

Diploma Thesis

Analytical Micromechanics with Macroscopic Strain Gradients, Motivated by Biological Materials

submitted in satisfaction of the requirements for the degree
Diplom-Ingenieur
of the TU Wien, Faculty of Civil and Environmental Engineering

Diplomarbeit

Analytische Mikromechanik mit makroskopischen Verzerrungsgradienten, motiviert durch biologische Materialien

ausgeführt zum Zwecke der Erlangung des akademischen Grads
Diplom-Ingenieur
eingereicht an der TU Wien, Fakultät für Bau- und Umweltingenieurwesen

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Wien, im Juni 2024



Abstract

The investigation of the mechanical properties of biological tissue is a topic of ever growing interest. One material that has been relatively little studied to date, but which has unique capabilities and some potentially useful applications compared to other biogenic substances, is the substance building up the jaws of polychaetes – better known as bristle worms. This material exhibits high hardness and stiffness due to its organometallic composition, and latest evidence has suggested that the material may be able to undergo dislocation-like deformations at the microscopic scale. This idea arises from recent nanoindentation testing which has shown that the measurement of mechanical properties is associated with size effects, namely indentation depths. Corresponding "loading sizes" can often be described by a "macroscopic" strain gradient, which means that measured mechanical quantities not only depend on the applied strain, but also on a measure of its gradient. The correspondingly arising, largely open, question concerns the link between the macroscopic strain gradient and the microscopic deformation pattern. This question is tackled herein in the context of analytical micromechanics.

Classical methods of micromechanics generally do not consider a strain gradient due to the requirement of scale separation, and more recent developments, where such a gradient is included, are often cumbersome and computationally expensive. Hence, the present work aims to introduce a measure of the strain gradient on the macroscale, which is connected via boundary conditions to a linear elastic microstructure. The goal is to maintain the applicability and versatility of classical micromechanics – and thus of most homogenization techniques, while extending the range of applications, especially regarding small scales and/or biological materials.

This thesis covers the first stage of this modeling process, by investigating the effect of a macroscopic strain gradient term on the mathematical pillars of micromechanics. Specifically, the strain average rule, the stress average rule and Eshelby's inhomogeneity problem are examined. It is shown that with the chosen formalism both averaging rules are applicable for a linear elastic medium on the microscale, and that the inhomogeneity problem has a solution. The latter is presented in the form of a Neumann series for the general case and as an approximated closed-form solution for a spherical, isotropic inhomogeneity of constant stiffness.

Kurzfassung

Die Erforschung der mechanischen Eigenschaften biologischer Gewebe stellt ein Thema von stetig wachsendem Interesse dar. Ein Material, das bis dato noch relativ wenig untersucht wurde, welches aber verglichen mit anderen biogenen Substanzen einzigartige Fähigkeiten und einige potenziell nützliche Anwendungsmöglichkeiten besitzt, baut die Kiefer von Polychaeten – besser bekannt als Borstenwürmer – auf. Wegen seiner charakteristischen metallorganischen Verbindungen weist dieses Material hohe Härten und Steifigkeiten auf, welche auf versetzungsartige Mikro-Deformationen schließen lassen. Ebenso haben neuere Nanoindentierungs-Versuche ergeben, dass die Messung von mechanischen Eigenschaften Größeneffekten unterworfen ist; die Messergebnisse hängen von der Indentierungstiefe ab. Solche Größeneffekte können oft mit einem Verzerrungsgradienten beschrieben werden, was bedeutet, dass gemessene mechanische Größen nicht nur von der eingebrachten Verzerrung, sondern auch von einem Maß für ihren Gradienten abhängen. Die sich dann stellende, weitgehend unbeantwortete Frage betrifft die Verknüpfung zwischen den makroskopischen Verzerrungsgradienten und den mikroskopischen Verformungsmustern. Diese Frage wird hier im Rahmen der analytischen Mikromechanik behandelt.

Da die klassischen Methoden der Mikromechanik durch die Voraussetzung der Skalentrennung im Allgemeinen keinen Verzerrungsgradienten berücksichtigen, und neuere Entwicklungen, wo ein solcher eingebunden wird, meist schwerfällig und rechnerisch sehr aufwendig sind, soll in dieser Arbeit ein Maß des Verzerrungsgradienten auf der Makroskala eingeführt werden, welches sich mittels Randbedingungen auf die sich linear elastisch verhaltende Mikrostruktur auswirkt. Damit wird angestrebt, die Anwendbarkeit und Vielseitigkeit der klassischen Mikromechanik – und damit der meisten Homogenisierungstechniken – zu erhalten, und gleichzeitig die Einsatzmöglichkeiten, besonders hinsichtlich kleinen Maßstäben und/oder biologischen Materialien, zu erweitern.

Als ersten Schritt dieser Modellbildung wird in der vorliegenden Arbeit die Auswirkung des makroskopischen Verzerrungsgradiententerms auf die Grundpfeiler der Mikromechanik untersucht. Konkret wird die Verzerrungsmittelungsregel, die Spannungsmittelungsregel und das Eshelby'sche Inhomogenitätenproblem behandelt.

Es wird gezeigt, dass mit dem gewählten Formalismus einerseits beide Mittelungsregeln für ein mikroskopisch linear elastisches Medium anwendbar sind, sowie, dass das Inhomogenitätenproblem eine Lösung besitzt. Letztere wird allgemein in Form einer Neumann-Reihe dargestellt und für den speziellen Fall einer sphärischen, isotropen Inhomogenität konstanter Steifigkeit als geschlossene, approximierbare Lösung präsentiert.

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Chapter 1

Introduction

1.1 Bristle Worms and Size Effects

The investigation of the mechanical behavior of biological materials has been a topic of ever-increasing interest over the past decades. Hierarchical, finely optimized structures together with a balanced chemical composition ensure impressive properties in a wide field of applications. In contrast to classical engineering materials, biogenic materials are made up of "energetically inexpensive" components, which usually results in a combination of organic and inorganic substances. Evolutionary reasons are decisive for this, since only ambient conditions and a constrained amount of certain elements were available throughout history. Compared to similar, synthetically manufactured materials, however, they mostly possess far superior properties, which is in part due to their highly hierarchical structure and the intricate molecular interactions occurring especially at the smaller length scales [1].

In nature, there are several ways in which hard, resilient materials can be produced. Polysaccharides, for example, of which cellulose and chitin are the most common representatives, are made up of long polymer chains, which dictate the properties of the macroscopic material through their degree of crosslinking and non-covalent interactions [2]. Several applications for both materials and their derivatives exist in the biomedical field, and a large body of literature has been acquired over the years.

Another type of hard tissue is mineralized tissue, often referred to as "calcified", when calcium salts are the main contributor, such as in bone, some types of cartilage, enamel, cementum and dentin, where hydroxyapatite deposits are precisely defined in orientation and size and thus shape material behavior [3]. Calcified tissue, especially bone, has been extensively researched over the years due to its direct translation into medical applications, so that knowledge of the mechanisms and influencing parameters of the mechanical behavior is already quite advanced.

One material that has not yet enjoyed such a level of attention, but which could have many interesting and unique potential biotechnological applications, is the jaw material of polychaetes. These marine inhabitants, better known as bristle worms, resemble a very old (dating back to the late Cambrian era [4]) and highly successful clade within the invertebrates, with over 80 families and well over 10.000 species [5]. While they generally have soft bodies, their (eponymous) bristles and especially their jaws are exceptional compared to the aforementioned hard tissues in several aspects. Recent discoveries have revealed that the bristles are produced by a "biological 3D printing" process: In special follicles, their shape is realized step by step through the continuous deposition of chitin along precisely modulated cell processes (microvilli) [6, 7]. The jaws of polychaetes, in turn, additionally contain a histidine-enriched protein matrix, which can complex with metals and halogen ions at regular intervals, markedly influencing their hardness and stiffness [8, 9]. The self-healing property of this type of bond, together with the results of indentation tests, has led to the interesting hypothesis that this material might perform dislocation-like movements upon loading [8, 10], which is illustrated in Figure 1.1.

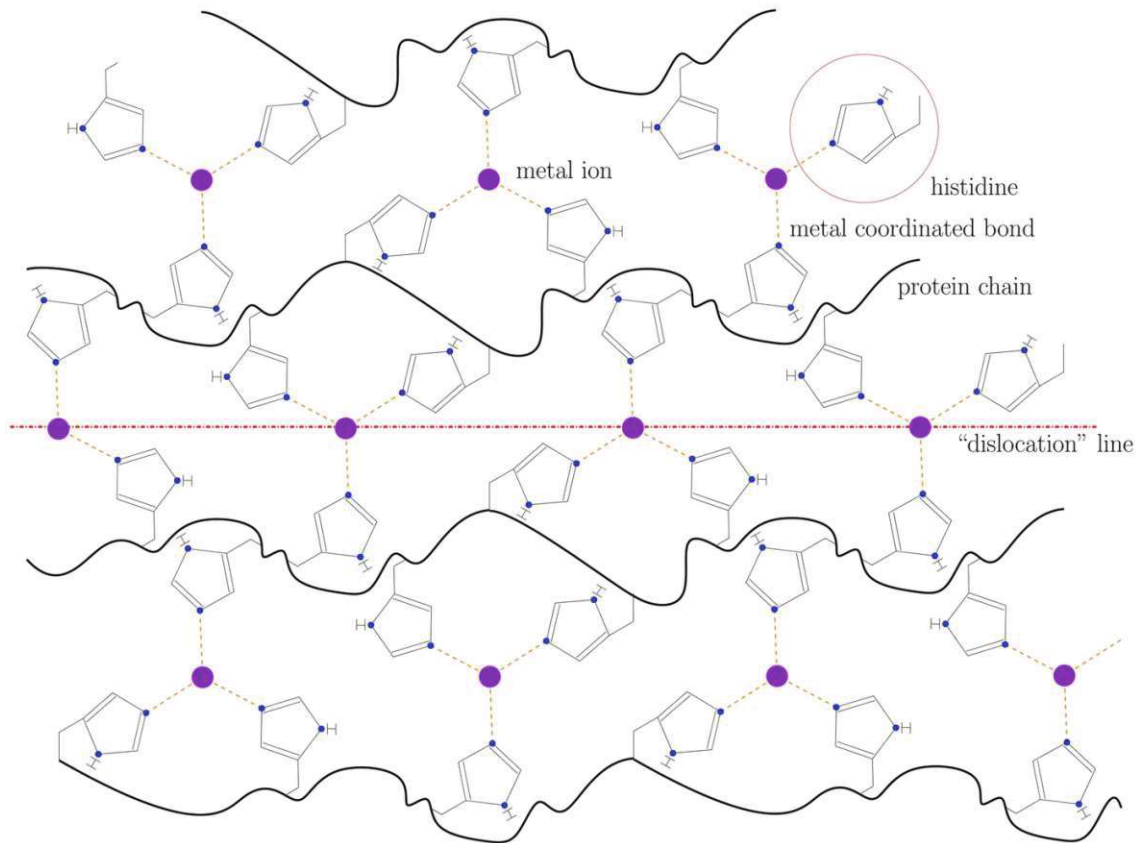


Fig. 1.1: Hypothesized dislocation lines in the jaw material of bristle worms: A histidine-enriched protein matrix is able to complex metal ions. The non-covalent and self-healing characteristic led to the assumption that dislocation movements can occur along the alignment of the coordination centres. Modified from [8], licensed under CC BY 4.0.

With regard to the indentation tests in particular, it was found that the difference in hardness exhibited by the jaws of different bristle worm species are not so much arising from chemical differences of the tested materials, but are rather due to a size effect, which has been well known for certain types of metals [8, 11, 12]. This size effect, named after the authors of the well-known paper from 1998 [13], W.D. Nix and H. Gao, describes the phenomenon that in indentation tests of crystalline metals, a lower indentation depth leads to a higher measured hardness.

The Nix-Gao-Size-Effect

The theoretical rationale for the derivation of this model is primarily based on previous experimental observations that for crystalline solids, strains alone were often not sufficient to describe the yield stress and dislocations during plastic deformations. It has been shown that the strain gradient also has an influence, particularly at small length scales (i.e., the micro- and sub-micrometer range), which is described as "gradient effects" [12, 13]. More precisely, those occur when the dimensions of the testing specimen come close to the dislocation spacing [11]. This effect can in part be understood by considering the principles of "statistically stored" and "geometrically necessary" dislocations:

Imagine a material that can undergo plastic flow. During straining, more and more dislocations will statistically occur in the body, where the material can glide. If these dislocations meet and accumulate, the dislocation density ρ_S increases and further gliding becomes more difficult, which

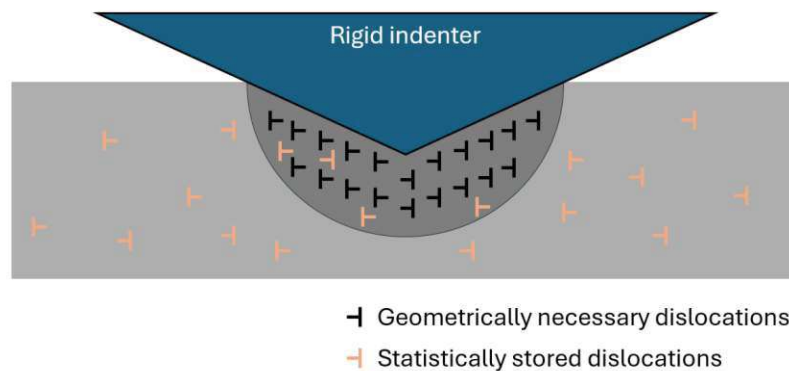


Fig. 1.2: Formation of geometrically necessary dislocations by a rigid indenter. The respective dislocation density ρ_G locally increases, as indicated by the circular region, and depends both on the shape of the tip and on the depth of indentation.

results in hardening [14]. This effect only depends on the average strain present [13]. However, if the material is loaded in a very localized fashion, for example through an indentation test (Figure 1.2), more dislocations must arise in the vicinity of the indented site, so that volume can be displaced. The stored geometrically necessary dislocations result in additional hardening taking place in this region. It is easy to imagine that the density of the geometrically necessary dislocations ρ_G and thus the increase in hardness, independently of ρ_S , depends not only on the geometry of the tip but also on the depth of indentation, or, more generally, on the applied strain gradient [11–13].

Based on these simple geometric considerations, Nix and Gao developed a model that allows, on the one hand, to relate the measured hardness to the penetration depth (specifically, the square of the hardness scales indirectly proportional with the indentation depth, $H^2 \propto h^{-1}$), as well as to derive a law for the flow stress in the presence of a strain gradient.

The fact that the strain gradient is of decisive importance for the measured mechanical properties on the microscale opens up the possibility to incorporate this phenomenon into theoretical micromechanical – and eventually multiscale – models. Actually, as will be described in the following chapters of the introduction, "conventional" continuum mechanics, and thus most micromechanics methods, are based on the concept of representative volume elements (RVEs), which usually are treated as free from the influence of a strain gradient. This is due to the fact that in most cases these RVEs can be chosen to be much larger than the deforming microstructure, so that gradient effects as those described above are negligible. In a material such as the jaws of bristle worms, however, it is inevitable that the RVE must be chosen so small, that this simplification is no longer valid. The subject of this thesis is therefore to lay the foundation for a continuum mechanics model that integrates a macroscopic strain gradient into the framework of classical linear elastic continuum micromechanics. Since over the years the latter has proven to be extremely useful in practice, it is intended that an extension of this theory will be created that is also practicable and relevant to applications. To get there, in the following chapters of the introduction, a refresher of some fundamental aspects of continuum mechanics will be given, followed by a description of the foundations of continuum micromechanics [15], which are dealt with in the thesis.

Tab. 1.1: Mathematical expressions and types of symbols used in this thesis.

a, Ψ, θ, \dots	scalar
$\underline{x}, \underline{Y}, \dots$ x_i, Y_j, \dots	vector
$\underline{\underline{\sigma}}, \underline{\underline{E}}, \dots$ $\sigma_{ij}, E_{kl}, \dots$	second-order tensor
$\underline{\underline{\underline{\mathcal{G}}}}, \underline{\underline{\underline{\mathcal{L}}}}, \dots$ $\mathcal{G}_{ijk}, \mathcal{L}_{lmn}, \dots$	third-order tensor
$\underline{\underline{\underline{\underline{\mathbb{C}}}}}, \underline{\underline{\underline{\underline{\mathbb{P}}}}}, \dots$ $\mathbb{C}_{ijkl}, \mathbb{P}_{mnop}, \dots$	fourth-order tensor
\cdot	dot product / single contraction
$:$	double dot product / double contraction
\otimes	dyadic product
\wedge	cross product
∇	Nabla operator
$\text{grad}(\cdot)$	gradient of (\cdot)
$\text{grad}^S(\cdot)$	symmetrized gradient of (\cdot)
$\text{div}(\cdot)$	divergence of (\cdot)
$\text{sym}(\cdot)$	symmetric part of (\cdot)

1.2 Notation

To present the topics as unambiguously as possible while trying not to unnecessarily overload the formulas, both intrinsic and index notation can be found in the derivations. The index notation (which is clearly the most frequently used) is replaced by intrinsic notation, whenever indices play no role and would be detrimental to the flow of reading, e.g., when new quantities are introduced. Furthermore, for the intrinsic notation, underlines are used to indicate the tensorial order. No underline would therefore characterize a scalar (tensor of order zero), one underline a vector (tensor of first order), two underlines a tensor of second order, etc. The list displayed in Table 1.1 summarizes the notations, operators and types of symbols used in this thesis.

1.3 Fundamental Aspects of Continuum Mechanics

1.3.1 Separation of Scales and Representative Volume Elements

For the description of continuum theories, the introduction of a continuous body is necessary. This body is characterized by its properties being continuously distributed over its volume. It is composed of so-called particles or material points, which – for the respective scale – are not separated any further and are therefore infinitesimally small from a mathematical point of view. However, it should already be noted that a large part of the work will be devoted to scale separation (see Chapter 1.4). This is to emphasize that infinitesimal in the mathematical sense does not mean that a particle is also physically infinitely small. Quite the contrary, such a particle in general has a distinct microstructure that is taken into account in homogenization and in multiscale modeling. It does allow, however, the introduction of mathematical tools like differential and integral calculus.

It must therefore be ensured that the quantities assigned to this particle, usually a volume element dV , are really representative of the highly complex material constituting this particle. Such constitutive material elements are called representative volume elements (RVEs) [15, 16]. There are certain structural conditions associated with this RVE: If the characteristic length of the heterogeneities or that of the deformation mechanisms (e.g., the dislocation spacing) within the RVE is denoted as d , and the size of the RVE itself as l , then d must be much smaller than l . Furthermore, l must generally be much smaller than the dimensions L of the body built up by many RVEs, and in any case, it needs to be very much smaller than the spatial changes of the loading, λ [15–17]. This can be written compactly as:

$$d \ll l \ll L \quad \cap \quad l \ll \lambda \quad (1.1)$$

In concrete terms, much smaller means that between d and l there must be at least a factor of two for spherical micro-heterogeneities (e.g., for a maximum error of 5% in the estimation of macroscopic moduli) [18], and between l and L or λ , a minimum factor of 5–10 is required [19]. If these requirements cannot be met, caution must be exercised with regard to calculations in the classical continuum mechanics framework. In such cases, adapted models, such as one for which the foundation is to be laid in this thesis, can be helpful to obtain meaningful results.

1.3.2 Kinematics of a Continuum

The derivations of the kinematic quantities of continuum mechanics are dealt with extensively in many works, see for example [20–23]. Only the most important aspects that are fundamental to this thesis will be dealt with briefly here.

A material particle with an infinitesimal volume dV , as described previously, is now assigned to a position (or location) \underline{x} with respect to a given frame, and so are associated field quantities, such as mass density or volume force density.

Consider that a continuous body can perform motion in space and, unless it is a rigid body, it can be deformed. This means that all quantities assigned to a particle can be specified for an initial (or material) configuration as well as for a deformed (or spatial) configuration. Here, all quantities associated with the initial configuration are indicated with a prime symbol $(\cdot)'$ (the very common upper and lower case formulation is deliberately avoided, as this is used later for micro- and macroscale expressions). With this, a displacement field \underline{u} can be defined in the Lagrangian sense:

$$\underline{u}(\underline{x}', t) = \underline{x}(\underline{x}', t) - \underline{x}' \quad (1.2)$$

This vector field therefore indicates how far individual particles are displaced from the initial position as a function of time. If a particle is now conceptually connected to a neighbouring particle, an infinitesimally small line element is obtained, for both the initial and deformed configuration: $d\underline{x}'$ and $d\underline{x}$. The change from $d\underline{x}'$ to $d\underline{x}$ is thus inherently related to changes in length and angle and is described by the deformation gradient $\underline{\underline{F}}$:

$$d\underline{x}(\underline{x}', t) = \underline{\underline{F}}(\underline{x}', t) \cdot d\underline{x}'$$

$$\underline{\underline{F}}(\underline{x}', t) = \frac{\partial \underline{x}(\underline{x}', t)}{\partial \underline{x}'} \quad (1.3)$$

This second-order tensor is in the general case asymmetrical, and not independent of rigid-body motion. To overcome these issues, strain tensors have been derived on the basis of the deformation gradient, one of the most common being the Green-Lagrange strain tensor $\underline{\underline{E}}$:

$$\underline{\underline{E}}(\underline{x}', t) = \frac{1}{2} [\underline{\underline{F}}^T(\underline{x}', t) \cdot \underline{\underline{F}}(\underline{x}', t) - \underline{\underline{I}}] \quad (1.4)$$

Here, $\underline{\underline{I}}$ denotes the second-order identity tensor.

1.3.3 Equilibrium of a Continuum

The displacements, deformations, and strains of a continuous body, as introduced above, generally arise from associated forces. However, since the introduction of discrete forces in a continuum of (mathematically speaking) infinitely many particles does not make much sense, appropriate quantities can be defined instead over the volume elements and surface elements in the deformed configuration: To a volume element dV , a volume force density \underline{f} can be assigned, which has the unit *force per volume*. The total volume force acting on the volume V of a body is therefore:

$$\underline{F}_f = \int_V \underline{f}(\underline{x}, t) dV(\underline{x}, t)$$

Similarly, surface forces (tractions) can act on surface elements dS . These tractions \underline{t} have *force per area* as unit and the force acting on a body's surface S is:

$$\underline{F}_t = \int_S \underline{t}(\underline{x}, \underline{n}, t) dS(\underline{x}, t)$$

Accordingly, the equilibrium conditions of forces for a continuous body reads as:

$$\underline{F}_f + \underline{F}_t = \int_V \underline{f}(\underline{x}, t) dV(\underline{x}, t) + \int_S \underline{t}(\underline{x}, \underline{n}, t) dS(\underline{x}, t) = 0 \quad (1.5)$$

Using the action-reaction law and the tetrahedron lemma (which dates back to the works of A.-L. Cauchy in the 1800's) [24], a connection can be established between the tractions on an infinitesimal surface element and the corresponding (Cauchy) stress tensor $\underline{\underline{\sigma}}$, which is generally known as Cauchy's stress theorem:

$$\underline{t}(\underline{x}, \underline{n}, t) = \underline{\underline{\sigma}}(\underline{x}, t) \cdot \underline{n}(\underline{x})$$

where \underline{n} is the unit surface normal vector, oriented outward. Inserting this relationship into the equilibrium conditions (1.5), and application of the divergence theorem leads to the alternative (local) formulation of equilibrium [20, 21, 23, 25]:

$$\text{div} \underline{\underline{\sigma}}(\underline{x}, t) + \underline{f}(\underline{x}, t) = 0 \quad (1.6)$$

This equation will be used extensively throughout this thesis. Due to the equilibrium conditions of moments, the stress tensor is symmetric.

1.3.4 Principle of Virtual Power

The principle of virtual power (PVP) is a very fundamental principle in continuum mechanics: On the one hand, it allows for the derivation of equilibrium conditions and equations of motion, either for the classical continuum and its extensions [26] or for structural mechanics theories

[27–29], and on the other hand, it is the basis for various numerical solution procedures, such as the finite element method [30]. The system of so-called *external forces*, as introduced in Chapter 1.3.3 as volume forces and tractions, generate power on virtual velocities $\hat{\underline{v}}$ [26]:

$$\mathcal{P}^{ext}(t) = \int_V f(\underline{x}, t) \cdot \hat{\underline{v}}(\underline{x}, t) dV(\underline{x}, t) + \int_S t(\underline{x}, \underline{n}, t) \cdot \hat{\underline{v}}(\underline{x}, t) dS(\underline{x}, t) \\ \forall \hat{\underline{v}}(\underline{x}) \in \mathbb{R}^3, \quad \text{with} \quad \exists \frac{\partial \hat{\underline{v}}}{\partial \underline{x}}(\underline{x}) \in \mathbb{R}^3 \otimes \mathbb{R}^3 \quad (1.7)$$

The hat symbol ($\hat{\cdot}$) indicates virtual quantities, which can be, within a certain mathematical set, arbitrarily chosen.

Moreover, *internal forces*, expressed by the stress tensor $\underline{\underline{\sigma}}$, generate power on virtual strain rates $\hat{\underline{\underline{d}}}$,

$$\mathcal{P}^{int}(t) = - \int_V \underline{\underline{\sigma}}(\underline{x}, t) : \hat{\underline{\underline{d}}}(\underline{x}, t) dV(\underline{x}, t), \quad (1.8)$$

whereby the virtual strain rates are defined as [17, 26]

$$\hat{\underline{\underline{d}}}(\underline{x}, t) = \frac{1}{2} \left[\frac{\partial \hat{\underline{v}}(\underline{x}, t)}{\partial \underline{x}} + \left(\frac{\partial \hat{\underline{v}}(\underline{x}, t)}{\partial \underline{x}} \right)^T \right]. \quad (1.9)$$

The power of internal forces \mathcal{P}^{int} is an objective quantity, which means that rigid body movements must not have any influence on its value [26].

For any system in equilibrium with respect to a given frame, the total mechanical power, i.e. the sum of the power of external and internal forces, is zero [26]:

$$\mathcal{P}^{ext} + \mathcal{P}^{int} = 0 \quad (1.10)$$

$$\int_V f(\underline{x}, t) \cdot \hat{\underline{v}}(\underline{x}, t) dV(\underline{x}, t) + \int_S t(\underline{x}, \underline{n}, t) \cdot \hat{\underline{v}}(\underline{x}, t) dS(\underline{x}, t) - \int_V \underline{\underline{\sigma}}(\underline{x}, t) : \hat{\underline{\underline{d}}}(\underline{x}, t) dV(\underline{x}, t) = 0$$

1.3.5 Linear Elasticity

The classical theory of linear elasticity as a branch of continuum mechanics has developed into one of the most established methods over the last two centuries through numerous applications in the engineering sciences. For example, models of linear elastic materials are being used extensively in civil engineering, mechanical engineering, biomedical engineering, and geology applications. In view of the fact that the theory has emerged in the 19th century, where the foundation was laid by the works of A.L. Cauchy and G. Lamé (although the initial, one-dimensional Hooke's law was already described in the 17th century [31]), the original purpose was to describe macroscopic materials and structures. In the course of the last century, however, it became apparent that the theory is also valid on much smaller length scales, as it is used for many micromechanical models [15].

The term elasticity specifies an idealized constitutive material property, which is characterized as follows [20, 23, 32]: If a load is applied to a body, it will deform. If the body returns to its original shape and size after the load is removed, the body is said to be elastic. This implies that there is no energy dissipation throughout this process. The recoverable potential energy per unit volume that is stored upon deformation in the body is a Helmholtz free-energy density, often

called strain energy density, Ψ , which only depends on a momentary state of deformation and not directly on the loading history, time, etc. [22, 23]

Restricting the kinematic description to small deformations allows for linearization and thus simplification of the elasticity concept. Recalling the definition of the deformation gradient (1.3), and utilizing the definition of the displacement (1.2) leads to the following form of the deformation gradient:

$$\underline{\underline{F}}(\underline{x}', t) = \frac{\partial \underline{u}(\underline{x}', t)}{\partial \underline{x}'} + \underline{\underline{I}} \quad (1.11)$$

Inserting this relationship into the definition of the Green-Lagrange strain tensor (1.4) leads to the well-known alternative expression thereof:

$$\underline{\underline{E}}(\underline{x}', t) = \frac{1}{2} \left[\frac{\partial \underline{u}(\underline{x}', t)}{\partial \underline{x}'} + \left(\frac{\partial \underline{u}(\underline{x}', t)}{\partial \underline{x}'} \right)^T + \left(\frac{\partial \underline{u}(\underline{x}', t)}{\partial \underline{x}'} \right)^T \cdot \frac{\partial \underline{u}(\underline{x}', t)}{\partial \underline{x}'} \right] \quad (1.12)$$

Through the assumption of small deformations, the quadratic terms in (1.12) can be neglected. Furthermore, the deformation field can be assumed approximately equal for the material and spatial description:

$$\underline{u}(\underline{x}, t) \approx \underline{u}(\underline{x}', t)$$

These conditions then lead to the definition of the linearized (infinitesimal) strain tensor $\underline{\underline{\varepsilon}}$ [20, 23, 25],

$$\underline{\underline{\varepsilon}}(\underline{x}, t) = \frac{1}{2} \left[\frac{\partial \underline{u}(\underline{x}, t)}{\partial \underline{x}} + \left(\frac{\partial \underline{u}(\underline{x}, t)}{\partial \underline{x}} \right)^T \right], \quad (1.13)$$

which is a suitable energy conjugate for the Cauchy stress tensor $\underline{\underline{\sigma}}$. As a small strain approximation of the strain rate tensor (1.9), the following simplification can be used [23]:

$$\underline{\underline{\dot{d}}}(\underline{x}, t) \approx \underline{\underline{\dot{\varepsilon}}}(\underline{x}, t) \quad (1.14)$$

where $\underline{\underline{\dot{\varepsilon}}}$ is the time derivative of the linearized strain tensor (1.13).

For classical linear elasticity, the strain energy density solely depends on the six independent components of $\underline{\underline{\varepsilon}}$. It can thus be written:

$$\Psi = \Psi(\underline{\underline{\varepsilon}}(\underline{x}, t)) \quad (1.15)$$

The total stored, recoverable, elastic energy \mathcal{E} , is then the strain energy density integrated over the body's volume

$$\mathcal{E}(t) = \int_V \Psi \, dV, \quad (1.16)$$

and its temporal derivative is related to the applied power (1.7)[22, 23], namely via

$$\mathcal{P}^{ext}(t) = -\mathcal{P}^{int}(t) = \dot{\mathcal{E}}(t) = \int_V \dot{\Psi} \, dV = \int_V \pi^{ext} \, dV = - \int_V \pi^{int} \, dV, \quad (1.17)$$

where π^{ext} and π^{int} are the power densities of external and internal forces, respectively. By means of (1.14), the applied power density can be written as:

$$\pi^{ext} = \underline{\underline{\sigma}}(\underline{x}, t) : \underline{\underline{\dot{\varepsilon}}}(\underline{x}, t) \quad (1.18)$$

and considering that all externally performed work is transformed into elastic energy, one arrives at

$$\underline{\underline{\sigma}}(\underline{x}, t) : \underline{\underline{\dot{\varepsilon}}}(\underline{x}, t) = \dot{\Psi} = \frac{\partial \Psi}{\partial \underline{\underline{\varepsilon}}} : \underline{\underline{\dot{\varepsilon}}}(\underline{x}, t). \quad (1.19)$$

This needs to hold for any $\underline{\underline{\dot{\varepsilon}}}$, yielding [23, 25]

$$\underline{\underline{\sigma}}(\underline{x}, t) = \frac{\partial \Psi}{\partial \underline{\underline{\varepsilon}}}. \quad (1.20)$$

For small $\underline{\underline{\varepsilon}}$, (1.20) can be expanded into a Taylor series, which leads to

$$\underline{\underline{\sigma}}(\underline{x}, t) = \frac{\partial^2 \Psi}{\partial \underline{\underline{\varepsilon}} \partial \underline{\underline{\varepsilon}}} : \underline{\underline{\varepsilon}}(\underline{x}, t) = \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}(\underline{x}, t), \quad (1.21)$$

with the fourth-order elasticity tensor $\underline{\underline{\underline{\underline{C}}}}$.

For the sake of completeness, the temporal dependency has been stated explicitly up to this point. For the sake of simplicity and readability, it is kept implicit for the rest of the thesis.

Expression (1.21) is the constitutive law for linear elasticity. For isotropy, the stiffness tensor is sufficiently described by two elastic parameters, e.g. the so-called Lamé parameters [25]:

$$\mathbb{C}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (1.22)$$

where λ is the first Lamé parameter, and μ is the shear modulus.

Different pairs of different elastic parameters can easily be converted [25]. E.g., the Poisson's ratio ν can be expressed in terms of λ and μ :

$$\nu = \frac{\lambda}{2(\mu + \lambda)} \quad (1.23)$$

1.4 Pillars of Micromechanics and the Bridge between the Micro- and Macro-World

Most industrial and engineering materials and essentially all biogenic materials are heterogeneous at certain length scales. The different components also have different mechanical properties, orientations, etc. and can in turn be made up of even smaller components [33]. In the field of engineering, for example, the emergence of new composite materials over the last century has led to the augmentation or replacement of "classic" engineering materials due to their versatility, configurability, and lightweight design. However, the introduction of multiple material phases also meant that conventional material models were often insufficient to predict the macroscopic behavior of heterogeneous materials.

Micromechanics can be considered as a set of theories developed to solve this problem by describing heterogeneous materials based on their individual constituents the properties of which are known [34, 35]. While the earlier motivation was largely driven by the development of advanced materials, over the years the theories have been successfully extended to completely different areas, such as biomedical engineering and the description of biocomposites (wood, bone, etc.) [35].

As earliest, preliminary theory for predicting the mechanical properties of heterogeneous materials is considered to be the work of W. Voigt at the end of the 19. century [36]. Together with the model introduced by A. Reuss [37], the well-known "rule of mixtures" delivers rigorous upper

and lower bounds for effective moduli as functions of the constituents' volume fractions [35]. Numerous other prominent micromechanical theories were subsequently developed (see e.g. [38]), but the foundation for "continuum micromechanics" (as per [15]) and successful homogenization methods was not laid until the mid 20th century.

With the landmark paper "*The Determination of the Elastic Field of an Ellipsoidal Inclusion, and Related Problems*" [39], J.D. Eshelby provided one of the most influential contributions to solid mechanics in 1957, which constitutes the basis for many modern theories of micromechanics. This work deals with two problems that would later become famous as the *first Eshelby problem* or *Eshelby's inclusion*, and the *second Eshelby problem* or *Eshelby's inhomogeneity*. A more detailed description of the topics is provided in the following (Chapter 1.4.2). On the basis of these derivations, various methods were developed, which can take into account the shape and orientation of inclusions representing the inhomogeneities making up the microstructure of the RVE; and which can thus either deliver much narrower bounds for the effective moduli, or predict estimates for the macroscopic elasticity of an RVE. These methods also include the very prominent *Mori-Tanaka scheme* [40]. A general overview of these and other available methods and a more detailed description thereof can be found, e.g., in [15, 34, 35].

1.4.1 Stress and Strain Average Rules

A fundamental aim of continuum micromechanics is the calculation of an RVE's effective mechanical properties from information about its components. This information can be of quantitative (volume fractions, moduli, etc.) or of qualitative (degree of anisotropy, phase distribution, etc.) nature [16], whereby both categories must be taken into account in the calculation. This estimation of an equivalent substitute medium is called homogenization. For this, the macroscopic stress and strain fields ($\underline{\underline{\Sigma}}$ and $\underline{\underline{E}}$) acting on the homogenized medium must be the same as the microscopic stress and strain fields ($\underline{\underline{\sigma}}$ and $\underline{\underline{\varepsilon}}$) averaged over the RVE [15]. This usually requires that the separation of scales (1.3.1) is fulfilled. The two averaging rules are generally referred to as the *stress* and *strain average rule*:

$$\underline{\underline{\Sigma}}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}} \underline{\underline{\sigma}}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) \quad (1.24)$$

$$\underline{\underline{E}}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}} \underline{\underline{\varepsilon}}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) \quad (1.25)$$

Here, lower case symbols represent the microscopic and upper case symbols the macroscopic formulation. The microscopic position, \underline{x} , is measured from the center of the RVE, and the RVE itself is located at the macroscopic position \underline{X} . This illustrates that, in principle, all microscopic variables can depend on \underline{X} , but macroscopic variables are constant over the RVE.

The validity of the two equations (1.24) and (1.25) is typically derived from boundary conditions for microscopic displacements associated with uniform macroscopic strains, or for microscopic traction forces associated with uniform macroscopic stresses. These types of boundary conditions are often called *Hashin boundary conditions* [17], attributed to Z. Hashin [41]. With $\underline{\underline{\Sigma}}$ and $\underline{\underline{E}}$ being constant at the boundary of the RVE [15], the Hashin displacement and traction boundary conditions read as [17, 41]:

$$\begin{aligned} \underline{u}(\underline{x}) &= \underline{\underline{E}}(\underline{X}) \cdot \underline{x} \\ \underline{t}(\underline{x}) &= \underline{\underline{\Sigma}}(\underline{X}) \cdot \underline{n}(\underline{x}) \end{aligned} \quad (1.26)$$

where \underline{u} and \underline{t} are microscopic displacements and tractions, respectively. However, simultaneous application of both boundary conditions (1.26) on the same RVE is not possible, leaving one of the

average rules as a mere definition [17]. An elegant way to circumvent this fundamental issue was proposed by Jiménez Segura et al. [17], by relating the stress average rule to virtual macroscopic and microscopic expressions of the internal power density. This formalism is employed in this thesis and outlined in more detail in Chapter 3.

1.4.2 The Eshelby Problems

When it comes to solid mechanics, the works of J.D. Eshelby are indispensable, as they have profoundly influenced our understanding of the mechanical behavior of heterogeneous materials. Pioneering contributions include the concepts of Eshelby's inclusion and Eshelby's inhomogeneity, which provide fundamental insights into the stress and strain distribution in heterogeneous materials.

The foundation for this was laid in the 1957 paper [39]: On the one hand, the elastic state of a region undergoing a transformation (such as martensitic phase transformation, thermal expansion etc.) in an elastic isotropic medium of infinite extent (matrix) is considered, with its shape change being restricted by the matrix (*Eshelby's inclusion*). On the other hand, *Eshelby's inhomogeneity* deals with an inclusion with different elastic properties than the matrix, which in turn is subjected to external load. Eshelby's inhomogeneity problem, which can be seen as a generalization of Eshelby's inclusion problem, serves as the basis for numerous important micromechanical theories and is of significance for this work. This is why an overview of both problems will be provided hereafter.

Eshelby's Inclusion

Consider an ellipsoidal region (inclusion) with volume V_I and surface S inside a matrix of infinite extent and stiffness \mathbb{C}^0 (Figure 1.3 a). An ellipsoidal inclusion is chosen because it was shown that the resulting stresses and strains with this geometry are homogeneous in the inclusion [39]. Closed-form solutions for other geometries are only possible in certain cases (some of which listed e.g., in [35]), which are not topic of this thesis. This inclusion is now subjected to a series of imaginary steps: The inclusion is removed from the matrix (Figure 1.3 b) and allowed to undergo a strain of the magnitude $\underline{\underline{\varepsilon}}^*$ (which is often referred to as an *eigenstrain* [34]), so that it is in a stress-free state. The corresponding stress, $\underline{\underline{\sigma}}^*$ (an *eigenstress*), which would be necessary to bring back the inclusion into the compressed state would be:

$$\sigma_{ij}^* = \mathbb{C}_{ijkl}^0 \varepsilon_{kl}^*$$

Applying a surface (traction) force \underline{t} , which is related to $\underline{\underline{\sigma}}^*$ via the surface normal \underline{n}

$$t_i(\underline{x}) = -\sigma_{ij}^* n_j(\underline{x})$$

re-compresses the inclusion to its original shape (Figure 1.3 c). Subsequent returning of the inclusion into the matrix and release of the traction force creates an opposite force distribution along S (Figure 1.3 d):

$$f_i(\underline{x}) = -t_i(\underline{x}) = \sigma_{ij}^* n_j(\underline{x})$$

The matrix as well as the inclusion are now in a constrained state with the strain $\underline{\underline{\varepsilon}}^c$. The corresponding constrained stress $\underline{\underline{\sigma}}^c$ is then:

$$\sigma_{ij}^c = \mathbb{C}_{ijkl}^0 [\varepsilon_{kl}^c - \varepsilon_{kl}^* \mathcal{H}(V_I)], \quad \mathcal{H}(V_I) = \begin{cases} 1 & \text{if } \underline{x} \in V_I \\ 0 & \text{if } \underline{x} \notin V_I \end{cases} \quad (1.27)$$

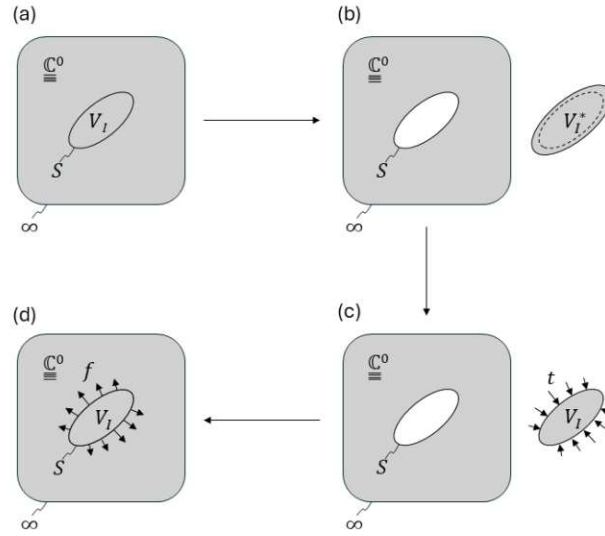


Fig. 1.3: Eshelby's inclusion problem.

Applying the equilibrium condition $\text{div}(\underline{\underline{\sigma}}) = 0$ to (1.27) yields:

$$\frac{\partial}{\partial x_i} (\sigma_{ij}^c) = 0 = \mathbb{C}_{ijkl}^0 \frac{\partial}{\partial x_i} (\varepsilon_{kl}^c) - \underbrace{\mathbb{C}_{ijkl}^0 \frac{\partial}{\partial x_i} [\varepsilon_{kl}^* \mathcal{H}(V_I)]}_{F_j}$$

where the second term on the right-hand side can be interpreted as a body force \underline{F} appearing inside of V_I due to the eigenstrain $\underline{\underline{\varepsilon}}^*$. With the formalism of Green's function for elasticity, the displacement field in the inclusion due to this body force can be written as [35]:

$$\begin{aligned} u_m(\underline{x}) &= - \int_{V_\infty} G_{mj}(\underline{x} - \underline{y}) \mathbb{C}_{ijkl}^0 \frac{\partial}{\partial y_i} [\varepsilon_{kl}^* \mathcal{H}(V_I)] dV(\underline{y}) = \\ &= - \int_{V_\infty} G_{mj}(\underline{x} - \underline{y}) \mathbb{C}_{ijkl}^0 \left[\frac{\partial}{\partial y_i} (\varepsilon_{kl}^*) \mathcal{H}(V_I) - \varepsilon_{kl}^* \delta(S) n_i \right] dV(\underline{y}) \end{aligned}$$

where $\underline{G}(\underline{x} - \underline{y})$ is the Green's function which gives the displacement at \underline{x} due to a point force located at \underline{y} (see Chapter 1.5), $\delta(\cdot)$ is the Dirac delta function and \underline{n} is the outward surface normal. Partial integration of the first term in the brackets, and subsequent application of the divergence theorem, while considering that the integrals vanish outside of V_I results in the second term canceling out [35]. Since the eigenstrain is homogeneous in an ellipsoidal inclusion [39], the following equation is obtained:

$$u_m(\underline{x}) = \mathbb{C}_{ijkl}^0 \varepsilon_{kl}^* \int_{V_I} \frac{\partial}{\partial y_i} [G_{mj}(\underline{x} - \underline{y})] dV(\underline{y}) \quad (1.28)$$

The symmetric gradient of (1.28) delivers the strain field in the constrained state resulting from a uniform eigenstress:

$$\varepsilon_{mn}^c = \mathbb{C}_{ijkl}^0 \varepsilon_{kl}^* \text{sym} \left\{ \frac{\partial}{\partial x_n} \int_{V_I} \frac{\partial}{\partial y_i} [G_{mj}(\underline{x} - \underline{y})] dV(\underline{y}) \right\} \quad (1.29)$$

Here, the fourth-order Hill Tensor \mathbb{P} is introduced (named after R. Hill, see e.g., [42]):

$$\mathbb{P}_{ijkl} = \text{sym} \left\{ \frac{\partial}{\partial x_j} \int_{V_I} \frac{\partial}{\partial y_k} [G_{il}(\underline{x} - \underline{y})] dV(\underline{y}) \right\} \quad (1.30)$$

With this, (1.29) can be written as:

$$\varepsilon_{mn}^c = \mathbb{C}_{ijkl}^0 \mathbb{P}_{ijmn} \varepsilon_{kl}^*$$

Or, in terms of the so-called Eshelby tensor \mathbb{S} :

$$\varepsilon_{ij}^c = \mathbb{S}_{ijkl} \varepsilon_{kl}^*$$

The Eshelby tensor therefore links the eigenstrain to the constrained (actual) strain. As indicated above, for ellipsoidal inclusions, the strain field due to a uniform eigenstress is also uniform. For other inclusions generally applies: $\mathbb{P} = \mathbb{P}(\underline{x})$, $\mathbb{S} = \mathbb{S}(\underline{x})$ and $\underline{\varepsilon}^c = \underline{\varepsilon}^c(\underline{x})$.

A description of analytical solutions for Hill tensors for various ellipsoidal inclusions is given, for example, in [34, 35].

Eshelby's Inhomogeneity

In the inhomogeneity problem, the (ellipsoidal) inclusion is of different stiffness \mathbb{C}^I than the surrounding matrix \mathbb{C}^0 . The general constitutive law can therefore be written as:

$$\sigma_{ij}^i(\underline{x}) = (\mathbb{C}_{ijkl}^0 + \Delta \mathbb{C}_{ijkl} \mathcal{H}(V_I)) \varepsilon_{kl}^i(\underline{x})$$

Where $\Delta \mathbb{C}$ is the difference between inclusion and matrix stiffness, i.e.:

$$\Delta \mathbb{C}_{ijkl} = \mathbb{C}_{ijkl}^i - \mathbb{C}_{ijkl}^0$$

The term $\Delta \mathbb{C} : \underline{\varepsilon}^i$ is often referred to as *polarization* or *polarization stresses* (e.g., [43]). Using the standard equilibrium conditions $\text{div}(\underline{\sigma}) = 0$ yields:

$$\begin{aligned} \frac{\partial}{\partial x_i} [\sigma_{ij}^i(\underline{x})] = 0 &= \mathbb{C}_{ijkl}^0 \frac{\partial}{\partial x_i} [\varepsilon_{kl}^i(\underline{x})] + \frac{\partial}{\partial x_i} [\Delta \mathbb{C}_{ijkl} \varepsilon_{kl}^i(\underline{x}) \mathcal{H}(V_I)] \\ \frac{\partial}{\partial x_i} [\mathbb{C}_{ijkl}^0 \varepsilon_{kl}^i(\underline{x})] &= - \underbrace{\frac{\partial}{\partial x_i} [\Delta \mathbb{C}_{ijkl} \varepsilon_{kl}^i(\underline{x}) \mathcal{H}(V_I)]}_{F_j} \end{aligned} \quad (1.31)$$

This equation resembles a non-homogeneous partial differential equation, for which a homogeneous and particulate solution is to be found depending on the boundary conditions [44]. For the particular solution, the term on the right-hand side of (1.31) can again be interpreted as a

fictional volume force \underline{F} present in the inclusion, this time caused by the difference in stiffness. The displacement solution thereof can be obtained via Green's functions.

1.5 Green's Functions for Elasticity

Generalities

Green's functions are the basis for an important method for solving differential equations, especially inhomogeneous, partial differential equations (PDEs). Such a PDE generally can have the form [45]:

$$L u(x) = f(x), \quad (1.32)$$

where L is a linear differential operator. E.g., let L be the Sturm-Liouville operator [45]:

$$L = \frac{d}{dx} \left(p(x) \frac{d}{dx} \right) + q(x) \quad (1.33)$$

with $p(x)$ and $q(x)$ being continuous function in an interval $[a, b]$. This problem is subject to homogeneous boundary conditions:

$$\begin{aligned} \alpha u(x) + \beta \left. \frac{du(x)}{d(x)} \right|_{x=a} &= 0 \\ \alpha u(x) + \beta \left. \frac{du(x)}{d(x)} \right|_{x=b} &= 0 \end{aligned} \quad (1.34)$$

with α and β being constants.

The Green's function for this set of problems then fulfills [45, 46]

$$L G(x, y) = \delta(x - y), \quad (1.35)$$

where $\delta(x - y)$ is the Dirac delta function with the properties [45, 46]:

$$\begin{aligned} \delta(x - y) &= 0 \quad \forall y \neq x \\ \delta(x - y) &= \infty \quad \text{if } y = x \\ \int_{-\infty}^{\infty} \delta(x - y) dx &= 1 \\ \int_{-\infty}^{\infty} \delta(x) dx &= 1 \\ \int_{-\infty}^{\infty} \delta(x - y) f(x) dx &= f(y) \\ \delta(x - y) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-y)} dp \end{aligned} \quad (1.36)$$

Considering the form of (1.35), multiplying both sides with a function $f(y)$ and integrating with respect to y yields [47]

$$L \left[\int_{-\infty}^{\infty} G(x, y) f(y) dy \right] = \int_{-\infty}^{\infty} \delta(x - y) f(y) dy = f(x).$$

Since the linear operator L is an operator on x it can be pulled out of the integral on the left-hand side. Comparing this with (1.32) shows that the solution of such a differential equation is [45, 46]:

$$u(x) = \int_{-\infty}^{\infty} G(x, y) f(y) dy$$

Finding a Green's function that satisfies the condition (1.35) and considering the respective boundary conditions leads to the solution of a differential equation (or to solutions of a set of similar differential equations).

Green's Functions for linear Elasticity

Recalling the equilibrium conditions for elasticity (1.6)

$$\frac{\partial}{\partial x_j} \sigma_{ij}(\underline{x}) + f_i(\underline{x}) = 0$$

and inserting the constitutive law for linear elasticity (1.21) yields

$$\mathbb{C}_{ijkl} \frac{\partial}{\partial x_j} \varepsilon_{kl}(\underline{x}) + f_i(\underline{x}) = 0.$$

Or, alternatively,

$$\mathbb{C}_{ijkl} \frac{\partial^2}{\partial x_l \partial x_j} u_k(\underline{x}) = -f_i(\underline{x}). \quad (1.37)$$

Due to the symmetry of $\underline{\underline{\mathbb{C}}}$ the gradient of $\underline{u}(\underline{x})$ does not have to be symmetrized.

Comparing this form with (1.32) shows that the operator to be solved with the Green's function is the following: $\mathcal{L} = \nabla [\nabla (\cdot)]$

The solution of these differential equations thus takes the following form, which can be regarded as the definition of Green's function for linear elasticity [48]:

$$u_i(\underline{x}) = G_{ij}(\underline{x} - \underline{y}) f_j(\underline{y}) \quad (1.38)$$

In this case, the Green's function is a second order tensor, which relates a point force \underline{f} at position \underline{y} to a displacement \underline{u} at position \underline{x} [34].

It must be noted that the form in which (1.38) is written (namely that $\underline{\underline{G}}$ solely depends on the distance between \underline{x} and \underline{y}) is only valid for homogeneous media. Furthermore, $\underline{\underline{G}}$ is a symmetric tensor, i.e. $G_{ij} = G_{ji}$, and $\underline{\underline{G}}(\underline{a}) = \underline{\underline{G}}(-\underline{a})$ [48].

The symmetric spatial derivative of (1.38) gives the corresponding strain at \underline{x} :

$$\varepsilon_{ik}(\underline{x}) = \text{sym} \frac{\partial}{\partial x_k} u_i(\underline{x}) = \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] f_j(\underline{y})$$

and together with the constitutive law the local stress is obtained:

$$\sigma_{lm}(\underline{x}) = \mathbb{C}_{lmik} \varepsilon_{ik}(\underline{x}) = \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] f_j(\underline{y}) \quad (1.39)$$

For any region with volume V_R , surface S , and surface outward normal \underline{n} , which contains the location of the point force \underline{y} , the equilibrium conditions must hold which can be expressed as [48]

$$\int_S \sigma_{lm}(\underline{x}) n_m dS(\underline{x}) + f_l(\underline{y}) = 0. \quad (1.40)$$

Insertion of (1.39) and application of the divergence theorem yields:

$$\int_{V_R} \frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] f_j(\underline{y}) \right\} dV(\underline{x}) + f_l(\underline{y}) = 0$$

The volume force can be pulled into the integral:

$$\begin{aligned} \int_{V_R} \left(\frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] f_j(\underline{y}) \right\} + \delta_{jl} \delta(\underline{x} - \underline{y}) f_j(\underline{y}) \right) dV(\underline{x}) &= 0 \\ \int_{V_R} \left(\frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] \right\} + \delta_{jl} \delta(\underline{x} - \underline{y}) \right) dV(\underline{x}) f_j(\underline{y}) &= 0 \end{aligned}$$

And, since equilibrium must hold for all regions inside the volume, the local form of the equation above reads as

$$\frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} [G_{ij}(\underline{x} - \underline{y})] \right\} + \delta_{jl} \delta(\underline{x} - \underline{y}) = 0. \quad (1.41)$$

This partial differential equation is the basis for solving with respect to \underline{G} . As the most prominent method to find solutions for this problem, the Fourier transform is used [35]. The Fourier transform of \underline{G} can be written as:

$$\hat{G}_{ij}(\underline{k}) = \int_{V_\infty} G_{ij}(\underline{x} - \underline{y}) e^{-i\underline{k}(\underline{x} - \underline{y})} dV(\underline{x}) \quad (1.42)$$

and the inverse Fourier transform follows as:

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{(2\pi)^3} \int_{V_\infty} \hat{G}_{ij}(\underline{k}) e^{i\underline{k}(\underline{x} - \underline{y})} dV(\underline{k}) \quad (1.43)$$

Here, \underline{k} denotes the (radially oriented) wave vector and i is the imaginary unit. Insertion of (1.43) into (1.41) gives [49]:

$$\begin{aligned} \frac{1}{(2\pi)^3} \frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \frac{\partial}{\partial x_k} \left[\int_{V_\infty} \hat{G}_{ij}(\underline{k}) e^{i\underline{k}(\underline{x} - \underline{y})} dV(\underline{k}) \right] \right\} + \delta_{jl} \delta(\underline{x} - \underline{y}) &= 0 \\ \frac{1}{(2\pi)^3} \frac{\partial}{\partial x_m} \left\{ \mathbb{C}_{lmik} \int_{V_\infty} \hat{G}_{ij}(\underline{k}) i k_k e^{i\underline{k}(\underline{x} - \underline{y})} dV(\underline{k}) \right\} + \delta_{jl} \delta(\underline{x} - \underline{y}) &= 0 \\ - \frac{1}{(2\pi)^3} \mathbb{C}_{lmik} \int_{V_\infty} \hat{G}_{ij}(\underline{k}) k_m k_k e^{i\underline{k}(\underline{x} - \underline{y})} dV(\underline{k}) + \delta_{jl} \delta(\underline{x} - \underline{y}) &= 0 \end{aligned}$$

which yields, for general \underline{k} [49]

$$\mathbb{C}_{lmik} k_m k_k \hat{G}_{ij}(\underline{k}) = I_{jl} \quad (1.44)$$

and with that

$$\hat{G}_{ij}(\underline{k}) = (\mathbb{C}_{lmik} k_m k_k)^{-1} I_{jl}. \quad (1.45)$$

This means, that knowledge of the inverse of tensor $\left(\underline{k} \cdot \underline{\underline{\mathbb{C}}} \cdot \underline{k} \right)$ and subsequent inverse Fourier transform gives the Green's function for (until here arbitrarily anisotropic) elasticity.

Isotropic elastic Materials

As described in Chapter 1.3.5, the isotropic stiffness tensor $\underline{\underline{\mathbb{C}}}^{iso}$ is fully determined by two constants, e.g., the Lamé constants λ and μ :

$$\mathbb{C}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{kj})$$

This means, that the tensor $\left(\underline{k} \cdot \underline{\underline{\mathbb{C}}} \cdot \underline{k} \right)$ can be written as:

$$\mathbb{C}_{lmik} k_m k_k = \lambda k_l k_i + \mu \delta_{li} k^2 + \mu k_l k_i = (\lambda + \mu) k_l k_i + \mu k^2 \delta_{li} \quad (1.46)$$

The inverse of this tensor can be calculated directly, or, more elegantly, as described e.g. in [48]: Namely, utilizing (1.44) and multiplying with k_l yields:

$$\begin{aligned} k_l \mathbb{C}_{lmik} k_m k_k \hat{G}_{ij}(\underline{k}) &= k_j \\ [(\lambda + \mu) k^2 + \mu k^2] k_i \hat{G}_{ij}(\underline{k}) &= k_j \\ k_i \hat{G}_{ij}(\underline{k}) &= \frac{k_j}{(\lambda + 2\mu) k^2} \end{aligned} \quad (1.47)$$

Re-substitution of (1.47) into (1.44) combined with (1.46) then results in:

$$\begin{aligned} \mu k^2 \delta_{li} \hat{G}_{ij}(\underline{k}) + \frac{(\lambda + \mu) k_l k_j}{(\lambda + 2\mu) k^2} &= \delta_{jl} \\ \hat{G}_{lj}(\underline{k}) &= \frac{\delta_{lj}}{\mu k^2} - \frac{(\lambda + \mu) k_l k_j}{(\lambda + 2\mu) \mu k^4} \end{aligned}$$

Application of the inverse Fourier transform (1.43) gives the Green's function for isotropic elasticity:

$$\begin{aligned} G_{ij}(\underline{x} - \underline{y}) &= \frac{1}{(2\pi)^3} \int_{V\infty} \left[\frac{I_{ij}}{\mu k^2} - \frac{(\lambda + \mu) k_i k_j}{(\lambda + 2\mu) \mu k^4} \right] e^{i\underline{k}(\underline{x} - \underline{y})} dV(\underline{k}) \\ &= \frac{1}{(2\pi)^3} \left[\frac{I_{ij}}{\mu} \int_{V\infty} \frac{e^{i\underline{k}(\underline{x} - \underline{y})}}{k^2} dV(\underline{k}) - \frac{(\lambda + \mu)}{(\lambda + 2\mu) \mu} \int_{V\infty} \frac{k_i k_j e^{i\underline{k}(\underline{x} - \underline{y})}}{k^4} dV(\underline{k}) \right] \end{aligned}$$

With the evaluation of these integrals, the closed form of Green's function for an isotropic elastic body of infinite extent is obtained [35, 48],

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{8\pi \mu (\lambda + 2\mu) |\underline{x} - \underline{y}|} \left[(\lambda + 3\mu) \delta_{ij} + (\lambda + \mu) \frac{(x_i - y_i)(x_j - y_j)}{|\underline{x} - \underline{y}|^2} \right], \quad (1.48)$$

with $|\underline{x} - \underline{y}| = \sqrt{(\underline{x} - \underline{y}) \cdot (\underline{x} - \underline{y})}$. In terms of μ and the Poisson ratio ν , (1.48) can be rewritten as

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{16\pi \mu (1 - \nu) |\underline{x} - \underline{y}|} \left[(3 - 4\nu) \delta_{ij} + \frac{(x_i - y_i)(x_j - y_j)}{|\underline{x} - \underline{y}|^2} \right].$$

Another alternative, equivalent expression (which will be used in this thesis) reads as [34]:

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{4\pi \mu} \frac{\delta_{ij}}{|\underline{x} - \underline{y}|} - \frac{1}{16\pi \mu (1 - \nu)} \frac{\partial^2}{\partial x_i \partial x_j} |\underline{x} - \underline{y}| \quad (1.49)$$

Closed-form solutions of Green's functions for higher degrees of anisotropy (regarding both matrix and inclusion) are only possible in some cases, a detailed overview is given e.g., in [35]. In this thesis, only the solution for the isotropic case, as derived, is utilized.

Chapter 2

Incorporation of a Higher Order Strain Measure and Strain Average Rule

As outlined in the previous chapter, the classical methods of micromechanics are to be extended by a measure for the macroscopic strain gradient. As a template, an excerpt from the prominent formalism for strain gradient elasticity by R.D. Mindlin [50] is employed and adapted. It is assumed that on the macroscopic level, in addition to the strain, a measure of the strain gradient is also responsible for displacements. The measure used is the macroscopic second gradient of the displacement $\underline{\underline{\mathcal{G}}}$:

$$\mathcal{G}_{ijk}(\underline{X}) = \frac{\partial^2 U_i(\underline{X})}{\partial X_j \partial X_k} \quad (2.1)$$

The second gradient of displacement is not only conceptually related to the actual strain gradient $\underline{\underline{\nabla E}}$, but they can be derived from each other via [51]:

$$\mathcal{G}_{ijk}(\underline{X}) = \nabla E_{ijk}(\underline{X}) + \nabla E_{ikj}(\underline{X}) - \nabla E_{jki}(\underline{X})$$

Explicitly written, $\underline{\underline{\nabla E}}$ reads as:

$$\nabla E_{ijk}(\underline{X}) = \frac{1}{2} \left(\frac{\partial^2 U_i(\underline{X})}{\partial X_j \partial X_k} + \frac{\partial^2 U_j(\underline{X})}{\partial X_i \partial X_k} \right)$$

The idea is now to incorporate this macroscopic $\underline{\underline{\mathcal{G}}}$ -tensor into the boundary value problem. Specifically, the Hashin displacement boundary conditions (1.26) are extended by a quadratic term, of the form given in [51]:

$$\underline{u}(\underline{x}, \underline{X}) = \underline{E}(\underline{X}) \cdot \underline{x} + \frac{1}{2} \underline{\underline{\mathcal{G}}}(\underline{X}) : (\underline{x} \otimes \underline{x}), \quad \underline{x} \in S_{RVE} \quad (2.2)$$

while we note in passing that quadratic forms have been prescribed at the boundary of an RVE for some 25 years (see e.g., [52]). This allows classical linear elasticity to be retained within the RVE, restricting gradient effects to the boundary (Figure 2.1). Correspondingly, very complicated and potentially impractical formulations arising from a strain-gradient-elastic microstructure are avoided.

We now investigate whether the new boundary conditions (2.2) are still consistent with the strain average rule (1.25); hence, whether

$$\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \underline{\underline{\varepsilon}}(\underline{x}, \underline{X}) \, dV(\underline{x}, \underline{X}) \stackrel{?}{=} \underline{E}(\underline{X}).$$

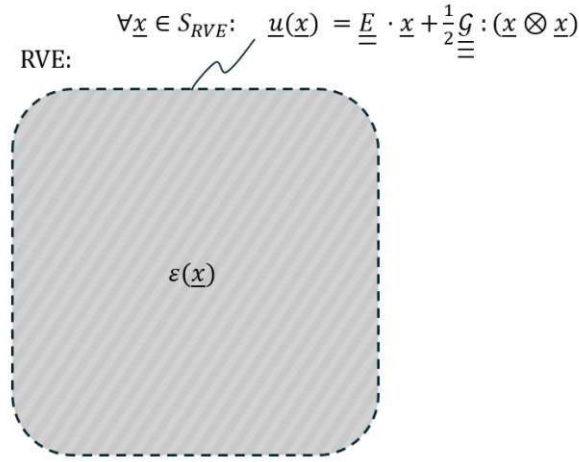


Fig. 2.1: Depiction of the boundary value problem for an RVE at position \underline{X} : The displacements at the boundary depend both on the macroscopic strain \underline{E} and on the macroscopic second gradient of displacement \underline{G} .

For this, the definition of the linearized strain tensor (1.13) is employed:

$$\int_{V_{RVE}} \varepsilon_{ij}(\underline{x}) dV(\underline{x}) = \frac{1}{2} \int_{V_{RVE}} \left(\frac{\partial u_i(\underline{x})}{\partial x_j} + \frac{\partial u_j(\underline{x})}{\partial x_i} \right) dV(\underline{x})$$

Application of the divergence theorem yields:

$$\int_{V_{RVE}} \varepsilon_{ij}(\underline{x}) dV = \frac{1}{2} \int_{S_{RVE}} [u_i(\underline{x}) n_j(\underline{x}) + u_j(\underline{x}) n_i(\underline{x})] dS(\underline{x})$$

Since the displacements are now specified at the boundary of the RVE, the boundary conditions (2.2) can be inserted for \underline{u} :

$$\begin{aligned} \int_{V_{RVE}(\underline{X})} \varepsilon_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) &= \frac{1}{2} \int_{S_{RVE}(\underline{X})} \left\{ \left[E_{ik}(\underline{X}) x_k + \frac{1}{2} \mathcal{G}_{ikl}(\underline{X}) x_l x_k \right] n_j(\underline{x}, \underline{X}) \right. \\ &\quad \left. + \left[E_{jk}(\underline{X}) x_k + \frac{1}{2} \mathcal{G}_{jkl}(\underline{X}) x_l x_k \right] n_i(\underline{x}, \underline{X}) \right\} dS(\underline{x}, \underline{X}) = \\ &= \frac{1}{2} E_{ik}(\underline{X}) \int_{S_{RVE}(\underline{X})} x_k n_j(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) + \frac{1}{4} \int_{S_{RVE}(\underline{X})} \mathcal{G}_{ikl}(\underline{X}) x_l x_k n_j(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) \\ &\quad + \frac{1}{2} E_{jk}(\underline{X}) \int_{S_{RVE}(\underline{X})} x_k n_i(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) + \frac{1}{4} \int_{S_{RVE}(\underline{X})} \mathcal{G}_{jkl}(\underline{X}) x_l x_k n_i(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) \end{aligned}$$

Taking $\underline{\underline{\mathcal{G}}}$ out of the integral and applying the divergence theorem once more yields

$$\begin{aligned} \int_{V_{RVE}(\underline{\mathbf{X}})} \varepsilon_{ij}(\underline{\mathbf{x}}, \underline{\mathbf{X}}) dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) &= \frac{1}{2} \left[E_{ik}(\underline{\mathbf{X}}) \int_{V_{RVE}(\underline{\mathbf{X}})} \frac{\partial x_k}{\partial x_j} dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) + E_{jk}(\underline{\mathbf{X}}) \int_{V_{RVE}(\underline{\mathbf{X}})} \frac{\partial x_k}{\partial x_i} dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) \right] \\ &\quad + \frac{1}{4} \left[\mathcal{G}_{ikl}(\underline{\mathbf{X}}) \int_{V_{RVE}(\underline{\mathbf{X}})} \frac{\partial}{\partial x_j} (x_l x_k) dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) + \mathcal{G}_{jkl}(\underline{\mathbf{X}}) \int_{V_{RVE}(\underline{\mathbf{X}})} \frac{\partial}{\partial x_i} (x_l x_k) dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) \right] = \\ &= \frac{1}{2} [E_{ik}(\underline{\mathbf{X}}) \delta_{kj} V_{RVE}(\underline{\mathbf{X}}) + E_{jk}(\underline{\mathbf{X}}) \delta_{ki} V_{RVE}(\underline{\mathbf{X}})] + \frac{1}{4} [T_{ij}(\underline{\mathbf{x}}, \underline{\mathbf{X}}) + T_{ji}(\underline{\mathbf{x}}, \underline{\mathbf{X}})] = \\ &= E_{ij}(\underline{\mathbf{X}}) V_{RVE}(\underline{\mathbf{X}}) + \frac{1}{2} \text{sym} [T_{ij}(\underline{\mathbf{x}}, \underline{\mathbf{X}})], \end{aligned}$$

where the expression $\mathcal{G}_{ikl} \int_{V_{RVE}} \frac{\partial}{\partial x_j} (x_l x_k) dV$ was abbreviated by T_{ij} .

It is obvious, that the strain average rule holds, when $\underline{\underline{\mathbf{T}}} = 0$. Explicitly writing the components of the third-order tensor $\frac{\partial}{\partial x_j} (x_l x_k)$ shows that $\underline{\mathbf{x}}$ only occurs linearly:

$$\begin{array}{ccc} \text{for } (l, k, j = 1) : & \text{for } (l, k, j = 2) : & \text{for } (l, k, j = 3) : \\ \frac{\partial}{\partial x_j} (x_l x_k) = & \begin{pmatrix} 2x_1 & x_2 & x_3 \\ x_2 & 0 & 0 \\ x_3 & 0 & 0 \end{pmatrix}, & \begin{pmatrix} 0 & x_1 & 0 \\ x_1 & 2x_2 & x_3 \\ 0 & x_3 & 0 \end{pmatrix}, & \begin{pmatrix} 0 & 0 & x_1 \\ 0 & 0 & x_2 \\ x_1 & x_2 & 2x_3 \end{pmatrix} \end{array}$$

With this, and in consideration of $\mathcal{G}_{ijk} = \mathcal{G}_{ikj}$, $\underline{\underline{\mathbf{T}}}$ reads as:

$$\begin{aligned} T_{ij}(\underline{\mathbf{x}}, \underline{\mathbf{X}}) &= \mathcal{G}_{ikl}(\underline{\mathbf{X}}) \int_{V_{RVE}(\underline{\mathbf{X}})} \frac{\partial}{\partial x_j} (x_l x_k) dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) = \\ &= \int_{V_{RVE}} \begin{pmatrix} 2x_1 \mathcal{G}_{111}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{112}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{113}(\underline{\mathbf{X}}) \\ +2x_2 \mathcal{G}_{112}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{122}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{123}(\underline{\mathbf{X}}) \\ +2x_3 \mathcal{G}_{113}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{123}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{133}(\underline{\mathbf{X}}) \\ \\ 2x_1 \mathcal{G}_{211}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{212}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{213}(\underline{\mathbf{X}}) \\ +2x_2 \mathcal{G}_{212}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{222}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{223}(\underline{\mathbf{X}}) \\ +2x_3 \mathcal{G}_{213}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{223}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{233}(\underline{\mathbf{X}}) \\ \\ 2x_1 \mathcal{G}_{311}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{312}(\underline{\mathbf{X}}) & 2x_1 \mathcal{G}_{313}(\underline{\mathbf{X}}) \\ +2x_2 \mathcal{G}_{312}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{322}(\underline{\mathbf{X}}) & +2x_2 \mathcal{G}_{323}(\underline{\mathbf{X}}) \\ +2x_3 \mathcal{G}_{313}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{323}(\underline{\mathbf{X}}) & +2x_3 \mathcal{G}_{333}(\underline{\mathbf{X}}) \end{pmatrix} dV(\underline{\mathbf{x}}, \underline{\mathbf{X}}) \end{aligned}$$

The integrand of every tensor component is a linear combination of the components of \underline{x} . The 11-component reads as:

$$T_{11}(\underline{x}, \underline{X}) = 2 \mathcal{G}_{111}(\underline{X}) \underbrace{\int_{V_{RVE}(\underline{X})} x_1 dV(\underline{x}, \underline{X})}_{I_1} + 2 \mathcal{G}_{112}(\underline{X}) \int_{V_{RVE}(\underline{X})} x_2 dV(\underline{x}, \underline{X}) + 2 \mathcal{G}_{113}(\underline{X}) \int_{V_{RVE}(\underline{X})} x_3 dV(\underline{x}, \underline{X})$$

The microscopic position \underline{x} is measured from the geometric center of the RVE. Thus, if a position vector \underline{x}' with arbitrary origin is introduced, it can be expressed as simple vector addition of \underline{x} with a constant vector \underline{x}^S that points from the same origin to the geometric center:

$$\underline{x}' = \underline{x} + \underline{x}^S \quad (2.3)$$

Evaluation of the integral I_1 , in consideration of (2.3) yields:

$$\begin{aligned} I_1 &= \int_{x_{1,a}}^{x_{1,b}} \int_{x_{2,a}(x_1)}^{x_{2,b}(x_1)} \int_{x_{3,a}(x_1,x_2)}^{x_{3,b}(x_1,x_2)} x_1' dx_3 dx_2 dx_1 - \int_{x_{1,a}}^{x_{1,b}} \int_{x_{2,a}(x_1)}^{x_{2,b}(x_1)} \int_{x_{3,a}(x_1,x_2)}^{x_{3,b}(x_1,x_2)} x_1^S dx_3 dx_2 dx_1 = \\ &= V_{RVE}(\underline{X}) \frac{x_{1,a} - x_{1,b}}{2} - V_{RVE}(\underline{X}) x_1^S = V_{RVE}(\underline{X}) x_1^S - V_{RVE}(\underline{X}) x_1^S = 0 \end{aligned}$$

Where $x_{i,a}$ and $x_{i,b}$ denote the boundaries of the RVE at position \underline{X} .

Since this calculation is analogous for all other components of \underline{T} , it can be stated that:

$$\underline{T} = 0$$

This result shows that the strain average rule (1.25) still holds for a linear elastic medium with the quadratic boundary conditions (2.2).

Chapter 3

Principle of Virtual Power and Stress Average Rule

In the previous chapter it was shown that the strain average rule still applies with the extended boundary conditions. Here, the stress average rule will be examined. As discussed by Jiménez Segura et al. [17], a simultaneous application of both Hashin boundary conditions (1.26) to the same RVE is not possible, which means that one of the average rules would always be treated as a definition. The proposed solution to this very fundamental issue, which will also be implemented here, was presented in the same paper, namely the utilization of the principle of virtual power (PVP) as put forward by P. Germain [26].

The basic aspects of the PVP for a general continuum, as described in Chapter 1.3.4 of the introduction, are applied here to an RVE, which represents an infinitesimal volume element on the macroscopic level, but is finite on the microscopic level. Thus, a connection between the macroscopically and microscopically formulated virtual quantities can be established [17].

In concrete terms, for every mechanical system in equilibrium, no matter the length scale, the total power of its forces on an arbitrary virtual velocity field characterizing the system, is zero:

$$\begin{aligned} \mathcal{P}(\hat{v}) = \mathcal{P}^{ext}(\hat{v}) + \mathcal{P}^{int}(\hat{v}) = 0 \quad \forall \hat{v}(\underline{x}), \quad \exists \frac{\partial \hat{v}(\underline{x})}{\partial \underline{x}} \\ \mathcal{P}^{int}(\hat{v}^{RB}) = 0 \quad \forall \hat{v}_T^{RB}, \hat{\omega}^{RB}; \text{ so that } \hat{v}^{RB}(\underline{x}) = \hat{v}_T^{RB} + \hat{\omega}^{RB} \wedge \underline{x} \end{aligned} \quad (3.1)$$

whereby \hat{v}^{RB} is a virtual velocity field associated with a rigid body motion, with \hat{v}_T^{RB} and $\hat{\omega}^{SK}$ denoting the translational and the rotational portion of the rigid body motion.

At the microscopic RVE level, where the classical linear elastic formulations are to be retained, the powers of the external and internal forces can be expressed as follows:

$$\mathcal{P}^{ext,\mu} = \int_{V_{RVE}} \underline{f}_i(\underline{x}) \hat{v}_i(\underline{x}) dV(\underline{x}) + \int_{S_{RVE}} \underline{t}_j(\underline{x}) \hat{v}_j(\underline{x}) dS(\underline{x}) \quad (3.2)$$

$$\mathcal{P}^{int,\mu} = - \int_{V_{RVE}} \underline{\sigma}_{ij}(\underline{x}) \hat{d}_{ij}(\underline{x}) dV(\underline{x}) \quad (3.3)$$

with \underline{f} and \underline{t} being microscopic volume and traction forces respectively, \hat{v} being the microscopic virtual velocity field, $\underline{\sigma}$ being the microscopic Cauchy stress tensor, and \hat{d} being the microscopic virtual strain rate tensor. The latter is defined as

$$\hat{d}_{ij}(\underline{x}) = \frac{1}{2} \left(\frac{\partial \hat{v}_i(\underline{x})}{\partial x_j} + \frac{\partial \hat{v}_j(\underline{x})}{\partial x_i} \right). \quad (3.4)$$

The incorporation of gradient effects is carried out in a comparable way to the previous chapter. Namely, geometrically compatible, quadratic boundary conditions are prescribed at the boundary of the RVE:

$$\hat{v}_i(\underline{x}, \underline{X}) = \hat{V}_i(\underline{X}) + \hat{D}_{ij}(\underline{X})x_j + \frac{1}{2}\hat{\mathcal{H}}_{ijk}(\underline{X})x_kx_j \quad \forall \underline{x} \in \partial V_{RVE} \quad (3.5)$$

where \hat{V} is the macroscopic virtual velocity field, \hat{D} is the macroscopic virtual strain rate tensor, defined as

$$\hat{D}_{ij}(\underline{X}) = \frac{1}{2} \left(\frac{\partial \hat{V}_i(\underline{X})}{\partial X_j} + \frac{\partial \hat{V}_j(\underline{X})}{\partial X_i} \right) \quad (3.6)$$

and $\hat{\mathcal{H}}$ is the macroscopic second gradient of virtual velocity, reading as

$$\hat{\mathcal{H}}_{ijk}(\underline{X}) = \frac{\partial^2 \hat{V}_i(\underline{X})}{\partial X_j \partial X_k}. \quad (3.7)$$

Equation (3.5) constitutes an extension of the boundary conditions described by Jiménez Segura et al. [17], and therefore a quite substantial generalization of the Hashin displacement boundary conditions (1.26).

With that, eqn. (3.5) can be interpreted as a modification of a second-order Taylor approximation of the macroscopic velocity field \hat{V} at position \underline{X} , that "radiates" into the microscale via \underline{x} ,

$$\hat{v}_i(\underline{x}, \underline{X}) = \hat{V}_i(\underline{X}) + \frac{\partial}{\partial X_j} [\hat{V}_i(\underline{X})] x_j + \frac{1}{2} \frac{\partial^2}{\partial X_j \partial X_k} [\hat{V}_i(\underline{X})] x_k x_j + \dots$$

Namely, due to reasons of objectivity, only the symmetric part of $\frac{\partial}{\partial X_j} [\hat{V}_i(\underline{X})]$, represented by \hat{D} as in (3.6), is used.

The introduction of $\hat{\mathcal{H}}$ also implies that the macroscopically formulated power of internal forces $\mathcal{P}^{int,M}$, is not only determined by the macroscopic stress tensor $\underline{\underline{\Sigma}}$ in combination with a macroscopic virtual strain rate tensor \hat{D} (analogous to (3.3)), but that $\hat{\mathcal{H}}$ must be included with a suitable energy conjugate as well. Therefore, macroscopic double stresses $\underline{\underline{\mathcal{S}}}$ are introduced:

$$\mathcal{P}^{int,M} = \int_V \pi^{int,M}(\underline{X}) dV(\underline{X}) = \int_V \left[-\Sigma_{ij}(\underline{X}) \hat{D}_{ij}(\underline{X}) - \mathcal{S}_{ijk}(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X}) \right] dV(\underline{X}) \quad (3.8)$$

Double stresses occur frequently in strain gradient elasticity theories, a practicable overview is given for example in [53].

Continuing in this vein, the macroscopically formulated power of external forces $\mathcal{P}^{ext,M}$ can be extended to

$$\begin{aligned} \mathcal{P}^{ext,M} = & \int_V F_i(\underline{X}) \hat{V}_i(\underline{X}) + \Phi_{ij}(\underline{X}) \hat{W}_{ij}(\underline{X}) + \Phi'_{ijk}(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X}) dV(\underline{X}) \\ & + \int_S T_i(\underline{X}) \hat{V}_i(\underline{X}) + M_{ij}(\underline{X}) \hat{W}_{ij}(\underline{X}) + M'_{ijk}(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X}) dS(\underline{X}), \end{aligned} \quad (3.9)$$

where $\underline{\Phi}$ denotes volumic double forces, $\underline{\Phi}'$ volumic triple forces, \underline{M} surface double tractions, \underline{M}' surface triple tractions, and $\underline{\hat{W}}$ is the (non-symmetrized) gradient of macroscopic virtual velocities:

$$\hat{W}_{ij}(\underline{X}) = \frac{\partial \hat{V}_i(\underline{X})}{\partial X_j}$$

Vanishing Internal Power for Virtual Rigid Body Motion

It must be verified, that $\underline{\hat{H}}$ is an objective quantity, i.e. rigid body motions do not affect the power of internal forces [26]: $\mathcal{P}^{int}(\underline{\hat{V}}^{RB}) = 0$ requires $\underline{\hat{H}}^{RB} = 0$.

A rigid body motion $\underline{V}^{RB}(\underline{x})$ can be written as

$$\underline{V}^{RB}(\underline{x}) = \underline{V}^T + \underline{\Omega} \wedge \underline{X}.$$

Where \underline{V}^T is the translational speed of the body's center of mass, $\underline{\Omega}$ is the angular velocity, and \underline{X} is the distance from the center of mass.

With the definition of $\underline{\hat{H}}$ (3.7) the following is obtained:

$$\hat{H}_{ijk} = \frac{\partial^2}{\partial X_j \partial X_k} [V_i^{RB}(\underline{X})] = \frac{\partial^2}{\partial X_j \partial X_k} (V_i^T + \epsilon_{lmi} \Omega_l X_m)$$

Here, $\underline{\epsilon}$ denotes the Levi-Civita symbol which performs the cross-product. Expressing the sum in the parentheses in matrix notation reveals that $\underline{\hat{H}}$ is indeed objective:

$$\hat{H}_{ijk} = \frac{\partial^2}{\partial X_j \partial X_k} \begin{pmatrix} V_1^T + \Omega_2 X_3 - \Omega_3 X_2 \\ V_2^T + \Omega_3 X_1 - \Omega_1 X_3 \\ V_3^T + \Omega_1 X_2 - \Omega_2 X_1 \end{pmatrix} = 0$$

Stress Average Rule

As formulated by Jiménez Segura et al. [17], the macroscopic power density of internal forces must be equal the corresponding power density of the RVE, averaged over its volume:

$$\pi^{int,M}(\underline{X}) \stackrel{!}{=} \pi_{RVE}^{int,\mu}(\underline{X})$$

In view of (3.3) and (3.8) this reads as

$$\Sigma_{ij}(\underline{X}) \hat{D}_{ij}(\underline{X}) + \mathcal{S}_{ijk}(\underline{X}) \hat{H}_{ijk}(\underline{X}) \stackrel{!}{=} \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) \hat{d}_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}). \quad (3.10)$$

This equivalence, together with classical linear elasticity at the microscale implies the following, most general form of $\underline{\hat{d}}$:

$$\hat{d}_{ij}(\underline{x}, \underline{X}) = A_{ijkl}^D(\underline{x}, \underline{X}) \hat{D}_{kl}(\underline{X}) + A_{ijklm}^H(\underline{x}, \underline{X}) \hat{H}_{klm}(\underline{X}), \quad (3.11)$$

and insertion of (3.11) into (3.10) yields

$$\pi_{RVE}^{int} = -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) \left[A_{ijkl}^D(\underline{x}, \underline{X}) \hat{D}_{kl}(\underline{X}) + A_{ijklm}^H(\underline{x}, \underline{X}) \hat{H}_{klm}(\underline{X}) \right] dV(\underline{x}, \underline{X}) \quad (3.12)$$

Moreover, analogously to the proof given in Chapter 2, it can be shown that the higher-order boundary conditions for virtual velocities (3.5) imply an average rule for the strain rates:

$$\hat{D}_{ij}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \hat{d}_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}). \quad (3.13)$$

The fourth-order tensor $\underline{\underline{\underline{\underline{A}}}}^D$ and the fifth-order tensor $\underline{\underline{\underline{\underline{A}}}}^H$ are downscaling tensor fields to be determined. From eqns. (3.11) and (3.13) it is obvious, that the volume averages of these tensor fields must be:

$$\frac{1}{V_{RVE}} \int_{V_{RVE}} \underline{\underline{\underline{\underline{A}}}}^D(\underline{x}, \underline{X}) dV = \underline{\underline{\underline{\underline{1}}}}; \quad \frac{1}{V_{RVE}} \int_{V_{RVE}} \underline{\underline{\underline{\underline{A}}}}^H(\underline{x}, \underline{X}) dV = 0. \quad (3.14)$$

An alternative expression for π_{RVE}^{int} is obtained from integration by parts as described by Jiménez Segura et al. [17] with their equations (16) and (18):

$$\pi_{RVE}^{int}(\underline{X}) = -\frac{1}{V_{RVE}(\underline{X})} \int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) \hat{v}_j(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) + \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \frac{\partial}{\partial x_l} \sigma_{kl}(\underline{x}, \underline{X}) \hat{v}_k(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X})$$

Inserting the boundary conditions (3.5) into the the first integral yields

$$\pi_{RVE}^{int}(\underline{X}) = -\frac{1}{V_{RVE}(\underline{X})} \underbrace{\int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) \left(\hat{V}_j(\underline{X}) + \hat{D}_{jk}(\underline{X}) x_k + \hat{H}_{jkl}(\underline{X}) x_l x_k \right) dS(\underline{x}, \underline{X})}_{I_1'} + \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \frac{\partial}{\partial x_j} \sigma_{ij}(\underline{x}, \underline{X}) \hat{v}_i(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}), \quad (3.15)$$

which in turn can be written as:

$$\begin{aligned} I_1' &= \int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) \left(\hat{V}_j(\underline{X}) + \hat{D}_{jk}(\underline{X}) x_k + \hat{H}_{jkl}(\underline{X}) x_l x_k \right) dS(\underline{x}, \underline{X}) = \\ &= \int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) dS(\underline{x}, \underline{X}) \hat{V}_j(\underline{X}) + \int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) x_k dS(\underline{x}, \underline{X}) \hat{D}_{jk}(\underline{X}) \\ &\quad + \int_{S_{RVE}(\underline{X})} n_i(\underline{x}, \underline{X}) \sigma_{ij}(\underline{x}, \underline{X}) x_l x_k dS(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}). \end{aligned}$$

Application of the divergence theorem gives

$$I'_1 = \int_{V_{RVE}(\underline{X})} \frac{\partial}{\partial x_i} \sigma_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) \hat{V}_j(\underline{X}) \\ + \int_{V_{RVE}(\underline{X})} \frac{\partial}{\partial x_i} [\sigma_{ij}(\underline{x}, \underline{X}) x_k] dV(\underline{x}, \underline{X}) \hat{D}_{jk}(\underline{X}) \\ + \int_{V_{RVE}(\underline{X})} \frac{\partial}{\partial x_i} [\sigma_{ij}(\underline{x}, \underline{X}) x_l x_k] dV(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}).$$

Considering the equilibrium conditions (1.6) and the product rule of differentiation, followed by rearrangement of terms results in

$$I'_1 = \int_{V_{RVE}(\underline{X})} -f_j(\underline{x}, \underline{X}) \left(\hat{V}_j(\underline{X}) + \hat{D}_{jk}(\underline{X}) x_k + \hat{H}_{jkl}(\underline{X}) x_l x_k \right) dV(\underline{x}, \underline{X}) \\ + \int_{V_{RVE}(\underline{X})} \sigma_{kj}(\underline{x}, \underline{X}) \hat{D}_{jk}(\underline{X}) dV(\underline{x}, \underline{X}) + \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}) \frac{\partial}{\partial x_i} (x_l x_k) dV(\underline{x}, \underline{X}).$$

Back-insertion into (3.15) gives:

$$\pi_{RVE}^{int}(\underline{X}) = -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[-f_j(\underline{x}, \underline{X}) \left(\hat{V}_j(\underline{X}) + \hat{D}_{jk}(\underline{X}) x_k + \hat{H}_{jkl}(\underline{X}) x_l x_k \right) \right. \\ \left. + \sigma_{kj}(\underline{x}, \underline{X}) \hat{D}_{jk}(\underline{X}) + \sigma_{ij}(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}) \frac{\partial}{\partial x_i} (x_l x_k) + f_j(\underline{x}, \underline{X}) \hat{v}_j(\underline{x}, \underline{X}) \right] dV(\underline{x}, \underline{X}) = \\ = -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[\sigma_{ij}(\underline{x}, \underline{X}) \hat{D}_{ji}(\underline{X}) + \sigma_{ij}(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}) \frac{\partial}{\partial x_i} (x_l x_k) \right. \\ \left. + f_j(\underline{x}, \underline{X}) \left(\hat{v}_j(\underline{x}) - \hat{V}_j(\underline{X}) - \hat{D}_{jk}(\underline{X}) x_k - \hat{H}_{jkl}(\underline{X}) x_l x_k \right) \right] dV(\underline{x}, \underline{X}) \\ \pi_{RVE}^{int}(\underline{X}) = -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} [\sigma_{ij}(\underline{x}, \underline{X})] dV(\underline{x}, \underline{X}) \hat{D}_{ji}(\underline{X}) \\ - \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[\sigma_{ij}(\underline{x}, \underline{X}) \hat{H}_{jkl}(\underline{X}) \frac{\partial}{\partial x_i} (x_l x_k) \right] dV(\underline{x}, \underline{X}) \\ - \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[f_j(\underline{x}, \underline{X}) \left(\hat{v}_j(\underline{x}, \underline{X}) - \hat{V}_j(\underline{X}) - \hat{D}_{jk}(\underline{X}) x_k - \hat{H}_{jkl}(\underline{X}) x_l x_k \right) \right] dV(\underline{x}, \underline{X}) \quad (3.16)$$

Comparing eqn. (3.16) with (3.12) leads to the result that $\underline{\underline{\underline{A}}}^D = \underline{\underline{\underline{I}}}$, and to an expression for $\underline{\underline{\underline{A}}}^H$:

$$\begin{aligned} & -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) \left[A_{ijkl}^D(\underline{x}, \underline{X}) \hat{D}_{kl}(\underline{X}) + A_{ijklm}^H(\underline{x}, \underline{X}) \hat{H}_{klm}(\underline{X}) \right] dV(\underline{x}, \underline{X}) = \\ & = -\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) \hat{D}_{ji}(\underline{X}) \\ & \quad - \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) \underbrace{\frac{\partial}{\partial x_i} x_l x_k \delta_{jm}}_{\underline{\underline{\underline{A}}}^H} dV(\underline{x}, \underline{X}) \hat{H}_{mkl}(\underline{X}) \\ & \underbrace{-\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[f_j(\underline{x}, \underline{X}) \left(\hat{v}_j(\underline{x}, \underline{X}) - \hat{V}_j(\underline{X}) - \hat{D}_{jk}(\underline{X})x_k - \hat{H}_{jkl}(\underline{X})x_l x_k \right) \right]}_{I_3} dV(\underline{x}, \underline{X}) \end{aligned}$$

$$A_{ijklm}^H(\underline{x}) = \frac{\partial}{\partial x_i} x_l x_k \delta_{jm}$$

When \underline{x} is measured from the RVEs geometrical center, the conditions (3.14) are met. Furthermore, a comparison of coefficients leads to the result that the third integral expression (I_3) must be zero:

$$I_3 = 0$$

This implies that for general volume forces, the expression in the parentheses must be equal to zero:

$$\hat{v}_j(\underline{x}, \underline{X}) - \hat{V}_j(\underline{X}) - \hat{D}_{jk}(\underline{X})x_k - \hat{H}_{jkl}(\underline{X})x_l x_k = 0$$

This shows, that the boundary conditions (3.5) are valid throughout the volume of the RVE:

$$\hat{v}_i(\underline{x}, \underline{X}) = \hat{V}_i(\underline{X}) + \hat{D}_{ij}(\underline{X})x_j + \hat{H}_{ijk}(\underline{X})x_k x_j \quad \forall \underline{x} \in V_{RVE} \quad (3.17)$$

With these results, the macroscopic stress can be expressed as the volume average of the microscopic stress, therefore the stress average rule (1.24) holds:

$$\Sigma_{ij}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \sigma_{ij}(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X})$$

Additionally, an average rule for the macroscopic double stress was obtained:

$$S_{klm}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \left[\sigma_{ij}(\underline{x}, \underline{X}) \frac{\partial}{\partial x_i} x_l x_k \delta_{jm} \right] dV(\underline{x}, \underline{X}) \quad (3.18)$$

Volume Force Average Rule

A similar procedure can be used to potentially obtain a volume force average rule. The power density of external forces, in particular volume forces, also must be equivalent for the macroscopic and microscopic point-of-view [17]:

$$\pi_{vol}^{ext, M}(\underline{X}) \stackrel{!}{=} \pi_{vol, RVE}^{ext, \mu}(\underline{X})$$

The respective, extended macroscopic power density of external forces reads as

$$\pi_{vol}^{ext,M}(\underline{X}) = F_i(\underline{X})\hat{V}_i(\underline{X}) + \Phi_{ij}(\underline{X})\hat{W}_{ij}(\underline{X}) + \Phi'_{ijk}(\underline{X})\hat{\mathcal{H}}_{ijk}(\underline{X}). \quad (3.19)$$

In the microscopic formulation, again, the classical form is conserved:

$$\pi_{vol, RVE}^{ext,\mu}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})\hat{v}_i(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}) \quad (3.20)$$

It was shown above, that the quadratic boundary conditions (3.5) are valid throughout the RVE (3.17), insertion into (3.20) delivers:

$$\begin{aligned} \pi_{vol, RVE}^{ext,\mu}(\underline{X}) &= \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})\hat{V}_i(\underline{X}) dV(\underline{x}, \underline{X}) \\ &\quad + \underbrace{\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})x_j dV(\underline{x}, \underline{X})}_{I'_2} \hat{W}_{ij}(\underline{X}) \\ &\quad + \underbrace{\frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})x_kx_j dV(\underline{x}, \underline{X})}_{I'_3} \hat{\mathcal{H}}_{ijk}(\underline{X}) \end{aligned} \quad (3.21)$$

Comparing (3.21) with (3.19) indicates, that

$$F_i(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X}) dV(\underline{x}, \underline{X}), \quad (3.22)$$

$$\Phi_{ij}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})x_j dV(\underline{x}, \underline{X}),$$

and

$$\Phi'_{ijk}(\underline{X}) = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} f_i(\underline{x}, \underline{X})x_kx_j dV(\underline{x}, \underline{X}). \quad (3.23)$$

It was shown [17], that – for unidirectional force fields and when the microscopic position \underline{x} is measured from the RVEs center of gravity – the integral expression I'_2 and with that $\underline{\Phi}$, is equal to zero. However, the integral I'_3 is in general not zero. The expression

$$I'_3 = \Phi'_{ijk}(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X})$$

reads for a unidirectional force field, such as the gravitational field, as

$$I'_3 = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} \rho(\underline{x}, \underline{X}) x_kx_j dV(\underline{x}, \underline{X}) g_i(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X}).$$

Due to the quadratic term, also for a microscopically uniform volume force field $\underline{f}(\underline{X})$ the integral does not vanish:

$$I'_3 = \frac{1}{V_{RVE}(\underline{X})} \int_{V_{RVE}(\underline{X})} x_kx_j dV(\underline{x}, \underline{X}) f_i(\underline{X}) \hat{\mathcal{H}}_{ijk}(\underline{X})$$

When \underline{x} is measured from the RVEs center of gravity, and a microscopic position vector $\bar{\underline{x}}$, which locates the center of gravity at \underline{x}^S , is adopted (comparable to (2.3)), the evaluation of the expression $\int_{V_{RVE}(\underline{X})} x_k x_j dV(\underline{x}, \underline{X})$ reads in matrix notation as:

$$\begin{aligned} \int_{V_{RVE}(\underline{X})} x_k x_j dV(\underline{x}, \underline{X}) &= \int_{V_{RVE}(\underline{X})} (\bar{x}_k - x_k^S) (\bar{x}_j - x_j^S) dV(\underline{x}, \underline{X}) = \\ &= \frac{1}{3} V_{RVE}(\underline{X}) \cdot \begin{pmatrix} (x_1^S)^2 & 0 & 0 \\ 0 & (x_2^S)^2 & 0 \\ 0 & 0 & (x_3^S)^2 \end{pmatrix} \neq 0 \end{aligned}$$

With the present formalism and the boundary conditions (3.5), in addition to an averaging rule for volume forces (3.22), an averaging rule for triple volume forces (3.23) is therefore also obtained.

Chapter 4

Matrix Inclusion Problem Subjected to Strain Gradient

4.1 General Derivation

Now that the validity of the strain and stress average rules was demonstrated in the two previous chapters, the macroscopic higher-order strain measure is to be incorporated into the matrix inclusion problem. In particular, the derivation of Eshelby's inhomogeneity, which was only briefly discussed in the introduction (Chapter 1.4.2), is revisited.

Consider an ellipsoidal inclusion with volume V_I and (for now arbitrary) stiffness $\underline{\underline{c}}^i$ in a matrix of infinite extent with constant stiffness $\underline{\underline{c}}^m$ (Figure 4.1). The elastic law can be expressed in terms of polarization stresses $\underline{\underline{\tau}}$ via the following relationships:

$$\begin{aligned} \sigma_{ij}(\underline{x}) &= \mathbb{c}_{ijkl}^i(\underline{x}) \varepsilon_{kl}(\underline{x}) = \mathbb{c}_{ijkl}^m \varepsilon_{kl}(\underline{x}) + \underbrace{[\mathbb{c}_{ijkl}^i(\underline{x}) \varepsilon_{kl}(\underline{x}) - \mathbb{c}_{ijkl}^m \varepsilon_{kl}(\underline{x})]}_{\underline{\underline{\tau}}} \mathcal{H}(V_I) \\ \tau_{ij}(\underline{x}) &= (\mathbb{c}_{ijkl}^i(\underline{x}) - \mathbb{c}_{ijkl}^m) \varepsilon_{kl}(\underline{x}) = \Delta \mathbb{c}_{ijkl}(\underline{x}) \varepsilon_{kl}(\underline{x}) \\ \sigma_{ij}(\underline{x}) &= \mathbb{c}_{ijkl}^m \varepsilon_{kl}(\underline{x}) + \tau_{ij}(\underline{x}) \mathcal{H}(V_I) \end{aligned} \tag{4.1}$$

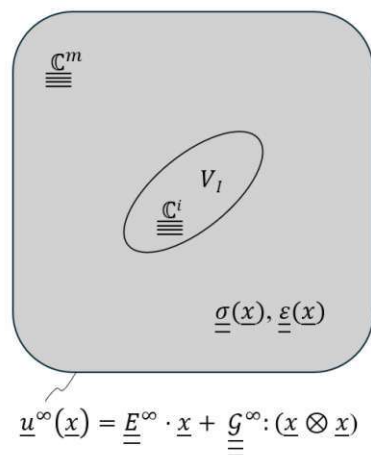


Fig. 4.1: Matrix inclusion problem incorporating the macroscopic higher-order strain measure \underline{G}^∞ via quadratic boundary conditions.

where $\mathcal{H}(V_I)$ is the Heaviside function, which is unity inside V_I and zero elsewhere. The strain field $\underline{\underline{\varepsilon}}$ is the symmetric gradient of the displacement field \underline{u} :

$$\varepsilon_{ij}(\underline{x}) = \text{sym} \left[\frac{\partial u_i(\underline{x})}{\partial x_j} \right]$$

Matrix and inclusion are subjected to a macroscopic – or "background" – strain \underline{E}^∞ and second gradient of displacement $\underline{\underline{\mathcal{G}}}^\infty$, extending the classic, well-known Eshelby's inhomogeneity problem by the latter term. The following "boundary" conditions are therefore specified:

$$u_i(\underline{x}) = E_{ij}^\infty \cdot x_j + \frac{1}{2} \mathcal{G}_{ikl}^\infty x_l x_k \quad \forall |\underline{x}| \rightarrow \infty \quad (4.2)$$

It is assumed that the polarization stresses dominate over general volume forces. If the equilibrium conditions $\text{div} \underline{\underline{\sigma}}(\underline{x}) = 0$ are applied in absence of a polarization (i.e., where either there is no inclusion or $\underline{\underline{\mathbb{C}}}^i = \underline{\underline{\mathbb{C}}}^m$), and where only the "background displacements" are present, the following term remains:

$$\begin{aligned} \frac{\partial}{\partial x_i} [\underline{\underline{\mathbb{C}}}_{ijkl}^m \varepsilon_{kl}(\underline{x})] &= \frac{\partial}{\partial x_i} \left\{ \underline{\underline{\mathbb{C}}}_{ijkl}^m \text{sym} \left[\frac{\partial u_k(\underline{x})}{\partial x_l} \right] \right\} \\ &= \frac{\partial}{\partial x_i} \left\{ \underline{\underline{\mathbb{C}}}_{ijkl}^m \text{sym} \left[\frac{\partial}{\partial x_l} \left(E_{km}^\infty \cdot x_m + \frac{1}{2} \mathcal{G}_{kmn}^\infty x_n x_m \right) \right] \right\} \\ &= \frac{1}{2} \frac{\partial}{\partial x_i} \left\{ \underline{\underline{\mathbb{C}}}_{ijkl}^m \text{sym} \left[\frac{\partial}{\partial x_l} (\mathcal{G}_{kmn}^\infty x_n x_m) \right] \right\} \end{aligned}$$

This means that due to the macroscopic higher-order strain measure $\underline{\underline{\mathcal{G}}}^\infty$ the equilibrium conditions leave a residue term. We therefore introduce a volume force correction term $\underline{f}^{\mathcal{G}}$, similarly to [51], which ensures that in absence of a polarization, the equilibrium conditions apply. Using $\text{div} \underline{\underline{\sigma}}(\underline{x}) = 0$ for eqn. (4.1) and introduction of the new term, leads to the following relationship:

$$\frac{\partial}{\partial x_i} [\underline{\underline{\mathbb{C}}}_{ijkl}^m \varepsilon_{kl}(\underline{x})] + \underbrace{\frac{\partial}{\partial x_i} \tau_{ij}(\underline{x}) \mathcal{H}(V_I)}_{\underline{f}^\tau} - f_j^{\mathcal{G}} = 0 \quad (4.3)$$

where

$$f_j^{\mathcal{G}} = \frac{1}{2} \frac{\partial}{\partial x_i} \left\{ \underline{\underline{\mathbb{C}}}_{ijkl}^m \text{sym} \left[\frac{\partial}{\partial x_l} (\mathcal{G}_{kmn}^\infty x_n x_m) \right] \right\} = \text{const.}$$

The term \underline{f}^τ can be interpreted as a body force field arising from the polarization $\underline{\underline{\tau}}$ inside the inclusion. Now, this partial differential equation (4.3) can be solved for $\underline{u}(\underline{x})$, which is the sum of a homogeneous and a particulate solution [44]:

$$u_i(\underline{x}) = u_i^h(\underline{x}) + u_i^p(\underline{x}) \quad (4.4)$$

The homogeneous solution thereby is the solution of:

$$\frac{\partial}{\partial x_i} \left[\underline{\underline{\mathbb{C}}}_{ijkl}^m \text{sym} \left(\frac{\partial u_k^h(\underline{x})}{\partial x_l} \right) \right] - f_j^{\mathcal{G}} = 0 \quad (4.5)$$

which satisfies the boundary conditions (4.2).

Obviously, this solution does not contain the contribution from the inclusion. Simply inserting the boundary conditions into (4.5) yields:

$$\begin{aligned} & \frac{\partial}{\partial x_i} \left\{ \mathfrak{c}_{ijkl}^m \operatorname{sym} \left[\frac{\partial}{\partial x_l} \left(E_{km}^\infty \cdot x_m + \frac{1}{2} \mathcal{G}_{kmn}^\infty x_n x_m \right) \right] \right\} - \frac{1}{2} \frac{\partial}{\partial x_i} \left\{ \mathfrak{c}_{ijkl}^m \operatorname{sym} \left[\frac{\partial}{\partial x_l} \left(\mathcal{G}_{kmn}^\infty x_n x_m \right) \right] \right\} \\ &= \frac{1}{2} \frac{\partial}{\partial x_i} \left\{ \mathfrak{c}_{ijkl}^m \operatorname{sym} \left[\frac{\partial}{\partial x_l} \left(\mathcal{G}_{kmn}^\infty x_n x_m \right) \right] \right\} - \frac{1}{2} \frac{\partial}{\partial x_i} \left\{ \mathfrak{c}_{ijkl}^m \operatorname{sym} \left[\frac{\partial}{\partial x_l} \left(\mathcal{G}_{kmn}^\infty x_n x_m \right) \right] \right\} = 0 \end{aligned}$$

This means that the homogeneous displacement solution, which resembles the solution in absence of a polarization, is simply:

$$u_i^h(\underline{x}) = u_i^\infty(\underline{x}) = E_{ij}^\infty \cdot x_j + \frac{1}{2} \mathcal{G}_{ikl}^\infty x_l x_k$$

The particulate solution is then the solution of the differential equation:

$$\frac{\partial}{\partial x_i} \left[\mathfrak{c}_{ijkl}^m \operatorname{sym} \left(\frac{\partial u_k^p(\underline{x})}{\partial x_l} \right) \right] = - \left\{ \frac{\partial}{\partial x_i} [\tau_{ij}(\underline{x}) \mathcal{H}(V_I)] - f_j^{\mathcal{G}} \right\} \quad (4.6)$$

with the boundary condition:

$$u_i^p = 0 \quad \forall |\underline{x}| \rightarrow \infty$$

The right-hand side of eqn. (4.6) can be interpreted as a "total" body force field acting inside the inclusion. To obtain the particulate displacement solution, the elastic Green's function is employed: As described in (1.5), in general, the displacement in i -direction at position \underline{x} due to a point force in j -direction (P_j) at position \underline{y} is given via the Green's function of elasticity G_{ij} :

$$u_i(\underline{x}) = G_{ij}(\underline{x} - \underline{y}) P_j(\underline{y})$$

Following the derivations described in the introduction, the integral formulation is used to incorporate the total body force field. The displacement solution of eqn. (4.3) is therefore:

$$\begin{aligned} u_i(\underline{x}) &= u_i^h(\underline{x}) + \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) \left\{ -f_k^{\mathcal{G}} + \frac{\partial}{\partial y_j} [\tau_{jk}(\underline{y}) \mathcal{H}(V_I)] \right\} dV(\underline{y}) = \\ &= E_{ij}^\infty \cdot x_j + \frac{1}{2} \mathcal{G}_{ikl}^\infty x_l x_k - \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) f_k^{\mathcal{G}} dV(\underline{y}) \\ &\quad + \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) \frac{\partial}{\partial y_j} [\tau_{jk}(\underline{y}) \mathcal{H}(V_I)] dV(\underline{y}) = \\ &= E_{ij}^\infty \cdot x_j + \frac{1}{2} \mathcal{G}_{ikl}^\infty x_l x_k - \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) f_k^{\mathcal{G}} dV(\underline{y}) \\ &\quad - \int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y})] [\tau_{jk}(\underline{y}) \mathcal{H}(V_I)] dV(\underline{y}) = \\ &= E_{ij}^\infty \cdot x_j + \frac{1}{2} \mathcal{G}_{ikl}^\infty x_l x_k - \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) f_k^{\mathcal{G}} dV(\underline{y}) \\ &\quad - \int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y})] [\Delta \mathfrak{c}_{jklm}(\underline{y}) \varepsilon_{lm}(\underline{y}) \mathcal{H}(V_I)] dV(\underline{y}) \end{aligned} \quad (4.7)$$

Here, the following relations were used:

1. product rule:

$$\int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) \frac{\partial}{\partial y_j} (\cdot)_{jk} dV(\underline{y}) = \int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y}) (\cdot)_{jk}] dV(\underline{y}) - \int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y})] (\cdot)_{jk} dV(\underline{y})$$

2. divergence theorem

$$\int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y}) (\cdot)_{jk}] dV(\underline{y}) = \int_{S^\infty} G_{ik}(\underline{x} - \underline{y}) (\cdot)_{jk} n_j^\infty dV(\underline{y})$$

3. the condition that $G_{ij}(\underline{x} - \underline{y}) \rightarrow 0 \quad \forall |\underline{x}, \underline{y}| \rightarrow \infty$

The symmetric gradient of the displacement (4.7) with respect to \underline{x} yields the corresponding strain field

$$\varepsilon_{in}(\underline{x}) = E_{in}^\infty + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial x_n} \mathcal{G}_{ikl}^\infty x_l x_k \right) - \text{sym} \left[\frac{\partial}{\partial x_n} \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) f_k^{\mathcal{G}} dV(\underline{y}) \right] - \text{sym} \left\{ \frac{\partial}{\partial x_n} \int_{V^\infty} \frac{\partial}{\partial y_j} [G_{ik}(\underline{x} - \underline{y})] [\Delta \mathbf{c}_{jklm}(\underline{y}) \varepsilon_{lm}(\underline{y}) \mathcal{H}(V_I)] dV(\underline{y}) \right\}.$$

This expression can be transformed to

$$\varepsilon_{in}(\underline{x}) = E_{in}^\infty + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial x_n} \mathcal{G}_{ikl}^\infty x_l x_k \right) - \text{sym} \left[\frac{\partial}{\partial x_n} \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}) f_k^{\mathcal{G}} dV(\underline{y}) \right] - \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}) \Delta \mathbf{c}_{jklm}(\underline{y}) \varepsilon_{lm}(\underline{y}) dV(\underline{y}), \quad (4.8)$$

where $\mathbb{G} = \nabla_x^s \nabla_y \underline{\underline{G}}$ is a fourth-order tensor.

Due to the last term on the right-hand side in (4.8), the equation can not be solved directly. Since the variable to be solved, the strain $\underline{\underline{\varepsilon}}$, occurs both inside and outside of an integral, this equation qualifies as a Fredholm integral equation of the second kind [46]. To obtain a solution, a Neumann series can be developed [45, 46], as it is described for a related example in [44]. For this, an infinitely repeated substitution of $\underline{\underline{\varepsilon}}(\underline{y})$ is performed: As the first step, in (4.8) the position variable \underline{y} is specified as $\underline{y} = \underline{y}^{(1)}$, yielding:

$$\varepsilon_{in}(\underline{x}) = E_{in}^\infty + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial x_n} \mathcal{G}_{ikl}^\infty x_l x_k \right) - \text{sym} \left[\frac{\partial}{\partial x_n} \int_{V^\infty} G_{ik}(\underline{x} - \underline{y}^{(1)}) f_k^{\mathcal{G}} dV(\underline{y}^{(1)}) \right] - \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \varepsilon_{lm}(\underline{y}^{(1)}) dV(\underline{y}^{(1)}) \quad (4.9)$$

If this equation is written for $\underline{x} = \underline{y}^{(1)}$ and $\underline{y}^{(1)} = \underline{y}^{(2)}$:

$$\begin{aligned} \varepsilon_{in}(\underline{y}^{(1)}) = & E_{in}^{\infty} + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial y_n^{(1)}} \mathcal{G}_{ikl}^{\infty} y_l^{(1)} y_k^{(1)} \right) \\ & - \text{sym} \left[\frac{\partial}{\partial y_n^{(1)}} \int_{V^{\infty}} G_{ik}(\underline{y}^{(1)} - \underline{y}^{(2)}) f_k^{\mathcal{G}} dV(\underline{y}^{(2)}) \right] \\ & - \int_{V_I} \mathbb{G}_{inkj}(\underline{y}^{(1)} - \underline{y}^{(2)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(2)}) \varepsilon_{lm}(\underline{y}^{(2)}) dV(\underline{y}^{(2)}) \end{aligned}$$

An expression for $\underline{\underline{\varepsilon}}(\underline{y}^{(1)})$ is obtained, which can be re-inserted into (4.9):

$$\begin{aligned} \varepsilon_{in}(\underline{x}) = & E_{in}^{\infty} + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial x_n} \mathcal{G}_{ikl}^{\infty} x_l x_k \right) - \text{sym} \left[\frac{\partial}{\partial x_n} \int_{V^{\infty}} G_{ik}(\underline{x} - \underline{y}^{(1)}) f_k^{\mathcal{G}} dV(\underline{y}^{(1)}) \right] \\ & - \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \left\{ E_{lm}^{\infty} + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial y_m^{(1)}} \mathcal{G}_{lop}^{\infty} y_p^{(1)} y_o^{(1)} \right) \right. \\ & - \text{sym} \left[\frac{\partial}{\partial y_m^{(1)}} \int_{V^{\infty}} G_{lo}(\underline{y}^{(1)} - \underline{y}^{(2)}) f_o^{\mathcal{G}} dV(\underline{y}^{(2)}) \right] \\ & \left. - \int_{V_I} \mathbb{G}_{lmoq}(\underline{y}^{(1)} - \underline{y}^{(2)}) \Delta \mathbf{c}_{qors}(\underline{y}^{(2)}) \varepsilon_{rs}(\underline{y}^{(2)}) dV(\underline{y}^{(2)}) \right\} dV(\underline{y}^{(1)}) \end{aligned}$$

$$\begin{aligned} \varepsilon_{in}(\underline{x}) = & \left\{ \mathbb{I}_{inlm} - \int_{V_I} \left[\mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \right] dV(\underline{y}^{(1)}) \right\} E_{lm}^{\infty} \\ & + \frac{1}{2} \text{sym} \left(\frac{\partial}{\partial x_n} \mathcal{G}_{ikl}^{\infty} x_l x_k \right) + \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \left\{ -\frac{1}{2} \text{sym} \left(\frac{\partial}{\partial y_m^{(1)}} \mathcal{G}_{lop}^{\infty} y_p^{(1)} y_o^{(1)} \right) \right\} dV(\underline{y}^{(1)}) \\ & - \text{sym} \left[\frac{\partial}{\partial x_n} \int_{V^{\infty}} G_{ik}(\underline{x} - \underline{y}^{(1)}) f_k^{\mathcal{G}} dV(\underline{y}^{(1)}) \right] \\ & + \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \left\{ \text{sym} \left[\frac{\partial}{\partial y_m^{(1)}} \int_{V^{\infty}} G_{lo}(\underline{y}^{(1)} - \underline{y}^{(2)}) f_o^{\mathcal{G}} dV(\underline{y}^{(2)}) \right] \right\} dV(\underline{y}^{(1)}) \\ & + \int_{V_I} \mathbb{G}_{inkj}(\underline{x} - \underline{y}^{(1)}) \Delta \mathbf{c}_{jklm}(\underline{y}^{(1)}) \left\{ \int_{V_I} \mathbb{G}_{lmoq}(\underline{y}^{(1)} - \underline{y}^{(2)}) \Delta \mathbf{c}_{qors}(\underline{y}^{(2)}) \varepsilon_{rs}(\underline{y}^{(2)}) dV(\underline{y}^{(2)}) \right\} dV(\underline{y}^{(1)}) \end{aligned}$$

Repeating this process, namely specifying (4.9) for $\underline{x} = \underline{y}^{(\alpha)}$ and $\underline{y}^{(1)} = \underline{y}^{(\alpha+1)}$ with $\alpha = 2, 3, \dots, N$ and consecutive re-insertion results in the following series expression:

$$\begin{aligned}
\underline{\underline{\underline{\varepsilon}}}(\underline{x}) &= \left(\underline{\underline{\underline{\mathbb{I}}}} - \int_{V_I} \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(1)}) : \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) + \sum_{n=2}^N \left\{ (-1)^n \int_{V_I} \dots \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) \right. \right. \\
&\quad \left. \left. : \prod_{i=2}^n \left[\underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(i-1)}) : \underline{\underline{\underline{G}}}(\underline{y}^{(i-1)} - \underline{y}^{(i)}) \right] : \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(n)}) \right\} dV(\underline{y}^{(2)}) \dots dV(\underline{y}^{(n)}) \right) \underline{\underline{\underline{E}}}^\infty \\
&\quad + \frac{1}{2} \underline{\underline{\underline{\nabla}}}_x^s \left[\underline{\underline{\underline{G}}}^\infty(\underline{x} \otimes \underline{x}) \right] - \frac{1}{2} \int_{V_I} \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(1)}) : \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) \underline{\underline{\underline{\nabla}}}_{\underline{y}^{(1)}}^s \left[\underline{\underline{\underline{G}}}^\infty(\underline{y}^{(1)} \otimes \underline{y}^{(1)}) \right] dV(\underline{y}^{(1)}) \\
&\quad + \frac{1}{2} \sum_{n=2}^N (-1)^n \int_{V_I} \dots \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^n \left[\underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(m-1)}) : \underline{\underline{\underline{G}}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \\
&\quad \quad \quad : \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(n)}) \underline{\underline{\underline{\nabla}}}_x^s \left[\underline{\underline{\underline{G}}}^\infty(\underline{y}^{(n)} \otimes \underline{y}^{(n)}) \right] dV(\underline{y}^{(2)}) \dots dV(\underline{y}^{(n)}) \\
&\quad - \underline{\underline{\underline{\nabla}}}_x^s \int_{V_\infty} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) \cdot \underline{\underline{\underline{f}}}^G dV(\underline{y}^{(1)}) \\
&\quad + \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) : \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(1)}) : \underline{\underline{\underline{\nabla}}}_x^s \int_{V_\infty} \underline{\underline{\underline{G}}}(\underline{y}^{(1)} - \underline{y}^{(2)}) \cdot \underline{\underline{\underline{f}}}^G dV(\underline{y}^{(2)}) dV(\underline{y}^{(1)}) \\
&\quad + \sum_{n=2}^N (-1)^{n-1} \int_{V_I} \dots \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^n \left[\underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(m-1)}) : \underline{\underline{\underline{G}}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(n)}) \\
&\quad \quad \quad : \underline{\underline{\underline{\nabla}}}_x^s \int_{V_\infty} \underline{\underline{\underline{G}}}(\underline{y}^{(n-1)} - \underline{y}^{(n)}) \cdot \underline{\underline{\underline{f}}}^G dV(\underline{y}^{(2)}) \dots dV(\underline{y}^{(n)}) \\
&\quad + (-1)^{N-1} \int_{V_I} \dots \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^N \left[\underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(m-1)}) : \underline{\underline{\underline{G}}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \\
&\quad \quad \quad : \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(N)}) : \underline{\underline{\underline{\varepsilon}}}(\underline{y}^{(N)}) dV(\underline{y}^{(2)}) \dots dV(\underline{y}^{(N)})
\end{aligned} \tag{4.10}$$

or, in more compact terms:

$$\underline{\underline{\underline{\varepsilon}}}(\underline{x}) = \underline{\underline{\underline{A}}}^0(\underline{x}) : \underline{\underline{\underline{E}}}^\infty + \frac{1}{2} \underline{\underline{\underline{A}}}^1(\underline{x}) + \underline{\underline{\underline{A}}}^2(\underline{x}) + (-1)^{N-1} \underline{\underline{\underline{Res}}}(\underline{x}, \underline{\underline{\underline{\varepsilon}}}(\underline{y}^{(N)})) \tag{4.11}$$

where

$$\underline{\underline{\underline{A}}}^0(\underline{x}) = \underline{\underline{\underline{\mathbb{I}}}} + \sum_{n=1}^N (-1)^n \underline{\underline{\underline{A}}}^0_n(\underline{x}) \tag{4.12}$$

$$\underline{\underline{\underline{A}}}^0_1(\underline{x}) = \int_{V_I} \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(1)}) : \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) \tag{4.13}$$

$$\text{for } n > 1 : \quad \underline{\underline{\underline{A}}}^0_n(\underline{x}) = \int_{V_I} \dots \int_{V_I} \underline{\underline{\underline{G}}}(\underline{x} - \underline{y}^{(1)}) : \prod_{i=2}^n \left[\underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(i-1)}) : \underline{\underline{\underline{G}}}(\underline{y}^{(i-1)} - \underline{y}^{(i)}) \right] \\
\quad \quad \quad : \underline{\underline{\underline{\Delta}}}\underline{\underline{\underline{C}}}(\underline{y}^{(n)}) dV(\underline{y}^{(2)}) \dots dV(\underline{y}^{(n)}) \tag{4.14}$$

$$\underline{\underline{A}}^1(\underline{x}) = \underline{\underline{A}}_0^1(\underline{x}) + \sum_{n=1}^N (-1)^n \underline{\underline{A}}_n^1(\underline{x}) \quad (4.15)$$

$$\underline{\underline{A}}_0^1(\underline{x}) = \nabla_x^s \left[\underline{\underline{G}}^\infty : (\underline{x} \otimes \underline{x}) \right] \quad (4.16)$$

$$\underline{\underline{A}}_1^1(\underline{x}) = \int_{V_I} \underline{\underline{\Delta c}}(\underline{y}^{(1)}) : \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) \nabla_{y^{(1)}}^s \left[\underline{\underline{G}}^\infty(\underline{y}^{(1)} \otimes \underline{y}^{(1)}) \right] dV(\underline{y}^{(1)}) \quad (4.17)$$

$$\text{for } n > 1: \quad \underline{\underline{A}}_n^1(\underline{x}) = \int_{V_I} \dots \int_{V_I} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^n \left[\underline{\underline{\Delta c}}(\underline{y}^{(m-1)}) : \underline{\underline{G}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \\ : \underline{\underline{\Delta c}}(\underline{y}^{(n)}) \nabla_x^s \left[\underline{\underline{G}}^\infty(\underline{y}^{(n)} \otimes \underline{y}^{(n)}) \right] dV(\underline{y}^{(n)}) \dots dV(\underline{y}^{(1)}) \quad (4.18)$$

$$\underline{\underline{A}}^2(\underline{x}) = -\underline{\underline{A}}_0^2(\underline{x}) + \sum_{n=1}^N (-1)^{n-1} \underline{\underline{A}}_n^2(\underline{x}) \quad (4.19)$$

$$\underline{\underline{A}}_0^2(\underline{x}) = \nabla_x^s \int_{V_\infty} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) \cdot \underline{f}^{\mathcal{G}} dV(\underline{y}^{(1)}) \quad (4.20)$$

$$\underline{\underline{A}}_1^2(\underline{x}) = \int_{V_I} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) : \underline{\underline{\Delta c}}(\underline{y}^{(1)}) : \nabla_x^s \int_{V_\infty} \underline{\underline{G}}(\underline{y}^{(1)} - \underline{y}^{(2)}) \cdot \underline{f}^{\mathcal{G}} dV(\underline{y}^{(2)}) dV(\underline{y}^{(1)}) \quad (4.21)$$

$$\text{for } n > 1: \quad \underline{\underline{A}}_n^2(\underline{x}) = \int_{V_I} \dots \int_{V_I} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^n \left[\underline{\underline{\Delta c}}(\underline{y}^{(m-1)}) : \underline{\underline{G}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \underline{\underline{\Delta c}}(\underline{y}^{(n)}) \\ : \nabla_x^s \int_{V_\infty} \underline{\underline{G}}(\underline{y}^{(n-1)} - \underline{y}^{(n)}) \cdot \underline{f}^{\mathcal{G}} dV(\underline{y}^{(n)}) \dots dV(\underline{y}^{(1)}) \quad (4.22)$$

$$\underline{\underline{Res}}(\underline{x}, \underline{\underline{\varepsilon}}(\underline{y}^{(N)})) = \int_{V_I} \dots \int_{V_I} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) : \prod_{m=2}^N \left[\underline{\underline{\Delta c}}(\underline{y}^{(m-1)}) : \underline{\underline{G}}(\underline{y}^{(m-1)} - \underline{y}^{(m)}) \right] \\ : \underline{\underline{\Delta c}}(\underline{y}^{(N)}) : \underline{\underline{\varepsilon}}(\underline{y}^{(N)}) dV(\underline{y}^{(N)}) \dots dV(\underline{y}^{(1)}).$$

The last term, $\underline{\underline{Res}}$, is the residue and for $N \rightarrow \infty$ it will approach zero, provided that [44]:

$$\int_{V_I} \mathbb{G}_{ijkl}(\underline{y}^{(n-1)} - \underline{y}^{(n)}) \Delta \mathbb{c}_{klmn}(\underline{y}^{(n)}) \mathbb{G}_{mnop}(\underline{y}^{(n)} - \underline{y}^{(n+1)}) dV(\underline{y}^{(n)}) < 1$$

4.2 Evaluation for a Spherical, Isotropic Inclusion with Constant Stiffness

As an example for evaluating the series expressions (4.11) - (4.22), an isotropic matrix of infinite extent with a spherical, isotropic inclusion of constant stiffness is chosen.

The second-order Green's tensor for an isotropic medium of infinite extent was described in the introduction (1.5) and is now employed:

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{4\pi\mu} \frac{\delta_{ij}}{|\underline{x} - \underline{y}|} - \frac{1}{16\pi\mu(1-\nu)} \frac{\partial^2}{\partial x_i \partial x_j} |\underline{x} - \underline{y}|$$

The fourth-order Green's tensor $\underline{\underline{\mathbb{G}}}$ therefore exhibits the following form in index notation [44]:

$$\begin{aligned} \mathbb{G}_{ijkl}(\underline{x} - \underline{y}) &= \frac{1}{8\pi\mu} \left[\frac{\partial^2}{\partial x_j \partial y_l} \left(\frac{\delta_{ik}}{|\underline{x} - \underline{y}|} \right) + \frac{\partial^2}{\partial x_i \partial y_l} \left(\frac{\delta_{jk}}{|\underline{x} - \underline{y}|} \right) \right] \\ &\quad - \frac{1}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_i \partial x_j \partial x_k \partial y_l} |\underline{x} - \underline{y}| \\ \mathbb{G}_{ijkl}(\underline{x} - \underline{y}) &= -\frac{1}{8\pi\mu} \left[\frac{\partial^2}{\partial x_j \partial x_l} \left(\frac{\delta_{ik}}{|\underline{x} - \underline{y}|} \right) + \frac{\partial^2}{\partial x_i \partial x_l} \left(\frac{\delta_{jk}}{|\underline{x} - \underline{y}|} \right) \right] \\ &\quad + \frac{1}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_i \partial x_j \partial x_k \partial x_l} |\underline{x} - \underline{y}| \quad (4.23) \end{aligned}$$

Strain-Related Contribution Term $\underline{\underline{\mathbb{A}}}^0$:

Since $\underline{\underline{\Delta}}_{\mathbb{C}} = \text{const.}$, this term can be moved out of the integrals appearing in (4.13) and (4.14).

This means that $\underline{\underline{\mathbb{A}}}^0$ can be written as:

$$\begin{aligned} \underline{\underline{\mathbb{A}}}^0(\underline{x}) &= \underline{\underline{\mathbb{I}}} - \int_{V_I} \underline{\underline{\mathbb{G}}}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) : \underline{\underline{\Delta}}_{\mathbb{C}} \\ &\quad + \int_{V_I} \left[\underline{\underline{\mathbb{G}}}(\underline{x} - \underline{y}^{(1)}) : \underline{\underline{\Delta}}_{\mathbb{C}} : \int_{V_I} \underline{\underline{\mathbb{G}}}(\underline{y}^{(1)} - \underline{y}^{(2)}) dV(\underline{y}^{(2)}) \right] dV(\underline{y}^{(1)}) : \underline{\underline{\Delta}}_{\mathbb{C}} - \dots \quad (4.24) \end{aligned}$$

The integral of the fourth-order Green's tensor is the Hill tensor, as described in the introduction (Chapter 1.4.2), which is constant for ellipsoidal (and therefore spherical) inclusions in an isotropic matrix [34]:

$$\int_{V_I} \underline{\underline{\mathbb{G}}}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) = \underline{\underline{\mathbb{P}}} = \text{const.}$$

Accordingly, $\underline{\underline{\mathbb{A}}}^0$ reads as

$$\underline{\underline{\mathbb{A}}}^0(\underline{x}) = \underline{\underline{\mathbb{I}}} - \underline{\underline{\mathbb{P}}} : \underline{\underline{\Delta}}_{\mathbb{C}} + \underline{\underline{\mathbb{P}}} : \underline{\underline{\Delta}}_{\mathbb{C}} : \underline{\underline{\mathbb{P}}} : \underline{\underline{\Delta}}_{\mathbb{C}} - \dots$$

If this series converges, for $N \rightarrow \infty$, it does so towards the limit [54]

$$\underline{\underline{\mathbb{A}}}^0 = \left(\underline{\underline{\mathbb{I}}} + \underline{\underline{\mathbb{P}}} : \underline{\underline{\Delta}}_{\mathbb{C}} \right)^{-1}, \quad (4.25)$$

which is the well-known "concentration" or "downscaling" tensor which relates strains at infinity ($\underline{\underline{E}}^\infty$) to strains inside the inclusion [15, 35, 49].

Strain-Gradient-Related Contribution Term $\underline{\underline{A}}^1$:

The development of the terms $\underline{\underline{A}}_n^1$ is considerably more complicated. Closer examination of (4.16) - (4.18) and comparison thereof with [46], Chapter 21, and [55], Chapter 13, reveals, that the term $\underline{\underline{A}}^1$ qualifies as a Neumann-type series expansion of the form

$$\varphi_N(x) = \sum_{i=n}^N \lambda^n \varphi_n(x), \quad (4.26)$$

where the individual series elements read as

$$\begin{aligned} \varphi_0(x) &= f(x) \\ \varphi_1(x) &= \int_a^b K(x, y) f(y) dy \\ \varphi_2(x) &= \int_a^b K(x, y^{(1)}) \left[\int_a^b K(y^{(1)}, y) f(y) dy \right] dy^{(1)} = \\ &= \int_a^b \left[\int_a^b K(x, y^{(1)}) K(y^{(1)}, y) dy^{(1)} \right] f(y) dy \\ \varphi_3(x) &= \dots \end{aligned} \quad (4.27)$$

The analogy between (4.27) and (4.16) - (4.18) is obvious.

Due to the occurrence of iterated kernels K , the resolvent formalism is to be utilized to solve for $\varphi(x) = \varphi_N(x)$ for $N \rightarrow \infty$ [55].

The n^{th} iterated Kernel can be expressed as

$$K^n(x, y) = \int_a^b \dots \int_a^b \left[K(x, y^{(1)}) K(y^{(1)}, y^{(2)}) \dots K(y^{(n-1)}, y) \right] dy^{(n-1)} \dots dy^{(1)} \quad (4.28)$$

and the resolvent R can be expressed as an infinite geometric series, reading as [55]

$$R(x, y, \lambda) = \sum_{n=0}^{\infty} \lambda^n K^{n+1}(x, y).$$

The solution is then

$$\varphi(x) = f(x) + \lambda \int_a^b R(x, y, \lambda) f(y) dy.$$

For the problem at hand, where the kernel corresponds to the fourth-order Green's function, doubly contracted with the difference in stiffness,

$$K(\underline{x}, \underline{y}^{(1)}) \hat{=} \underline{\underline{G}}(\underline{x} - \underline{y}^{(1)}) : \underline{\underline{\Delta c}}$$

the execution of the iteration steps (4.28) is computationally very expensive. In this thesis, a first-order approximate solution, $\underline{\underline{A}}^1 \approx \underline{\underline{A}}_0^1 + \underline{\underline{A}}_1^1$, is presented:

The first iterated series element, $\underline{\underline{A}}_1^1$ reads as

$$A_{1,ij}^1 = \int_{V_I} \mathbb{G}_{ijkn}(\underline{x} - \underline{y}^{(1)}) \Delta c_{nkml} \text{sym} \left(\frac{\partial}{\partial y_m^{(1)}} \mathcal{G}_{lop}^{\infty} y_p^{(1)} y_o^{(1)} \right) dV(\underline{y}^{(1)}). \quad (4.29)$$

Evaluating its 11-component, describing a contribution to the normal strain, yields the following:

$$\begin{aligned}
A_{1,11}^1 = \int_{V_I} \left\{ & -\frac{c_1 y_1^{(1)} + c_2 y_2^{(1)} + c_3 y_3^{(1)}}{4\pi\mu} \frac{\partial^2}{\partial x_1^2} \left(\frac{1}{|\underline{x} - \underline{y}^{(1)}|} \right) \right. \\
& + \frac{c_1 y_1^{(1)} + c_2 y_2^{(1)} + c_3 y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1^4} |\underline{x} - \underline{y}^{(1)}| \\
& + \frac{c_4 y_1^{(1)} + c_5 y_2^{(1)} + c_6 y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1^2 \partial x_2^2} |\underline{x} - \underline{y}^{(1)}| + \frac{c_7 y_1^{(1)} + c_8 y_2^{(1)} + c_9 y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1^2 \partial x_3^2} |\underline{x} - \underline{y}^{(1)}| \\
& + 2 \frac{c_{10} y_1^{(1)} + c_{11} y_2^{(1)} + c_{12} y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1 \partial x_1 \partial x_2 \partial x_3} |\underline{x} - \underline{y}^{(1)}| \\
& - \frac{c_{13} y_1^{(1)} + c_{14} y_2^{(1)} + c_{15} y_3^{(1)}}{4\pi\mu} \frac{\partial^2}{\partial x_1 \partial x_3} \left(\frac{1}{|\underline{x} - \underline{y}^{(1)}|} \right) \\
& + \frac{c_{13} y_1^{(1)} + c_{14} y_2^{(1)} + c_{15} y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1 \partial x_1 \partial x_1 \partial x_3} |\underline{x} - \underline{y}^{(1)}| \\
& - \frac{c_{16} y_1^{(1)} + c_{17} y_2^{(1)} + c_{18} y_3^{(1)}}{4\pi\mu} \frac{\partial^2}{\partial x_1 \partial x_2} \left(\frac{1}{|\underline{x} - \underline{y}^{(1)}|} \right) \\
& + \frac{c_{16} y_1^{(1)} + c_{17} y_2^{(1)} + c_{18} y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1 \partial x_1 \partial x_1 \partial x_2} |\underline{x} - \underline{y}^{(1)}| \\
& \left. + \frac{c_{16} y_1^{(1)} + c_{17} y_2^{(1)} + c_{18} y_3^{(1)}}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial x_1 \partial x_1 \partial x_1 \partial x_2} |\underline{x} - \underline{y}^{(1)}| \right\} dV(\underline{y}^{(1)})
\end{aligned} \tag{4.30}$$

The constant factors containing the components of $\underline{\underline{\mathcal{G}}}^\infty$ were abbreviated as follows:

$$\begin{aligned}
c_1 &= 2 (\Delta c_{1111} \mathcal{G}_{111}^\infty + \Delta c_{1122} \mathcal{G}_{212}^\infty + \Delta c_{1133} \mathcal{G}_{313}^\infty) = 2 (\Delta c_{1111} \mathcal{G}_{111}^\infty + \Delta c_{1122} \mathcal{G}_{212}^\infty + \Delta c_{1122} \mathcal{G}_{313}^\infty) \\
c_2 &= 2 (\Delta c_{1111} \mathcal{G}_{112}^\infty + \Delta c_{1122} \mathcal{G}_{222}^\infty + \Delta c_{1133} \mathcal{G}_{323}^\infty) = 2 (\Delta c_{1111} \mathcal{G}_{112}^\infty + \Delta c_{1122} \mathcal{G}_{222}^\infty + \Delta c_{1122} \mathcal{G}_{323}^\infty) \\
c_3 &= 2 (\Delta c_{1111} \mathcal{G}_{113}^\infty + \Delta c_{1122} \mathcal{G}_{223}^\infty + \Delta c_{1133} \mathcal{G}_{333}^\infty) = 2 (\Delta c_{1111} \mathcal{G}_{113}^\infty + \Delta c_{1122} \mathcal{G}_{223}^\infty + \Delta c_{1122} \mathcal{G}_{333}^\infty) \\
c_4 &= 2 (\Delta c_{1122} \mathcal{G}_{111}^\infty + \Delta c_{2222} \mathcal{G}_{212}^\infty + \Delta c_{2233} \mathcal{G}_{313}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{111}^\infty + \Delta c_{1111} \mathcal{G}_{212}^\infty + \Delta c_{1122} \mathcal{G}_{313}^\infty) \\
c_5 &= 2 (\Delta c_{1122} \mathcal{G}_{112}^\infty + \Delta c_{2222} \mathcal{G}_{222}^\infty + \Delta c_{2233} \mathcal{G}_{323}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{112}^\infty + \Delta c_{1111} \mathcal{G}_{222}^\infty + \Delta c_{1122} \mathcal{G}_{323}^\infty) \\
c_6 &= 2 (\Delta c_{1122} \mathcal{G}_{113}^\infty + \Delta c_{2222} \mathcal{G}_{223}^\infty + \Delta c_{2233} \mathcal{G}_{333}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{113}^\infty + \Delta c_{1111} \mathcal{G}_{223}^\infty + \Delta c_{1122} \mathcal{G}_{333}^\infty) \\
c_7 &= 2 (\Delta c_{1133} \mathcal{G}_{111}^\infty + \Delta c_{2233} \mathcal{G}_{212}^\infty + \Delta c_{3333} \mathcal{G}_{313}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{111}^\infty + \Delta c_{1122} \mathcal{G}_{212}^\infty + \Delta c_{1111} \mathcal{G}_{313}^\infty) \\
c_8 &= 2 (\Delta c_{1133} \mathcal{G}_{112}^\infty + \Delta c_{2233} \mathcal{G}_{222}^\infty + \Delta c_{3333} \mathcal{G}_{323}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{112}^\infty + \Delta c_{1122} \mathcal{G}_{222}^\infty + \Delta c_{1111} \mathcal{G}_{323}^\infty) \\
c_9 &= 2 (\Delta c_{1133} \mathcal{G}_{113}^\infty + \Delta c_{2233} \mathcal{G}_{223}^\infty + \Delta c_{3333} \mathcal{G}_{333}^\infty) = 2 (\Delta c_{1122} \mathcal{G}_{113}^\infty + \Delta c_{1122} \mathcal{G}_{223}^\infty + \Delta c_{1111} \mathcal{G}_{333}^\infty) \\
c_{10} &= \Delta c_{2323} (\mathcal{G}_{213}^\infty + \mathcal{G}_{312}^\infty) = \Delta c_{1212} (\mathcal{G}_{213}^\infty + \mathcal{G}_{312}^\infty) \\
c_{11} &= \Delta c_{2323} (\mathcal{G}_{223}^\infty + \mathcal{G}_{322}^\infty) = \Delta c_{1212} (\mathcal{G}_{223}^\infty + \mathcal{G}_{322}^\infty) \\
c_{12} &= \Delta c_{2323} (\mathcal{G}_{233}^\infty + \mathcal{G}_{323}^\infty) = \Delta c_{1212} (\mathcal{G}_{233}^\infty + \mathcal{G}_{323}^\infty) \\
c_{13} &= \Delta c_{1313} (\mathcal{G}_{113}^\infty + \mathcal{G}_{311}^\infty) = \Delta c_{1212} (\mathcal{G}_{113}^\infty + \mathcal{G}_{311}^\infty) \\
c_{14} &= \Delta c_{1313} (\mathcal{G}_{123}^\infty + \mathcal{G}_{312}^\infty) = \Delta c_{1212} (\mathcal{G}_{123}^\infty + \mathcal{G}_{312}^\infty) \\
c_{15} &= \Delta c_{1313} (\mathcal{G}_{133}^\infty + \mathcal{G}_{313}^\infty) = \Delta c_{1212} (\mathcal{G}_{133}^\infty + \mathcal{G}_{313}^\infty) \\
c_{16} &= \Delta c_{1212} (\mathcal{G}_{112}^\infty + \mathcal{G}_{211}^\infty) \\
c_{17} &= \Delta c_{1212} (\mathcal{G}_{122}^\infty + \mathcal{G}_{212}^\infty) \\
c_{18} &= \Delta c_{1212} (\mathcal{G}_{123}^\infty + \mathcal{G}_{213}^\infty)
\end{aligned} \tag{4.31}$$

Here, it was considered that $\mathcal{G}_{ijk}^\infty = \mathcal{G}_{ikj}^\infty$ and that in the isotropic case $\Delta c_{1111} = \Delta c_{2222} = \Delta c_{3333}$, $\Delta c_{1122} = \Delta c_{1133} = \Delta c_{2233}$, and $\Delta c_{1212} = \Delta c_{1313} = \Delta c_{2323}$.

The integration of the first two terms in (4.30) can be performed as described in the following: Performing a variable change $\underline{x} - \underline{y}^{(1)} = -\underline{z}$ yields

$$\begin{aligned}
& \int_{V_I} \left[-\frac{c_1 (x_1 + z_1) + c_2 (x_2 + z_2) + c_3 (x_3 + z_3)}{4\pi \mu} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{-z}|} \right) \right. \\
& \quad \left. + \frac{c_1 (x_1 + z_1) + c_2 (x_2 + z_2) + c_3 (x_3 + z_3)}{16\pi\mu(1-\nu)} \frac{\partial^4}{\partial z_1^4} |\underline{-z}| \right] dV(\underline{z}) = \\
& = -\frac{1}{8\pi \mu} \int_{V_I} (c_1 x_1 + c_2 x_2 + c_3 x_3 + c_1 z_1 + c_2 z_2 + c_3 z_3) \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{-z}|} \right) dV(\underline{z}) \\
& \quad + \frac{1}{32\pi\mu(1-\nu)} \int_{V_I} (c_1 x_1 + c_2 x_2 + c_3 x_3 + c_1 z_1 + c_2 z_2 + c_3 z_3) \frac{\partial^4}{\partial z_1^4} |\underline{-z}| dV(\underline{z}) =
\end{aligned}$$

$$\begin{aligned}
&= -\frac{c_1x_1 + c_2x_2 + c_3x_3}{8\pi\mu} \int_{V_I} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|-z|} \right) dV(\underline{z}) \\
&\quad - \frac{1}{8\pi\mu} \int_{V_I} (c_1z_1 + c_2z_2 + c_3z_3) \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|-z|} \right) dV(\underline{z}) \\
&\quad + \frac{c_1x_1 + c_2x_2 + c_3x_3}{32\pi\mu(1-\nu)} \int_{V_I} \frac{\partial^4}{\partial z_1^4} |-z| dV(\underline{z}) \\
&\quad + \frac{1}{32\pi\mu(1-\nu)} \int_{V_I} (c_1z_1 + c_2z_2 + c_3z_3) \frac{\partial^4}{\partial z_1^4} |-z| dV(\underline{z}), \quad (4.32)
\end{aligned}$$

where $|-z| = |z|$ and therefore $\frac{1}{|-z|} = \frac{1}{|z|}$. The occurring derivatives read as:

$$\begin{aligned}
\frac{\partial}{\partial z_1} \left(\frac{1}{|z|} \right) &= \frac{\partial}{\partial z_1} (z_1^2 + z_2^2 + z_3^2)^{-\frac{1}{2}} = -\frac{z_1}{|z|^3} \\
\frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|z|} \right) &= \frac{2z_1^2 - z_2^2 - z_3^2}{|z|^5} \\
\frac{\partial^4}{\partial z_1^4} |z| &= \frac{3(4z_1^2 - z_2^2 - z_3^2)(z_2^2 + z_3^2)}{|z|^7}
\end{aligned}$$

The four integrals in (4.32) are now to be solved individually. Clearly, all integral expressions show a singularity at $|z| = 0$, i.e., $\underline{x} = \underline{y}$. A suitable tool for this problem is the Cauchy principal value analysis. This splits an integral containing a singularity into two terms, where, in three-dimensional space, one may represent a sphere with radius ϵ around the singularity, and the second one contains the remaining space [44]. If the singular point is kept out of the integration domain while $\epsilon \rightarrow 0$, the integral can be solved.

First integral:

$$\int_{V_I} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|z|} \right) dV(\underline{z}) = \int_{V_I} \left(\frac{2z_1^2 - z_2^2 - z_3^2}{|z|^5} \right) dV(\underline{z}) \quad (4.33)$$

Denoting the volume of a sphere with radius ϵ as V_ϵ and splitting up (4.33) into two portions yields:

$$\int_{V_I} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|z|} \right) dV(\underline{z}) = \underbrace{\int_{V_\epsilon} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|z|} \right) dV(\underline{z})}_{\rightarrow 0 \text{ for } \epsilon \rightarrow 0} + \int_{V_I \setminus V_\epsilon} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|z|} \right) dV(\underline{z}) \quad (4.34)$$

A change to spherical coordinates, where

$$\begin{aligned}
z_1 &= \rho \cos(\eta) \sin(\theta) \\
z_2 &= \rho \sin(\eta) \sin(\theta) \\
z_3 &= \rho \cos(\theta) \\
dV(\underline{z}) &= \rho^2 \sin(\theta) d\eta d\theta d\rho,
\end{aligned} \quad (4.35)$$

and insertion into (4.34) gives

$$\begin{aligned} & \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \left(\frac{2[\rho \cos(\eta) \sin(\theta)]^2 - [\rho \sin(\eta) \sin(\theta)]^2 - [\rho \cos(\theta)]^2}{\rho^5} \right) \rho^2 \sin(\theta) d\eta d\theta d\rho = \\ & = \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \left(\frac{2 \cos(\eta)^2 \sin(\theta)^2 \sin(\theta) - \sin(\eta)^2 \sin(\theta)^3 - \cos(\theta)^2 \sin(\theta)}{\rho} \right) d\eta d\theta d\rho. \end{aligned}$$

Obviously, the definite integral $\int_{\epsilon}^{r_I} \frac{1}{\rho} d\rho$ does not converge for $\epsilon \rightarrow 0$. A simple way to keep the singularity out of the integration domain is to use the divergence theorem as described by Jiménez Segura et al. [44]. The solution for this integral is then

$$\int_{V_I} \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{z}|} \right) dV(\underline{z}) = \int_S \frac{\partial}{\partial z_1} \left(\frac{1}{|\underline{z}|} \right) n_1 dS(\underline{z}) = - \int_{\theta=0}^{\pi} \sin(\theta)^3 d\theta \int_{\eta=0}^{2\pi} \cos(\eta)^2 d\eta = -\frac{4}{3}\pi,$$

with

$$\begin{aligned} n_1 &= \cos(\eta) \sin(\theta) \\ dS &= \rho^2 \sin(\theta) d\eta d\theta. \end{aligned} \quad (4.36)$$

Second integral:

Again, the integral is split up into two portions, one containing the singularity in V_{ϵ} and one without this spherical region. Following the steps described e.g., in [56], p. 54, where $\phi(\underline{z}) = c_1 z_1 + c_2 z_2 + c_3 z_3$ yields

$$\begin{aligned} \int_{V_I} \phi(\underline{z}) \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{z}|} \right) dV(\underline{z}) &= \underbrace{\int_{V_{\epsilon}} [\phi(\underline{z}) - \phi(0)] \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{z}|} \right) dV(\underline{z})}_{\rightarrow 0 \text{ for } \epsilon \rightarrow 0} + \int_{V_I \setminus V_{\epsilon}} \phi(\underline{z}) \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{z}|} \right) dV(\underline{z}) \\ \int_{V_I} \phi(\underline{z}) \frac{\partial^2}{\partial z_1^2} \left(\frac{1}{|\underline{z}|} \right) dV(\underline{z}) &= \int_{V_I \setminus V_{\epsilon}} (c_1 z_1 + c_2 z_2 + c_3 z_3) \left(\frac{2 z_1^2 - z_2^2 - z_3^2}{|\underline{z}|^5} \right) dV(\underline{z}). \end{aligned} \quad (4.37)$$

A simple change to spherical coordinates then reveals

$$\begin{aligned} & \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} [c_1 \rho \cos(\eta) \sin(\theta) + c_2 \rho \sin(\eta) \sin(\theta) + c_3 \rho \cos(\theta)] \\ & \quad \times \left[\frac{2\rho^2 \cos(\eta)^2 \sin(\theta)^2 - \rho^2 \sin(\eta)^2 \sin(\theta)^2 - \rho^2 \cos(\theta)^2}{\rho^5} \right] \rho^2 \sin(\theta) d\eta d\theta d\rho = \\ & = \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} [c_1 \cos(\eta) \sin(\theta) + c_2 \sin(\eta) \sin(\theta) + c_3 \cos(\theta)] \\ & \quad \times [2 \cos(\eta)^2 \sin(\theta)^2 - \sin(\eta)^2 \sin(\theta)^2 - \cos(\theta)^2] \sin(\theta) d\eta d\theta d\rho = 0. \end{aligned}$$

The third integral can be evaluated similarly to the first one, namely by means of the divergence theorem:

$$\begin{aligned} \int_{V_I} \frac{\partial^4}{\partial z_1^4} |z| \, dV(z) &= \int_S \frac{\partial^3}{\partial z_1^3} (|z|) \, n_1 \, dS(z) = \int_S \left(\frac{3z_1^3}{|z|^5} - \frac{3z_1}{|z|^3} \right) n_1 \, dS(z) = \\ &= \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \left(\frac{3[\rho \cos(\eta) \sin(\theta)]^3}{\rho^5} - \frac{3\rho \cos(\eta) \sin(\theta)}{\rho^3} \right) \cos(\eta) \sin(\theta)^2 \rho^2 \, d\eta \, d\theta = -\frac{8\pi}{5} \end{aligned}$$

And the fourth integral can be treated similarly to the second integral:

$$\begin{aligned} \int_{V_I} (c_1 z_1 + c_2 z_2 + c_3 z_3) \frac{\partial^4}{\partial z_1^4} |z| \, dV(z) &= \\ &= \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} [c_1 \rho \cos(\eta) \sin(\theta) + c_2 \rho \sin(\eta) \sin(\theta) + c_3 \rho \cos(\theta)] \\ &\quad \times \frac{[12\rho^2 \cos(\eta)^2 \sin(\theta)^2 - 3\rho^2 \sin(\eta)^2 \sin(\theta)^2 - 3\rho^2 \cos(\theta)^2] [\rho^2 \sin(\eta)^2 \sin(\theta)^2 + \rho^2 \cos(\theta)^2]}{\rho^7} \\ &\quad \times \rho^2 \sin(\theta) \, d\eta \, d\theta \, d\rho = \\ &= \int_{\rho=\epsilon}^{r_I} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} [c_1 \cos(\eta) \sin(\theta) + c_2 \sin(\eta) \sin(\theta) + c_3 \cos(\theta)] \\ &\quad \times [12 \cos(\eta)^2 \sin(\theta)^3 - 3 \sin(\eta)^2 \sin(\theta)^3 - 3 \cos(\theta)^2 \sin(\theta)] [\sin(\eta)^2 \sin(\theta)^2 + \cos(\theta)^2] \, d\eta \, d\theta \, d\rho = 0 \end{aligned}$$

Evaluation of all integrals in (4.30) according to this procedure gives the result:

$$A_{1,11}^1(\underline{x}) = \frac{c_1 x_1 + c_2 x_2 + c_3 x_3}{6\mu} - \frac{c_1 x_1 + c_2 x_2 + c_3 x_3}{20\mu(1-\nu)} - \frac{c_4 x_1 + c_5 x_2 + c_6 x_3}{60\mu(1-\nu)} - \frac{c_7 x_1 + c_8 x_2 + c_9 x_3}{60\mu(1-\nu)} \quad (4.38)$$

Specification of (4.29) for the other normal-strain-related components and re-iteration of this process gives:

$$A_{1,22}^1(\underline{x}) = \frac{c_4 x_1 + c_5 x_2 + c_6 x_3}{6\mu} - \frac{c_4 x_1 + c_5 x_2 + c_6 x_3}{20\mu(1-\nu)} - \frac{c_1 x_1 + c_2 x_2 + c_3 x_3}{60\mu(1-\nu)} - \frac{c_7 x_1 + c_8 x_2 + c_9 x_3}{60\mu(1-\nu)} \quad (4.39)$$

$$A_{1,33}^1(\underline{x}) = \frac{c_7 x_1 + c_8 x_2 + c_9 x_3}{6\mu} - \frac{c_7 x_1 + c_8 x_2 + c_9 x_3}{20\mu(1-\nu)} - \frac{c_1 x_1 + c_2 x_2 + c_3 x_3}{60\mu(1-\nu)} - \frac{c_4 x_1 + c_5 x_2 + c_6 x_3}{60\mu(1-\nu)} \quad (4.40)$$

and, for the shear-strain-related components,

$$A_{1,12}^1(\underline{x}) = \frac{c_{16} x_1 + c_{17} x_2 + c_{18} x_3}{6\mu} - \frac{c_{16} x_1 + c_{17} x_2 + c_{18} x_3}{30\mu(1-\nu)} \quad (4.41)$$

$$A_{1,13}^1(\underline{x}) = \frac{c_{13} x_1 + c_{14} x_2 + c_{15} x_3}{6\mu} - \frac{c_{13} x_1 + c_{14} x_2 + c_{15} x_3}{30\mu(1-\nu)} \quad (4.42)$$

$$A_{1,23}^1(\underline{x}) = \frac{c_{10} x_1 + c_{11} x_2 + c_{12} x_3}{6\mu} - \frac{c_{10} x_1 + c_{11} x_2 + c_{12} x_3}{30\mu(1-\nu)}. \quad (4.43)$$

Volume-Force-Related Contribution Term $\underline{\underline{A}}^2$:

As described above, the volume force correction term $\underline{f}^{\mathcal{G}}$ is constant and can be pulled out of the integrals. The term $\underline{\underline{A}}_0^2$ therefore reads as

$$\underline{\underline{A}}_0^2(\underline{x}) = \nabla_x^s \int_{V_\infty} \underline{G}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) \cdot \underline{f}^{\mathcal{G}}.$$

Thus, the second-order Green's function is required:

$$G_{ij}(\underline{x} - \underline{y}) = \frac{1}{4\pi \mu} \frac{\delta_{ij}}{|\underline{x} - \underline{y}|} - \frac{1}{16\pi\mu(1-\nu)} \frac{\partial^2}{\partial x_i \partial x_j} |\underline{x} - \underline{y}|$$

Differentiation and subsequent integration of the individual components of \underline{G} can be performed in a similar way as before:

$$\begin{aligned} & \frac{\partial}{\partial x_1} \int_{V_\infty} G_{11}(\underline{x} - \underline{y}^{(1)}) dV(\underline{y}^{(1)}) f_1^{\mathcal{G}} = \\ & = \frac{f_1^{\mathcal{G}}}{4\pi \mu} \frac{\partial}{\partial x_1} \int_{V_\infty} \frac{1}{|\underline{x} - \underline{y}^{(1)}|} dV(\underline{y}^{(1)}) - \frac{f_1^{\mathcal{G}}}{16\pi \mu (1-\nu)} \frac{\partial}{\partial x_1} \int_{V_\infty} \frac{(x_2 - y_2^{(1)})^2 + (x_3 - y_3^{(1)})^2}{|\underline{x} - \underline{y}^{(1)}|^3} dV(\underline{y}^{(1)}) \end{aligned}$$

Evaluation of the first integral in spherical coordinates gives

$$\begin{aligned} & \frac{f_1^{\mathcal{G}}}{4\pi \mu} \int_{V_\infty} \frac{\partial}{\partial x_1} \frac{1}{|\underline{x} - \underline{y}^{(1)}|} dV(\underline{y}^{(1)}) = \frac{f_1^{\mathcal{G}}}{4\pi \mu} \int_S \frac{1}{|\underline{x} - \underline{y}^{(1)}|} n_1 dS(\underline{y}^{(1)}) = \\ & = \frac{f_1^{\mathcal{G}}}{4\pi \mu} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \frac{1}{\rho} \cos(\eta) \sin(\theta)^2 \rho^2 d\eta d\theta = \frac{f_1^{\mathcal{G}}}{4\pi \mu} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \cos(\eta) \sin(\theta)^2 \rho d\eta d\theta = 0. \end{aligned}$$

Similarly, for the second integral

$$\begin{aligned} & \frac{f_1^{\mathcal{G}}}{16\pi \mu (1-\nu)} \int_{V_\infty} \frac{\partial}{\partial x_1} \frac{(x_2 - y_2^{(1)})^2 + (x_3 - y_3^{(1)})^2}{|\underline{x} - \underline{y}^{(1)}|^3} dV(\underline{y}^{(1)}) = \\ & = \frac{f_1^{\mathcal{G}}}{16\pi \mu (1-\nu)} \int_{V_\infty} -\frac{3(x_1 - y_1^{(1)}) [(y_2^{(1)} - x_2)^2 + (y_3^{(1)} - x_3)^2]}{|\underline{x} - \underline{y}|^5} dV(\underline{y}^{(1)}) = \\ & = \frac{f_1^{\mathcal{G}}}{16\pi \mu (1-\nu)} \int_{\rho=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\eta=0}^{2\pi} \frac{3\rho \cos(\eta) \sin(\theta) [\rho^2 \sin(\eta)^2 \sin(\theta)^2 + \rho^2 \cos(\theta)^2]}{\rho^5} \rho^2 \sin(\theta) d\eta d\theta d\rho = 0. \end{aligned}$$

The same applies to all other components to be evaluated, which means that $\underline{\underline{A}}_0^2 = 0$, and, subsequently, $\underline{\underline{A}}^2 = 0$.

Consequently, considering the first iteration for \underline{A}^1 , for an isotropic medium and a spherical inclusion of constant stiffness, the strain can be calculated via

$$\underline{\underline{\epsilon}}(\underline{x}) = \left(\underline{\underline{\mathbb{I}}} + \underline{\underline{\mathbb{P}}} : \underline{\underline{\Delta c}} \right)^{-1} : \underline{\underline{E}} + \frac{1}{2} \left\{ \underline{\underline{\nabla}}_x^s \left[\underline{\underline{\mathcal{G}}}^\infty : (\underline{x} \otimes \underline{x}) \right] - \underline{\underline{A}}_1^1(\underline{x}) \right\}, \quad (4.44)$$

with the components of $\underline{\underline{A}}_1^1$ listed in (4.38) - (4.43), and the constants (4.31).

Potential for Simplification:

It was described that finding a general limit value for $\underline{\underline{A}}^1$ is computationally very expensive and is beyond the scope of this thesis. However, if simplifications are introduced with regard to the components of $\underline{\underline{\mathcal{G}}}^\infty$, it can be comparatively straightforward to find limits. As an illustrative example, consider the following condition:

$$A_{1,11}^1 = A_{1,22}^1 = A_{1,33}^1$$

so that

$$c_1 = c_4 = c_7$$

$$c_2 = c_5 = c_8$$

$$c_3 = c_6 = c_9$$

and therefore

$$\mathcal{G}_{111}^\infty = \mathcal{G}_{212}^\infty = \mathcal{G}_{313}^\infty$$

$$\mathcal{G}_{112}^\infty = \mathcal{G}_{222}^\infty = \mathcal{G}_{323}^\infty$$

$$\mathcal{G}_{113}^\infty = \mathcal{G}_{223}^\infty = \mathcal{G}_{333}^\infty.$$

Then, performing additional iterations, e.g., for the 11-component of $\underline{\underline{A}}_n^1$ shows, that

$$A_{3,11}^1 = A_{2,11}^1 \times f = A_{1,11}^1 \times f^2, \quad (4.45)$$

with

$$f = \Delta c_{1111} \left(\frac{1}{6\mu} - \frac{1}{20\mu(1-\nu)} - \frac{2}{60\mu(1-\nu)} \right) + 2 \Delta c_{1122} \left(\frac{1}{6\mu} - \frac{1}{20\mu(1-\nu)} - \frac{2}{60\mu(1-\nu)} \right).$$

If the series converges, the limit value of A_{11}^1 can then be determined via

$$A_{11}^1 = A_{0,11}^1 + \frac{A_{1,11}^1}{1-f}. \quad (4.46)$$

Chapter 5

Discussion

The aim of the present work was to incorporate a macroscopic measure of the strain gradient into the classical formulations of continuum micromechanics, and to investigate how this macroscopic strain gradient affects the basic pillars of micromechanics. The additional term should ensure that gradient effects, which can occur as a type of size effect in material tests on small length scales, can be taken into account. Such a corresponding model could therefore be particularly suitable for use in biomechanics, as gradient effects might be especially pronounced due to the inherent hierarchical structures.

As measure of the strain gradient, the second gradient of displacement $\underline{\underline{\underline{\mathcal{G}}}}$ was introduced on the macroscale. The total elastic energy stored in the medium therefore depends not only on the macroscopic strain $\underline{\underline{E}}$, but also on $\underline{\underline{\underline{\mathcal{G}}}}$. This formalism essentially corresponds to *Form I* of Mindlin's strain gradient elasticity theory [50], although its application in this thesis is different: Instead of constructing a strain-gradient-elastic material on the microscale, it was attempted to transfer the macroscopically introduced elastic energy via boundary conditions into a classically linear elastic microscopic medium:

$$\Psi^M(\underline{\underline{E}}, \underline{\underline{\underline{\mathcal{G}}}}) \rightarrow \Psi^\mu(\underline{\underline{\underline{\varepsilon}}})$$

Therefore, it was intended to extend the established and highly useful methods of (linear elastic) micromechanics towards the incorporation of gradient effects. As e.g., discussed in [57] and [50], instead of $\underline{\underline{\underline{\mathcal{G}}}}$, other strain-gradient-related terms may be incorporated – such as the gradient of the strain, $\underline{\underline{\underline{\nabla E}}}$, or the gradient of the rotation in combination with the gradient of the strain. Since the components of these terms are simply linear combinations of $\underline{\underline{\underline{\mathcal{G}}}}$ [57], it is expected that they do not exhibit fundamentally different properties.

As for the identification of appropriate force quantities at the macroscopic scale, we employ the principle of virtual power as formulated by P. Germain [26]. It is based on virtual velocity-type quantities associated, to some degree, with the mathematical structure of the actual deformations, but arbitrary in magnitude. The power of internal forces needs to vanish for virtual rigid body motions, and this is indeed the case for the virtual second gradient of velocity $\underline{\underline{\underline{\hat{H}}}}$, the mathematical analogon to $\underline{\underline{\underline{\mathcal{G}}}}$ in the virtual realm. This corresponding proof is found in Chapter 3. Imposing such displacement boundary conditions on the RVE, which depend not only on the macroscopic strain tensor $\underline{\underline{E}}$, but also on the second-order macroscopic displacement gradient $\underline{\underline{\underline{\mathcal{G}}}}$, as also described by Yvonnet et al. [51], may be regarded as an extension of the classical boundary conditions named after Z. Hashin [41], where only $\underline{\underline{E}}$ enters as a macroscopic quantity. In fact, the generalization may be seen as a kind of a second-order Taylor approximation, with the Hashin boundary conditions qualifying as respective first-order approximation. However, the macroscopic displacement itself is not included in the Hashin boundary conditions, because it typically does not have any implications on the material behavior which is to be homogenized. Similar deliberations hold for the virtual velocity-related boundary conditions depending on the

macroscopic virtual strain rate $\underline{\hat{D}}$ and the macroscopic virtual second gradient of velocity $\underline{\hat{H}}$, where the original proposition of Jiménez-Segura et al. [17] was extended. The latter reference, however, did introduce the macroscopic virtual velocity as well, hence providing a "more complete" version of a Taylor series expression.

In Chapter 2 it was shown that the strain average rule (1.25) with the adapted boundary conditions is still valid for a linear elastic RVE if the microscopic position is measured from the geometric center. Since simultaneous application of strain and stress boundary conditions on the same RVE is mathematically not possible, only strain boundary conditions, implying the strain average rule, were applied, while the stress average rule was derived from the very fundamental formalism of the principle of virtual power according to P. Germain [26] (this was described in Chapter 3). Following [17], the equivalence of macroscopically and microscopically formulated power densities of the internal forces was required. As a result, the classical stress average rule was found, together with a rule connecting microscopic Cauchy stresses to a macroscopic double stress.

Finally, Eshelby's inhomogeneity problem, the fundamental matrix inclusion problem, was dealt with in Chapter 4. Solutions of this problem form the basis for the development of many homogenization techniques, not least the very prominent Mori-Tanaka scheme [40]. In addition to the conventional "boundary" or "background" strain \underline{E}^∞ , the strain gradient measure \underline{G}^∞ was added similarly to the previously described boundary conditions. Solving the problem resulted in a Fredholm integral equation of the second kind, where a Neumann series was developed to receive possible solutions. With a spherical, isotropic inclusion of constant stiffness, it was shown that on the one hand the classical concentration tensor could be obtained, referred to here as \underline{A}^0 , which establishes a connection between \underline{E}^∞ and the microscopic strains. In addition, a Neumann series representation of a concentration-like tensor \underline{A}^1 was obtained, which maps the components of \underline{G}^∞ onto the microscopic strains. Due to the more intricate form originating from additional dependencies on position, finding a limit value for this series is a more difficult task and was beyond the scope of this thesis. Instead, a first-order approximation for \underline{A}^1 was presented and the possibility of finding limits more directly by simplification was demonstrated.

It was thus shown that Eshelby's inhomogeneity problem with an additional background strain-gradient-term is generally solvable.

It is therefore evident that finding a limit for \underline{A}^1 is the topic of following research, as well as evaluation for other types of inclusions. Furthermore, the incorporation of this formalism in homogenization techniques and the resulting behavior is to be investigated.

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