{(0)})} \quad (3.34)$$

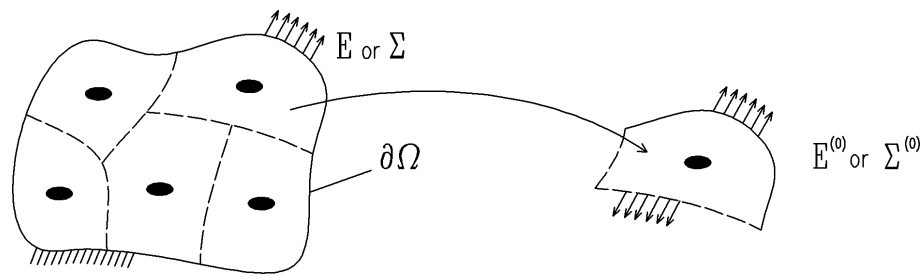


Figure 3.2: Interaction of inhomogeneities in the Mori-Tanaka model [9]

. The effective bulk and shear moduli can be then expressed as

$$K^{\text{eff}} = \frac{c^{(0)}K^{(0)} + \sum_{r=1}^n c^{(r)}K^{(r)}A_{\text{dil},K}^{(r)}}{c^{(0)} + \sum_{r=1}^n c^{(r)}A_{\text{dil},K}^{(r)}} \quad \text{and} \quad G^{\text{eff}} = \frac{c^{(0)}G^{(0)} + \sum_{r=1}^n c^{(r)}G^{(r)}A_{\text{dil},G}^{(r)}}{c^{(0)} + \sum_{r=1}^n c^{(r)}A_{\text{dil},G}^{(r)}} \quad (3.35)$$

# Chapter 4

## Homogenization with Coated Particles

This section is devoted to the evaluation of the dilute concentration factors for individual layers of coated particles. Herve and Zaoui [12] found an analytical solution for derivation of the elastic strain and stress fields in an infinite medium constituted of an  $n$ -layered isotropic spherical inclusion, embedded in a matrix subjected to uniform stress or strain conditions at infinity. The integration constants were found using the continuity conditions and equilibrium of stresses on the interface of individual phases. Since the Harve-Zaoui scheme describes an infinite domain consisting of  $n + 1$  inclusions, it belongs to the family of self-consistent schemes. The geometrical and material isotropy allows separation of the volumetric and deviatoric part.

### 4.1 Dilute Concentration Factors by Herve-Zaoui Scheme

Only the determination of the dilute concentration factors for a coated particle and its coating is presented here. The whole derivation by Herve and Zaoui of the elastic strain and stress fields in an infinite medium constituted of an  $n$ -layered spherical inclusion, embedded in a matrix and subjected to uniform stress or strain conditions at infinity can be found in [12]. The problem is illustrated in Figure 4.1. Each phase of the composite from the Figure ?? is represented by its radius (except for the matrix),  $r^i$ , Poisson's ratio,  $\nu^i$ , bulk and shear moduli,  $K^i$  and  $G^i$ .

Note that the layers are marked by subscript  $i$  attaining the values from 1 (representing the inner sphere) to  $n$  (representing the outer layer of the inclusion) and  $n + 1$  representing the matrix. This notation is used for the determination of concentration factors next.

#### 4.1.1 Volumetric Part

The volumetric part of the dilute concentration factors for individual layers of the spherical inclusion can be found as elements of a vector  $\mathbf{F}$ :

$$A_{\text{dil,K}}^{(i)} = F_i \quad (4.1)$$

where the first term is determined as

$$F_1 = \frac{1}{Q_{11}^{(n)}} \quad (4.2)$$

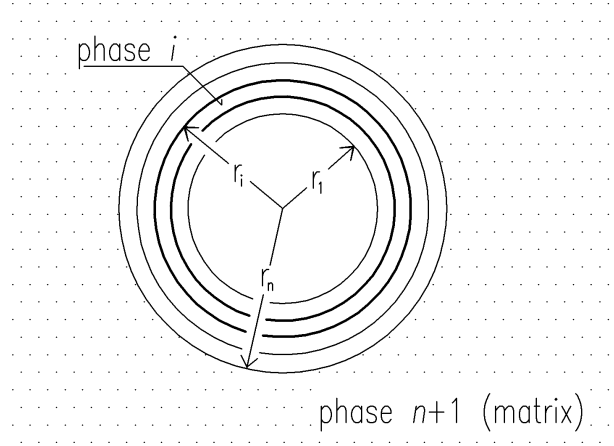


Figure 4.1: The  $n$ -layered spherical inclusion considered in Harve-Zaoui scheme

and the remaining terms as

$$F_i = \frac{Q_{11}^{(i-1)}}{Q_{11}^{(n)}} \quad \text{for } i = 2, \dots, n \quad (4.3)$$

The determination of matrices  $\mathbf{Q}^{(i)}$ , representing individual layers of the composite inclusion, can be found in Appendix, Section A.1.

### 4.1.2 Deviatoric Part

The deviatoric part of the dilute concentration factor for the inner sphere ( $i = 1$ ) can be found as:

$$A_{\text{dil,G}}^{(1)} = A_1 - \frac{21}{5} \frac{r^{(1)2}}{1 - 2\nu^{(1)}} B_1 \quad (4.4)$$

and for the other layers as

$$A_{\text{dil,G}}^{(i)} = A_i - \frac{21}{5} \frac{r^{(i)5} - r^{(i-1)5}}{(1 - 2\nu^{(i)})(r^{(i)3} - r^{(i-1)3})} B_i \quad \text{for } i = 2, \dots, n \quad (4.5)$$

The determination of vectors  $\mathbf{A}^{(i)}$  and  $\mathbf{B}^{(i)}$ , representing individual layers of the composite inclusion, can be found in Appendix, Section A.2.

## 4.2 Modification of Mori-Tanaka Model

For the calculation of the effective moduli,  $K^{\text{eff}}$  and  $G^{\text{eff}}$ , the coated particle and its coating(s) are in equation (3.35) represented by the dilute concentration factors  $A_{\text{dil,K}}^{(i)}$  and  $A_{\text{dil,G}}^{(i)}$  evaluated according to equations (4.1), (4.4) and (4.5) instead of concentration factors  $A_{\text{dil,K}}^{(r)}$  and  $A_{\text{dil,G}}^{(r)}$  calculated according to equation (3.34). Otherwise there is no change in the procedure of the effective stiffness estimation.

## Chapter 5

### Strength Estimation

The strength estimation is based on the  $J_2$  yield criterion, i.e. that only the deviatoric part of the imposed load can cause a failure of the material. Therefore, it is necessary to calculate the deviatoric stress in individual components, which can be afterwards compared with a critical stress. Such approach was used by [1] and it turned out to be suitable for an estimation of the compressive strength in cementitious materials.

Due to the assumed elastic linear behavior of the RVE, all imposed work is stored at each point as an elastic energy density,  $W_e = \frac{1}{2} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}$ , which can be decomposed into the volumetric and deviatoric part:

$$W_e = \frac{1}{2} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \frac{1}{2} (\mathbf{s} + \sigma_m \boldsymbol{\delta}) : (\mathbf{e} + \varepsilon_m \boldsymbol{\delta}) = \frac{1}{2} \mathbf{s} : \mathbf{e} + \frac{1}{2} \sigma_m \varepsilon_m \boldsymbol{\delta} : \boldsymbol{\delta} = \frac{1}{2} \mathbf{s} : \mathbf{e} + \frac{1}{2} \sigma_m \varepsilon_m \quad (5.1)$$

knowing that  $W_e = \frac{1}{2} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{L} : \boldsymbol{\varepsilon}$  and that the elastic stiffness tensor can be also decomposed as  $\mathbf{L} = 3K\mathbf{I}_V + 2G\mathbf{I}_D$ , we can express the deviatoric part of the imposed work as

$$W_{eD} = \frac{1}{2} \mathbf{s} : \mathbf{e} = \frac{1}{4G} \mathbf{s} : \mathbf{s} \quad (5.2)$$

which is proportional to the second invariant of the stress deviator,  $J_2$ , where

$$J_2 = \frac{1}{2} \mathbf{s} : \mathbf{s} \quad (5.3)$$

and therefore  $W_{eD} = J_2/(2G)$ . The quadratic average of the deviatoric stress is then  $\|\mathbf{s}\| = \sqrt{2J_2}$ .

#### 5.1 Quadratic Strain Averages

The expression for the quadratic average of the deviatoric strain field over a general phase,  $r$ , can be derived using the Hill's lemma, which expresses the equality between the average strain energy density,  $\langle W_e \rangle$ , in the RVE by means of the microscopic or macroscopic quantities [9]. From equation (3.9) the following equality can be obtained:

$$\mathbf{E} : \mathbf{L}^{\text{eff}} : \mathbf{E} = \frac{1}{|\Omega|} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) : \mathbf{L}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \, dx \quad (5.4)$$

where  $\Omega$  stands for the domain of the entire RVE, opposed to  $\Omega^{(r)}$  denoting the domain of the single inclusion (inhomogeneity). The local strain  $\boldsymbol{\varepsilon}(\mathbf{x})$  can be then decomposed into its volumetric and deviatoric part (responsible for the material failure):

$$\mathbf{E} : \mathbf{L}^{\text{eff}} : \mathbf{E} = \frac{1}{|\Omega|} \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) : [3K(\mathbf{x})\mathbf{I}_V + 2G(\mathbf{x})\mathbf{I}_D] : \boldsymbol{\varepsilon}(\mathbf{x}) \, d\mathbf{x} \quad (5.5)$$

To extract the deviatoric part, it is convenient to differentiate the entire expression (5.5) with respect to  $G^{(r)}$ . The volumetric part vanishes and we obtain

$$\mathbf{E} : \frac{\partial \mathbf{L}^{\text{eff}}}{\partial G^{(r)}} : \mathbf{E} = \frac{1}{|\Omega|} \sum_{r=0}^n \int_{\Omega^{(r)}} 2 \mathbf{e}^{(r)}(\mathbf{x}) : \mathbf{e}^{(r)}(\mathbf{x}) \, d\mathbf{x} \quad (5.6)$$

which can be after a simple manipulation:

$$\frac{1}{2} \mathbf{E} : \frac{\partial \mathbf{L}^{\text{eff}}}{\partial G^{(r)}} : \mathbf{E} = \frac{1}{|\Omega|} \frac{|\Omega^{(r)}|}{|\Omega^{(r)}|} \sum_{r=0}^n \int_{\Omega^{(r)}} \mathbf{e}^{(r)}(\mathbf{x}) : \mathbf{e}^{(r)}(\mathbf{x}) \, d\mathbf{x} \quad (5.7)$$

knowing that  $c^{(r)} = |\Omega^{(r)}|/|\Omega|$ , even more simplified:

$$\frac{1}{2} \mathbf{E} : \frac{\partial \mathbf{L}^{\text{eff}}}{\partial G^{(r)}} : \mathbf{E} = c^{(r)} \frac{1}{|\Omega^{(r)}|} \int_{\Omega^{(r)}} \mathbf{e}^{(r)}(\mathbf{x}) : \mathbf{e}^{(r)}(\mathbf{x}) \, d\mathbf{x} \quad (5.8)$$

The quadratic average of the deviatoric strain field over a general phase,  $r$ , is defined as [1]

$$\|\mathbf{e}^{(r)}\| = \sqrt{\frac{1}{|\Omega^{(r)}|} \int_{\Omega^{(r)}} \frac{1}{2} \mathbf{e}^{(r)}(\mathbf{x}) : \mathbf{e}^{(r)}(\mathbf{x}) \, d\mathbf{x}} \quad (5.9)$$

and obviously from equation (5.8), it can be also expressed as

$$\|\mathbf{e}^{(r)}\| = \sqrt{\frac{1}{4c^{(r)}} \mathbf{E} : \frac{\partial \mathbf{L}^{\text{eff}}}{\partial G^{(r)}} : \mathbf{E}} \quad (5.10)$$

The related quadratic average of the deviatoric stress field (see (5.3)) is used as an estimate for deviatoric stress peaks [1]:

$$\|\mathbf{s}^{(r)}\| = \sqrt{\frac{1}{|\Omega^{(r)}|} \int_{\Omega^{(r)}} \frac{1}{2} \mathbf{s}^{(r)}(\mathbf{x}) : \mathbf{s}^{(r)}(\mathbf{x}) \, d\mathbf{x}} = 2G^{(r)} \|\mathbf{e}^{(r)}\| \quad (5.11)$$

Assuming the elasto-brittle behavior, the elastic response can be expected until the quadratic deviatoric stress averages over each of the phases remain below a critical strength [1]:

$$\|\mathbf{s}^{(r)}\| \leq s_{\text{crit}}^{(r)} \quad (5.12)$$

## **Part II**

# **APPENDIX**

# Appendix A

## Herve-Zaoui Solution

The individual matrices, needed for the calculation of the dilute concentration factors in Herve-Zaoui scheme ( $n$ -layered spherical inclusion problem, see Section 4.1), are presented next.

### A.1 Volumetric Part

The matrices  $\mathbf{Q}^{(i)}$ , needed for the determination of the volumetric part of the dilute concentration factors for the individual layers of the spherical inclusion can be found as

$$\mathbf{Q}^{(i)} = \mathbf{N}^{(i)} \quad \text{for } i = 1 \quad (\text{A.1})$$

and

$$\mathbf{Q}^{(i)} = \mathbf{N}^{(i)} \mathbf{Q}^{(i-1)} \quad \text{for } i = 2, \dots, n \quad (\text{A.2})$$

The matrices  $\mathbf{N}^{(i)}$  are calculated as

$$\mathbf{N}^{(i)} = \frac{1}{3K^{(i+1)} + G^{(i+1)}} \begin{pmatrix} 3K^{(i)} + 4G^{(i+1)} & \frac{4}{r^{(i)3}}(G^{(i+1)} - G^{(i)}) \\ 3r^{(i)3}(K^{(i+1)} - K^{(i)}) & 3K^{(i+1)} + 4G^{(i)} \end{pmatrix} \quad (\text{A.3})$$

### A.2 Deviatoric Part

The vectors  $\mathbf{A}^{(i)}$  (having the number of elements  $n$ ), needed for the determination of the volumetric part of the dilute concentration factors for the individual layers of the spherical inclusion can be found as

$$\mathbf{A}^{(i)} = \frac{P_{22}^{(n)}}{P_{11}^{(n)} P_{22}^{(n)} - P_{12}^{(n)} P_{21}^{(n)}} \quad \text{for } i = 1 \quad (\text{A.4})$$

and

$$\mathbf{A}^{(i)} = W_1^{(i)} \quad \text{for } i = 2, \dots, n \quad (\text{A.5})$$





with

$$a^{(i)} = \frac{G^{(i)}}{G^{(i+1)}}(7 + 5G^{(i)})(7 - 10G^{(i+1)}) - (7 - 10G^{(i)})(7 + 5G^{(i+1)}) \quad (\text{A.12a})$$

$$b^{(i)} = \frac{G^{(i)}}{G^{(i+1)}}(7 + 5G^{(i)}) + 4(7 - 10G^{(i)}) \quad (\text{A.12b})$$

$$c^{(i)} = (7 - 5G^{(i+1)}) + 2(4 - 5G^{(i+1)})\frac{G^{(i)}}{G^{(i+1)}} \quad (\text{A.12c})$$

$$d^{(i)} = (7 + 5G^{(i+1)}) + 4(7 - 10G^{(i+1)})\frac{G^{(i)}}{G^{(i+1)}} \quad (\text{A.12d})$$

$$e^{(i)} = 2(4 - 5G^{(i)}) + \frac{G^{(i)}}{G^{(i+1)}}(7 - 5G^{(i)}) \quad (\text{A.12e})$$

$$f^{(i)} = (4 - 5G^{(i)})(7 - 5G^{(i+1)}) - \frac{G^{(i)}}{G^{(i+1)}}(4 - 5G^{(i+1)})(7 - 5G^{(i)}) \quad (\text{A.12f})$$

$$\alpha^{(i)} = \frac{G^{(i)}}{G^{(i+1)}} - 1 \quad (\text{A.12g})$$

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