

DISSERTATION

Numerical Simulation of the Thermal and Thermomechanical Behaviour of Metal Matrix Composites

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*A mis padres y
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Abstract

The thermal conduction and thermomechanical properties of materials used for making thermal management devices often constitute bottlenecks in the development of new technologies in many important fields, such as the development of faster microprocessors, of fusion nuclear reactors, or more efficient heat engines, amongst others. There is an urgent need for new materials than can withstand increasingly extreme working conditions.

The present thesis is devoted to the development of computer tools for supporting the design and manufacturing of new materials. Analytical, semi-analytical and numerical continuum-level descriptions for studying the macroscopic and local thermophysical and thermomechanical behaviours of discontinuously reinforced composites that contain reinforcements of non-ellipsoidal shapes and general size distributions are reviewed, extended and/or developed. An issue of special interest are the effects of thermally imperfect interfaces between the constituents on the macroscopic thermal conduction behaviour. The methods are applied to diamond reinforced metal matrix composites (DRMMCs).

The use of semi-analytical “replacement tensor” Mori–Tanaka methods for estimating the effective conductivity of DRMMCs at moderate and elevated particle volume fractions is validated. Windowing methods using essential, natural and mixed uniform boundary conditions as well as Periodic Microfield Approaches (PMAs) are applied to computer-generated volume elements for studying the thermal conduction of DRMMCs. Good agreement between the results obtained with the different approaches is found, which supports the validity of the different modeling approaches.

Semianalytical methods and PMAs are used for extracting the macroscopic elasticity and coefficient of thermal expansion tensors of DRMMCs, with good agreement between the predictions of the two approaches. Unit cell analyses of the thermoelastoplastic behaviour of DRMMCs indicate a tendency towards yielding of the matrix for rather moderate temperature excursions. In addition, incremental Mori–Tanaka methods for studying the behaviour of components made of inhomogeneous materials exposed to thermal cycling

are implemented.

The modelling methods reviewed, extended or developed in this work contribute a set of tools for the assessment of the macroscopic conductivity of inhomogeneous materials. These tools cover considerable ranges of detail that can be resolved and of numerical requirements. Moreover, they help in achieving an improved understanding of the local thermomechanical and thermophysical behavior of these composites at the microscale.

Kurzfassung

Das Wärmeleitungs- und thermomechanische Verhalten von Werkstoffen, die in Vorrichtungen zum Temperaturmanagement zum Einsatz kommen, kann bei der Entwicklung neuer Technologien in vielen wichtigen Bereichen eine Schlüsselrolle spielen. Beispiele dafür sind Hochleistungsmikroprozessoren, Fusionsreaktoren oder hocheffiziente Wärmekraftmaschinen. Daher besteht ein dringender Bedarf an neuen Werkstoffen, die bei extremen Bedingungen eingesetzt werden können.

Die vorliegende Dissertation ist auf die Entwicklung computergestützter Werkzeuge zur Unterstützung der Entwicklung und Herstellung neuer Werkstoffe ausgerichtet. Analytische, semianalytische und numerische Beschreibungen auf Kontinuummebene, die zur Untersuchung des thermophysikalischen und thermomechanischen Verhaltens diskontinuierlich verstärkter Verbundwerkstoffe dienen, werden diskutiert, erweitert und/oder entwickelt. Das Schwergewicht liegt dabei auf Verbunden, deren diskontinuierliche Verstärkungen nichtellipsoidale Formen und beliebige Größenverteilungen haben. Von besonderem Interesse sind dabei die Auswirkungen nicht idealer Interfaces zwischen den Konstituenten auf das makroskopische Wärmeleitungsverhalten. Die Methoden werden auf diamantverstärkte Metallmatrix-Verbundwerkstoffe (DRMMCs) angewendet.

Der Einsatz semianalytischer “Ersatztensor”-Mori–Tanaka-Methoden zur Abschätzung der effektiven Wärmeleitfähigkeit von DRMMCs mit moderaten bis hohen Partikelvolumenfraktionen wird validiert. Windowing-Methoden, die notwendige, natürliche und gemischte gleichförmige Randbedingungen verwenden, sowie Verfahren auf Basis periodischer Mikrofelder (PMAs) werden auf computergenerierte Volumenelemente angewandt, um die Wärmeleitung in DRMMCs zu modellieren. Eine gute Übereinstimmung der mit den verschiedenen Methoden errechneten Resultate konnte festgestellt werden, was die Gültigkeit dieser Modellierungszugänge stützt.

Weiters werden semianalytische und PMA-Methoden zur Bestimmung der makroskopischen Elastizitäts- und Wärmeausdehnungstensoren von DRMMCs herangezogen, wobei

wiederum eine gute Übereinstimmung der Vorhersagen der beiden Verfahren beobachtet wird. Einheitszellenanalysen des thermoelastoplastischen Verhaltens von DRMMCs weisen auf eine Tendenz dieser Werkstoffe hin, bereits bei relativ geringen Temperaturänderungen Plastifizieren der Matrix zu zeigen. Weiters werden Mori–Tanaka-Methoden implementiert, um das Verhalten von aus inhomogenen Werkstoffen hergestellten Komponenten unter dem Einfluss thermisch-zyklischer Belastungen zu studieren.

Die in der vorliegenden Arbeit besprochenen, erweiterten bzw. entwickelten Modellierungsmethoden stellen einen Satz von Werkzeugen dar, mit dem das makroskopische Verhalten inhomogener Werkstoffe voraussagend beurteilt werden kann. Die Werkzeuge decken einen breiten Bereich sowohl hinsichtlich des Detaillierungsgrads als auch der numerischen Anforderungen ab. Sie helfen beim Erreichen eines besseren Verständnisses des thermomechanischen und thermophysikalischen Verhaltens inhomogener Werkstoffe auf der Mikroskala.

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Notation

In this work, both tensorial and engineering notations are used. In tensorial notation the order of the tensors is denoted by the number of subscripts of the variables whereas in engineering notation the tensors do not have any subscript denoting the order of the tensors.

Tensors up to rank four are used, denoted as follows in engineering notation:

- Scalars: lowercase or uppercase Italic letters, non–bold Greek lower case letters, or any letters with indices. Examples: $a, b, A, B, \alpha, \beta, \mathbf{a}(i), \mathbf{B}(i, j)$
- Tensors of rank one: lowercase bold Roman letters. Examples: $\mathbf{a}, \mathbf{b}$
- Tensors of rank two: bold Greek lower case letters or uppercase calligraphic letters. Examples: $\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathcal{A}, \mathcal{B}$
- Tensors of rank four: boldface uppercase Roman letters. Examples: $\mathbf{A}, \mathbf{B}$

Throughout this thesis, mechanical and heat conduction problems are studied. The orders of the tensors involved in the above problems are different and the engineering notation used for them, too.

In heat conduction problems, tensors up to rank two are used, which can be represented by matrices, vectors and scalars, without loss of information.

In mechanical problems symmetric tensors of rank 4 and 2 appear. There are several engineering notations that take advantage of these symmetries to represent these tensors reducing their order, e.g. Nye notation (also called Voigt notation) or Mandel notation (also called Kelvin notation), see [35]. In this work the second order tensors are represented

following Nye notation. In this notation the strain and stress tensors, $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ read:

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon(1) \\ \varepsilon(2) \\ \varepsilon(3) \\ \varepsilon(4) \\ \varepsilon(5) \\ \varepsilon(6) \end{pmatrix} = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{13} \\ \gamma_{23} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma(1) \\ \sigma(2) \\ \sigma(3) \\ \sigma(4) \\ \sigma(5) \\ \sigma(6) \end{pmatrix} = \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix}$$

respectively, where ε_{ij} and σ_{ij} are the components of the strain and stress tensors, respectively, and $\gamma_{ij} = 2\varepsilon_{ij}$ are the shear angles. Every second order tensor is represented like the stress tensor, the only exception are strain tensors. Fourth order tensors are represented as matrices, e.g. the elasticity tensor, $\mathbf{E}$:

$$\mathbf{E} = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1112} & E_{1113} & E_{1123} \\ E_{2211} & E_{2222} & E_{2233} & E_{2212} & E_{2213} & E_{2223} \\ E_{3311} & E_{3322} & E_{3333} & E_{3312} & E_{3313} & E_{3323} \\ E_{1211} & E_{1222} & E_{1233} & E_{1212} & E_{1213} & E_{1223} \\ E_{1311} & E_{1322} & E_{1333} & E_{1312} & E_{1313} & E_{1323} \\ E_{2311} & E_{2322} & E_{2333} & E_{2312} & E_{2313} & E_{2323} \end{pmatrix}$$

where E_{ijkl} are the components of the elasticity tensor. For a more thorough description of the engineering notation used and a comparison with tensorial notation, see [appendix A](#).

If tensorial notation is used, the rank of the tensor equals the number of subscripts

- Engineering notation: $a, \mathbf{a}, \boldsymbol{\alpha}, \mathcal{A}, \mathbf{A}$
- Tensorial notation: $a, a_i, \alpha_{ij}, A_{ij}, A_{ijkl}$

In tensorial notation, all variables without subscripts are scalars.

Unless stated otherwise, the Einstein convention is used in this work for tensorial notation. If a subscript occurs twice in any term, it is understood that the index has to be summed from 1 to 3. If a subscript occurs once in a term, it is called a “free suffix”. Square brackets are used to clarify the order of the tensor within them, by indicating the free-suffixes after the right square bracket. Einstein convention does not apply to these indices.

The tensorial product of second order tensors, which is usually denoted in the literature as $\otimes$, it is defined as follows:

$$A_{ijkl} = b_{ij}c_{kl} \quad (1)$$

This operation is distributive and associative but not commutative.

The double contraction operation of a fourth order tensor and a second order tensor will be denoted as follows:

$$\begin{aligned} a_{ij} &= B_{ijkl}c_{lk} \\ d_{ij} &= c_{lk}B_{klij} \end{aligned} \quad (2)$$

and for tensors of order two:

$$a = b_{ij}c_{ji} = c_{ij}b_{ji} \quad (3)$$

The double contraction operation is distributive and associative but not commutative, with the exception of cases where both tensors are of second order.

The Kronecker delta, δ_{ij} , is defined as:

$$\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases} \quad (4)$$

Using the Kronecker delta, the second and fourth order symmetric identity tensors, I_{ij} and 1_{ijkl} respectively, are defined as:

$$\begin{aligned} I_{ij} &= \delta_{ij} \\ 1_{ijkl} &= \delta_{ik}\delta_{jl} \end{aligned} \quad (5)$$

The unit fourth order tensor has the important property:

$$1_{ijkl}a_{lk} = a_{ij} = a_{lk}1_{klij} \quad (6)$$

The volumetric and deviatoric operators follow as:

$$\begin{aligned}
1_{ijkl}^{\text{vol}} &= \frac{1}{3} I_{ij} I_{kl} \\
1_{ijkl}^{\text{dev}} &= 1_{ijkl} - 1_{ijkl}^{\text{vol}}
\end{aligned} \tag{7}$$

Every second order tensor, a_{ij} , can be decomposed into its deviatoric part, a_{ij}^{dev} , and its volumetric part, a_{ij}^{vol} :

$$a_{ij} = a_{lk} 1_{kl ij}^{\text{dev}} + a_{lk} 1_{kl ij}^{\text{vol}} = 1_{ijkl}^{\text{dev}} a_{lk} + 1_{ijkl}^{\text{vol}} a_{lk} = a_{ij}^{\text{dev}} + a_{ij}^{\text{vol}} \tag{8}$$

A fourth-tensor rank tensor A_{ijkl} is said to have major symmetry if:

$$A_{ijkl} = A_{klij} \tag{9}$$

and minor symmetry if:

$$A_{ijkl} = A_{jikl} = A_{ijlk} \tag{10}$$

As the tensors 1_{ijkl} and 1_{ijkl}^{dev} have major but not minor symmetry, it is sometimes useful to work with the symmetrized fourth order tensors:

$$\begin{aligned}
1_{ijkl}^{\text{s}} &= \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \\
1_{ijkl}^{\text{dev,s}} &= 1_{ijkl}^{\text{s}} - 1_{ijkl}^{\text{vol}}
\end{aligned} \tag{11}$$

These tensors exhibit major and minor symmetry, but fulfill equations (6) and (8) only if a_{ij} is symmetric.

The three basic invariants of any second order tensor are defined as:

$$\begin{aligned}
j^{(1)}(a_{ij}) &= a_{ij} \delta_{ij} = a_{ii} \\
j^{(2)}(a_{ij}) &= \frac{1}{2} a_{ij} a_{ji} \\
j^{(3)}(a_{ij}) &= \det |a_{ij}|
\end{aligned} \tag{12}$$

Chapter 1

Introduction

The rapid growth of thermal management requirements necessitates the development of new materials that can withstand extreme working conditions with good reliability. This is a major goal of the European Integrated Project EXTREMAT [54], which supported a large part of this study.

Thermal management devices have a wide range of applications. In this chapter, some of them in the fields of energy and power microelectronics are presented. It is worth noting that thermal management devices play an important role and in some cases are the bottleneck in important fields of engineering.

1.1 Motivation

1.1.1 Fusion Power

It is expected that the world population will increase by 50% in the next 40 years [37]. Consequently, the energy requirements will increase. Furthermore, the developing countries will want to improve the standards of life of their inhabitants.

At present some 85% of energy requirements are covered by fossil energy sources such as coal or oil [7]. The reserves of these materials are limited and, although estimates vary [1; 36; 136], they are not expected to last more than 100 years. Furthermore the green-house effect penalizes the use of these energy sources.

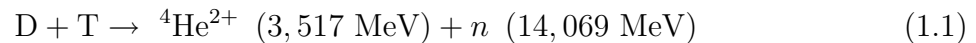
It is obvious that new alternative energy sources for the mid to long term must be



Figure 1.1: Operator standing on the divertor of a tokamak nuclear fusion reactor, (courtesy of IPP).

found. One of these possible alternatives is nuclear fusion.

Nuclear fusion is the process by which multiple particles join together to form a heavier nucleus. During this process energy is released or absorbed. The fusion of two nuclei lighter than iron or nickel releases energy. Therefore, typical fuels are isotopes of hydrogen, deuterium (D) and tritium (T). The fusion of these hydrogen isotopes, according to the reaction:



produces 17.6 MeV of Energy [142].

In order to bring together two nuclei, a substantial energy barrier (Coulomb barrier) must be overcome. Once they are close enough the nuclear force is sufficiently strong and fusion is achieved.

One way of overcoming the Coulomb barrier is by heating the particles, temperature being a measure of the average kinetic energy of particles. The temperatures needed for overcoming the barrier are huge, e.g. for the case of the deuterium-tritium fuel, 50 million K [142]. At these temperatures the gas exists as a macroscopically neutral collection of ions and unbound electrons which is called a plasma. However, two effects reduce the actual temperature needed. One is the fact that temperature is determined by the average kinetic energy, and this energy is not homogeneous within a plasma. The other one is quantum tunneling [135]. The nuclei do not need to have enough energy to overcome the barrier, it is sufficient if they have nearly enough energy.

Heating a plasma up to suitable temperatures and confining it so that a net positive energy balance can be achieved are the main milestones of nuclear fusion.

A fusion plasma cannot be maintained at thermonuclear temperatures if it comes into contact with the walls of the confinement. Additionally, the confinement materials would not survive these temperatures. One way of overcoming this problem are magnetic fields. Usually, magnetic field lines are configured to remain completely within the confinement chamber. The simplest such configuration is the torus. In this case, however, the field produces some forces that would, if uncompensated, cause the particles to hit the walls. A poloidal magnetic field must be superimposed to avoid this effect. This may be produced by a toroidal current flowing in the plasma (tokamak fusion reactor, see fig. 1.1) or by external coils as in the case of the stellarator fusion reactor.

Developing materials for fusion reactors is challenging. Huge neutron fluxes, large cyclic mechanical loads and extreme temperatures must be withstood by these new materials, see [21; 22]. The divertor of a fusion reactor (see fig. 1.1) is a device that removes some fusion products as well as some impurities from the plasma. It removes these particles during operation of the reactor, allowing continuous fusion. Due to the collision with these particles, the divertor is heavily loaded thermally. The divertor is expected to remove heat fluxes of 5 MW/m² in the tokamak machine ITER, 10 MW/m² for the stellarator device Wendelstein 7-X, and this value may reach up to 20 MW/m² under quasistatic conditions in future fusion reactors [166; 167].

Realistic material testing for these conditions is very complicated, therefore modeling is needed. One of the goals of this thesis is the development of a material law than can be implemented into a finite element code which is to be used in the development and study of components of fusion reactors made of inhomogeneous materials, such as a divertor.

1.1.2 Heat sinks

A heat sink is an environment or object that absorbs and dissipates heat from another object using thermal contact. Heat sinks are nowadays widely used in electronics. They have become essential to modern integrated circuits (See fig. 1.2).

The key points in the selection of a material for a heat sink application are:

- High thermal conductivity
- Suitable Coefficient of Thermal Expansion (CTE)
- Stability during thermal cycling



Figure 1.2: Standard application of a heat sink: heat sink of a PC

If the CTE of the heat sink approaches that of the substrate material used (typically silicon) the macroscopic thermal stresses and strains during cycling are kept low, which increases the life of the material. A high thermal conductivity increases the heat removed per unit of time. Additional requirements depend on the final application, e.g. low weight for aerospace applications.

Diamond reinforced metal matrix composites (DRMMCs) are promising candidate materials for attaining elevated thermal conductivities, up to 2000 W/mK [164]. They combine the good thermal conductivity of the metallic matrix with the excellent thermal conductivity of the diamonds. Furthermore, the small CTE of the diamond can be used to tailor the overall CTE of the composite. The large mismatch between the CTEs of the metal and the diamonds, however, tends to lead to high thermal stresses on the microscale and may be a drawback for the thermal stability and mechanical behaviour of the composite.

An important objective of this thesis is the development of computational tools for assessing of the thermal conduction behaviour of particle reinforced MMCs, such as DRMMCs. Furthermore, the thermomechanical behaviour of these materials is modeled.

Chapter 2

Plasticity

As stated in the introduction, one field of interest of the present work is the thermomechanical behaviour of MMCs. During service the matrices of MMCs are often exposed to loads beyond their elastic limit, e.g., in the divertor of a fusion reactor, see section 1.1.1. Therefore, the modeling of the elastic-plastic behaviour of ductile matrix composites is of major interest for the present work. Accordingly, some models for describing the non-cyclic and cyclic elastoplastic behaviour of metallic materials are presented. The discussion is based on the course notes by Jirásek [88].

2.1 General Remarks

In this chapter, the rate independent theory of plasticity is reviewed. Only small strains are considered. Throughout this chapter the microstructure of a material refers to the microscopic description of the crystal structure of a material. For the case of metals, microstructure refers to the dislocation structure, grain structure, precipitates, defects,... and the interaction between them. The microstructure in this sense does not necessarily refer to the microgeometry of the material in the sense of continuum micromechanics.

The Hooke's elasticity tensor for isotropic materials, E_{ijkl} , can be written as:

$$E_{ijkl} = 3k1_{ijkl}^{\text{vol}} + 2g1_{ijkl}^{\text{dev, s}} \quad (2.1)$$

where k and g are the bulk and shear moduli of the material, respectively.

Most plasticity models make use of the volumetric-deviatoric decomposition of the

stress and strain tensors:

$$\begin{aligned}\sigma_{ij} &= \sigma^m \delta_{ij} + \sigma_{ij}^{\text{dev}} \\ \varepsilon_{ij} &= \varepsilon^m \delta_{ij} + \varepsilon_{ij}^{\text{dev}}\end{aligned}\tag{2.2}$$

where $\sigma^m = \sigma_{kk}/3$ and $\varepsilon^m = \varepsilon_{kk}/3$ are the mean stress and strain, respectively, and σ_{ij}^{dev} and $\varepsilon_{ij}^{\text{dev}}$ the stress and strain deviator tensors.

Combining equations 2.1 and 2.2 gives:

$$\begin{aligned}\sigma^m &= 3k\varepsilon^m \\ \sigma_{ij}^{\text{dev}} &= 2g\varepsilon_{ij}^{\text{dev}}\end{aligned}\tag{2.3}$$

2.2 Basic equations

The classical flow theory of plasticity is based on the work of Tresca [154] and von Mises [156]. As only small strains are considered, the total strain can be decomposed additively into the elastic and the plastic strains, equation (2.4). Furthermore, it is assumed that the current state of a volume element is fully described by the plastic strain, the elastic strain and some variables, the hardening variables, describing the changes in the microstructure of the material.

The principal equations of a flow theory model are:

- The elastic-plastic decomposition:

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p\tag{2.4}$$

- The stress-strain law for the elastic behaviour:

$$\sigma_{ij} = E_{ijkl}\varepsilon_{lk}^e\tag{2.5}$$

- The yield condition:

$$y(\sigma_{ij}, Z_*^r) \leq 0\tag{2.6}$$

- The flow rule:

$$\dot{\varepsilon}_{ij}^p = \dot{l} [\phi(\sigma_{ij}, Z_*^r)]_{,ij}\tag{2.7}$$

- The hardening model, which consists of two parts:
 - The definition of the hardening variables, Z_*^h , usually in the form of rate equations:

$$\dot{h}_{ij\dots n}^{(x)} = l \left[i^{(x)}(\sigma_{ij}, Z_*^h) \right]_{ij\dots n} \quad (2.8)$$

$$\forall h_{ij\dots n}^{(x)} \in Z_*^h = \left\{ h_i^{(1)}, \dots, h_i^{(q_1)}, \dots, h_{ij\dots n}^{(\sum_{k=1}^{n-1} (q_k)+1)}, \dots, h_{ij\dots n}^{(\sum_{k=1}^n (q_k))}, \dots \right\}$$
 - and the dependence of the variables Z_*^r appearing in equations (2.6) and (2.7) on the hardening variables, the hardening laws:

$$r_{ij\dots n}^{(y)} = [o^{(y)}(Z_*^h)]_{ij\dots n} \quad (2.9)$$

$$\forall r_{ij\dots n}^{(y)} \in Z_*^r = \left\{ r_i^{(1)}, \dots, r_i^{(t_1)}, \dots, r_{ij\dots n}^{(\sum_{k=1}^{n-1} (t_k)+1)}, \dots, r_{ij\dots n}^{(\sum_{k=1}^n (t_k))}, \dots \right\}$$

where ε_{ij}^e and ε_{ij}^p represent the elastic and the plastic contribution to the strain tensor, respectively; y is the yield function, ϕ is a function specifying the direction of plastic flow; the functions $i^{(x)}$ and $o^{(y)}$ describe the influence of the microstructure on the hardening; l is the plastic multiplier; Z_*^h and Z_*^r are sets of tensors of different orders; and $h_{ij\dots n}^{(x)}$ and $r_{ij\dots n}^{(y)}$ are tensors belonging to the sets Z_*^h and Z_*^r , respectively. A dot over a symbol denotes differentiation with respect to a formal parameter that controls the loading process. It is worth noting that theories described by equations (2.4)–(2.9) are rate independent, and therefore this parameter does not need to have the meaning of real physical time. The set of variables Z_*^r could be eliminated by substituting eqn. (2.9) into equations (2.6) and (2.7). However, as they have a clear physical meaning that helps to understand the model, usually, they are not eliminated. Recall that in the thermodynamical formulation of plasticity, the variables Z_*^r appear naturally as the thermodynamic forces conjugate with the hardening variables Z_*^h , and equations (2.8) are the corresponding state laws, see [95].

The yield function, y , defines the elastic domain in stress space, which is surrounded by the yield surface. Stress states for which $y < 0$ are elastic states, for $y = 0$ they are plastic, and $y > 0$ is not possible. Of course, as the microstructure changes Z_*^h and Z_*^r evolve, which may expand and/or translate the yield surface.

Plastic flow can occur only if the current state is plastic, which is expressed as:

$$ly(\sigma_{ij}, Z_*^r) = 0 \quad (2.10)$$

If the material is in an elastic stress state, $y < 0$, equation (2.10) implies that the rate of the plastic multiplier is equal to zero and, therefore, the plastic strain and the hardening

variables remain constant. If the material is in a plastic state, equation (2.10) does not restrict the rate of the plastic multiplier. However, as the rate of the plastic strain should be greater than zero in a uniaxial tensile test, the rate of the plastic multiplier should never be negative, because ϕ_{ij} in equation (2.7) specifies the oriented direction of evolution. This is described by an additional restriction:

$$\dot{l} \geq 0 \quad (2.11)$$

Equation (2.11) together with equations (2.6) and (2.10) provide the loading/unloading conditions in the so called Kuhn-Tucker form [88].

Once the current values of all variables and the rate of the total strain are known, equations (2.4)–(2.11) make it possible to obtain the rates of all variables.

If the current stress state is elastic, then the rate of the plastic multiplier as well as the rates of the plastic strain are zero and the hardening variables remain constant, as discussed above. In this case, the model is governed by the elastic law.

If the current stress state is plastic, the rate of the plastic multiplier may be zero or positive. The latter case describes a plastic loading. The former case represents an elastic unloading, $\dot{y} < 0$, or the so called neutral loading, $\dot{y} = 0$, both governed by the elastic law.

If plastic loading takes place, the rate of the yield function can be written as:

$$\dot{y} = \left[\frac{\partial y}{\partial \sigma_{ij}} \right]_{ij} \dot{\sigma}_{ji} + \left[\frac{\partial y}{\partial Z_*^r} \right]_* \dot{Z}_*^r = 0 \quad (2.12)$$

Combining the rate form of equation (2.5) with the flow rule and the additive split of the total strain, equations (2.4) and (2.7), we get:

$$\dot{\sigma}_{ij} = E_{ijkl}(\dot{\epsilon}_{lk} - \dot{l}\phi_{lk}) \quad (2.13)$$

The rate form of equation (2.8) combined with equation (2.9), gives rise to:

$$\dot{Z}_*^r = \left[\frac{\partial o_*}{\partial Z_*^h} \right]_* \dot{h}_* = \dot{l} \left[\frac{\partial o_*}{\partial Z_*^h} \right]_* i_* \quad (2.14)$$

Substituting equations (2.13) and (2.14) into (2.12), the rate of the plastic multiplier is obtained as:

$$\dot{\epsilon}_{nm} = \frac{N_{ij} E_{jimn} \dot{\epsilon}_{nm}}{N_{ij} E_{jimn} \phi_{nm} - Z_*^{y,r} Z_*^{o,h} \dot{\epsilon}_{nm}} \quad (2.15)$$

where $N_{ij} = \left[\frac{\partial y}{\partial \sigma_{ij}} \right]_{ij}$, $Z_*^{y,r} = \left[\frac{\partial y}{\partial Z_*^r} \right]_*$, and $Z_*^{o,h} = \left[\frac{\partial \phi}{\partial h_*} \right]_*$. Finally, substituting this result into equation (2.13), leads to the rate form of the elastoplastic stress-strain law:

$$\dot{\sigma}_{ij} = \left[E_{ijkl} - \frac{E_{ijmn} \phi_{nm} N_{op} E_{pokl}}{N_{qr} E_{rqmn} \phi_{nm} - Z_*^{y,r} Z_*^{o,h} \dot{\epsilon}_{nm}} \right]_{ijkl} \dot{\epsilon}_{lk} \quad (2.16)$$

where the tensor in square brackets, is the so called elastoplastic stiffness tensor or tangent tensor, which is a tensor of rank four. It does not posses, in general, major symmetry, except when $\phi_{ij} = N_{ij}$. In this case, the flow rule is said to be associated.

Note that all operations in which one of the members has a star as a subscript, have to be interpreted in a general way, because the variables Z_*^r can be a collection of tensors of different orders. For example, the Chaboche–Marquis model, see section 2.6.2, uses $Z_*^r = \{s^y, X_{ij}\}$. The product $Z_*^{y,r} \dot{Z}_*^r$ for this case is:

$$Z_*^{y,r} \dot{Z}_*^r = \left[\frac{\partial y}{\partial s^y} \right] s^y + \left[\frac{\partial y}{\partial X_{ij}} \right]_{ij} \dot{X}_{ji} \quad (2.17)$$

2.3 Yield criteria

The yield criterion, y , is a scalar function of the stresses tensor and some other variables, which defines the elastic region of a given material element. In other words:

$$\begin{aligned} y(\sigma_{ij}, Z_*^r) &< 0 && \text{if } \sigma_{ij} \text{ is in the elastic regime} \\ y(\sigma_{ij}, Z_*^r) &= 0 && \text{if } \sigma_{ij} \text{ leads to the yielding of the material element} \end{aligned}$$

Experimentally, it has been verified for most materials that the yield surface is convex in stress space.

There exist several yield criteria for different materials. Due to the nature of MMCs' matrices, only criteria for isotropic pressure independent materials are considered. Nevertheless, when a metallic material is reinforced, the homogenized yielding of the MMC may be affected by hydrostatic loads, see e.g. [118].

2.3.1 Isotropic metallic materials

The following discussion is restricted to isotropic elastoplastic materials, i.e., the properties of the material are taken to be independent of the chosen loading direction. This assumption is valid for many polycrystalline metallic materials. In consequence, the yield criterion is invariant to rotations of the system of reference. Accordingly, y must be a symmetric function of the principal stresses or a function of the invariants of the stresses tensor.

Then, for an isotropic material, the elastic region can be defined in the space of the principal stresses, and the surface of this region must be symmetrical with respect to the bisector planes between coordinate axes in this space.

In the case of metallic materials, it has been observed experimentally that yielding is not affected by hydrostatic loads. In other words, the yield criterion for an element of a metallic material it is not a function of the whole stress state of the element, but only of the deviatoric stress tensor, σ_{ij}^{dev} . And, as the first invariant of the stress deviator tensor, $j^{(1)}(\sigma_{ij}^{\text{dev}})$, is zero, it can be deduced that the form of the yield criterion must be:

$$y(j^{(2)}(\sigma_{ij}^{\text{dev}}), j^{(3)}(\sigma_{ij}^{\text{dev}}), Z_*^r) \quad (2.18)$$

where $j^{(2)}(\sigma_{ij}^{\text{dev}})$ and $j^{(3)}(\sigma_{ij}^{\text{dev}})$ are the second and the third invariant of the stress deviator tensor.

For the sake of simplicity, in the following is assumed that the yield function does not depend on Z_*^r .

2.3.1.1 Geometrical representation

The yield criterion can be represented in the space of the principal stresses as a surface with several symmetries. For metallic materials, the criterion does not depend on the hydrostatic component of the stress tensor, so that the yield surface must be a cylinder the axis of which is parallel to the hydrostatic axis, and therefore perpendicular to the plane $\sigma_1 + \sigma_2 + \sigma_3 = 0$, where σ_1 , σ_2 and σ_3 are the principal stresses, $\sigma_1 \geq \sigma_2 \geq \sigma_3$.

This plane is known as deviatoric plane, and it contains the deviatoric stress quasi-vectors. The yield surface intersects the deviatoric plane in a curve that is known as the yield curve.

This curve must be symmetric with respect to the projections of the axes due to the

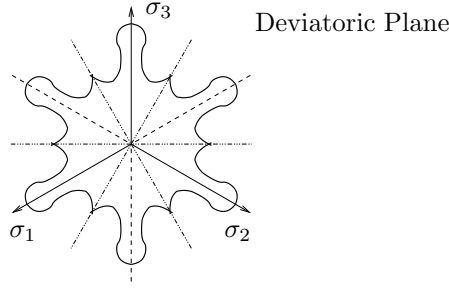


Figure 2.1: Symmetries of the yield curve for metallic materials.

symmetries of the yield surface. Also, the property of the equality of the yield limit in tension and compression can be generalized such that if a point is situated on the yield curve, it also will be if the signs of the stress components are changed. In other words, the yield curve is symmetric with respect to the origin. Therefore, the yield curve can be described by a small portion of the curve that is symmetrically repeated every 60 degrees, see figure 2.1.

2.3.1.2 Tresca and von Mises yield criteria

Several yield criteria have been proposed, but most of them have been forgotten due to their limited correlation with the behaviour of real materials. For metallic materials, the criteria most used nowadays are those proposed by Tresca and by von Mises.

The Tresca criterion assumes that yielding takes place when the maximum value of the shear stress reaches a critical value $c^{\text{cr,Tr}}$. This can be expressed as:

$$\frac{\sigma_1 - \sigma_3}{2} = c^{\text{cr,Tr}} \quad (2.19)$$

The critical value can be obtained from a uniaxial test, because in this test only one principal stress is different from zero, and yielding happens when this stress reaches the limit so that:

$$c^{\text{cr,Tr}} = \frac{s^y}{2} \quad (2.20)$$

where s^y is the uniaxial yield stress.

The yield function can be expressed as:

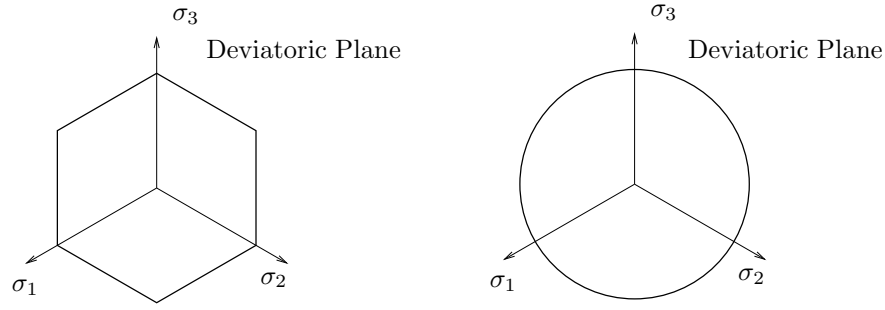


Figure 2.2: Yield curves for the Tresca (left) and von Mises (right) criteria.

$$y(\sigma_{ij}) \equiv \text{Sup}|\sigma_i - \sigma_j - s^y| = 0 \quad i, j = 1, 2, 3 \quad (2.21)$$

Accordingly, the yield surface in the space of principal stresses is a regular hexagonal prism, the axis of which is parallel to the hydrostatic axis. Its section with the deviatoric plane is a regular hexagon, see figure 2.2 (left).

The von Mises criterion is based on the idea that yielding happens when the second invariant of the stress deviator reaches the square of a prescribed value, $c^{\text{cr,VM}}$:

$$j^{(2)}(\sigma_{ij}^{\text{dev}}) = (c^{\text{cr,VM}})^2 \quad (2.22)$$

Evidently, the von Mises criterion is a simplification of the general criterion for metallic materials, equation (2.18). It is easy to verify that if the stress state is a pure shear stress τ , yielding takes place when τ reaches $c^{\text{cr,VM}}$. But, if the stress state is simple tension or compression, yielding takes place when the applied stress is equal to $\sqrt{3}c^{\text{cr,VM}}$, and therefore the maximum shear stress, $\frac{\sqrt{3}}{2}c^{\text{cr,VM}}$, is lower than the shear stress that produces yielding in pure shear. This is the most important difference between the two criteria, and reality typically lies between the two.

The von Mises yield function can be written as:

$$y(\sigma_{ij}) \equiv \sqrt{\frac{3}{2}\sigma_{ij}^{\text{dev}}\sigma_{ji}^{\text{dev}}} - s^y = 0 \quad (2.23)$$

In the space of the principal stresses, the von Mises yield surface is a regular circular cylinder, the axis of which is parallel to the hydrostatic axis and its section with the deviatoric plane is a circle, see figure 2.2 (right).

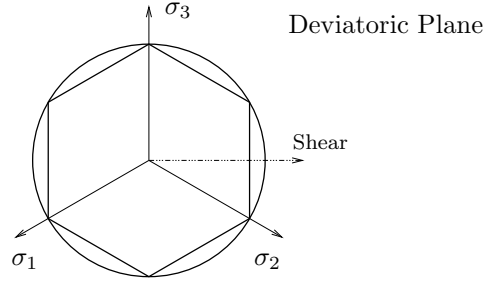


Figure 2.3: Comparison between Tresca and von Mises yield criteria

The differences between the two criteria can be observed in figure 2.3.

2.4 Flow Rules

As long as the stress remains within the elastic region, the deformation process is purely elastic and is governed by the elastic stress-strain law, equation (2.1). Plastic flow begins once the stress state reaches the yield surface. During plastic flow the stress state remains on the yield surface and therefore the condition $y(\sigma_{ij}, Z_*^r) = 0$ is satisfied. The yield condition does not contain enough information to obtain the whole plastic strain tensor, which has six independent components (recall that this tensor is symmetric). Therefore, an additional rule governing the evolution of the plastic flow, the flow rule, must be postulated.

The flow rule should be deduced experimentally. From the theoretical point of view it is convenient to use a rule that preserves the principle of maximum plastic dissipation. This principle for perfectly plastic materials reads:

Let $\dot{\varepsilon}_{ij}^p$ be a given plastic strain rate. Among all possible stress states σ_{ij}^{pos} satisfying the yield condition, the power $\sigma_{ij}^{\text{pos}} \dot{\varepsilon}_{ji}^p$ is maximized by the actual stress, σ_{ij} :

$$\sigma_{ij} \dot{\varepsilon}_{ji}^p = \max_{y(\sigma_{ij}^{\text{pos}}) \leq 0} (\sigma_{ij}^{\text{pos}} \dot{\varepsilon}_{ji}^p) \quad (2.24)$$

Equation (2.24) means that the projection of admissible stress states onto the direction of the plastic strain rate is maximized by the actual stress state. It holds if:

- The elastic domain is convex
- The direction of the plastic strain rate is normal to the yield surface

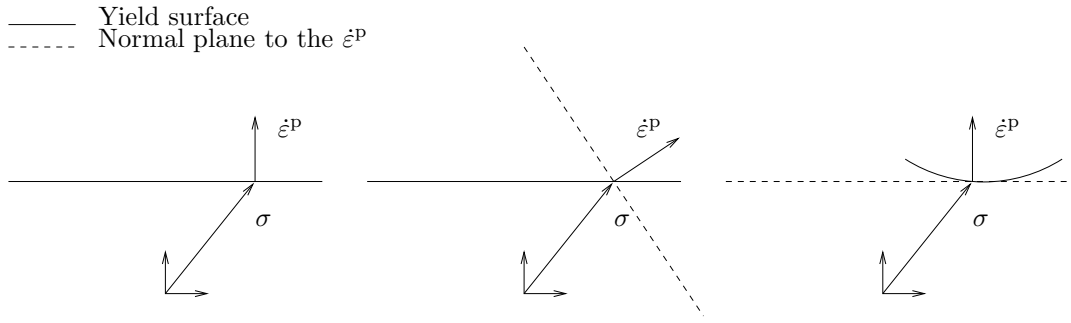


Figure 2.4: Ideal yield surfaces and plastic strain rate situations.

This can be easily understood observing figure 2.4, recall that the double contraction of these tensors has a similar meaning as the dot product of vectors. In figure 2.4 (left), a planar yield surface is sketched. It is obvious that the dot product of the plastic strain rate and any admissible stress state in the yield surface is constant and proportional to the distance of the origin to the planar yield surface, so that planar surfaces normal to the rate of the plastic strain act as isoplanes of the scalar field $\sigma_{ij}\dot{\epsilon}_{ji}^P$. If the rate of the plastic strain were not normal to the yield surface, figure 2.4 (center), the principle of maximum plastic dissipation would not be fulfilled. The same would happen if the yield surface were not convex, see figure 2.4 (right).

The yield surface in stress space is a graphical representation of $y(\sigma_{ij}, Z_*^r) = 0$, therefore the gradient of y with respect to σ_{ij} determines the direction normal to the yield surface, and the flow rule follows as:

$$\dot{\epsilon}_{ij}^P = \dot{l} \left[\frac{\partial y(\sigma_{kl}, Z_*^r)}{\partial \sigma_{ij}} \right]_{ij} = \dot{l} N_{ij} \quad (2.25)$$

which is called the normality rule or the associated flow rule. Note, that for a given stress state the gradient N_{ij} is a fixed tensor specifying the direction of the rate of the plastic strain. The magnitude of this rate is not specified by the plastic flow rule, and it must be determined using the yield function, because during plastic flow the stress state remains on the yield surface.

The behaviour of most metals can be well described using an associated flow rule. Nevertheless, for some pressure-sensitive materials an associated flow rule can be unrealistic, and it must be replaced by a more general flow rule, see equation 2.7, where $\phi(\sigma_{ij}, Z_*^r)$ is the so called plastic potential.

2.5 Hardening models

The microstructure of a material evolves as plastic flow continues, resulting in a change of the properties observable at the macroscale. It is known that in many materials the yield stress is not constant.

Under uniaxial loading the stress transmitted by a yielding material may increase, known as hardening, or decrease, referred to as softening. During hardening or softening, the elastic domain undergoes a certain evolution. The initial yield surface of a virgin material is called the elastic limit envelope. The boundary of the yield surface at an intermediate state is usually called a loading surface.

In this section two hardening models, isotropic hardening and linear kinematic hardening, are presented. With some exceptions, the hardening behaviour of most materials usually appears to be well described by a combination of both, the so called mixed hardening. The suitability of a hardening model depends not only on the material, but the phenomena studied play a role, too. An isotropic hardening model may be suitable for studying the behaviour of a material exposed to uniaxial tensile loading, but completely inadequate for studying the behaviour of the same material under thermomechanical cycling.

2.5.1 Isotropic hardening model

Isotropic hardening is the simplest approach to characterizing the effect of hardening. It uses only one parameter to describe the evolution of the yield surface.

In this model, the yield surface may change only its size. The size of the yield surface is governed by the current yield stress:

$$Z_*^r = \{s^y\} \quad (2.26)$$

The evolution of the yield stress during plastic flow must be described by an additional equation, a hardening law, see equation (2.9). If the hardening law describes the evolution of the yield limit under uniaxial stress as a function of the equivalent plastic strain, it is referred to in the following as hardening equation.

One possible way to achieve this is using the equivalent plastic strain, p :

$$s^y = o^{(1)}(p) \quad (2.27)$$

with:

$$p(t) = \sqrt{\frac{2}{3}} \int_0^t \|\dot{\varepsilon}_{ij}^p(s)\| ds \quad (2.28)$$

and therefore the rate of the equivalent plastic strain is:

$$\dot{p} = \sqrt{\frac{2}{3}} \|\dot{\varepsilon}_{ij}^p\| = \sqrt{\frac{2}{3} \dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ji}^p} = \dot{l} \sqrt{\frac{2}{3} \phi_{ij} \phi_{ji}} \quad (2.29)$$

The equivalent plastic strain is a better choice than e.g. the norm of the plastic strain, because the latter does not always increase during plastic flow, whereas the equivalent plastic strain does. The factor $\sqrt{\frac{2}{3}}$ is chosen such that under monotonic uniaxial loading, $\dot{p}$ coincides with the component $\dot{\varepsilon}_{11}^p$ of $\dot{\varepsilon}_{ij}^p$. The isotropic hardening model assumes that the yield stress depends on the accumulated equivalent plastic strain.

The function $o^{(1)}$ is a hardening equation. Its derivative with respect to the equivalent plastic strain is called the plastic modulus. The hardening equation can be an analytical function, a piecewise linear function or any other interpolation of experimental data. A considerable number of hardening equations have been proposed in the literature. The simplest one is the elastic perfectly plastic material, in which $o^{(1)}(p)$ is constant and the plastic modulus is zero. Among the more complex (and more realistic) hardening equations found in the literature is the Voce law [155]:

$$s^y = c^{(1),\text{Voce}} - c^{(2),\text{Voce}} e^{pc^{(3),\text{Voce}}} \quad (2.30)$$

which is used in the following. In equation 2.30 $c^{(1),\text{Voce}}$ is the saturation stress, $c^{(2),\text{Voce}}$ is a modulus-like parameter, and $c^{(3),\text{Voce}}$ is a dimensionless exponent.

An alternative to the strain-hardening hypothesis is the work hardening, w^p , hypothesis:

$$s^y = o^{(2)}(w^p) \quad (2.31)$$

with

$$\dot{w}^p = \sigma_{ij} \dot{\varepsilon}_{ji}^p = \dot{l} \sigma_{ij} \phi_{ji} \quad (2.32)$$

The choice between strain hardening and work hardening depends on multiaxial experiments. Both are widely used and even lead to similar results in many multiaxial situations. For associated J_2 plasticity they are completely equivalent.

2.5.2 Kinematic hardening model

For some cases, i.e. unloading or cyclic loading, more complicated hardening models are necessary. For unreinforced metals the Bauschinger effect cannot be modelled using an isotropic hardening model. The simplest model for studying this phenomenon is linear kinematic hardening, in which the current loading surface is assumed not to expand but to move in stress space.

To describe the shift of the yield surface a new variable, the so called back stress, X_{ij} , is introduced. The back stress represents the center of the shifted elastic domain. Therefore in this model:

$$Z_*^r = \{X_{ij}\} \quad (2.33)$$

and the yield function can be rewritten as:

$$y(\sigma_{ij}, X_{ij}) \equiv y(\sigma_{ij} - X_{ij}) - s^y = 0 \quad (2.34)$$

It is worth noting that X_{ij} is the thermodynamic conjugate force of the hardening variable ϱ_{ij} , the kinematic hardening (see [38]). Equation (2.9) takes the form:

$$X_{ij} = c^{(1),\text{Kin}} \varrho_{ij} \quad (2.35)$$

where $c^{(1),\text{Kin}}$ is a material parameter. Often ϱ_{ij} is not used in the literature.

Now, we need a kinematic hardening law that governs the evolution of the back stress. Melan [105] and Prager [133] proposed:

$$\dot{X}_{ij} = c^{(2),\text{Kin}} \dot{\varepsilon}_{ij}^p \quad (2.36)$$

where $c^{(2),\text{Kin}}$ is a factor proportional to the plastic modulus, see section 2.5.1. According to this proposal the rate of the back stress is proportional to the plastic strain rate.

Ziegler [169] observed that if the Prager law, equation (2.36), is reduced to a subspace of the stress space, the yield surface does not always move in the direction of its normal

at the current stress point. In some cases the yield surface even deforms. Of course, the complete yield surface in stress space does not deform but as it moves, the shape of the intersection with a given subspace of the stress space may change.

Furthermore, Ziegler observed that the von Mises yield surface always moves in the direction of the vector that goes from its center to the current stress point. Therefore he suggested the following kinematic hardening law:

$$\dot{X}_{ij} = \dot{c}^{(3),\text{Kin}}(\sigma_{ij} - X_{ij}) \quad (2.37)$$

where $\dot{c}^{(3),\text{Kin}}$ is the rate of a new multiplier. A new unknown has been introduced and therefore a supplementary condition is needed. Studying the consistency condition, Ziegler postulated that the projection of the stress rate onto the direction of the normal to the yield surface be proportional to the projection of the plastic strain rate:

$$\dot{\sigma}_{ij}N_{ij} = c^{(2),\text{Kin}}\dot{\epsilon}_{ij}^p N_{ij} \quad (2.38)$$

This condition is also satisfied by the Prager law. Thus the parameter $c^{(2),\text{Kin}}$ has the same meaning as in the Prager rule. Using equations (2.38) and (2.37), together with the elastic stress-strain law, the flow rule and the consistency condition, the rate of the plastic multiplier can be obtained as:

$$\dot{l} = \frac{N_{ij}E_{jimn}\dot{\epsilon}_{nm}}{N_{ij}E_{jimn}\phi_{nm} + c^{(2),\text{Kin}}N_{ij}N_{ji}} \quad (2.39)$$

and the rate of the multiplier, $\dot{c}^{(3),\text{Kin}}$, follows as:

$$\dot{c}^{(3),\text{Kin}} = c^{(2),\text{Kin}} \frac{N_{ij}N_{ji}}{N_{ij}(\sigma_{ji} - X_{ji})} \frac{N_{ij}E_{jimn}\dot{\epsilon}_{nm}}{N_{ij}E_{jimn}\phi_{nm} + c^{(2),\text{Kin}}N_{ij}N_{ji}} \quad (2.40)$$

The rate of the plastic multiplier, $\dot{l}$, can, also, be calculated using equation (2.15), once the scale factor $c^{(2),\text{Kin}} \frac{N_{ij}N_{ji}}{N_{ij}(\sigma_{ji} - X_{ji})}$ between the plastic multiplier and $\dot{c}^{(3),\text{Kin}}$ is known. Note that $N_{ij} = -Z_{*}^{y,r}$ in the present case.

For the Von-Mises yield criteria, Ziegler's and Prager's hardening models, understood here to mean linear kinematic hardening models using Ziegler's or Prager's hardening law, respectively, lead to exactly the same results. In Ziegler's model the yield surface moves in the direction connecting its current center with the current stress point, and this remains true in any subspace.

2.6 Examples

In order to clarify concepts two of the most widely used plasticity models for isotropic metals are developed in this section; elasto-plasticity with isotropic hardening and the Chaboche-Marquis model.

2.6.1 J2 elasto-plasticity model with isotropic hardening

This is one of the simplest and most used plasticity models for metals, because of its simplicity and accuracy. Usually it is a good choice for describing the plastic behaviour of metals that are not exposed to cyclic loading so that the Bauschinger effect need not be accounted for. The model is rate independent, follows a Von-Mises type yield criterion, has an associative flow rule, and hardening is purely isotropic.

As $Z_*^r = \{s^y\}$ and the model has a Von-Mises type yield criterion, the yield condition can be formulated as:

$$y(\sigma_{ij}, s^y) \equiv \sqrt{\frac{3}{2} \sigma_{ij}^{\text{dev}} \sigma_{ji}^{\text{dev}}} - s^y \leq 0 \quad (2.41)$$

The derivative of $y(\sigma_{ij}, s^y)$ with respect to the stress tensor is:

$$N_{ij} = \left[\frac{\partial y(\sigma_{kl}, s^y)}{\partial \sigma_{ij}} \right]_{ij} = \left[\frac{\partial}{\partial \sigma_{ij}} \left(\sqrt{\frac{3}{2} \sigma_{kl}^{\text{dev}} \sigma_{lk}^{\text{dev}}} - s^y \right) \right]_{ij} = \frac{3}{2 \sqrt{\frac{3}{2} \sigma_{kl}^{\text{dev}} \sigma_{lk}^{\text{dev}}}} \sigma_{ij}^{\text{dev}} \quad (2.42)$$

The flow rule, equation (2.7), which is associative, can then be rewritten as:

$$\dot{\varepsilon}_{ij}^p = \dot{l} \left[\frac{\partial y(\sigma_{kl}, s^y)}{\partial \sigma_{ij}} \right]_{ij} = \frac{3 \dot{l}}{2 \sqrt{\frac{3}{2} \sigma_{kl}^{\text{dev}} \sigma_{lk}^{\text{dev}}}} \sigma_{ij}^{\text{dev}} \quad (2.43)$$

Combining the definition of the rate of the equivalent plastic strain, equation (2.29), with the flow rule (2.43), the plastic multiplier is obtained as:

$$\dot{p} = \sqrt{\frac{2}{3} \dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ji}^p} = \dot{l} \sqrt{\frac{2}{3} \frac{3}{2}} \sqrt{\frac{\sigma_{ij}^{\text{dev}} \sigma_{ji}^{\text{dev}}}{\frac{3}{2} \sigma_{kl}^{\text{dev}} \sigma_{lk}^{\text{dev}}}} = \dot{l} \quad (2.44)$$

To summarize, the basic equations of this model, the equivalents to equations (2.4)-(2.9), are the elastic plastic decomposition and the stress-strain law for the elastic part, equations (2.4)-(2.5), together with the yield condition, equation (2.41) and:

- The flow rule:

$$\dot{\varepsilon}_{ij}^p = \frac{3\dot{p}}{2\sqrt{\frac{3}{2}\sigma_{kl}^{\text{dev}}\sigma_{lk}^{\text{dev}}}}\sigma_{ij}^{\text{dev}} \quad (2.45)$$

- The two “ingredients” of the hardening model:

- The definition of the hardening variables, $Z_*^h = \{p, \varepsilon_{ij}^p\}$:

$$\begin{aligned} \dot{p} &= \dot{l} \\ \dot{\varepsilon}_{ij}^p &= \dot{l} \frac{3}{2\sqrt{\frac{3}{2}\sigma_{kl}^{\text{dev}}\sigma_{lk}^{\text{dev}}}}\sigma_{ij}^{\text{dev}} \end{aligned} \quad (2.46)$$

- and the dependence of the variables, $Z_*^r = \{s^y\}$, on the hardening variables, equation (2.27).

Using equation (2.16), the elastoplastic stiffness tensor, F_{ijkl} , is obtained as:

$$F_{ijkl} = E_{ijkl} - \frac{\frac{(3g)^2}{\frac{3}{2}\sigma_{mn}^{\text{dev}}\sigma_{nm}^{\text{dev}}}}{3g + \frac{d\sigma^{(1)}(p)}{dp}}\sigma_{ij}^{\text{dev}}\sigma_{kl}^{\text{dev}} \quad (2.47)$$

Recall that in this plasticity model $N_{ij}N_{ji} = \frac{3}{2}$ and that N_{ij} is a deviatoric tensor, and, therefore, taking into account equation (2.1), $E_{ijkl}N_{lk} = N_{kl}E_{lkij} = 2gN_{ij}$. Furthermore, for the isotropic hardening model:

$$Z_*^{y,r} Z_*^{o,h} i_* = \frac{dy}{ds^y} \left[\frac{\partial s^y}{\partial p} 1 + \frac{\partial s^y}{\partial \varepsilon_{ij}^p} \frac{3}{2\sqrt{\frac{3}{2}\sigma_{kl}^{\text{dev}}\sigma_{lk}^{\text{dev}}}}\sigma_{ij}^{\text{dev}} \right] \quad (2.48)$$

2.6.2 Chaboche-Marquis hardening model

This is one of the most widely used models in the literature for studying cyclic plasticity in metals. The model is rate independent, follows a Von-Mises type yield criterion, has an associative flow rule, and uses mixed hardening. In its more general form, the model has

multiple back stresses. The multiple back stresses were introduced by Chaboche [26] to extend the capability of the original Armstrong–Frederick model [8] for larger strain range. These back stresses evolve according a similar rule defined by different material constants, thus allowing saturation of hardening to take place at different strain levels. The present example is developed for a single back stress.

Linear isotropic hardening and kinematic hardening can be easily combined to form the yield condition:

$$y(\sigma_{ij}, Z_*^r) \equiv \sqrt{3j^{(2)}(1_{ijkl}^{\text{dev}}(\sigma_{lk} - X_{lk}))} - s^y \leq 0 \quad (2.49)$$

where $Z_*^r = \{X_{ij}, s^y\}$, and the derivative with respect to the stress tensor becomes:

$$N_{ij} = \left[\frac{\partial y(\sigma_{mn}, Z_*^r)}{\partial \sigma_{ij}} \right]_{ij} = \frac{3}{2\sqrt{3j^{(2)}(1_{mnkl}^{\text{dev}}(\sigma_{lk} - X_{lk}))}} (\sigma_{ij}^{\text{dev}} - X_{ij}^{\text{dev}}) \quad (2.50)$$

Recall that the position of the yield surface, X_{ij} , is independent of the actual stress state, and that:

$$\left[\frac{d\sigma_{ij}^{\text{dev}}}{d\sigma_{kl}} \right]_{ijkl} = 1_{ijkl} - 1_{ijkl}^{\text{vol}} \quad (2.51)$$

Since $N_{ij}N_{ji} = \frac{3}{2}$, combining the definition of the rate of the equivalent plastic strain with the the associative flow rule, the plastic multiplier is obtained as:

$$\dot{p} = \dot{l} \quad (2.52)$$

The basic equations of this model, the equivalents to equations (2.4)–(2.9), are the elastic plastic decomposition, the stress-strain law for the elastic part and the yield condition, equations (2.4)–(2.5) and (2.49), together with:

- The flow rule:

$$\dot{\varepsilon}_{ij}^p = \frac{3\dot{p}}{2\sqrt{\frac{3}{2}(\sigma_{kl}^{\text{dev}} - X_{kl}^{\text{dev}})(\sigma_{lk}^{\text{dev}} - X_{lk}^{\text{dev}})}} (\sigma_{ij}^{\text{dev}} - X_{ij}^{\text{dev}}) \quad (2.53)$$

- The two parts of the hardening model:

- The definition of the hardening variables, $Z_*^h = \{p, \varepsilon_{ij}^p, \varrho_{ij}\}$:

$$\begin{aligned}\dot{p} &= \dot{l} \\ \dot{\varepsilon}_{ij}^p &= \dot{l} \frac{3}{2\sqrt{\frac{3}{2}(\sigma_{kl}^{\text{dev}} - X_{kl}^{\text{dev}})(\sigma_{lk}^{\text{dev}} - X_{lk}^{\text{dev}})}} (\sigma_{ij}^{\text{dev}} - X_{ij}^{\text{dev}}) \\ \dot{\varrho}_{ij} &= \dot{l} \left(N_{ij} - \frac{c^{(2),\text{C-M}}}{c^{(1),\text{C-M}}} X_{ij} \right)\end{aligned}\tag{2.54}$$

- and the dependence of the variables, $Z_*^r = \{s^y, X_{ij}\}$, on the hardening variables, equations (2.27) and:

$$X_{ij} = c^{(1),\text{C-M}} \varrho_{ij}\tag{2.55}$$

where $c^{(1),\text{C-M}}$ and $c^{(2),\text{C-M}}$ are material constants.

Usually equations (2.35) and (2.54) are combined to remove the variable ϱ_{ij} , obtaining:

$$\dot{X}_{ij} = c^{(1),\text{C-M}} \dot{\varepsilon}_{ij}^p - c^{(2),\text{C-M}} X_{ij} \dot{p}\tag{2.56}$$

which is known as the Frederick–Armstrong equation.

Together with equations (2.50) and (2.53), equation (2.56) shows clearly that if the initial value of X_{ij} is deviatoric, e.g. $X_{ij} = 0$, X_{ij} is deviatoric, and therefore it can be often found in the literature that equation (2.50) is written as:

$$N_{ij} = \frac{3}{2\sqrt{3j^{(2)}(\sigma_{lk} - X_{lk})}} (\sigma_{ij}^{\text{dev}} - X_{ij})\tag{2.57}$$

The finite element code ABAQUS, [2], uses a similar model with the same equations, but with a different hardening law. Instead of equation (2.56) it uses:

$$\dot{X}_{ij} = \frac{c^{(1),\text{ABA}}}{s^y} (\sigma_{ij} - X_{ij}) \dot{p} - c^{(2),\text{ABA}} X_{ij} \dot{p}\tag{2.58}$$

where $c^{(1),\text{ABA}}$ and $c^{(2),\text{ABA}}$ are material parameters.

This model leads exactly to the same results, although the two models are not strictly equivalent. Notice that equation (2.58) can be rewritten as:

$$\dot{X}_{ij}^{\text{dev}} = \frac{c^{(1),\text{ABA}}}{s^y} (\sigma_{ij}^{\text{dev}} - X_{ij}^{\text{dev}}) \dot{p} - c^{(2),\text{ABA}} X_{ij}^{\text{dev}} \dot{p}\tag{2.59}$$

$$\dot{X}_{ij}^{\text{vol}} = \frac{c^{(1),\text{ABA}}}{s^y} (\sigma_{ij}^{\text{vol}} - X_{ij}^{\text{vol}}) \dot{p} - c^{(2),\text{ABA}} X_{ij}^{\text{vol}} \dot{p}\tag{2.60}$$

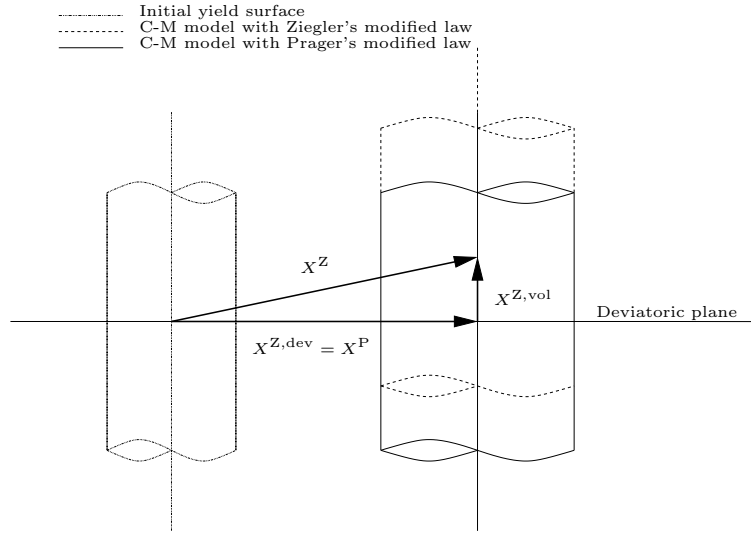


Figure 2.5: Evolution of the yield surface in the Chaboche–Marquis criterion for different kinematic hardening laws: Prager’s modified law, equation (2.56), and Ziegler’s modified law, equation (2.58).

whenever plastic flow takes place, $s^y = \sqrt{3j^{(2)}(\sigma_{lk}^{dev} - X_{lk}^{dev})}$ because the yield function equals zero. If the yield function is less than zero, the rate of the plastic multiplier is zero, and therefore the rate of the hardening variables equals zero, recall equation (2.8). Equation (2.59), can then be rewritten as:

$$\dot{X}_{ij}^{dev} = \frac{2c^{(1),ABA}}{3}\dot{\varepsilon}_{ij}^p - c^{(2),ABA}X_{ij}^{dev}\dot{p} \quad (2.61)$$

and by setting $c^{(1),ABA} = \frac{3}{2}c^{(1),C-M}$ and $c^{(2),ABA} = c^{(2),C-M}$ equation (2.59) is equivalent to equation (2.56).

Furthermore, the volumetric part of X_{ij} does not have any influence on the yield surface. This can be easily understood in figure (2.5). Both models describe the movement of a cylinder. In the Chaboche–Marquis model, the cylinder moves normally to the deviatoric axis, whereas for the ABAQUS model, the cylinder, in addition, moves along its axis. But, as we have a cylinder the two surfaces coincide.

Using equation 2.16, the elastoplastic stiffness tensor, F_{ijkl} , is obtained:

$$F_{ijkl} = E_{ijkl} - \frac{(2g)^2}{3g + \frac{do^{(1)}(p)}{dp} + 3/2c^{(1),C-M} - c^{(2),C-M}N_{mn}X_{nm}}N_{ij}N_{kl} \quad (2.62)$$

This is, normally, done as follows:

$$\mathbf{g}(\mathbf{x}) = \mathbf{x} - \mathcal{A}(\mathbf{x})\mathbf{a}(\mathbf{x}) \quad (2.66)$$

If $\mathcal{A}(\mathbf{x})$ is chosen such that it equals the inverse of the Jacobian of $\mathbf{a}(\mathbf{x})$, $\mathcal{J}(\mathbf{x})$:

$$\mathcal{A}(\mathbf{x}) = (\mathcal{J}(\mathbf{x}))^{-1}; \quad \mathcal{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial a_1}{\partial x_1} & \cdots & \frac{\partial a_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_n}{\partial x_1} & \cdots & \frac{\partial a_n}{\partial x_n} \end{pmatrix} \quad (2.67)$$

then the root of the succession $\{\mathbf{x}^{(m)}\}_{m=0}^{\infty}$, where $\mathbf{x}^{(m+1)} = \mathbf{g}(\mathbf{x}^{(m)})$, is unique [59]. This is the well known Newton-Raphson method for systems of equations:

$$\mathbf{x}^{(m+1)} = \mathbf{x}^{(m)} - (\mathcal{J}(\mathbf{x}^{(m)}))^{-1} \mathbf{a}(\mathbf{x}^{(m)}) \quad (2.68)$$

Of course, in order to avoid difficulties, $\mathcal{J}$ must not be singular at the solution of the system (2.64), and the partial derivatives of $(a_1, a_2, \dots, a_n)$ must be continuous. Furthermore, if $\mathbf{a}$ is C^2 , a function with 2 continuous derivatives, in an interval that contains the solution, then the method will converge for every initial value within a neighborhood of the solution.

To avoid the calculation of the inverse of the Jacobian, equation (2.68) is rewritten as:

$$\mathcal{J}(\mathbf{x}^{(m)}) (\mathbf{u}^{(m)}) = -\mathbf{a}(\mathbf{x}^{(m)}) \quad (2.69)$$

where $\mathbf{u}^{(m)} = \mathbf{x}^{(m+1)} - \mathbf{x}^{(m)}$ is the unique unknown of the system. Once the system is solved $\mathbf{x}^{(m+1)}$ can be easily calculated as:

$$\mathbf{x}^{(m+1)} = \mathbf{x}^{(m)} + \mathbf{u}^{(m)} \quad (2.70)$$

2.7.2 Generalized trapezoidal rule

The flow rule, equation (2.7), is a differential equation that must be integrated numerically:

$$\dot{\epsilon}_p = l\phi(\sigma) \quad (2.71)$$

Formal integration leads to the formula:

$$\Delta \boldsymbol{\varepsilon}_p = \int_{l_{(n)}}^l \boldsymbol{\phi}(\boldsymbol{\sigma}(s)) ds \quad (2.72)$$

where the integral is evaluated from the value of the plastic multiplier at the beginning of the increment, $l_{(n)}$, to the value of the plastic multiplier at the end of the increment, l . This equation can be solved approximately using the generalized trapezoidal rule:

$$\Delta \boldsymbol{\varepsilon}_p = \Delta l [(1 - c^{\text{Trap}}) \boldsymbol{\phi}(\boldsymbol{\sigma}(l_{(n)})) + c^{\text{Trap}} \boldsymbol{\phi}(\boldsymbol{\sigma}(l))] \quad (2.73)$$

where c^{Trap} is an adjustable weight factor. Ortiz and Popov [121] showed that when the increment size tends to zero $c^{\text{Trap}} = 0.5$ would be the best choice, but, when the increment size increases this may not be the case. According to their analysis for von Mises plasticity the closest point projection, $c^{\text{Trap}} = 1$, is probably optimal.

2.7.3 Stress return algorithm

The basic task of the stress return algorithm is to provide the values of all the variables at the end of a generic increment, knowing the respective values at the beginning of the increment, denoted by subscripts $_{(n)}$, and the increment of the total strain. If a variable does not have a subscript, it will be computed at the end of the increment. In this section a stress return algorithm for handling isotropic elasto-plasticity models, compare section 2.6, is described.

The main equations of this elasto-plasticity model can be rewritten as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p \quad (2.74)$$

$$\boldsymbol{\sigma} = \mathbf{E} \boldsymbol{\varepsilon}^e \quad (2.75)$$

$$y \equiv \sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev}}]^T \boldsymbol{\sigma}^{\text{dev}} \right]^M} - s^y = 0 \quad (2.76)$$

$$\boldsymbol{\varepsilon}^p - \boldsymbol{\varepsilon}_{(n)}^p = (p - p_{(n)}) \frac{3}{2} \frac{\boldsymbol{\sigma}^{\text{dev}}}{\sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev}}]^T \boldsymbol{\sigma}^{\text{dev}} \right]^M}} \quad (2.77)$$

$$s^y = o(p) \quad (2.78)$$

where $\llbracket^M$ are the modified products described in appendix A.

The flow rule is evaluated at the end of the increment which means that the algorithm corresponds to the backward Euler scheme.

The unloading/loading conditions, equations (2.6), (2.10) and (2.11), can be replaced by:

$$y(\boldsymbol{\sigma}) \leq 0, \quad (l - l_n)y(\boldsymbol{\sigma}) = 0, \quad l - l_n \geq 0 \quad (2.79)$$

The first step consists of the evaluation of a trial stress state, $\boldsymbol{\sigma}^{\text{tr}}$. This trial stress state is calculated under the assumption that no plastic flow occurs during the increment:

$$\boldsymbol{\sigma}^{\text{tr}} = \mathbf{E}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{(n)}^p) = \boldsymbol{\sigma}_{(n)} + \mathbf{E}\Delta\boldsymbol{\varepsilon} \quad (2.80)$$

If the trial stress satisfies the yield condition, it is accepted as the solution. If not, plastic flow occurs during the increment and the set of equations (2.74–2.78) must be solved using an iterative solution procedure, e.g., the Newton-Raphson method. The set of equations (2.74–2.78) can be easily reduced to one equation with one unknown, Δp :

$$\sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev, tr}}]^T \boldsymbol{\sigma}^{\text{dev, tr}} \right]^M} - s^y - \Delta p 3g = 0 \quad (2.81)$$

Recall that in this model:

$$\mathcal{N} = \frac{\boldsymbol{\sigma}^{\text{dev}}}{\sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev}}]^T \boldsymbol{\sigma}^{\text{dev}} \right]^M}} = \frac{\boldsymbol{\sigma}^{\text{dev, tr}}}{\sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev, tr}}]^T \boldsymbol{\sigma}^{\text{dev, tr}} \right]^M}} \quad (2.82)$$

where $\boldsymbol{\sigma}^{\text{dev, tr}}$ is the deviatoric part of the trial stress state.

Applying the Newton-Raphson method to equation (2.81) gives:

$$\Delta p = \Delta p + \frac{\sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev, tr}}]^T \boldsymbol{\sigma}^{\text{dev, tr}} \right]^M} - s^y - \Delta p 3g}{3g + \frac{ds^y}{dp}} \quad (2.83)$$

and when Δp is known, the rest of the variables can be easily updated using equations (2.74–2.78). Once all the variables are evaluated the algorithmic Jacobian (see subsection 2.7.4) can be calculated using equation (2.88).

An algorithm following this scheme can be found e.g. in [2]. Observe that in the nomenclature of the ABAQUS sample user material subroutine for isotropic elasto-plasticity $\text{SYIELD} = \sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev}}]^T \boldsymbol{\sigma}^{\text{dev}} \right]^M}$ and $\text{SMISES} = \sqrt{\frac{3}{2} \left[[\boldsymbol{\sigma}^{\text{dev, tr}}]^T \boldsymbol{\sigma}^{\text{dev, tr}} \right]^M}$. For the Chaboche-Marquis model with one back stress tensor an algorithm can be found in [38], for multiple back stresses see [138].

2.7.4 Algorithmic stiffness and tangent material stiffnesses

There are two types of elastoplastic stiffness tensors, the algorithmic and the tangent stiffnesses. The latter was explained and obtained for some plasticity models in the previous sections. It describes the change of the stress tensor produced by an infinitesimal change of the strain tensor. The algorithmic stiffness, in contrast, describes the change of the stress tensor produced by a finite change of the strain tensor. In general the two stiffnesses are different for finite increments.

The tangent elastoplastic stiffness is obtained by differentiation of the constitutive law, whilst the algorithmic elastoplastic stiffness is obtained by differentiation of the numerical algorithm. Some authors refer to the algorithmic stiffness tensor as the consistent tensor. This name is not optimally chosen because both stiffnesses are derived consistently. A quadratic rate of convergence of the Newton-Raphson equilibrium iteration is obtained only when using the algorithmic stiffness [39]. Nevertheless, the converged results may be the same using algorithmic or tangent elastoplastic stiffness.

The algorithmic tangent stiffness is obtained by letting all the variables vary slightly around the converged solution. In the following, it is obtained for the isotropic elasto-plasticity model, section 2.6.1.

Combining the elastic-plastic decomposition, the stress-strain law, the yield condition and the flow rule, equations (2.4), (2.5), (2.41) and (2.45), the following relationship is obtained:

$$\left(1 + \frac{3g}{s_y} \Delta p \right) \sigma_{ij}^{\text{dev}} = 2g \left(\varepsilon_{ij,(n)}^{\text{dev,e}} + \Delta \varepsilon_{ij}^{\text{dev}} \right) \quad (2.84)$$

where $\varepsilon_{ij,(n)}^{\text{dev,e}}$ is the deviatoric part of the elastic strain tensor at the beginning of the increment.

Taking the variation of equation (2.84) with respect to all the variables at the end of

the increment gives:

$$\left(1 + \frac{3g}{s^y} \Delta p\right) \partial \sigma_{ij}^{\text{dev}} + \frac{3g}{s^y} \left(\partial p - \frac{\Delta p}{s^y} \partial s^y\right) \sigma_{ij}^{\text{dev}} = 2g \partial \left(Z_{ij}^{\text{Alg}}\right) \quad (2.85)$$

where $Z_{ij}^{\text{Alg}} = \varepsilon_{ij,(n)}^{\text{dev,e}} + \Delta \varepsilon_{ij}^{\text{dev}}$

The differentials of the equivalent plastic strain and the yield stress can be obtained as functions of Z_{ij} , using equations (2.27) and (2.84), which leads to:

$$\partial \sigma_{ij}^{\text{dev}} = \left(c^{(1),\text{Alg}} 1_{ijkl}^s - c^{(2),\text{Alg}} \sigma_{ij}^{\text{dev}} \sigma_{kl}^{\text{dev}}\right) \partial Z_{lk}^{\text{Alg}} \quad (2.86)$$

$$\text{where } c^{(1),\text{Alg}} = \frac{(2/3) s^y}{\sqrt{(2/3) Z_{mn}^{\text{Alg}} Z_{nm}^{\text{Alg}}}} \text{ and } c^{(2),\text{Alg}} = \frac{1}{s^y \sqrt{(2/3) Z_{mn}^{\text{Alg}} Z_{nm}^{\text{Alg}}}} \frac{1 - \frac{\Delta p}{s^y} \frac{ds^y}{dp}}{1 + \frac{ds^y}{dp} / 3g}.$$

Since:

$$\partial Z_{ij}^{\text{Alg}} = 1_{ijkl}^{\text{dev,s}} \partial \varepsilon_{lk} \quad (2.87)$$

combining equation (2.2) with (2.86) leads to:

$$\partial \sigma_{ij} = \left[c^{(1),\text{Alg}} 1_{ijkl}^s + (3k - c^{(1),\text{Alg}}) 1_{ijkl}^{\text{vol}} - c^{(2),\text{Alg}} \sigma_{ij}^{\text{dev}} \sigma_{kl}^{\text{dev}}\right]_{ijkl} \partial \varepsilon_{lk} \quad (2.88)$$

where the tensor in square brackets is the algorithmic stiffness.

Chapter 3

Continuum Micromechanics

The tools employed in this thesis to study the thermomechanical or thermal conduction behaviour of inhomogeneous materials are based on continuum models, an approach that is usually referred to as continuum micromechanics. Therefore in the following the basic concepts of the continuum micromechanics are revisited. This chapter follows several reports by Böhm [17; 18].

3.1 General Considerations

In this chapter, some basic issues and some approaches in the field of continuum micromechanics of materials are discussed. The treatment concentrates on the thermo-mechanical and thermal conduction behaviour of two-phase materials showing a matrix-inclusion topology, and, especially, to metal matrix composites. Source terms, such as body forces and heat production are not considered. Dynamical effects and transient thermal conduction are excluded. Non-uniform phase properties are not considered, either. In order to bring out similarities and differences, elasticity and heat conduction are presented in parallel, see table 3.1.

Recall that some of the numerical approaches described in this chapter, see section 3.3, can account for the presence of source terms as well as non-uniform phase properties. Such conditions, however, are not accounted for in this thesis.

Whenever engineering notation is used throughout this chapter for mechanical problems, the correction terms, see appendix A, are not shown to simplify the notation. Never-

Elasticity	Thermal conduction
$\boldsymbol{\varepsilon}$ Strain tensor	$\mathbf{d}$ Thermal gradient vector
$\boldsymbol{\sigma}$ Stress tensor	$\mathbf{q}$ Heat flux vector
$\mathbf{C}$ Compliance tensor	$\mathcal{R}$ Thermal resistivity tensor
$\mathbf{E}$ Elasticity tensor	$\mathcal{K}$ Thermal conductivity tensor
$\mathbf{u}$ Displacement vector	t Temperature

Table 3.1: Analogous variables used in thermal conduction and elasticity.

theless, they may be taken into account when implementing an algorithm. Some authors use Nye notation instead. In Nye notation, the tensors have a slightly different notation, and they are written so that the corrections are avoided, e.g., the symmetric unit tensor is represented using the unit matrix. Nye notation is equivalent to engineering notation if the tensors of rank four involved in the equations have the following structure:

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 & 0 \\ A_{21} & A_{22} & A_{23} & 0 & 0 & 0 \\ A_{31} & A_{32} & A_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & A_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{66} \end{pmatrix} \quad (3.1)$$

If the structure is different, e.g., for the Eshelby tensor of an ellipsoidal particle embedded in a matrix with lower than orthotropic symmetry, Nye notation may lead to incorrect results. In fact, for any symmetry lower than isotropy the tensors must be given in principal orientation

3.1.1 Inhomogeneous materials and length scales

Most industrial and engineering materials are inhomogeneous; they consist of dissimilar constituents that are distinguishable at some length scale. Each constituent has different material properties and/or material orientations, and may itself be inhomogeneous at some smaller scale. Typical examples of such materials are composites, steel, concrete, laminates, bones, wood . . . Important aims of theoretical studies of inhomogeneous materials lie in homogenization and localization. Homogenization consists in deducing the overall behaviour from the geometrical arrangements of the constituents, their material properties and the interfaces between them. Localization consists in deducing the local state from the geometrical arrangements of the constituents, their material properties, the interfaces between them and the macroscopic loading the inhomogeneous material is exposed to.

Description of the properties of inhomogeneous materials have to account for at least two length scales:

- Macroscale: the length scale of the component, structure or sample.
- Microscale: the length scale at which the constituents are distinguishable.

In many cases, however, the constituents may be inhomogeneous at a lower length scale.

In micromechanical approaches the strain, stress, temperature gradient and heat flux fields, $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$, $\mathbf{d}$, $\mathbf{q}$, in an inhomogeneous material are split into contributions corresponding to different length scales. It is assumed that these length scales are sufficiently different so that:

- Fluctuations of the strain, stress, temperature gradient and heat flux at the microscale (microfields, fast variables) influence the macroscopic behaviour only via their volume averages.
- Gradients of strain, stress, temperature gradient and heat flux at the macroscale (macrofields, slow variables) are not significant at the microscale, where these fields appear to be locally constant, and can be described in terms of uniform applied or far field strains, stresses, temperature gradients or heat fluxes.

Formally, this splitting can be written as:

$$\begin{aligned}\boldsymbol{\varepsilon}(\mathbf{x}) &= \langle \boldsymbol{\varepsilon} \rangle + \boldsymbol{\varepsilon}'(\mathbf{x}) & \mathbf{d}(\mathbf{x}) &= \langle \mathbf{d} \rangle + \mathbf{d}'(\mathbf{x}) \\ \boldsymbol{\sigma}(\mathbf{x}) &= \langle \boldsymbol{\sigma} \rangle + \boldsymbol{\sigma}'(\mathbf{x}) & \mathbf{q}(\mathbf{x}) &= \langle \mathbf{q} \rangle + \mathbf{q}'(\mathbf{x})\end{aligned}\tag{3.2}$$

where $\langle \boldsymbol{\varepsilon} \rangle$, $\langle \boldsymbol{\sigma} \rangle$, $\langle \mathbf{d} \rangle$ and $\langle \mathbf{q} \rangle$ are the macroscopic fields, and $\boldsymbol{\varepsilon}'$, $\boldsymbol{\sigma}'$, $\mathbf{d}'$ and $\mathbf{q}'$ denote the microscopic fluctuations.

The term “composite” is used in this thesis whenever the microtopology of the inhomogeneous material is of the matrix-inclusion type.

For different homogenization methods that can be used when the above conditions are not fulfilled (e.g. marked compositional or load gradients, insufficiently separated length scales, ...), see e.g. [56; 93].

3.1.2 Homogenization and localization

For any region of an inhomogeneous material the microscopic fields and the macroscopic response can be linked by localization relations of the type:

$$\begin{aligned}\boldsymbol{\varepsilon}(\mathbf{x}) &= \mathbf{A}(\mathbf{x}) \langle \boldsymbol{\varepsilon} \rangle & \mathbf{d}(\mathbf{x}) &= \mathcal{A}(\mathbf{x}) \langle \mathbf{d} \rangle \\ \boldsymbol{\sigma}(\mathbf{x}) &= \mathbf{B}(\mathbf{x}) \langle \boldsymbol{\sigma} \rangle & \mathbf{q}(\mathbf{x}) &= \mathcal{B}(\mathbf{x}) \langle \mathbf{q} \rangle\end{aligned}\tag{3.3}$$

where $\mathbf{A}$, $\mathbf{B}$, $\mathcal{A}$ and $\mathcal{B}$ are the mechanical strain, mechanical stress, thermal gradient and heat flux concentration tensors. The above equations are directly applicable only for linear elastic and steady state heat conduction behaviour, respectively. Nevertheless, equations (3.3) can be modified to cover thermoelastic behaviour, compare equations (3.17).

If, in addition, the region is sufficiently large and contains no significant macroscopic gradients of strain, stress, temperature, heat fluxes or composition, homogenization relations can be defined as:

$$\begin{aligned}\langle \boldsymbol{\varepsilon} \rangle &= \frac{1}{v} \int_v \boldsymbol{\varepsilon}(\mathbf{x}) \, dv & \langle \mathbf{d} \rangle &= \frac{1}{v} \int_v \mathbf{d}(\mathbf{x}) \, dv \\ \langle \boldsymbol{\sigma} \rangle &= \frac{1}{v} \int_v \boldsymbol{\sigma}(\mathbf{x}) \, dv & \langle \mathbf{q} \rangle &= \frac{1}{v} \int_v \mathbf{q}(\mathbf{x}) \, dv\end{aligned}\tag{3.4}$$

where v stands for the volume of the region under consideration.

For perfectly bonded constituents and in the absence of cracks the divergence theorem can be applied to equations (3.4). In this case the mean strains and stresses in v are fully determined by the surface displacements and tractions, and the mean temperature gradients and heat fluxes are determined by the surface temperatures and the normal components of the heat fluxes at the surface.

For inhomogeneous materials that show sufficient separation between the macro- and micro-scales the relation:

$$\int_v [\boldsymbol{\sigma}^*(\mathbf{x})]^T \boldsymbol{\varepsilon}^*(\mathbf{x}) dv = \int_v [\boldsymbol{\sigma}^*(\mathbf{x})]^T dv \int_v \boldsymbol{\varepsilon}^*(\mathbf{x}) dv \quad (3.5)$$

can be shown to hold for general admissible stress fields, $\boldsymbol{\sigma}^*$, and kinematically admissible strain fields, $\boldsymbol{\varepsilon}^*$. This equation is known as Hill's macrohomogeneity condition or the Mandel-Hill condition, see [83]. For the special case of homogeneous stress and strain boundary conditions, it is referred as Hill's lemma. So, homogenization can be interpreted as finding a homogeneous comparison material that is energetically equivalent to a given microstructured material. Hill's lemma represents one of the basic principles in homogenization of statistically homogeneous and ergodic random and periodic materials [77]. Hill's condition can be extended to heat conduction, see [90]:

$$\int_v [\mathbf{q}^*(\mathbf{x})]^T \mathbf{d}^*(\mathbf{x}) dv = \int_v [\mathbf{q}^*(\mathbf{x})]^T dv \int_v \mathbf{d}^*(\mathbf{x}) dv \quad (3.6)$$

Note that for the heat conduction case, the equation does not have energy units.

The microgeometries of real inhomogeneous materials are usually highly complex. Accordingly, exact expressions for most of the terms in the previous equations cannot realistically be provided and approximations have to be introduced. Typically, the inhomogeneous material is assumed to be statistically homogeneous. Thus, sufficiently large subvolumes selected randomly within a sample are taken to give rise to the same averaged material properties which, in turn, correspond to the overall or effective material properties.

Ideally, the homogenization volume should be chosen to be a proper representative volume element (RVE), a subvolume of the sample that is statistically representative of the microgeometry of the material. Such a volume element must be sufficiently large to allow a meaningful sampling of the microfields and sufficiently small for the influence of macroscopic gradients to be negligible and for an analysis of the microfields to be possible.

3.1.3 Overall behaviour, material symmetries

The homogenized fields in an inhomogeneous material obtained with the previous equations can be linked by effective compliance, $\mathbf{C}^*$, elasticity, $\mathbf{E}^*$, resistivity, $\mathcal{R}^*$, and conductivity,

$\mathcal{K}^*$, tensors:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle &= \mathbf{C}^* \langle \boldsymbol{\sigma} \rangle & \langle \mathbf{d} \rangle &= -\mathcal{R}^* \langle \mathbf{q} \rangle \\ \langle \boldsymbol{\sigma} \rangle &= \mathbf{E}^* \langle \boldsymbol{\varepsilon} \rangle & \langle \mathbf{q} \rangle &= -\mathcal{K}^* \langle \mathbf{d} \rangle \end{aligned} \quad (3.7)$$

These tensors, the effective tensors, may be viewed as the elastic or thermal conduction tensors of an appropriate equivalent homogeneous material.

The resulting homogenized behaviour of many multiphase materials can be idealized as being statistically isotropic, or statistically transversely isotropic. Thus, effective elastic and thermal conduction tensors have the same restrictions as the elastic and thermal conduction tensors of homogeneous materials for the same symmetries. For example, if the inhomogeneous material is considered as statistically isotropic, the elastic tensor can be described with two independent parameters, and one is required for the effective thermal conduction behaviour in the linear range (recall that the elastic and thermal conduction tensors have different ranks).

3.1.4 Basic modeling strategies in continuum micromechanics of materials

Homogenization procedures aim at finding a volume element's responses to prescribed thermomechanical or thermal loads and at deducing from them the corresponding overall properties. The most straightforward applications of such studies are materials characterization and constitutive models. Besides materials characterization and constitutive modeling, there are a number of other important applications like the study of local phenomena in inhomogeneous materials, such as the initiation and evolution of microscopic damage, the nucleation and growth of cracks, hot spots, the stresses at intersections between macroscopic interfaces and free surfaces... For the latter behaviours, details of the microstructure tend to be of major importance. Because for realistic phase distributions the analysis of the spatial variations of the microfields in sufficiently large reference volumes tends to be beyond present capabilities, approximations have to be used. The available models can be treated as falling into two groups. The first of them comprises methods that describe the microgeometries of inhomogeneous materials on the basis of statistical information:

- Mean Field Approaches (MFAs): The microfields within each constituent are approximated by their phase averages $\langle \boldsymbol{\varepsilon} \rangle^{(p)}$, $\langle \boldsymbol{\sigma} \rangle^{(p)}$, $\langle \mathbf{d} \rangle^{(p)}$ and $\langle \mathbf{q} \rangle^{(p)}$. Such descriptions typically use information on the microscopic topology, microscopic geometry (volume

fraction) and microscopic symmetry. Mean field approaches tend to be formulated in terms of the phase concentration tensors, they pose relatively low computational requirements, and they have been highly successful in describing the thermoelastic and thermal conduction response of inhomogeneous materials.

- **Variational Bounding Methods:** Variational principles are used to obtain upper and, in many cases, lower bounds on the overall physical properties of inhomogeneous materials, e.g., elastic bulk and shear moduli or thermal conductivities. Bounds, aside of their intrinsic interest, are important tools for assessing other models of inhomogeneous materials.

The second group of approximations is based on studying discrete microstructures and includes:

- **Periodic Microfield Approaches (PMAs) or Unit Cell Methods:** The real inhomogeneous material is approximated by an infinitely extended model material with a periodic phase arrangement. The corresponding periodic microfields are usually evaluated by analyzing unit cells via analytical or numerical methods. Unit cells are typically used for performing characterization of inhomogeneous materials in the non-linear range, but they can also be employed as micromechanically based constitutive models. The high resolution of the microfields provided by PMAs can be very useful for studying the initiation of microdamage on the microscale. However, they are not well suited for investigating macroscopic cracks. Periodic microfield approaches can give detailed information on the local strain, stress, thermal gradient and heat flux fields within a given unit cell, but they tend to be computationally expensive.
- **Embedded Cell Approaches (ECAs):** The real inhomogeneous material is approximated by a model that consists of a core containing a discrete phase arrangement that is embedded within some outer region to which far field loads, displacements or temperatures are applied. ECAs can be used for materials characterization, and they are usually the best choice for studying regions of special interest, such as crack tips and their surroundings, in inhomogeneous materials or for studying the heat conduction behaviour of inhomogeneous materials with temperature dependent properties. Like PMAs, ECAs can resolve local fields in the core region at high detail, but tend to be computational expensive.
- **Windowing approaches:** Rectangular or hexahedral subregions are chosen from a given phase arrangement and subjected to macrohomogeneous boundary conditions

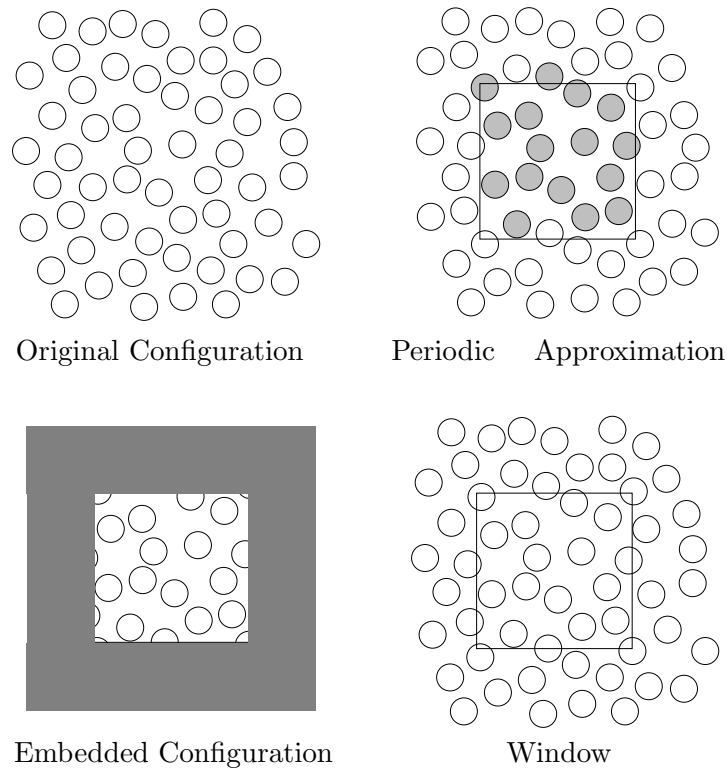


Figure 3.1: Representation of a hypothetical microstructure, and the modified microgeometries used to model it by PMA, ECA and windowing approaches.[18]

to obtain estimates as well as lower and upper bounds for the overall behaviour of the material. Homogeneous strain and stress boundary conditions are applied to obtain lower and upper estimates on the mechanical behaviour, and homogeneous temperature gradient and heat flux boundary conditions are applied to obtain lower and upper estimates on the thermal conduction behaviour. Bounds can be obtained by ensemble averaging. Mixed uniform boundary conditions can be applied, too, to obtain estimates of the macroscopic behaviour of the material, see [86; 123].

Schematic representations of the different discrete microstructure approximations are given in fig. 3.1. For studying materials that are inhomogeneous at a number of length scales, hierarchical procedures that use homogenization at more than one level are a natural extension of the above concepts.

3.2 Analytical and Semianalytical Approaches

In this section some approaches belonging to the first group of methods listed in section 3.1.4 are discussed. The description is not a review of all pertinent methods in the literature, and only some methods of interest for studying the problems outlined in the introduction are covered. For a more thorough description see e.g. [17; 18] and the references therein. The present treatment is divided into three parts, the first one reviews classical methods, whereas the second and the third parts discuss more specific methods for studying the thermo-elastoplastic behaviour of metal matrix composites, which may be used in the divertor of a nuclear reactor, see section 1.1.1, and the thermal conduction behaviour of DRMMCs, see section 1.1.2, respectively.

The volume fraction of any phase is defined as:

$$f^{(p)} = \frac{v^{(p)}}{\sum_{(k)} v^{(k)}} \quad (3.8)$$

where k is an index that represents all the phases and $v^{(k)}$ is the volume pertinent to phase k . For the special case of matrix-inclusion topologies with only one type of inclusion, the superscript ⁽ⁱ⁾ refers to the inclusion, and the superscript ^(m) to the matrix. For this case the convention:

$$\begin{aligned} f^{(i)} &= f \\ f^{(m)} &= 1 - f \end{aligned} \quad (3.9)$$

is used.

3.2.1 General approaches for linear elasticity and steady state heat conduction

In this section only two-phase materials are covered explicitly, with the exception of multiphase Mori–Tanaka methods, section 3.2.1.2.3, and some variational bounds in section 3.2.1.3. Nevertheless, most of the methods may be extended to multiphase composites without difficulty. Perfect bonding between phases is assumed. For mechanical problems the material behaviour of all the phases is taken to be linear thermo-elastic, and for heat transfer problems linear conductivity is assumed.

3.2.1.1 Classical Approaches

The rules of mixture (ROM) are probably the best known classical approach. They produce estimates for some scalar effective physical property, a^* , of a two phase composite from the phase values of this property and the volume fractions of the composite. In the general case they take the form:

$$a^* = \left[f (a^{(i)})^b + (1 - f) (a^{(m)})^b \right]^{1/b} \quad (3.10)$$

The ROM do not contain any information on the microtopology of the material studied and therefore their results may be inaccurate in many situations. Furthermore, there is no clear physical interpretation for cases with $b \neq \{-1, 1\}$. Nevertheless, for some microtopologies the rules of mixture can successfully describe some macroscopic properties.

For mechanical properties, the ROM have been widely used to estimate the Young's modulus in longitudinal direction (fiber direction), $E^*(1, 1)$, and transverse direction, $E^*(2, 2)$, of long-fiber reinforced composites. These are the well known Voigt and Reuss estimates:

$$\begin{aligned} E^*(1, 1) &= f E^{(i)}(1, 1) + (1 - f) E^{(m)}(1, 1) \\ E^*(2, 2) &= \frac{E^{(i)}(2, 2) E^{(m)}(2, 2)}{f E^{(i)}(2, 2) + (1 - f) E^{(m)}(2, 2)} \end{aligned} \quad (3.11)$$

that are obtained by setting $b = 1$ and $b = -1$ in equation (3.10). Voigt expressions correspond to full strain coupling of the phases (springs in parallel), whilst Reuss expressions correspond to full stress coupling (springs in series), i.e. they describe the in plane and out-of-plane behaviour of layered materials the constituents of which have the same Poisson contractions. The Voigt rule is a good estimate for the axial stiffness of long fiber reinforced composites, but the Reuss model is not that accurate. Instead of it some other models have been used, see e.g. [66].

For heat conduction properties, the equivalents of Voigt and Reuss expressions can be used as well for long fiber reinforced composites, for estimating the thermal conductivity in fiber direction, $K^*(1, 1)$ and transverse direction, $K^*(2, 2)$:

$$\begin{aligned} K^*(1, 1) &= f K^{(i)}(1, 1) + (1 - f) K^{(m)}(1, 1) \\ K^*(2, 2) &= \frac{K^{(i)}(2, 2) K^{(m)}(2, 2)}{f K^{(i)}(2, 2) + (1 - f) K^{(m)}(2, 2)} \end{aligned} \quad (3.12)$$

which, in fact, are particular cases of the Wiener bounds, see section 3.2.1.3.1. Equations (3.12) give an excellent estimate for the thermal conductivity of long fiber reinforced composites in the direction of the fiber.

ROM can be used to generate effective elastic tensors and conductivity tensors. However, as they do not account for the relationship between the moduli, such procedures tend to lead to inconsistent results in the former case. A better approach that generates consistent elasticity tensors for unidirectionally reinforced composites is the Vanishing Fiber Diameter (VFD) model of Dvorak [49]. However, the VFD-model generally does not fulfill Hill's relationships for unidirectional long fiber reinforced composites, see [81]. The composite sphere assemblage (CSA) and the composite cylinder assemblage (CCA) give exact expressions for some effective elastic engineering moduli of special particle reinforced and aligned continuously reinforced composites, but the complete effective tensors cannot be generated with these approaches, see [67].

3.2.1.2 Mean Field Approaches

This section concentrates mainly on Mori-Tanaka methods, which may be viewed as the simplest mean field approaches for inhomogeneous materials that encompass the full physical range of phase volume fractions. Additionally, some other mean field methods such as the differential scheme are described.

It is assumed that the inclusions are distributed homogeneously in the matrix. Equations are derived for aligned ellipsoidal inclusions. Approximations for using Mean-Field methods with non-ellipsoidal inclusions are described in detail in section 3.2.2.2.

3.2.1.2.1 General relations For linear materials the overall strain-stress and thermal gradient-heat flux relations can be denoted in the form:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle &= \mathbf{C}^* \langle \boldsymbol{\sigma} \rangle + \boldsymbol{\alpha}^* \Delta t & \langle \mathbf{d} \rangle &= -\mathcal{R}^* \langle \mathbf{q} \rangle \\ \langle \boldsymbol{\sigma} \rangle &= \mathbf{E}^* \langle \boldsymbol{\varepsilon} \rangle + \boldsymbol{\omega}^* \Delta t & \langle \mathbf{q} \rangle &= -\mathcal{K}^* \langle \mathbf{d} \rangle \end{aligned} \quad (3.13)$$

where Δt is a temperature increment with respect to a stress free temperature, and $\boldsymbol{\alpha}^*$, $\boldsymbol{\omega}^*$ are the overall coefficient of thermal expansion tensor and the overall specific thermal stress

tensor, respectively. The overall specific thermal stress tensor gives the overall response of the fully constrained material to a purely thermal unit load, $\boldsymbol{\omega}^* = -\mathbf{E}^* \boldsymbol{\alpha}^*$. The constituents are also taken to behave linearly:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle^{(p)} &= \mathbf{C}^{(p)} \langle \boldsymbol{\sigma} \rangle^{(p)} + \boldsymbol{\alpha}^{(p)} \Delta t & \langle \mathbf{d} \rangle^{(p)} &= -\mathcal{R}^{(p)} \langle \mathbf{d} \rangle^{(p)} \\ \langle \boldsymbol{\sigma} \rangle^{(p)} &= \mathbf{E}^{(p)} \langle \boldsymbol{\varepsilon} \rangle^{(p)} + \boldsymbol{\omega}^{(p)} \Delta t & \langle \mathbf{q} \rangle^{(p)} &= -\mathcal{K}^{(p)} \langle \mathbf{q} \rangle^{(p)} \end{aligned} \quad (3.14)$$

where the subscript $^{(p)}$ represents either the matrix, $^{(m)}$, or the inclusion, $^{(i)}$.

When the microfields within each constituent are approximated by their phase averages, the homogenization relations for each phase become:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle^{(p)} &= \frac{1}{v^{(p)}} \int_{v^{(p)}} \boldsymbol{\varepsilon}(\mathbf{x}) dv & \langle \mathbf{d} \rangle^{(p)} &= \frac{1}{v^{(p)}} \int_{v^{(p)}} \mathbf{d}(\mathbf{x}) dv \\ \langle \boldsymbol{\sigma} \rangle^{(p)} &= \frac{1}{v^{(p)}} \int_{v^{(p)}} \boldsymbol{\sigma}(\mathbf{x}) dv & \langle \mathbf{q} \rangle^{(p)} &= \frac{1}{v^{(p)}} \int_{v^{(p)}} \mathbf{q}(\mathbf{x}) dv \end{aligned} \quad (3.15)$$

From the definition of volume averaging, equation (3.4), and equation (3.15), one obtains the following relations:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle &= f \langle \boldsymbol{\varepsilon} \rangle^{(i)} + (1-f) \langle \boldsymbol{\varepsilon} \rangle^{(m)} = \boldsymbol{\varepsilon}_a & \langle \mathbf{d} \rangle &= f \langle \mathbf{d} \rangle^{(i)} + (1-f) \langle \mathbf{d} \rangle^{(m)} = \mathbf{d}_a \\ \langle \boldsymbol{\sigma} \rangle &= f \langle \boldsymbol{\sigma} \rangle^{(i)} + (1-f) \langle \boldsymbol{\sigma} \rangle^{(m)} = \boldsymbol{\sigma}_a & \langle \mathbf{q} \rangle &= f \langle \mathbf{q} \rangle^{(i)} + (1-f) \langle \mathbf{q} \rangle^{(m)} = \mathbf{q}_a \end{aligned} \quad (3.16)$$

where $\boldsymbol{\varepsilon}_a$, $\boldsymbol{\sigma}_a$, $\mathbf{d}_a$ and $\mathbf{q}_a$ are the applied (far field) strain, stress, temperature gradient and heat flux. These equations hold provided no displacement jumps are present in the composite. For the heat conduction case, interfacial temperature jumps are studied in section 3.3.2.2.3.

The phase averaged fields can be related to the overall fields by concentration tensors, so that:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle^{(p)} &= \bar{\mathbf{A}}^{(p)} \langle \boldsymbol{\varepsilon} \rangle + \bar{\boldsymbol{\iota}}^{(p)} \Delta t & \langle \mathbf{d} \rangle^{(p)} &= \bar{\mathcal{A}}^{(p)} \langle \mathbf{d} \rangle \\ \langle \boldsymbol{\sigma} \rangle^{(p)} &= \bar{\mathbf{B}}^{(p)} \langle \boldsymbol{\sigma} \rangle + \bar{\boldsymbol{\theta}}^{(p)} \Delta t & \langle \mathbf{q} \rangle^{(p)} &= \bar{\mathcal{B}}^{(p)} \langle \mathbf{q} \rangle \end{aligned} \quad (3.17)$$

where $\bar{\mathbf{A}}^{(p)}$, $\bar{\boldsymbol{\iota}}^{(p)}$, $\bar{\mathbf{B}}^{(p)}$ and $\bar{\boldsymbol{\theta}}^{(p)}$ are the elastic and thermal phase strain and stress concentration tensors, and $\bar{\mathcal{A}}^{(p)}$ and $\bar{\mathcal{B}}^{(p)}$ are the phase temperature gradient and heat flux concentration tensors. Recall that in MFAs the microfields within each phase are approximated by their phase averages and therefore the concentration tensors are not position dependent within each phase. Combining equations (3.16) and (3.17), the following equations are

obtained:

$$\begin{aligned}
 f \bar{\mathbf{A}}^{(i)} + (1-f) \bar{\mathbf{A}}^{(m)} &= \mathbf{1}^s \\
 f \bar{\mathbf{B}}^{(i)} + (1-f) \bar{\mathbf{B}}^{(m)} &= \mathbf{1}^s & f \bar{\mathcal{A}}^{(i)} + (1-f) \bar{\mathcal{A}}^{(m)} &= \mathcal{I} \\
 f \bar{\boldsymbol{\epsilon}}^{(i)} + (1-f) \bar{\boldsymbol{\epsilon}}^{(m)} &= \mathcal{O} & f \bar{\boldsymbol{\beta}}^{(i)} + (1-f) \bar{\boldsymbol{\beta}}^{(m)} &= \mathcal{I} \\
 f \bar{\boldsymbol{\theta}}^{(i)} + (1-f) \bar{\boldsymbol{\theta}}^{(m)} &= \mathcal{O}
 \end{aligned} \tag{3.18}$$

where $\mathcal{O}$ is the second order zero tensor. These equations show that the concentration tensors of matrix and inclusions are not independent. Thus, if the strain or thermal gradient concentration tensor of the matrix is known, the strain or thermal gradient concentration tensor of the inclusions is known, too, and vice versa.

Combining equations (3.4) with the definition of concentration tensors for mean field methods (3.17), it is easy to obtain the effective elastic or thermal conductivity tensors of the composite as:

$$\begin{aligned}
 \mathbf{C}^* &= f \mathbf{C}^{(i)} \bar{\mathbf{B}}^{(i)} + (1-f) \mathbf{C}^{(m)} \bar{\mathbf{B}}^{(m)} & \mathcal{R}^* &= f \mathcal{R}^{(i)} \bar{\boldsymbol{\beta}}^{(i)} + (1-f) \mathcal{R}^{(m)} \bar{\boldsymbol{\beta}}^{(m)} \\
 \mathbf{E}^* &= f \mathbf{E}^{(i)} \bar{\mathbf{A}}^{(i)} + (1-f) \mathbf{E}^{(m)} \bar{\mathbf{A}}^{(m)} & \mathcal{K}^* &= f \mathcal{K}^{(i)} \bar{\mathcal{A}}^{(i)} + (1-f) \mathcal{K}^{(m)} \bar{\mathcal{A}}^{(m)}
 \end{aligned} \tag{3.19}$$

The effective thermal expansion coefficient tensor and the effective thermal stress tensor can be written as:

$$\boldsymbol{\alpha}^* = f \left(\mathbf{C}^{(i)} \bar{\boldsymbol{\theta}}^{(i)} + \boldsymbol{\alpha}^{(i)} \right) + (1-f) \left(\mathbf{C}^{(m)} \bar{\boldsymbol{\theta}}^{(m)} + \boldsymbol{\alpha}^{(m)} \right) \tag{3.20}$$

$$\boldsymbol{\omega}^* = f \left(\mathbf{E}^{(i)} \bar{\boldsymbol{\epsilon}}^{(i)} + \boldsymbol{\omega}^{(i)} \right) + (1-f) \left(\mathbf{E}^{(m)} \bar{\boldsymbol{\epsilon}}^{(m)} + \boldsymbol{\omega}^{(m)} \right) \tag{3.21}$$

The overall coefficients of thermal expansion can be obtained, too, using the Mandel-Levin formula [100]:

$$\boldsymbol{\alpha}^* = (1-f) [\bar{\mathbf{B}}^{(m)}]^T \boldsymbol{\alpha}^{(m)} + f [\bar{\mathbf{B}}^{(i)}]^T \boldsymbol{\alpha}^{(i)} \tag{3.22}$$

Furthermore the following relationships can be found, see e.g. [17]:

$$\begin{aligned}
 \bar{\mathbf{A}}^{(m)} &= \mathbf{C}^{(m)} \bar{\mathbf{B}}^{(m)} \mathbf{E}^* & \bar{\mathcal{A}}^{(m)} &= \mathcal{R}^{(m)} \bar{\boldsymbol{\beta}}^{(m)} \mathcal{K}^* \\
 \bar{\mathbf{B}}^{(m)} &= \mathbf{E}^{(m)} \bar{\mathbf{A}}^{(m)} \mathbf{C}^* & \bar{\boldsymbol{\beta}}^{(m)} &= \mathcal{K}^{(m)} \bar{\mathcal{A}}^{(m)} \mathcal{R}^*
 \end{aligned} \tag{3.23}$$

Expressions connecting the thermal strain and stress concentration tensors of a given phase with the elastic strain and stress concentration tensors can be found e.g. in [13]:

$$\bar{\boldsymbol{\epsilon}}^{(m)} = (\mathbf{1}^s - \bar{\mathbf{A}}^{(m)}) (\mathbf{E}^{(i)} - \mathbf{E}^{(m)})^{-1} (\boldsymbol{\omega}^{(m)} - \boldsymbol{\omega}^{(i)}) \tag{3.24}$$

$$\bar{\boldsymbol{\theta}}^{(m)} = (\mathbf{1}^s - \bar{\mathbf{B}}^{(m)}) (\mathbf{C}^{(i)} - \mathbf{C}^{(m)})^{-1} (\boldsymbol{\alpha}^{(m)} - \boldsymbol{\alpha}^{(i)}) \tag{3.25}$$

From equations (3.18 – 3.25) is obvious that the full thermoelastic behaviour of two-phase inhomogeneous materials is fully described by the knowledge of one elastic phase concentration tensor and that the thermal conduction behaviour is fully described by the knowledge of one thermal conduction phase concentration tensor.

3.2.1.2.2 Eshelby tensor and dilute matrix-inclusion composites A large proportion of the mean field descriptions used in continuum micromechanics of materials are based on the work of Eshelby [51], who studied the stress and strain distributions in a homogeneous medium containing a subregion (inclusion) that spontaneously changes its shape and/or size so that it no longer fits into its previous space in the parent medium. Eshelby's results show that if an elastic homogeneous ellipsoidal inclusion in an infinite linear elastic matrix is subjected to a uniform strain $\boldsymbol{\varepsilon}_t$ (called the stress-free strain, unconstrained strain, eigenstrain, or transformation strain), a uniform strain, $\boldsymbol{\varepsilon}_c$, is induced in the constrained inclusion (the constrained strain) which is related to the stress-free strain, $\boldsymbol{\varepsilon}_t$, by the expression:

$$\boldsymbol{\varepsilon}_c = \mathbf{S}\boldsymbol{\varepsilon}_t \quad (3.26)$$

where $\mathbf{S}$ is called the Eshelby tensor. For this equation to hold, the stress-free strain may be any kind of eigenstrain which is uniform over the inclusion.

For mean field descriptions of dilute matrix-inclusion composites it is the stress and strain fields of inhomogeneous inclusions embedded in a matrix that are of interest. Such cases can be handled by introducing the concept of equivalent homogeneous inclusions. This process can be visualized as consisting of cutting and welding operations as shown in fig. 3.2. The concept of an equivalent homogeneous inclusion can be extended to cases where a uniform mechanical strain or external stress is applied to a perfectly bonded inhomogeneous inclusion in an infinite matrix. It allows dilute stress and strain concentration tensors to be evaluated as [82]:

$$\bar{\mathbf{A}}_{\text{dil}}^{(i)} = [\mathbf{1}^s + \mathbf{S}\mathbf{C}^{(m)} (\mathbf{E}^{(i)} - \mathbf{E}^{(m)})]^{-1} \quad (3.27)$$

$$\bar{\mathbf{B}}_{\text{dil}}^{(i)} = [\mathbf{1}^s + \mathbf{E}^{(m)} (\mathbf{1}^s - \mathbf{S}) (\mathbf{C}^{(i)} - \mathbf{C}^{(m)})]^{-1} \quad (3.28)$$

Expressions of this type are derived under the hypothesis that the inclusions are dilutely dispersed in the matrix and thus do not feel any effects due to their neighbors. Accordingly, they are independent of the phase volume fractions. It must be kept in mind, however,

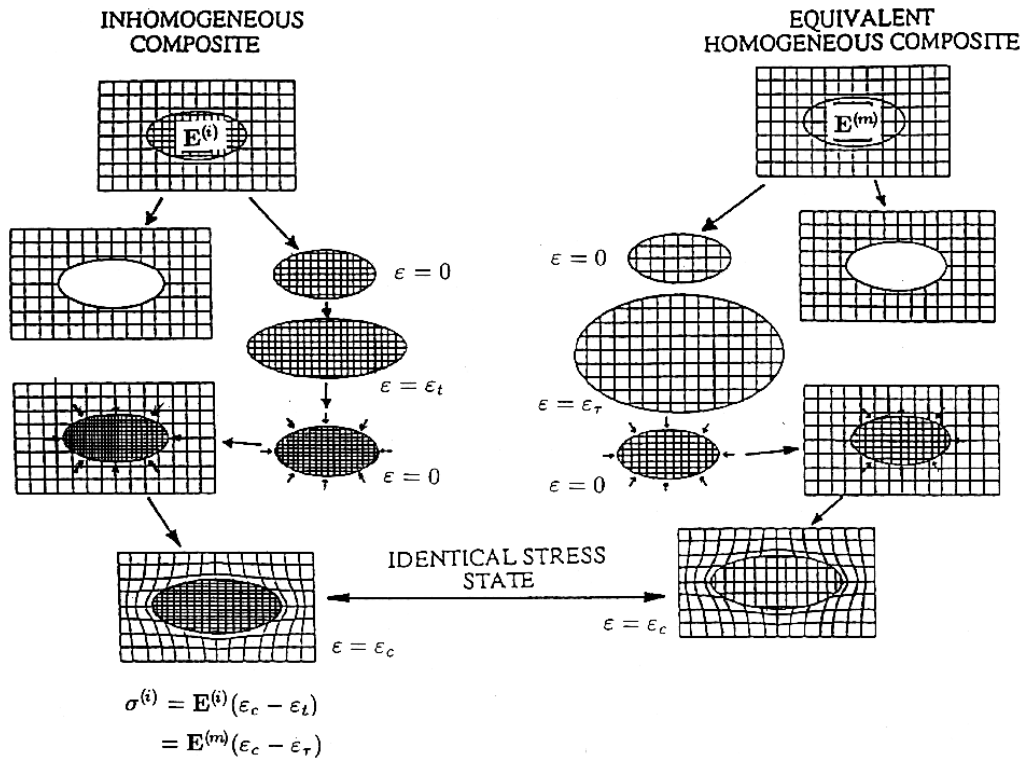


Figure 3.2: Equivalent inclusion procedure [33].

that the dilute expressions are strictly valid only for vanishingly small inclusion volume fractions and should be used only for $f \ll 0.1$.

The Eshelby tensor, $\mathbf{S}$, depends only on the material properties of the matrix and on the aspect ratio of the inclusions. Expressions for the Eshelby tensor of spheroidal inclusions embedded in an isotropic matrix can be found e.g. in [115; 124; 146]. Closed form expressions for the Eshelby tensor have also been reported for spheroidal inclusions in a matrix of transversely isotropic [163] or cubic [115] material symmetry. For other matrix symmetries where no analytical formula is available, the Eshelby tensor can be computed numerically, see [60].

The Eshelby's concept can be extended for studying effective transport properties in homogeneous materials such as steady state heat conduction, see [75]. In analogy to eqns. (3.27)–(3.28), the dilute temperature gradient and heat flux concentration tensors can be obtained as:

$$\begin{aligned}\bar{\mathcal{A}}_{\text{dil}}^{(i)} &= [\mathcal{I} + \mathcal{S}\mathcal{R}^{(m)} (\mathcal{K}^{(i)} - \mathcal{K}^{(m)})]^{-1} \\ \bar{\mathcal{B}}_{\text{dil}}^{(i)} &= [\mathcal{I} + \mathcal{K}^{(m)} (\mathcal{I} - \mathcal{S}) (\mathcal{R}^{(i)} - \mathcal{R}^{(m)})]^{-1}\end{aligned}\tag{3.29}$$

where $\mathcal{S}$ is the Eshelby tensor for the thermal conduction problem. Expressions for $\mathcal{S}$ for the case of ellipsoidal particles embedded in an isotropic matrix are collected in appendix B, see [75; 91] for details. For this case, in contrast to elasticity, the Eshelby tensor for heat conduction depends only on the shape of the reinforcement and not on the properties of the matrix. For other cases, numerical integration in analogy to the elastic case, [60], may be used.

It is well known that the Eshelby property holds only for ellipsoidal inclusions [99]. As a consequence, the Eshelby tensor and dilute concentration tensors are position dependent within non-ellipsoidal inclusions. Analytical solutions are available only for some non-ellipsoidal inclusion shapes, see [115]. One straightforward solution for overcoming this problem is the use of averaged Eshelby or dilute inclusion concentration tensors, recall that these approaches are not equivalent. Averaged replacement concentration tensors can be obtained by setting up numerical models with a single dilute inhomogeneity, generating solutions for six, in elasticity, or 3, in heat conduction, linearly independent load cases. For details see section 3.2.2.2.

Theoretical descriptions of the overall behaviour of composites with inclusion volume fractions of more than a few percent must explicitly account for the interaction between

inclusions. These interactions give rise to inhomogeneous fields within each inhomogeneity (intra-phase fluctuations), and they cause the levels of averaged fields in individual inhomogeneities to differ (inter-phase fluctuations). Inhomogeneous fields are present in the matrix even at dilute reinforcement fractions [52]. There are a number of approximations in the literature, the most important of which are effective field approaches, such as Mori-Tanaka methods, and effective medium approaches, such as self-consistent and differential schemes. These methods account for the intra-phase and inter-phase interactions in an averaged (mean field) sense.

3.2.1.2.3 Mori-Tanaka Estimates One way of accounting for the inter- and intra-phase interactions consists of approximating the stresses or heat fluxes acting on an inclusion, which may be viewed as the perturbation stresses or heat fluxes caused by the presence of other inclusions superimposed on the applied far field stress or heat flux, by an appropriate average matrix stress or heat flux. Effective field theories of this type are generically called Mori-Tanaka methods or, for the elastic case, “Equivalent Inclusion Average Stress” (EIAS) approaches. The idea of combining the average-stress field in the matrix with the Eshelby theory can already be found in the works of Brown [24] and Mori and Tanaka [113].

The central assumption involved in Mori-Tanaka approaches can be denoted for the isothermal elastic and the steady heat conduction problems as [11]:

$$\begin{aligned} \langle \boldsymbol{\varepsilon} \rangle^{(i)} &= \bar{\mathbf{A}}_{\text{dil}}^{(i)} \langle \boldsymbol{\varepsilon} \rangle^{(m)} = \bar{\mathbf{A}}_{\text{dil}}^{(i)} \bar{\mathbf{A}}_{\text{M}}^{(m)} \langle \boldsymbol{\varepsilon} \rangle & \langle \mathbf{d} \rangle^{(i)} &= \bar{\mathcal{A}}_{\text{dil}}^{(i)} \langle \mathbf{d} \rangle^{(m)} = \bar{\mathcal{A}}_{\text{dil}}^{(i)} \bar{\mathcal{A}}_{\text{M}}^{(m)} \langle \mathbf{d} \rangle \\ \langle \boldsymbol{\sigma} \rangle^{(i)} &= \bar{\mathbf{B}}_{\text{dil}}^{(i)} \langle \boldsymbol{\sigma} \rangle^{(m)} = \bar{\mathbf{B}}_{\text{dil}}^{(i)} \bar{\mathbf{B}}_{\text{M}}^{(m)} \langle \boldsymbol{\sigma} \rangle & \langle \mathbf{q} \rangle^{(i)} &= \bar{\mathcal{B}}_{\text{dil}}^{(i)} \langle \mathbf{q} \rangle^{(m)} = \bar{\mathcal{B}}_{\text{dil}}^{(i)} \bar{\mathcal{B}}_{\text{M}}^{(m)} \langle \mathbf{q} \rangle \end{aligned} \quad (3.30)$$

where the concentration tensors with the subscript M are the so called Mori-Tanaka concentration tensors. These equations can be viewed as modifications of equations (3.3), in which the applied fields are replaced by the unknown matrix fields according to the Mori-Tanaka strategy.

Very simple and straightforward Mori-Tanaka-type expressions for the matrix concentration tensors follow from equations (3.16) and (3.30):

$$\begin{aligned} \bar{\mathbf{A}}_{\text{M}}^{(m)} &= \left[(1-f) \mathbf{1}^s + f \bar{\mathbf{A}}_{\text{dil}}^{(i)} \right]^{-1} & \bar{\mathcal{A}}_{\text{M}}^{(m)} &= \left[(1-f) \mathcal{I} + f \bar{\mathcal{A}}_{\text{dil}}^{(i)} \right]^{-1} \\ \bar{\mathbf{B}}_{\text{M}}^{(m)} &= \left[(1-f) \mathbf{1}^s + f \bar{\mathbf{B}}_{\text{dil}}^{(i)} \right]^{-1} & \bar{\mathcal{B}}_{\text{M}}^{(m)} &= \left[(1-f) \mathcal{I} + f \bar{\mathcal{B}}_{\text{dil}}^{(i)} \right]^{-1} \end{aligned} \quad (3.31)$$

The corresponding relations for the inclusion concentration tensors then follow from equation (3.30):

$$\begin{aligned}\bar{\mathbf{A}}_{\text{M}}^{(i)} &= \bar{\mathbf{A}}_{\text{dil}}^{(i)} \left[(1-f) \mathbf{1}^s + f \bar{\mathbf{A}}_{\text{dil}}^{(i)} \right]^{-1} & \bar{\mathcal{A}}_{\text{M}}^{(i)} &= \bar{\mathcal{A}}_{\text{dil}}^{(i)} \left[(1-f) \mathcal{I} + f \bar{\mathcal{A}}_{\text{dil}}^{(i)} \right]^{-1} \\ \bar{\mathbf{B}}_{\text{M}}^{(i)} &= \bar{\mathbf{B}}_{\text{dil}}^{(i)} \left[(1-f) \mathbf{1}^s + f \bar{\mathbf{B}}_{\text{dil}}^{(i)} \right]^{-1} & \bar{\mathcal{B}}_{\text{M}}^{(i)} &= \bar{\mathcal{B}}_{\text{dil}}^{(i)} \left[(1-f) \mathcal{I} + f \bar{\mathcal{B}}_{\text{dil}}^{(i)} \right]^{-1}\end{aligned}\quad (3.32)$$

By construction the Mori–Tanaka concentration tensors fulfill equations (3.18).

A number of authors gave different but essentially equivalent Mori–Tanaka-type expressions for the phase concentration tensors and effective elastic tensors of inhomogeneous materials, see e.g. [124; 147; 157]. Alternatively, the Mori–Tanaka method can be formulated to directly give the overall Mori–Tanaka elasticity, $\mathbf{E}_{\text{M}}^*$, [146] or conductivity tensor, $\mathcal{K}_{\text{M}}^*$, as:

$$\begin{aligned}\mathbf{E}_{\text{M}}^* &= \mathbf{E}^{(\text{m})} \left\{ \mathbf{1}^s - f \left[(\mathbf{E}^{(i)} - \mathbf{E}^{(\text{m})}) (\mathbf{S} - f (\mathbf{S} - \mathbf{1}^s)) + \mathbf{E}^{(\text{m})} \right]^{-1} [\mathbf{E}^{(i)} - \mathbf{E}^{(\text{m})}] \right\}^{-1} \\ \mathcal{K}_{\text{M}}^* &= \mathcal{K}^{(\text{m})} \left\{ \mathcal{I} - f \left[(\mathcal{K}^{(i)} - \mathcal{K}^{(\text{m})}) (\mathcal{S} - f (\mathcal{S} - \mathcal{I})) + \mathcal{K}^{(\text{m})} \right]^{-1} [\mathcal{K}^{(i)} - \mathcal{K}^{(\text{m})}] \right\}^{-1}\end{aligned}\quad (3.33)$$

In accordance with their derivation, Mori–Tanaka type theories at all volume fractions describe composites consisting of aligned ellipsoidal inclusions embedded in a matrix, compare fig. 3.3. Mori–Tanaka methods have been successfully “extended” for studying non-aligned composites, see e.g. [12; 45; 109; 127]. However, in some cases these methods may lead to unphysical results [55]. Mori–Tanaka methods can also be extended for studying elastoplastic composites or composites with imperfect interfaces, see sections 3.2.2 and 3.2.3. Mori–Tanaka methods do not have an intrinsic length scale, but this can be introduced through the material properties, see e.g. section 3.2.2.2. Mori–Tanaka methods can be extended to studying multi-phase materials, in this case equations (3.32) take the form:

$$\bar{\mathbf{A}}_{\text{M}}^{(\text{p})} = \bar{\mathbf{A}}_{\text{dil}}^{(\text{p})} \left[(f^{(\text{m})}) \mathbf{1}^s + \sum_{j=1}^N f^{(j)} \bar{\mathbf{A}}_{\text{dil}}^{(j)} \right]^{-1} \quad \bar{\mathcal{A}}_{\text{M}}^{(\text{p})} = \bar{\mathcal{A}}_{\text{dil}}^{(\text{p})} \left[(f^{(\text{m})}) \mathcal{I} + \sum_{j=1}^N f^{(j)} \bar{\mathcal{A}}_{\text{dil}}^{(j)} \right]^{-1} \quad (3.34)$$

and the effective elasticity or conductivity tensors can be written as:

$$\begin{aligned}\mathbf{E}_{\text{M}}^* &= \mathbf{E}^{(\text{m})} + \sum_{j=1}^N f^{(j)} (\mathbf{E}^{(j)} - \mathbf{E}^{(\text{m})}) \bar{\mathbf{A}}_{\text{M}}^{(j)} \\ \mathcal{K}_{\text{M}}^* &= \mathcal{K}^{(\text{m})} + \sum_{j=1}^N f^{(j)} (\mathcal{K}^{(j)} - \mathcal{K}^{(\text{m})}) \bar{\mathcal{A}}_{\text{M}}^{(j)}\end{aligned}\quad (3.35)$$

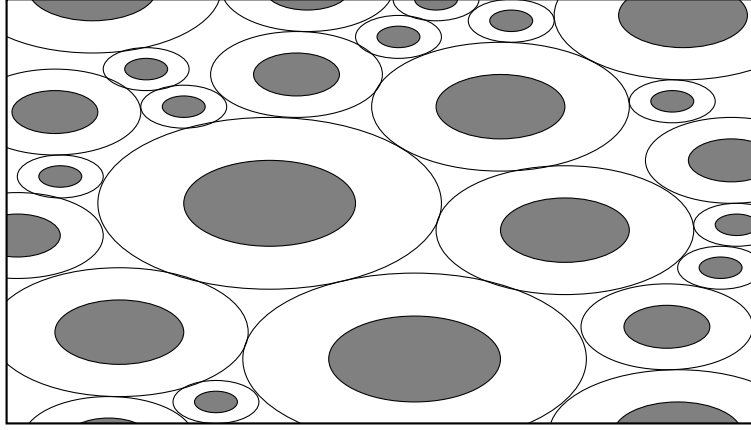


Figure 3.3: Example of aligned composite material described by Mori-Tanaka method.[18]

where the relationship $f^{(m)} + \sum_{j=1}^N f^{(j)} = 1$ holds.

Mori–Tanaka predictions for the overall elastic moduli of composites reinforced by stiff aligned or spherical reinforcements are stiffer than the matrix. In high contrast cases they tend to considerably underestimate the effective elastic properties of typical matrix–inclusion composites. Similarly, they tend to underpredict the macroscopic conductivities of composites reinforced with inclusions that have a higher conductivity than the matrix.

Mori-Tanaka type theories can be implemented into computer programs in a straightforward way. Because they are explicit algorithms, all that is required are matrix additions, multiplications, and inversions plus expressions for the Eshelby tensor. Together with their good accuracy this makes them important tools for evaluating the stiffness, thermal expansion and heat conduction properties of inhomogeneous materials that show a matrix–inclusion topology with aligned inclusions or voids.

3.2.1.2.4 Differential schemes The differential scheme, [104; 120], takes into account the interaction between inclusions by repeatedly adding a small concentration of inhomogeneities followed by homogenizing, the starting point being the pure matrix. Following [68], the overall tensors can be defined by the sets of differential equations:

$$\begin{aligned} \frac{d\mathbf{C}_D^*}{df} &= \frac{1}{(1-f)} (\mathbf{C}^{(i)} - \mathbf{C}_D^*) \bar{\mathbf{B}}_{\text{dil}}^{(i)} & \frac{d\mathcal{R}_D^*}{df} &= \frac{1}{(1-f)} (\mathcal{R}^{(i)} - \mathcal{R}_D^*) \bar{\mathcal{B}}_{\text{dil}}^{(i)} \\ \frac{d\mathbf{E}_D^*}{df} &= \frac{1}{(1-f)} (\mathbf{E}^{(i)} - \mathbf{E}_D^*) \bar{\mathbf{A}}_{\text{dil}}^{(i)} & \frac{d\mathcal{K}_D^*}{df} &= \frac{1}{(1-f)} (\mathcal{K}^{(i)} - \mathcal{K}_D^*) \bar{\mathcal{A}}_{\text{dil}}^{(i)} \end{aligned} \quad (3.36)$$

where the subscript $_{\text{D}}$ denotes the overall tensors evaluated according to the differential scheme. The initial conditions are $\mathbf{C}_{\text{D}}^* = \mathbf{C}^{(\text{m})}$ and $\mathbf{E}_{\text{D}}^* = \mathbf{E}^{(\text{m})}$ at $f = 0$ for the elastic case and $\mathcal{R}_{\text{D}}^* = \mathcal{R}^{(\text{m})}$ and $\mathcal{K}_{\text{D}}^* = \mathcal{K}^{(\text{m})}$ at $f = 0$ for the heat conduction case. Recall that the material is homogenized after every small addition of reinforcements and, therefore, at the beginning of each cycle, the effective “matrix” material is different. As a consequence, the Eshelby and the dilute concentration tensors are not constant and they must be recalculated. The dilute concentration tensors read

$$\begin{aligned} \bar{\mathbf{A}}_{\text{dil}}^{(\text{i})} &= [\mathbf{1}^{\text{s}} + \mathbf{S}_{\text{D}} \mathbf{C}_{\text{D}}^* (\mathbf{E}^{(\text{i})} - \mathbf{E}_{\text{D}}^*)]^{-1} & \bar{\mathcal{A}}_{\text{dil}}^{(\text{i})} &= [\mathcal{I} + \mathcal{S}_{\text{D}} \mathcal{R}_{\text{D}}^* (\mathcal{K}^{(\text{i})} - \mathcal{K}_{\text{D}}^*)]^{-1} \\ \bar{\mathbf{B}}_{\text{dil}}^{(\text{i})} &= [\mathbf{1}^{\text{s}} + \mathbf{E}_{\text{D}}^* (\mathbf{1}^{\text{s}} - \mathbf{S}_{\text{D}}) (\mathbf{C}^{(\text{i})} - \mathbf{C}_{\text{D}}^*)]^{-1} & \bar{\mathcal{B}}_{\text{dil}}^{(\text{i})} &= [\mathcal{I} + \mathcal{K}_{\text{D}}^* (\mathcal{I} - \mathcal{S}_{\text{D}}) (\mathcal{R}^{(\text{i})} - \mathcal{R}_{\text{D}}^*)]^{-1} \end{aligned} \quad (3.37)$$

in analogy to equation (3.28). Combining equations (3.36) and (3.37) one obtains:

$$\begin{aligned} \left[(\mathbf{E}^{(\text{i})} - \mathbf{E}_{\text{D}}^*)^{-1} + \mathbf{S}_{\text{D}} \mathbf{C}_{\text{D}}^* \right] \frac{d\mathbf{E}_{\text{D}}^*}{df} &= \frac{1}{(1-f)} \mathbf{1}^{\text{s}} \\ \left[(\mathcal{K}^{(\text{i})} - \mathcal{K}_{\text{D}}^*)^{-1} + \mathcal{S}_{\text{D}} \mathcal{R}_{\text{D}}^* \right] \frac{d\mathcal{K}_{\text{D}}^*}{df} &= \frac{1}{(1-f)} \mathcal{I} \end{aligned} \quad (3.38)$$

which are differential equations that can be solved by separation of variables. The main problem in solving these equations is the dependence of the Eshelby tensor on the elasticity or conductivity tensor of the matrix. In heat conduction, though, when the matrix is isotropic and the reinforcements are spherical, the Eshelby tensor does not depend on the conductivity tensor of the matrix and the differential equation can be solved analytically, see [151].

The differential schemes describe matrix-inclusion topologies with a wide range of reinforcements sizes. Their results comply with the appropriate Hashin-Shtrikman bounds.

3.2.1.3 Variational Bounding Methods

Variational bounding methods are restricted to homogenization, in contrast to the numerical approaches or mean field methods. In the following, only outlines of the methods are given.

3.2.1.3.1 Hill and Wiener Bounds The Hill [80] and Wiener [161] bounds can be seen as the most universal and simple bounds for elasticity and heat conduction, respec-

tively. Both methods use minimum potential energy principles to bound the effective elasticity and conductivity tensors, respectively:

$$\begin{aligned} \left[\sum_{\langle p \rangle} f^{(p)} \mathbf{C}^{(p)} \right]^{-1} &\leq \mathbf{E}^* \leq \sum_{\langle p \rangle} f^{(p)} \mathbf{E}^{(p)} \\ \left[\sum_{\langle p \rangle} f^{(p)} \mathcal{R}^{(p)} \right]^{-1} &\leq \mathcal{K}^* \leq \sum_{\langle p \rangle} f^{(p)} \mathcal{K}^{(p)} \end{aligned} \quad (3.39)$$

These bounds, although universal and very simple, do not contain any information on the microgeometry of the material except the volume fractions, and are typically too slack for practical purposes. Nevertheless, they hold for volume elements that are too small to be proper RVEs. The Hill bounds coincide with the Reuss and Voigt expressions if the Poisson numbers of the constituents fulfill special conditions.

3.2.1.3.2 Hashin–Shtrikman Bounds Much tighter bounds can be obtained using the variational formulation of Hashin and Shtrikman [69; 70]. For two-phase composites with isotropic constituents and isotropic overall behaviour, the effective elasticity tensor lower bound, $\mathbf{E}_{\text{HS}}^{*,\text{l.b.}}$, and the effective conductivity tensor lower bound, $\mathcal{K}_{\text{HS}}^{*,\text{l.b.}}$, can be expressed in terms of the Mori–Tanaka concentration tensors [160] as:

$$\begin{aligned} \mathbf{E}_{\text{HS}}^{*,\text{l.b.}} &= \mathbf{E}^{(\text{m})} + f (\mathbf{E}^{(\text{i})} - \mathbf{E}^{(\text{m})}) \bar{\mathbf{A}}_{\text{M}}^{(\text{i})} \\ \mathcal{K}_{\text{HS}}^{*,\text{l.b.}} &= \mathcal{K}^{(\text{m})} + f (\mathcal{K}^{(\text{i})} - \mathcal{K}^{(\text{m})}) \bar{\mathcal{A}}_{\text{M}}^{(\text{i})} \end{aligned} \quad (3.40)$$

whilst the upper bounds, $\mathbf{E}_{\text{HS}}^{*,\text{u.b.}}$ and $\mathcal{K}_{\text{HS}}^{*,\text{u.b.}}$, can be obtained after a “color inversion” or in other words after changing the roles of the matrix and the inclusion:

$$\begin{aligned} \mathbf{E}_{\text{HS}}^{*,\text{u.b.}} &= \mathbf{E}^{(\text{i})} + (1 - f) \left[(\mathbf{E}^{(\text{i})} - \mathbf{E}^{(\text{m})})^{-1} + f \mathbf{S}^{(\text{i})} \mathbf{C}^{(\text{i})} \right]^{-1} \\ \mathcal{K}_{\text{HS}}^{*,\text{u.b.}} &= \mathcal{K}^{(\text{i})} + (1 - f) \left[(\mathcal{K}^{(\text{i})} - \mathcal{K}^{(\text{m})})^{-1} + f \mathcal{S}^{(\text{i})} \mathcal{R}^{(\text{i})} \right]^{-1} \end{aligned} \quad (3.41)$$

Equations (3.40) and (3.41) apply to materials that additionally fulfill the condition $(k^{(\text{i})} - k^{(\text{m})}) (g^{(\text{i})} - g^{(\text{m})}) > 0$ and $K^{(\text{i})}(i, i) > K^{(\text{m})}(i, i)$ respectively. These equations can be applied, too, to transversely isotropic materials that fulfill similar conditions, see [67].

Kohn and Milton [92] extended the method to anisotropic composites for heat conduction. For the case of oriented anisotropic inclusions of ellipsoidal shape, Walpole [158] and Willis [162] derived bounds on the elastic moduli.

It is worth noting that Hashin-Shtrikman bounds are the tightest bounds that can be given for the type of geometrical information used, i.e. phase volume fractions and overall symmetry.

3.2.1.3.3 Improved Bounds The more information we have about the geometry, the better bounds we can generate. Improved bounds that are significantly tighter than Hashin-Shtrikman type expressions can be obtained by using more complex trial functions in variational bounding. These functions require statistical information on the phase arrangement in the form of n -point correlation functions for their optimization, see [63; 151].

Three-point bounds for the elastic behaviour of two-phase isotropic materials can be formulated such that the information about the phase arrangement statistics is contained in two microstructural parameters, only one of these parameters is needed for conductivity. The evaluation of these parameters is a considerable task. However, analytical or tabular data as a function of the reinforcement volume fraction, f , are available, see [151], for some important microgeometries. Among them are statistically homogeneous isotropic materials containing identical, bidisperse and polydisperse impenetrable spheres as well as monodisperse interpenetrating spheres, and statistically homogeneous transversely isotropic materials reinforced by impenetrable or interpenetrating aligned cylinders. This allows to study a good number of cases that range from matrix-inclusion composites to interwoven composites.

3.2.2 Approaches for studying composites with imperfect interfaces and/or non-ellipsoidal reinforcements

In this section, some micromechanical approaches for studying the heat conduction behaviour of composites with imperfect interfaces are presented. Additionally, extensions of the mean-field methods for studying the mechanical and heat conduction behaviour of composites reinforced with non-ellipsoidal inclusions are discussed. Only two-phase materials are covered explicitly and the material behaviour of all the phases is taken to be linear elastic for mechanical problems, or linear for heat transfer problems.

3.2.2.1 Basic theories for heat conduction: Hasselman–Johnson method

Hasselman and Johnson [74] studied the effective conductivity of composites with interfacial thermal barrier resistance, by modifying the original theories of Rayleigh [134] and Maxwell [103]. They gave results for composites consisting of a continuous matrix phase containing inhomogeneities with spherical, cylindrical and platelet geometry.

For spherical reinforcements of radius r , interfacial conductance h_β and isotropic thermal conductivity $\mathcal{K}^{(i)}$ embedded in an isotropic matrix of thermal conductivity $\mathcal{K}^{(m)}$, the elements of the resulting effective conductivity tensor, $\mathcal{K}^*$, read:

$$K^*(i, i) = K^{(m)}(i, i) \frac{\left[2 \left(\frac{K^{(i)}(i, i)}{K^{(m)}(i, i)} - \frac{K^{(i)}(i, i)}{rh_\beta} - 1 \right) f + \frac{K^{(i)}(i, i)}{K^{(m)}(i, i)} + \frac{2K^{(i)}(i, i)}{rh_\beta} + 2 \right]}{\left[\left(1 - \frac{K^{(i)}(i, i)}{K^{(m)}(i, i)} + \frac{K^{(i)}(i, i)}{rh_\beta} \right) f + \frac{K^{(i)}(i, i)}{K^{(m)}(i, i)} + \frac{2K^{(i)}(i, i)}{rh_\beta} + 2 \right]} \quad (3.42)$$

From equation (3.42) is trivial to obtain the critical radius for spherical reinforcements, r_c^s . The critical radius is the radius at which the effective conductivity of the composite equals the conductivity of the matrix. Therefore, by setting $K^*(i, i) = K^{(m)}(i, i)$ in equation 3.42, it follows:

$$r_c^s = \frac{K^{(i)}(i, i)K^{(m)}(i, i)}{h_\beta (K^{(i)}(i, i) - K^{(m)}(i, i))} \quad (3.43)$$

The Hasselman-Johnson method has been widely used for estimating the thermal conductivity of particle reinforced composites, even at high volume fractions, see e.g. [53; 62; 71; 72; 73]. It is worth noting that Hasselman and Johnson stated explicitly that their theory is valid only for “dilute” volume fractions for which interactions between the temperature field of neighboring dispersions is negligible. Nevertheless, equation (3.42) can be derived using a modified MTM approach, see 3.2.2.2, which is a theory that does account for collective interactions between inclusions (but not for pair-wise ones).

3.2.2.2 Mean Field Methods: Replacement Tensor Algorithm

Mean-field methods can be extended to handle inhomogeneities of non-ellipsoidal shape as well as finite interfacial thermal conductances (for which the Eshelby equivalent inclusion theory no longer holds) by introducing phase averaged dilute “replacement” inhomogeneity elasticity or conductivity tensors, $\mathbf{E}^{(i,r)}$ or $\mathcal{K}^{(i,r)}$, and the associated dilute “replacement”

inhomogeneity strain or gradient concentration tensors, $\bar{\mathbf{A}}_{\text{dil}}^{(i,r)}$ or $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$. The replacement tensors must fulfill the consistency conditions:

$$\begin{aligned}\mathbf{E}^{(i,r)} &= \mathbf{E}^{(m)} + \frac{1}{f_{\text{dil}}}(\mathbf{E}_{\text{dil}}^* - \mathbf{E}^{(m)})(\bar{\mathbf{A}}_{\text{dil}}^{(i,r)})^{-1} \\ \mathcal{K}^{(i,r)} &= \mathcal{K}^{(m)} + \frac{1}{f_{\text{dil}}}(\mathcal{K}_{\text{dil}}^* - \mathcal{K}^{(m)})(\bar{\mathcal{A}}_{\text{dil}}^{(i,r)})^{-1}\end{aligned}\quad (3.44)$$

which follow from eqn. (3.19) for the dilute case. Here $\mathbf{E}_{\text{dil}}^*$ and $\mathcal{K}_{\text{dil}}^*$ are the effective elasticity and the effective conductivity of a composite with dilute reinforcement volume fraction f_{dil} . The replacement tensors $\mathbf{E}^{(i,r)}$, $\mathcal{K}^{(i,r)}$, $\bar{\mathbf{A}}_{\text{dil}}^{(i,r)}$ and $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ can be inserted into any mean-field scheme in lieu of $\mathbf{E}^{(i)}$, $\mathcal{K}^{(i)}$, $\bar{\mathbf{A}}_{\text{dil}}^{(i)}$ and $\bar{\mathcal{A}}_{\text{dil}}^{(i)}$, respectively, see e.g. [47; 119]. Extensions to multiphase materials can be found, e.g. in [20].

For heat conduction in the presence of finite interfacial conductances between the phases, the replacement tensors depend on the size of the reinforcements, so that an absolute length scale is introduced into the Mori–Tanaka scheme. A number of authors also modeled the mechanical behaviour of composites with imperfect interfaces by assigning replacement stiffnesses to partially or fully debonded particles, compare e.g. [149]. In the present study, however, only the elastic behaviour of polyhedral particles with mechanically perfect interfaces is considered, for which the replacement tensor approach may be viewed as an alternative to the compliance contribution formalism of Kachanov et al. [89].

It is worth noting that combining equations (3.29) and (3.33) with the heat conduction Eshelby tensor for non-perfectly bonded spheres embedded in an isotropic matrix, see [47], the Hasselman-Johnson relationship, equation (3.42), is obtained.

3.2.2.3 Improved Bounds for heat conduction

Torquato and Rintoul [152] developed three-point bounds on the effective thermal conductivity of dispersions that are given in terms of the phase contrast between the inclusion and matrix, the conductance of the interface, volume fraction and some higher-order morphological information.

3.2.3 Mean Field Approaches for studying inelastic composites

Descriptions for inelastic microstructured materials are closely related to those for elastic composites see [67]. The extension of mean field estimates and bounding methods to elastoplastic inhomogeneous materials, however, has been found to be challenging.

The main aim of mean field models of microstructured materials with at least one elastoplastic constituent, besides materials characterization, consists in providing accurate estimates for the material response for any load state and load history at reasonable computational cost. The main difficulties in attaining this goal lie in the typically strong intra-phase fluctuations of the stress and strain fields in elastoplastic inhomogeneous materials and in the hereditary path dependent nature of plasticity. The responses of elastoplastic constituents can thus vary markedly at the microscale, with each point following its own trajectory in stress space. Accordingly, a two-phase elastoplastic composite effectively behaves as a multiphase material and phase averages are less useful descriptors than in the linear elastic case.

Mean field models of elastoplastic inhomogeneous materials typically are based on solving sequences or sets of linearized problems in terms of linear reference media. Accordingly, choices have to be made with respect to the linearization procedure, the linear homogenization model, and the phase-wise equivalent stresses and strains to be used in evaluating the elastoplastic constituent material behaviour. In the literature several lines of development of mean field approaches for elastoplastic inhomogeneous materials can be found. Historically, the most important of them have been secant plasticity concepts based on deformation theory, and incremental plasticity models. In addition, tangent concepts [112], and the affine formulation [101] have been proposed.

3.2.3.1 Secant methods

Secant models aim at directly arriving at solutions in terms of the overall response for a given load state. They are based on the deformation theory of plasticity and can be formulated in terms of potentials, which allows for a concise mathematical presentation [144]. Secant plasticity models are limited to monotonic loading and radial trajectories of the constituents in stress space during loading, which precludes their use as micromechanically based constitutive models in multi-scale analyses.

The secant formulation determines for each elastoplastic phase, $^{(\text{ep})}$, a secant operator, $\mathbf{E}_S^{(\text{ep})}$, that relates the average strain and the average stress tensors in every phase. If macroscopic isotropy is assumed, the secant operator reads:

$$\langle \boldsymbol{\sigma} \rangle^{(\text{ep})} = \mathbf{E}_S^{(\text{ep})} \langle \boldsymbol{\varepsilon} \rangle^{(\text{ep})} \quad \mathbf{E}_S^{(\text{ep})} = 3k^{(\text{ep})} \mathbf{1}^{\text{vol}} + 2g_S^{(\text{ep})} \mathbf{1}^{\text{dev},s} \quad (3.45)$$

where $g_S^{(\text{ep})}$ is the secant shear modulus, which is a function of the phase-wise reference

equivalent strain $\varepsilon_{\text{REF}}^{(\text{ep})}$. There are several methods to define the phase-wise equivalent strain, the classical one being:

$$\varepsilon_{\text{REF}}^{(\text{ep})} = \left(\frac{2}{3} \left[\mathbf{1}^{\text{dev},s} \langle \boldsymbol{\varepsilon} \rangle^{(\text{ep})} \right]^T \mathbf{1}^{\text{dev},s} \langle \boldsymbol{\varepsilon} \rangle^{(\text{ep})} \right)^{1/2} \quad (3.46)$$

Other methods for determining the equivalent reference strain can be found in [25; 130].

Once the equivalent reference strains are determined, the effective elastoplastic tensor can be determined by using a linear homogenized scheme defined by its strain concentration tensor, equation (3.19). Secant methods can be formulated, too, in terms of reference stresses instead of reference strains, [65], both formulations being equivalent [143].

A common problem to all mean field approaches for elastoplastic composites lies in handling the intra-phase variations of the stress and strain fields within the assumption of phase-wise uniformity. Improvements in this respect have been obtained by evaluating the phase averages of the von Mises equivalent stress from energy considerations, or by using statistically based theories. Such algorithms, however, have been limited to secant plasticity approaches, leading to modified secant models. Excellent agreement has been reported between the latter method and multi-particle unit cell models in a materials characterization context [140].

3.2.3.2 Incremental methods

Incremental methods are another alternative for predicting the macroscopic and local (averaged) behaviour of non-linear materials. This is done incrementally over several “time” steps. In contrast to secant methods, incremental methods can deal with any elastoplastic model and any load-path. In these methods the rates of the stress and strain tensors of the elastoplastic phases are linked through algorithmic or tangent material stiffness tensors, compare section 2.7.4. From the state of deformation at the beginning of the time step, homogenization models can be applied to obtain the effective algorithmic stiffness tensor.

In what follows, the Incremental Mori-Tanaka (IMT) model of Pettermann [126] is reviewed. Incremental mean field methods can be formulated in terms of phase averaged strain and stress rate tensors, $d \langle \boldsymbol{\varepsilon} \rangle^{(\text{p})}$ and $d \langle \boldsymbol{\sigma} \rangle^{(\text{p})}$, which can be expressed in analogy with the elastic case, equation (3.17), as:

$$\begin{aligned} d \langle \boldsymbol{\varepsilon} \rangle^{(\text{p})} &= \bar{\mathbf{A}}_t^{(\text{p})} d \langle \boldsymbol{\varepsilon} \rangle + \bar{\boldsymbol{\varepsilon}}_t^{(\text{p})} dt \\ d \langle \boldsymbol{\sigma} \rangle^{(\text{p})} &= \bar{\mathbf{B}}_t^{(\text{p})} d \langle \boldsymbol{\sigma} \rangle + \bar{\boldsymbol{\sigma}}_t^{(\text{p})} dt \end{aligned} \quad (3.47)$$

where $d\langle\boldsymbol{\varepsilon}\rangle$ stands for the instantaneous macroscopic mechanical strain rate tensor, and $d\langle\boldsymbol{\sigma}\rangle$ for the instantaneous macroscopic stress rate tensor. $\bar{\mathbf{A}}_t^{(p)}$, $\bar{\mathbf{B}}_t^{(p)}$, $\bar{\mathbf{t}}_t^{(p)}$ and $\bar{\boldsymbol{\theta}}_t^{(p)}$ are the instantaneous elastic and thermal phase strain and stress concentration tensors, respectively. Using the assumption that the inclusions show elastic and the matrix elastoplastic material behaviour, the overall instantaneous (tangent) stiffness tensor, $\mathbf{E}_t$, can be written in terms of the phase properties and the instantaneous concentration tensors as:

$$\mathbf{E}_t^* = \mathbf{E}^{(i)} + (1 - f) \left(\mathbf{E}_t^{(m)} - \mathbf{E}^{(i)} \right) \bar{\mathbf{A}}_t^{(m)} \quad (3.48)$$

This equation is formulated so that $\mathbf{E}_t$ is a continuum tangent operator.

In analogy to equation (3.31), the instantaneous matrix concentration tensors take the form:

$$\bar{\mathbf{A}}_t^{(m)} = \left[(1 - f) \mathbf{1}^{\text{dev},s} + f \left[\mathbf{1}^{\text{dev},s} + \mathbf{S}_t \mathbf{C}_t^{(m)} \left(\mathbf{E}^{(i)} - \mathbf{E}_t^{(m)} \right) \right]^{-1} \right]^{-1} \quad (3.49)$$

$$\bar{\mathbf{B}}_t^{(m)} = \left[(1 - f) \mathbf{1}^{\text{dev},s} + f \left[\mathbf{1}^{\text{dev},s} + \mathbf{E}_t^{(m)} \left(\mathbf{1}^{\text{dev},s} - \mathbf{S}_t \right) \left(\mathbf{C}^{(i)} - \mathbf{C}_t^{(m)} \right) \right]^{-1} \right]^{-1} \quad (3.50)$$

where $\mathbf{S}_t$ is the instantaneous Eshelby tensor. It depends on the current state of the matrix material and in general has to be evaluated numerically due to the anisotropic structure of the instantaneous tangent stiffness tensor of the matrix, $\mathbf{E}_t^{(m)}$. If the symmetry of the Eshelby tensor is lower than orthotropic Nye notation may lead to incorrect results.

Formulations of the previous equations that are directly suitable for implementation as micromechanically based constitutive models at the integration point level within Finite Element codes can be obtained by replacing rates such as $d\langle\boldsymbol{\varepsilon}\rangle^{(p)}$ with finite increments such as $\Delta\langle\boldsymbol{\varepsilon}\rangle^{(p)}$. It is worth noting that in the resulting incremental Mori-Tanaka methods no assumptions on the overall yield locus and the overall flow potential are made, the effective material behaviour being entirely determined by the incremental mean field equations and the constitutive behaviour of the phases. However, mapping of the stresses onto the yield surface cannot be handled at the level of the homogenized material and the stress return mapping algorithm has to be applied to the matrix at the microscale instead. Accordingly, the constitutive equations describing the overall behaviour cannot be integrated directly, and iterative algorithms are required. For example, Pettermann [126] used an implicit Euler scheme in an implementation of an incremental Mori-Tanaka method as a user supplied material routine (UMAT) for the commercial Finite Element code ABAQUS. Algorithms of this type can also handle thermal expansion effects and temperature dependent material parameters.

Due to their combination of usually reasonable accuracy, flexibility in terms of inclusion geometries, and relatively low computational requirements, incremental Mori-Tanaka methods can be useful as micromechanically based constitutive laws within Finite Element codes for analyzing components and structures made of elastoplastic composite materials such as metal matrix composites.

Furthermore, incremental plasticity approaches are not subject to limitations with respect to loading paths. However, especially for matrix deformation dominated models they tend to markedly overestimate the overall strain hardening in the post-yield regime. Recent algorithmic improvements are reported to markedly reduce this weakness, see Doghri's modification below. Using this algorithm, incremental Mori-Tanaka methods can handle large strains, see [84].

3.2.3.2.1 Doghri's modification The algorithmic and tangent tensors, see section 2.7.4, obtained with the isotropic elasto-plasticity, see section 2.6.1, or the Chaboche plasticity, see section 2.6.2, models are anisotropic. Numerical experience has shown, however, that good predictions with the IMT method are obtained only when modified tensors, isotropized or transversely-isotropized, are used instead, see Doghri [41]. Evidently, this holds if the global symmetry of the composite is isotropic or transversely isotropic. For anisotropic elastoplastic tensors, Z_{ijkl} , Doghri proposed four methods for modifying:

- Isotropic generalized projection method:

The isotropic part, Z_{ijkl}^{Iso} , of Z_{ijkl} is defined as :

$$Z_{ijkl}^{\text{Iso}} = (1_{ijkl}^{\text{vol}} Z_{lkji}) 1_{ijkl}^{\text{vol}} + \frac{1}{5} \left(1_{ijkl}^{\text{dev,s}} Z_{lkji} \right) 1_{ijkl}^{\text{dev,s}} \quad (3.51)$$

- Isotropic spectral decomposition:

This method applies to anisotropic tangent operators which are a linear combination of 1_{ijkl}^{vol} , $1_{ijkl}^{\text{dev,s}}$ and $N_{ij}N_{kl}$, where N_{ij} satisfies the relations:

$$N_{ij} = N_{ji}; \quad N_{ii} = 0; \quad N_{ij}N_{ji} = \frac{3}{2} \quad (3.52)$$

For isotropic elasto-plasticity, the algorithmic and the tangent tensors satisfy all the conditions. For the Chaboche-Marquis model, the conditions are satisfied by the tangent tensor in all cases, and by the algorithmic tensor when $c^{(2),\text{C-M}} = 0$. For

those cases, Ponte Castañeda [132] proposed the following form of the elastoplastic tensor:

$$Z_{ijkl} = 3c^{(1),SD} 1_{ijkl}^{\text{vol}} + 2c^{(2),SD} \left[1_{ijkl}^{\text{dev},s} - \frac{2}{3} N_{ij} N_{ji} \right] + 2c^{(3),SD} N_{ij} N_{ji} \quad (3.53)$$

where $c^{(1),SD}$, $c^{(2),SD}$ and $c^{(3),SD}$ are constants.

The isotropic spectral decomposition of the tensor, $Z_{ijkl}^{\text{Iso, Spe}}$, is defined as:

$$Z_{ijkl}^{\text{Iso, Spe}} = 3c^{(1),SD} 1_{ijkl}^{\text{vol}} + 2c^{(3),SD} 1_{ijkl}^{\text{dev},s} \quad (3.54)$$

- Transversely isotropic generalized projection method:

Any transversely isotropic second-order tensor, λ_{ij} , with direction of anisotropy, w_i , can be written as:

$$\lambda_{ij} = c^s \varsigma_{ij} + c^T \tau_{ij} \quad (3.55)$$

where $\varsigma_{ij} = w_i w_j$ and $\tau_{ij} = 1 - \varsigma_{ij}$.

The transversely isotropized part of Z_{ijkl} , Z_{ijkl}^{TrIso} , can be written as (see [23]):

$$\begin{aligned} Z_{ijkl}^{\text{TrIso}} &= \left[Z_{ijkl}^{(B_1)} Z_{lkij} \right] Z_{ijkl}^{(B_1)} + \left[Z_{ijkl}^{(B_2)} Z_{lkij} \right] Z_{ijkl}^{(B_2)} + \\ &+ \frac{1}{2} \left[Z_{ijkl}^{(B_3)} Z_{lkij} \right] Z_{ijkl}^{(B_3)} + \frac{1}{2} \left[Z_{ijkl}^{(B_4)} Z_{lkij} \right] Z_{ijkl}^{(B_4)} + \\ &+ \frac{1}{2} \left[Z_{ijkl}^{(B_5)} Z_{lkij} \right] Z_{ijkl}^{(B_5)} + \frac{1}{2} \left[Z_{ijkl}^{(B_6)} Z_{lkij} \right] Z_{ijkl}^{(B_6)} \end{aligned} \quad (3.56)$$

where:

$$Z_{ijkl}^{(B_1)} = \frac{1}{2} \tau_{ij} \tau_{kl} \quad (3.57)$$

$$Z_{ijkl}^{(B_2)} = \varsigma_{ij} \varsigma_{kl} \quad (3.58)$$

$$Z_{ijkl}^{(B_3)} = \frac{1}{2} (\tau_{ik} \tau_{jl} + \tau_{jk} \tau_{il} - \tau_{ij} \tau_{kl}) \quad (3.59)$$

$$Z_{ijkl}^{(B_4)} = \frac{1}{2} (\varsigma_{ik} \varsigma_{jl} + \tau_{il} \varsigma_{jk} + \tau_{jl} \varsigma_{ik} + \tau_{jk} \varsigma_{il}) \quad (3.60)$$

$$Z_{ijkl}^{(B_5)} = \varsigma_{ij} \varsigma_{kl} \quad (3.61)$$

$$Z_{ijkl}^{(B_6)} = \tau_{ij} \varsigma_{kl} \quad (3.62)$$

- Transversely isotropic spectral method:

For elasto–plasticity with isotropic hardening, the transversely isotropic spectral part of Z_{ijkl} , $Z_{ijkl}^{\text{TrIso, Spe}}$, is:

$$Z_{ijkl}^{\text{TrIso, Spe}} = Z_{ijkl} - c^K \frac{(2g)^2}{3g + \frac{d\phi^{(1)}(p)}{dp}} N_{ij} N_{kl} \quad (3.63)$$

where c^K is a softening factor.

Doghri rewrote equations (3.48)–(3.50) as:

$$\mathbf{E}_t = \mathbf{E}^{(i)} + (1 - f) \left(\mathbf{E}_t^{(m),C} - \mathbf{E}^{(i)} \right) \bar{\mathbf{A}}_t^{(m)} \quad (3.64)$$

$$\bar{\mathbf{A}}_t^{(m)} = \left[(1 - f) \mathbf{1}^{\text{dev,s}} + f \left[\mathbf{1}^{\text{dev,s}} + \mathbf{S}_t \mathbf{C}_t^{(m),D} \left(\mathbf{E}^{(i)} - \mathbf{E}_t^{(m),C} \right) \right]^{-1} \right]^{-1} \quad (3.65)$$

where the Eshelby tensor is calculated using $\mathbf{E}_t^{(m),E}$, $\mathbf{S}_t = \mathbf{S}_t \left(\mathbf{E}_t^{(m),E} \right)$. $\mathbf{E}_t^{(m),C}$, $\mathbf{E}_t^{(m),D}$ and $\mathbf{E}_t^{(m),E}$ are modified elastoplastic tensors of the matrix. In the IMT of Pettermann, a fourth modified elastoplastic tensor, $\mathbf{E}_t^{(m),F}$, is introduced to deal with the thermal concentration tensor, so that equation 3.25 is rewritten as:

$$\bar{\boldsymbol{\theta}}^{(m)} = (\mathbf{1}^s - \bar{\mathbf{B}}^{(m)}) \left(\mathbf{C}^{(i)} - \left[\mathbf{E}_t^{(m),F} \right]^{-1} \right)^{-1} (\boldsymbol{\alpha}^{(m)} - \boldsymbol{\alpha}^{(i)}) \quad (3.66)$$

The “classical” IMT method corresponds to:

$$\mathbf{E}_t^{(m),C} = \mathbf{E}_t^{(m),D} = \mathbf{E}_t^{(m),E} = \mathbf{E}_t^{(m),F} = \mathbf{E}_t^{(m)} \quad (3.67)$$

Softer and better predictions are obtained by using:

$$\begin{aligned} \mathbf{E}_t^{(m),E} &= \mathbf{E}_t^{(m),\text{Iso}} \\ \mathbf{E}_t^{(m),D} &= \mathbf{E}_t^{(m),C} = \mathbf{E}_t^{(m),F} = \mathbf{E}_t^{(m)} \end{aligned} \quad (3.68)$$

see [41; 40; 118].

Alternatively, Chaboche [27] obtained good predictions with the following set of elastoplastic tensors:

$$\begin{aligned}
\mathbf{E}_t^{(m),E} &= \mathbf{E}_t^{(m),D} = \mathbf{E}_t^{(m),\text{Iso, spe}} \\
\mathbf{E}_t^{(m),C} &= \mathbf{E}_t^{(m),F} = \mathbf{E}_t^{(m)}
\end{aligned} \tag{3.69}$$

The best set of modified tensors to be used for a given composite depends on its macroscopic symmetry. For a detailed description of the most suitable sets for different composites, see e.g. [129].

3.2.3.3 Variational bounds

In analogy to mean-field estimates for elastoplastic materials, non-linear bounds are obtained by evaluating a sequence of linear bounds. Talbot and Willis [145] extended the Hashin-Shtrikman variational principle to obtain upper or lower bounds, depending on the material combination, on the non-linear mechanical behaviour of inhomogeneous materials. Ponte Castañeda [131] derived a variational principle that allows to obtain upper bounds on the effective non-linear behaviour of inhomogeneous materials, on the basis of upper bounds for the elastic response. Analogous bounds to the Hill Bounds were presented by Bishop and Hill [16].

3.3 Numerical Approaches

3.3.1 General remarks on approaches based on discrete microgeometries

Broadly speaking, micromechanical approaches based on discrete microgeometries trade off restrictions to the generality of the microstructures that can be studied for the capabilities of using fine grained geometrical models and of resolving details of the microfields at the length scale of the inhomogeneities. The main fields of application of such methods are studying the nonlinear behaviour of inhomogeneous materials and evaluating the microscopic fields of model materials at high resolution. This information may be required when the local fields fluctuate strongly and this information is important, too, for understanding behaviours that depend on details of the microgeometry, such as damage or failure behaviour.

There are two, often complementary, philosophies for modeling inhomogeneous materials via discrete microgeometries. One of them is based on studying generic phase arrangements, which may vary from simple periodic arrays of fibers to highly complex microgeometries involving a considerable number of reinforcements. Complex phase arrangements of the latter type can be generated by appropriate statistically based algorithms. Model microgeometries of this type tend to employ idealized inclusion shapes, equiaxed particles embedded in a matrix, for example, being often represented by spheres [19; 141].

Alternatively, microgeometries may be chosen to follow as closely as possible the phase arrangement of a given sample of the material to be modeled, obtained from metallographic sections, serial sections, or tomographic data, . . . The resulting descriptions are termed real structure or digital image based (DIB) models [9; 28].

Unless materials with simple periodic phase arrangements are considered, for both modeling strategies the question immediately arises of how complex (and thus large) the model geometry must be in order to adequately capture the physical behaviour of the material to be studied. For the case of elastic statistically isotropic composites with matrix-inclusion topology and sphere-like particles, Drugan and Willis [42] estimated that for approximating the overall elastic moduli with errors of less than 5% or less than 1%, respectively, volume elements with sizes of approximately two or five inclusion diameters are sufficient for any volume fraction. In addition, the adequacy of the size of a volume element may be judged on the basis of deviations from the required symmetry of the overall response. At present, however, there appears to be no reliable method for directly assessing the representativeness of the microscopic field distributions obtained from a given volume element.

For nonlinear behaviour a number of numerical studies have indicated that substantially larger volume elements are necessary for satisfactorily approximating the required overall symmetry and for obtaining good agreement between the macroscopic responses of statistically equivalent phase arrangements, especially for mechanical analysis at elevated overall inelastic strains [64; 87; 170]. The reason for this behaviour lies in the marked inhomogeneity of the microfields typically found in these regimes, which may introduce a new length scale into the problem. Accordingly, the size of satisfactory multi-inclusion unit cells depends markedly on the phase material behaviour.

The majority of published micromechanical analyses of discrete microstructures have employed standard numerical engineering methods for resolving the microfields. Studies using Finite Difference algorithms [6], spring lattice models [122], the boundary element

method [97], the Finite Element Method, techniques using Fast Fourier Transforms and Discrete Fourier Transforms [114], as well as FE-based discrete dislocation models [32] have been reported. Generally speaking, spring lattice models tend to have advantages in handling traction boundary conditions and in modeling the progress of microcracks due to local (brittle) fracture. Boundary elements tend to be at their best in studying geometrically complex linear elastic problems. For all the above methods the characteristic length of the discretization must, of course, be considerably smaller than the microscale of a given problem in order to obtain spatially well resolved results.

At present the FEM is the most commonly used numerical scheme for evaluating discrete microgeometries, especially in the nonlinear range, where its flexibility and capability of supporting a wide range of constitutive models for the constituents and for the interfaces between them are specially appreciated. An additional asset of the FEM in the context of continuum micromechanics is its ability to handle discontinuities in the strain, stress, temperature gradient and heat flux components (which typically occur at interfaces between different constituents) in a natural way via appropriately placed element boundaries.

In most published works, the phase arrangements are discretized by an often high number of standard continuum elements, the mesh being designed in such a way that element boundaries are positioned at all interfaces between constituents. Such an approach has the advantage that in principle any microgeometry can be handled and that readily available commercial FE packages may be used. However the actual modeling of complex phase configurations in many cases requires sophisticated and/or specialized preprocessors for generating the mesh, a task that has been tricky to automatize. The resulting stiffness matrices may show unfavorable conditioning due to suboptimal element shapes. Satisfactory resolution of the microfields at local hot spots can lead to very large models indeed.

3.3.2 Periodic microfield approaches

Periodic microfield approaches (PMAs) aim to describe the macroscopic and microscopic behaviour of inhomogeneous materials by studying model materials that have periodic microstructures.

In the following discussion the main emphasis is on the small strain elastoplastic behaviour and on the heat conduction behaviour of materials the properties of which are temperature independent. Homogenization methods for finite strain problems are discussed in e.g. [108; 148].

3.3.2.1 Basic concepts of unit cell models

Periodic microfield approaches analyze the behaviour of infinite (one-, two- or three-dimensional) periodic arrangements of constituents making up a given inhomogeneous material under the action of far field mechanical or thermal loads. They describe a micro-geometry by a periodically repeating unit cell to which the investigations may be limited without loss of information or generality, at least for steady state analyses.

A wide variety of unit cells have been employed in published PMA studies, ranging from geometries used to describe simple periodic arrays of inclusions to highly complex phase arrangements, such as multi-inclusion cells. For simple periodic phase arrangements it may also be possible to find analytical solutions via series expansions [34] or potential methods [159].

Most PMA studies have used standard numerical engineering methods, but some more specialized approaches for evaluating microscopic stress and strain fields use somewhat different methods, e.g the method of the cells, [3; 4; 5], or Transformation Field Analysis [50].

In typical periodic microfield approaches the fields are split into constant macroscopic contributions, $\langle \boldsymbol{\varepsilon} \rangle$, $\langle \boldsymbol{\sigma} \rangle$, $\langle \mathbf{d} \rangle$ and $\langle \mathbf{q} \rangle$ (slow variables), and periodically varying microscopic fluctuations, $\boldsymbol{\varepsilon}'(\mathbf{z})$, $\boldsymbol{\sigma}'(\mathbf{z})$, $\mathbf{d}'(\mathbf{z})$ and $\mathbf{q}'(\mathbf{z})$ (fast variables), in analogy to equation (3.2). The position vectors are denoted here as $\mathbf{z}$ to indicate that the unit cells “lives” on the microscale. The volume integrals used to obtain averages must, of course, be solved over the volume of the unit cell, v_{UC} . Formal derivations of the above relationships for periodically varying microstrains and microstresses, show that the work done by the fluctuating strains and stresses vanishes [107]. Analogously, for periodically varying micro thermal gradients and micro heat fluxes, the product of thermal gradients and heat fluxes vanishes, see [151].

Evidently in periodic microfield approaches each unit of periodicity (unit cell) contributes the same displacement or temperature increment and the macroscopic displacements or temperatures vary (multi)linearly. In fig. 3.4 an idealized depiction of such a situation in elasticity is presented, which shows the variation of the strains $\boldsymbol{\varepsilon}_\beta(z_\beta) = \langle \boldsymbol{\varepsilon}_\beta \rangle + \boldsymbol{\varepsilon}'_\beta(z_\beta)$ and of the corresponding displacements $\mathbf{u}_\beta(z_\beta) = \langle \boldsymbol{\varepsilon}_\beta \rangle z_\beta + \mathbf{u}'_\beta(z_\beta)$ along some section line β in a hypothetical periodic two-phase material consisting of constituents A and B. The periodicity of the strains and of the displacements is immediately apparent, the unit of periodicity in direction β and the corresponding displacement increment being marked as c^{U} and Δu_β , respectively (note that $\Delta u_\beta = \langle \boldsymbol{\varepsilon}_\beta \rangle c^{\text{U}}$ for linear displacement-strain

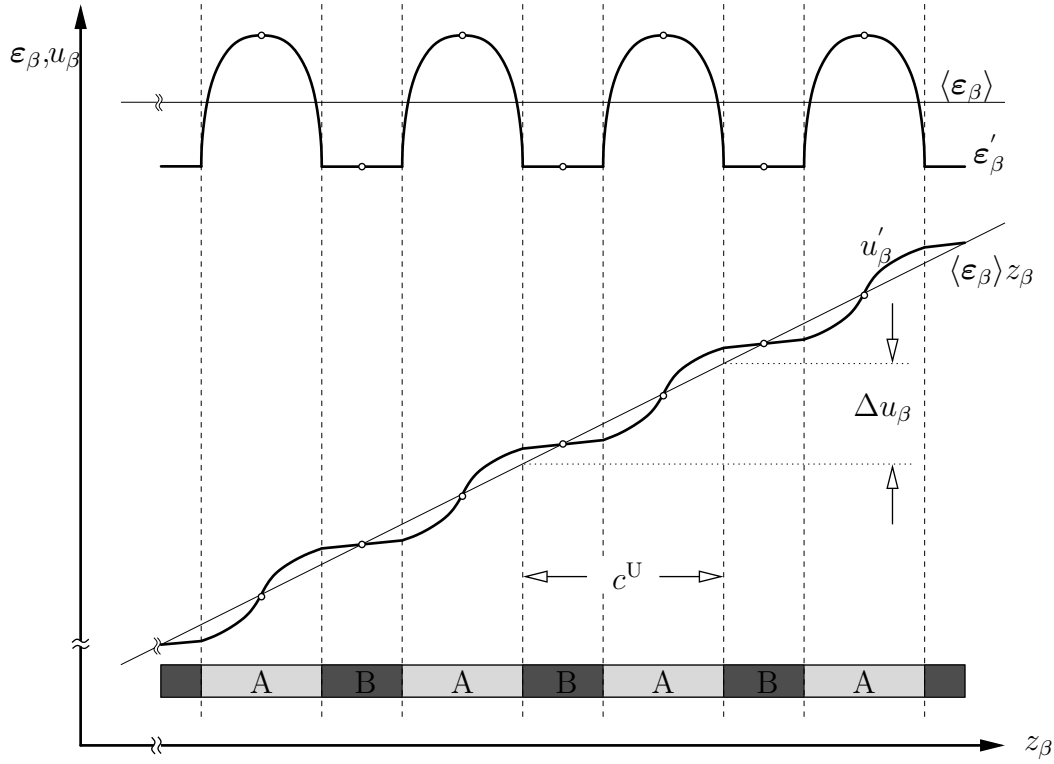


Figure 3.4: Scheme of the strain variation and displacements along a linear section in an hypothetical inhomogeneous material made of constituents A and B. [17]

relations). In addition symmetry points of $\epsilon_\beta(z_\beta)$ and $u_\beta(z_\beta)$ are indicated by small circles. The same plot holds for heat conduction, by replacing the variables by their analogs, see table 3.1. A difference between thermomechanical and thermal conduction problems is worth noting at this point. In thermomechanics material nonlinearities typically involve dependencies of the materials parameters on stress, strain and temperature, i.e. on variables the averages of which do not vary from unit cell to unit cell. In thermal conduction material nonlinearities typically take the form of dependencies on the temperature, the average of which varies from unit cell to unit cell in such problems. Furthermore, the temperature varies from $-\infty$ to ∞ .

Accordingly, even though the average conductivity of unit cells with temperature dependent material parameters can be evaluated, for this case PMAs may not be free of contradictions.

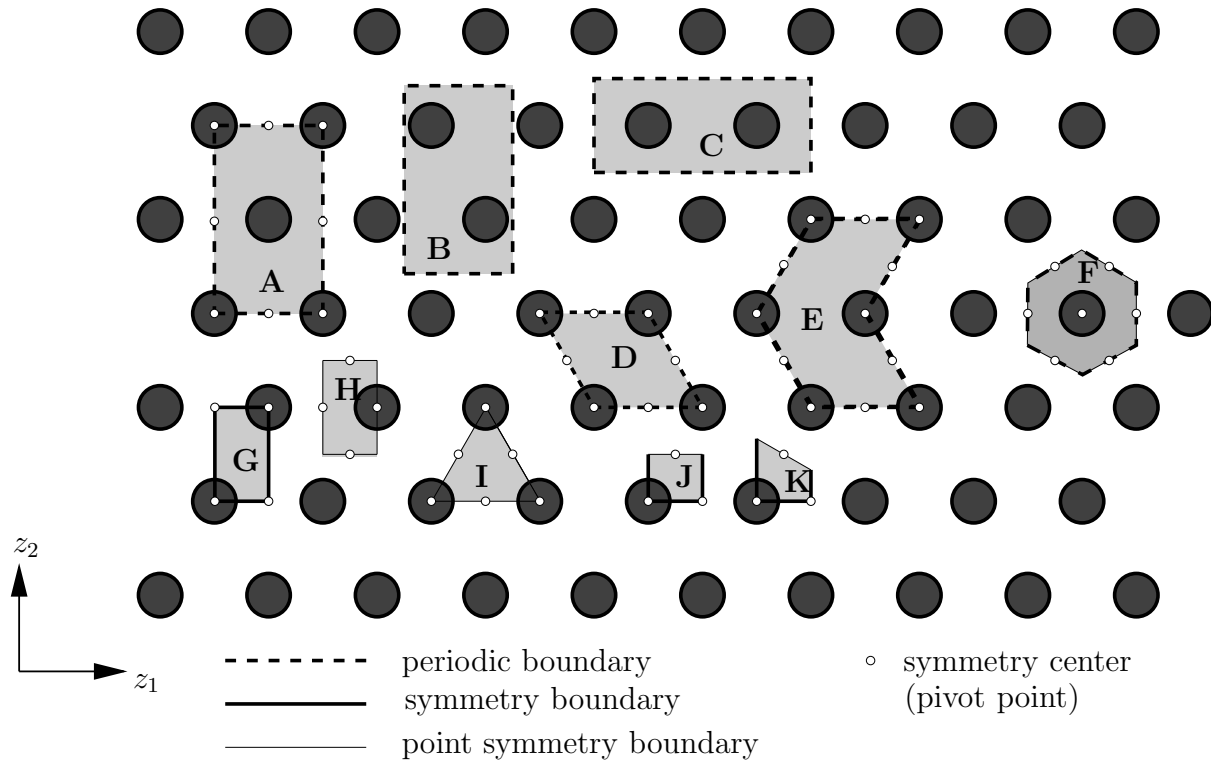


Figure 3.5: Two-dimensional unit cells for a periodic hexagonal array. [17]

3.3.2.2 Boundary conditions, application of loads, evaluation of microfields

3.3.2.2.1 Boundary Conditions The proper use of unit cell based methods requires that the cells together with the boundary conditions prescribed on them generate valid tilings both for the undeformed geometry and for all deformed states pertinent to the investigation for mechanical problems and that temperature profiles are compatible on the unit cell's faces for all possible temperature gradients in conduction problems. In order to achieve this, the boundary conditions for the unit cells must be specified in such a way that all deformation modes or temperature profiles appropriate for the load cases to be studied can be attained. The three major types of boundary conditions used in periodic microfield analyses of the mechanical and thermal conduction behaviour of periodic model materials are periodicity, symmetry, and antisymmetry boundary conditions. In this thesis, only periodicity boundary conditions are used with PMAs.

Periodicity boundary conditions are the most general boundary conditions for unit cells, they can handle any possible deformation state or temperature profile of the cell and, consequently, of the inhomogeneous material to be modeled. In fig.3.5, cells A to F

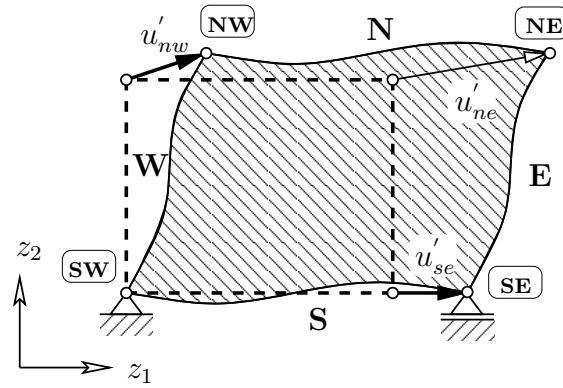


Figure 3.6: Mechanical periodicity boundary conditions for a two-dimensional unit cell. [18]

belong to this group. Because such unit cells tile the computational space by translation, neighboring cells must fit into each other like parts of a jigsaw puzzle in both unloaded and loaded states. For the case of two-dimensional unit cells with even number of faces this can be achieved by pairing opposite faces and linking the corresponding degrees of freedom from each pair of faces.

Using the conventions for naming the vertices and faces shown in figs. 3.6 and 3.7, the resulting equations for the periodically varying displacement vectors at the boundaries, $\mathbf{u}'$, and periodically varying temperatures, t' , at the boundaries can be symbolically written as:

$$\begin{aligned} \mathbf{u}'_{\mathbf{N}}(\tilde{z}_1) &= \mathbf{u}'_{\mathbf{S}}(\tilde{z}_1) + \mathbf{u}'_{\mathbf{NW}} & t'_{\mathbf{N}}(\tilde{z}_1) &= t'_{\mathbf{S}}(\tilde{z}_1) + t'_{\mathbf{NW}} \\ \mathbf{u}'_{\mathbf{E}}(\tilde{z}_2) &= \mathbf{u}'_{\mathbf{W}}(\tilde{z}_2) + \mathbf{u}'_{\mathbf{SE}} & t'_{\mathbf{E}}(\tilde{z}_2) &= t'_{\mathbf{W}}(\tilde{z}_2) + t'_{\mathbf{SE}} \end{aligned} \quad (3.70)$$

Here $\tilde{z}_1$ and $\tilde{z}_2$ denote corresponding positions on the **N** and **S** faces and on the **E** and **W** faces of the unit cell, respectively. From equations (3.70), it follows that the displacements and the temperatures of nodes on faces **N** and **E** depend on or are “slaved” to the displacements and temperatures of the nodes **SE** and **NW**, respectively. These nodes control the displacement and temperatures of the nodes on faces **N** and **E** and are called “master nodes”, whilst the dependent nodes are the so called “slaved nodes”. In principle, all variables (in example for mechanical analyses the displacements, strain and stresses and for thermal analyses temperature, temperature gradients and fluxes) must be linked by appropriate periodicity conditions. When a displacement or a temperature based FE code is used, however, such conditions (including where appropriate, rotation D.O.F.s)

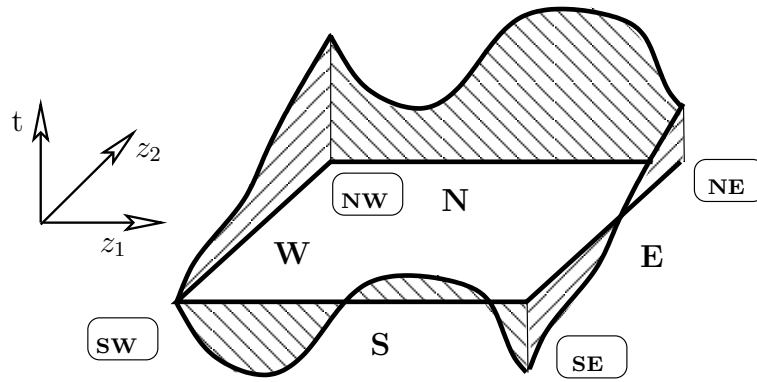


Figure 3.7: Temperature periodicity boundary conditions for a two-dimensional unit cell for studying heat conduction

can be specified explicitly only for the displacement components and temperatures, and the periodicity of the strains, stresses, temperature gradients and heat fluxes is only fulfilled approximately. In mechanical problems, for periodicity boundary conditions, the main error is due to the fact that in typical implementations the nodal stresses and strains are not averaged across cell boundaries, even though they ought to be. The same holds for heat fluxes and temperature gradients in conductivity. Note also that when stresses are periodic, unit cell boundary tractions are antiperiodic.

Periodicity boundary conditions generally are the least restrictive option for periodic multi-inclusion unit cells models using phase arrangements obtained by statistically based algorithms or by experimental techniques. In practice FE-based unit cell studies using periodicity boundary conditions can be rather expensive in terms of computing time and memory requirements, because the multipoint constraints required for implementing equations (3.70) tend to degrade the band structure of the system matrix, especially in three-dimensional problems. In addition it is worth noting that considerable care may be required to prevent over- and underconstraining due to inappropriate selection of regions with periodicity boundary conditions [128].

All the previous equations refer to the usual case where standard material behaviour is used on the macroscale and the scale transition is handled via homogenized stress and strain fields. Periodicity boundary conditions that are conceptually similar to the previous equation can be devised for cases where gradient theories are employed on the macroscale and higher order stresses as well as strain gradients figure in coupling the length scales [61].

Obviously, the description of real materials, which in general are not periodic, by periodic model materials entails some geometrical approximations. These take the form of periodicity constraints on computer generated phase arrangements or of appropriate modifications in the case of real structure microgeometries. The effects of such approximations in the vicinity of the cell surfaces, of course, diminish in importance with growing size of the model.

3.3.2.2.2 Linking macroscale and microscale The primary practical challenge in using periodic microfield approaches for modeling inhomogeneous materials lies in choosing and generating suitable unit cells that, in combination with appropriate boundary conditions, allow a realistic representation of the actual microgeometries within available computational resources. The unit cells must then be subjected to appropriate macroscopic strains, stresses, or temperature excursions for mechanical analyses and thermal gradients or heat fluxes for heat conduction analyses. Whereas homogeneous temperature excursions for studying the effective thermal expansion behaviour do not pose major difficulties, applying far field strains, stresses, temperature gradients or heat fluxes may be difficult.

There are two main strategies for linking the macroscale and the microscale in unit cell analysis, asymptotic homogenization [125; 168] and the method of macroscopic degrees of freedom [106]. In this work, only the latter one is used.

In the method of macroscopic degrees of freedom, the loads are prescribed by assigning appropriate displacements, loads, temperatures or heat flows to the master nodes. For example a uniaxial strain state is obtained in the unit cell of the figure 3.6, by applying a displacement in z_1 direction to the master node **SE** or a displacement in direction z_2 to the master node **NW**. Equivalently, a thermal gradient in z_1 is obtained in the unit cell of figure 3.7 by fixing the nodal temperature of the node **NW** equal to the temperature of node **SW**, and specifying different nodal temperatures for the nodes **SE** and **SW**.

3.3.2.2.3 Evaluation of averaged microfields For evaluating the phase averaged quantities from unit cells models in the absence of imperfect interfaces, it is possible to use direct integration of eqns (3.4). This can be done in every FE code by integrating numerically these equations according to:

$$\begin{aligned}
 \langle \boldsymbol{\varepsilon} \rangle &= \frac{1}{v} \int_v \boldsymbol{\varepsilon}(\mathbf{x}) dv \approx \frac{1}{v} \sum_{i=1}^N \boldsymbol{\varepsilon}_i v_i & \langle \mathbf{d} \rangle &= \frac{1}{v} \int_v \mathbf{d}(\mathbf{x}) dv \approx \frac{1}{v} \sum_{i=1}^N \mathbf{d}_i v_i \\
 \langle \boldsymbol{\sigma} \rangle &= \frac{1}{v} \int_v \boldsymbol{\sigma}(\mathbf{x}) dv \approx \frac{1}{v} \sum_{i=1}^N \boldsymbol{\sigma}_i v_i & \langle \mathbf{q} \rangle &= \frac{1}{v} \int_v \mathbf{q}(\mathbf{x}) dv \approx \frac{1}{v} \sum_{i=1}^N \mathbf{q}_i v_i
 \end{aligned} \tag{3.71}$$

where the subscripts $_i$ denote the value of the respective variables at the integration point and v_i is the volume associated with the integration point. In the case of rectangular or hexahedral unit cells that are aligned with the coordinate axes, averaged engineering strain and stress components can be evaluated by dividing the displacements at the master nodes by the appropriate cell lengths and by dividing the applied or reaction forces at the master nodes by the appropriate surface areas, respectively. The averaged temperature gradient and heat fluxes can be evaluated by dividing the temperature difference at the master nodes by the appropriate cell lengths and by dividing the applied concentrated heat flow components at the master nodes by the appropriate surface areas, respectively. For example, for extracting the Young modulus in z_1 direction, E_{z_1} , of the unit cell depicted in figure 3.6, when a load, c^{Load} , is applied at node **SE** in z_1 direction, the next formula can be applied:

$$E_{z_1} = \frac{\frac{c^{\text{Load}}}{c^{\mathbf{E}}e}}{\frac{u(1)}{c^{\mathbf{S}}}} \tag{3.72}$$

where, $c^{\mathbf{E}}$ is the length of the face “E”, $c^{\mathbf{S}}$ the length of the face “S”, and e the thickness of the unit cell.

In the presence of imperfect interfaces, the evaluation cannot, in general, be done using equations (3.71). In this thesis, imperfect interfaces are considered in thermal conduction, only. In order to evaluate the phase averaged temperature gradient or heat flux, the following procedures are used.

Consider a generic composite like the one depicted in figure 3.8. Its volume is divided into three parts. The first one is formed by “shells” of finite thickness, e^{IF} , containing the imperfect interfaces, v^{IF} . The second one contains all the matrix material that does not belong to the first part, v^{M} , and the last one contains all the inclusion material that does not belong to the first part v^{I} . In this case the volume integrals can be written without loss of generality as:

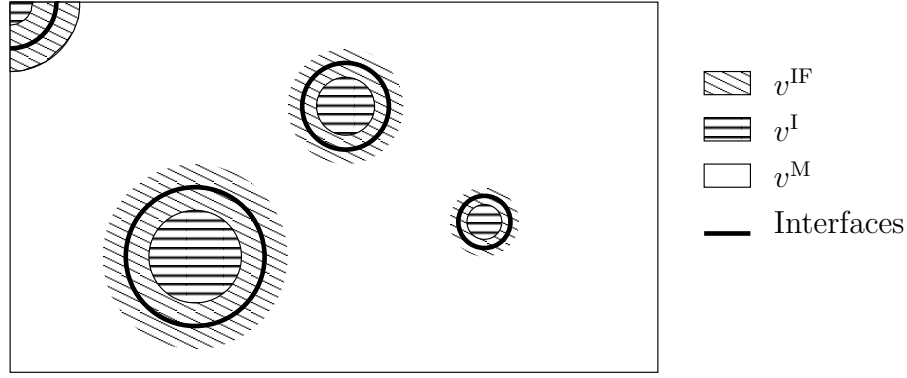


Figure 3.8: Idealized composite material divided into three regions

$$\begin{aligned}
 \int_{v^{UC}} \mathbf{d}(\mathbf{x}) dv &= \int_{v^{IF}} \mathbf{d}(\mathbf{x}) dv + \int_{v^M} \mathbf{d}(\mathbf{x}) dv + \int_{v^I} \mathbf{d}(\mathbf{x}) dv \\
 \int_{v^{UC}} \mathbf{q}(\mathbf{x}) dv &= \int_{v^{IF}} \mathbf{q}(\mathbf{x}) dv + \int_{v^M} \mathbf{q}(\mathbf{x}) dv + \int_{v^I} \mathbf{q}(\mathbf{x}) dv
 \end{aligned} \quad (3.73)$$

Note that the volumes above can always be obtained as the sum of connected volumes.

If the thickness of the shells tends to zero, see figure 3.9, equation (3.73) can be written as:

$$\int_{v^{UC}} \mathbf{d}(\mathbf{x}) dv = \lim_{e^{IF} \rightarrow 0} \left\{ \int_{v^{IF}} \mathbf{d}(\mathbf{x}) dv \right\} + \int_{v^{(m)}} \mathbf{d}(\mathbf{x}) dv + \int_{v^{(i)}} \mathbf{d}(\mathbf{x}) dv \quad (3.74)$$

$$\int_{v^{UC}} \mathbf{q}(\mathbf{x}) dv = \lim_{e^{IF} \rightarrow 0} \left\{ \int_{v^{IF}} \mathbf{q}(\mathbf{x}) dv \right\} + \int_{v^{(m)}} \mathbf{q}(\mathbf{x}) dv + \int_{v^{(i)}} \mathbf{q}(\mathbf{x}) dv \quad (3.75)$$

Furthermore, the thermal gradient in the shells tends to $\frac{\Delta t^{IF}}{e^{IF}} \mathbf{n}$ and the heat flux to $[[\mathbf{q}]^T \mathbf{n}] \mathbf{n}$, when their thickness tends to zero, where Δt^{IF} is the temperature jump at the interface and $\mathbf{n}$ is a unit vector normal to the surface going from the inclusion to the matrix. Then it follows:

$$\begin{aligned}
 \lim_{e^{IF} \rightarrow 0} \left\{ \int_{v^{IF}} \mathbf{d}(\mathbf{x}) dv \right\} &= \int_{s^{IF}} \lim_{e^{IF} \rightarrow 0} \left\{ \int_{e^{IF}} \frac{\Delta t^{IF}}{e^{IF}} \mathbf{n} de \right\} ds \\
 \lim_{e^{IF} \rightarrow 0} \left\{ \int_{v^{IF}} \mathbf{q}(\mathbf{x}) dv \right\} &= \int_{s^{IF}} \lim_{e^{IF} \rightarrow 0} \left\{ \int_{e^{IF}} [[\mathbf{q}]^T \mathbf{n}] \mathbf{n} de \right\} ds
 \end{aligned} \quad (3.76)$$

where s^{IF} represents the boundaries of the interface. As the variations in the normal component are of vanishing importance as the thickness goes to zero, it follows that:

$$\begin{aligned} \lim_{e^{\text{IF}} \rightarrow 0} \left\{ \int_{v^{\text{IF}}} \mathbf{d}(\mathbf{x}) dv \right\} &= \int_{s^{\text{IF}}} \Delta t^{\text{IF}} \mathbf{n} ds \\ \lim_{e^{\text{IF}} \rightarrow 0} \left\{ \int_{v^{\text{IF}}} \mathbf{q}(\mathbf{x}) dv \right\} &= 0 \end{aligned} \quad (3.77)$$

Inserting this result into equation (3.73), and applying the divergence theorem to the integrals of the gradients within each phase the following result is obtained:

$$\begin{aligned} \int_{v^{\text{UC}}} \mathbf{d}(\mathbf{x}) dv &= \int_{s^{\text{IF}}} \Delta t^{\text{IF}} \mathbf{n} ds + \int_{s^{(\text{m})}} t \mathbf{n} ds + \int_{s^{(\text{i})}} t \mathbf{n} ds \\ \int_{v^{\text{UC}}} \mathbf{q}(\mathbf{x}) dv &= \int_{v^{(\text{i})}} \mathbf{q}(\mathbf{x}) dv + \int_{v^{(\text{m})}} \mathbf{q}(\mathbf{x}) dv \end{aligned} \quad (3.78)$$

Therefore the effective heat flux can be calculated following the same procedure as in equations (3.71). The phase average of the thermal gradient equation can be rewritten as:

$$\int_{v^{\text{UC}}} \mathbf{d}(\mathbf{x}) dv = \int_{s^{\text{EXT}}} t \mathbf{n} ds + \int_{s^{\text{INT}}} t \mathbf{n} ds + \int_{s^{\text{IF}}} \Delta t^{\text{IF}} \mathbf{n} ds \quad (3.79)$$

where s^{EXT} are the external surfaces of the unit cell, and s^{INT} the internal surfaces, compare figure 3.9 (left). In figure 3.9 (right) a detail of the internal surfaces, the interfaces and their normals is depicted. As observed, there are two points A' and B' for every “section” of the interface, so that the temperature jump at the interface is $t^{B'} - t^{A'}$. Furthermore, for the point A' there is a point A in the inclusion surface with the same temperature, and the same applies for the point B' and B on the interface and on the matrix's surface. Therefore for every “section” of the interface:

$$\underbrace{t^A - t^B}_{(t\mathbf{n})_{s^{\text{INT}}}} + \underbrace{t^{B'} - t^{A'}}_{(\Delta t^{\text{IF}}\mathbf{n})_{s^{\text{IF}}}} = 0 \quad (3.80)$$

In other words, the contributions of the external surfaces and the interfaces to the phase average of the thermal gradient cancel out and, consequently, it follows that:

$$\int_{v^{\text{UC}}} \mathbf{d}(\mathbf{x}) dv = \int_{s^{\text{EXT}}} t \mathbf{n} ds \quad (3.81)$$

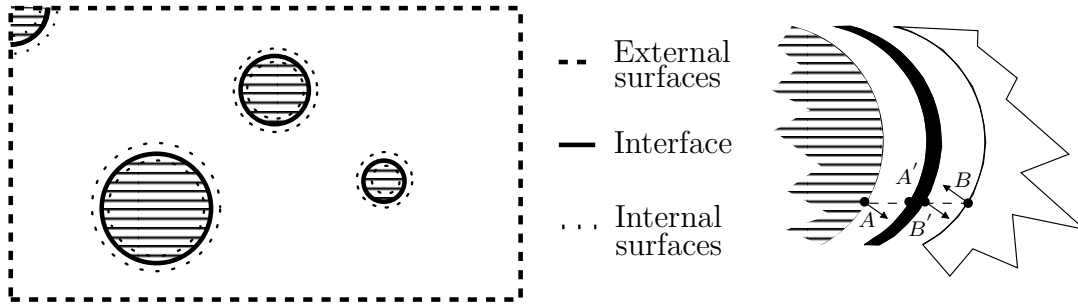


Figure 3.9: Surfaces of the idealized composite depicted in figure 3.8 (left), and detail of these surfaces and their normals (right).

which coincides with the result obtained if the Gauss theorem is applied to a material with perfect interfaces. Note that there is no such behaviour in elasticity.

3.3.3 Windowing methods

In windowing approaches appropriate boundary conditions are applied to simply shaped mesoscopic regions (typically right hexahedral) “cut out” at random positions and orientations from an inhomogeneous material, compare figure 3.10, to calculate the properties of these mesoscopic regions. These properties are called the apparent properties [85] of the inhomogeneous sample. They allow to estimate or bound the effective behaviour of the inhomogeneous material. It is worth noting that, if the boundary conditions applied are periodic, the properties obtained are called effective rather than apparent, because the mesoscopic region together with the boundary conditions represent an infinite periodic material and not a mesoscopic region of an inhomogeneous material. If the mesoscopic region is big enough to be a representative volume element, the properties obtained are independent of the boundary conditions used.

Using variational principles [151], it can be shown that the ensemble average of the apparent properties obtained with a number of equally sized “non-pathological” volume elements, $\mathbf{E}^{\text{appar, NAT}}$, $\mathbf{E}^{\text{appar, ESS}}$, $\mathcal{K}^{\text{appar, NAT}}$, and $\mathcal{K}^{\text{appar, ESS}}$, obtained using uniform essential:

$$\mathbf{u}_i(\mathbf{x}_j) = \langle \boldsymbol{\varepsilon} \rangle_{ik} \mathbf{x}_k \quad t(\mathbf{x}) = [\langle \mathbf{d} \rangle]^T \mathbf{x} \quad (3.82)$$

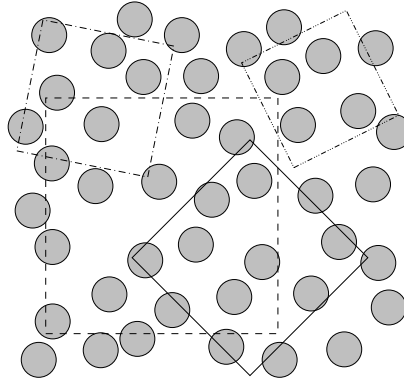


Figure 3.10: Different windows in an inhomogeneous material.

and uniform natural boundary conditions:

$$\sigma_{ij}(\mathbf{x}_k) \mathbf{n}_j = \langle \sigma \rangle_{ik} \mathbf{n}_k \quad [\mathbf{q}(\mathbf{x})]^T \mathbf{n} = [\langle \mathbf{q} \rangle]^T \mathbf{n} \quad (3.83)$$

bound the effective elasticity and conductivity tensors for a given microgeometry [85]:

$$\begin{aligned} \mathbf{E}^{\text{appar, ESS}} &\geq \mathbf{E}^* \geq \mathbf{E}^{\text{appar, NAT}} \\ \mathcal{K}^{\text{appar, ESS}} &\geq \mathcal{K}^* \geq \mathcal{K}^{\text{appar, NAT}} \end{aligned} \quad (3.84)$$

Here the order relation $\mathbf{E}^{\text{appar, ESS}} \geq \mathbf{E}^{\text{appar, NAT}}$ and $\mathcal{K}^{\text{appar, ESS}} \geq \mathcal{K}^{\text{appar, NAT}}$ means that:

$$\begin{aligned} [\mathcal{Z}^{\text{any}}]^T (\mathbf{E}^{\text{appar, ESS}} - \mathbf{E}^{\text{appar, NAT}}) \mathcal{Z}^{\text{any}} &\geq 0 \\ [\mathbf{z}^{\text{any}}]^T (\mathcal{K}^{\text{appar, ESS}} - \mathcal{K}^{\text{appar, NAT}}) \mathbf{z}^{\text{any}} &\geq 0 \end{aligned} \quad (3.85)$$

for any second order symmetric tensor, $\mathcal{Z}^{\text{any}}$, or any vector, $\mathbf{z}^{\text{any}}$, different from the zero second order tensor or the zero vector, respectively.

Alternatively, mixed uniform boundary conditions (MUBCs) may be used. MUBCs fulfill the Hill macrohomogeneity condition, eqn. (3.5), for elasticity or its equivalent for heat conduction, eqn. (3.6). For example, for the heat conduction case, MUBCs applied to a right hexahedron consist of essential boundary conditions on two parallel faces of the volume and natural conditions to the other faces or vice versa. It can be shown, [79; 87], that the apparent properties obtained using the MUBC lie between the natural and the essential apparent properties.

The previous results hold for perfect interfaces or imperfect interfaces provided there is no discontinuity of the vector $\mathbf{x} \otimes \mathbf{n}$ on the interface, see [78], where $\otimes$ represents the tensor

product. They can be extended to imperfect interfaces where there is a discontinuity of $\mathbf{x} \otimes \mathbf{n}$, but additional terms must be taken into account.

All the boundary conditions described fulfill the Hill condition, which for the heat conduction case can be rewritten as:

$$\int_{s^{\text{UC}}} \left([\mathbf{q}(\mathbf{x})]^T \mathbf{n} - \langle \mathbf{q} \rangle^T \mathbf{n} \right) (t(\mathbf{x}) - \langle \mathbf{d} \rangle \mathbf{x}) \, ds = 0 \quad (3.86)$$

where $\mathbf{x}$ is the position vector.

Chapter 4

Study of the thermal conduction behaviour of Diamond Reinforced Metal Matrix Composites using Micromechanics of Materials

In this chapter some of the methods described in chapter 3 are applied to studying the thermal conduction behaviour of Diamond Reinforced Metal Matrix Composites (DRMMCs). The discussion takes into account several aspects of the microgeometry of the material, such as volume fraction, imperfect interfaces between the constituents, and size, shape and orientation of the particles. Furthermore, monodisperse and polydisperse particle size distributions are studied.

4.1 Literature review

The effective heat conduction properties of composites are mainly affected by the following factors:

- Heat conduction properties of the constituents
- Volume fractions of the constituents
- Shapes of the reinforcements

- Sizes of the reinforcements
- Orientations of the reinforcements
- Interfaces between the constituents

Numerical methods as e.g. PMAs, see section 3.3.2, can, in principle, take into account all of these factors and some others, such as the arrangement of the particles, but they are computationally expensive, see [47; 102; 119].

Analytical or semi-analytical methods, can be used instead. Whilst some methods that take into account a number of the previous factors but the interfaces can be found in the literature, see e.g. [44; 91] and the references therein, works considering imperfect thermal interfaces are less numerous, and works taking into account all of the factors are scarce, see [119].

The effects of the interfaces are mainly captured by using an interface of zero thickness or by using an interphase model of finite thickness.

Examples of works using the concept of zero-thickness interface can already be found in the pioneering works of Benveniste and Miloh [14] or Hasselman and Johnson [74]. Hasselman and Johnson extended the work of Maxwell to non-ideal interfaces for obtaining estimates of the effective conductivity of composite materials reinforced with spheres or aligned continuous fibers, see section 3.2.2.1. Benveniste and Miloh studied the effective conductivity of dilute composites reinforced with spheroidal inclusions the interfaces of which are imperfect. Extensions to non-dilute volume fractions were done by Benveniste [10] by using a generalized self consistent scheme and a Mori-Tanaka approach, and by Chiew and Glandt [30] using a second order approximation. Different approximations and/or development of the previous methods were done by Lu, Chen, Duschlbauer, Ganapathy, Duan et al. as well as Böhm and Nogales. Lu [98] proposed an equivalent inclusion model for studying the thermal conductivity of composites reinforced by aligned spheroids having the same size, shape and constant interfacial parameter. Chen [29] studied the thermal conduction behaviour of a circular inclusion with variable interfacial parameter. Duschlbauer et al. [48] analyzed the effect of the imperfect interfaces by replacing the inclusion with the imperfect interface by an inclusion with perfect interface but reduced conductivity, extensions of this method are used in the present work. Ganapathy et al. [58] combined effective medium theory and the finite difference method for studying composites reinforced with cylindrical particles. Duan et al. [43] used the average t -matrix approximation of the multiple-scattering approach to take into account the effect of three

types of imperfect bonding. Böhm and Nogales [20] extended the work of Duschlbauer to studying non-ellipsoidal particle shapes and size distributions.

Works capturing the effect of the interfacial barrier using a coating of finite thickness with very low conductivity are less numerous. Benveniste and Miloh [15] investigated coated ellipsoidal inclusions, the coating being represented by two confocal ellipsoids. Dunn and Taya [46] combined the coating concept, corresponding to a variable interface parameter, with a Mori–Tanaka approach for studying the thermal conduction of composites with imperfect interfaces. Nan et al. [117] estimated the effective thermal conductivity by using coatings of constant thickness. Zou [171] derived analytical expressions for the transverse thermal conductivities of unidirectional fibre composites with thermal barrier by using an electrical analogy and unit cell models.

4.2 Material studied

Throughout this chapter, the same set of thermophysical constituent material parameters, which correspond to diamond particles embedded in matrix of commercially pure aluminum, was used for all simulations.

Table 4.1 lists the thermal conductivities, $\mathcal{K}$, used for the constituents. Diamond has cubic symmetry and, accordingly, has isotropic conduction properties. Therefore, both constituents have isotropic conductivity. The conductances for the $\{100\}$ and $\{111\}$ faces, see figure 4.1 (left), of synthetic diamond particles embedded in aluminum given in table 4.2 are preliminary estimates that aim at accounting for differences in the behaviour of the two sets of faces, the lower reactivity of the $\{111\}$ faces leading to reduced bonding and to a lower interfacial conductance [137].

Table 4.1: Thermal conductivities of the constituents.

	$\mathcal{K}(i, i)$ [W/Km]
Diamond	1800
Aluminum	237

4.3 Monodisperse particle size distributions

In this section only composites reinforced with particles of the same size and shape are studied. Two geometries are considered for the reinforcements, spheres and regular cubo-octahedra, the latter being depicted in figure 4.1 (left), and the real particles in figure 4.1 (right). The radius of the cubo-octahedral particles, r , is defined as the radius of the sphere into which the cubo-octahedra can be inscribed. In the first part, some analytical/semianalytical methods for obtaining the effective properties of these composites are studied. In the second part, some numerical methods are used to test the results obtained with the analytical methods and for studying in detail the local behaviour of these composites.

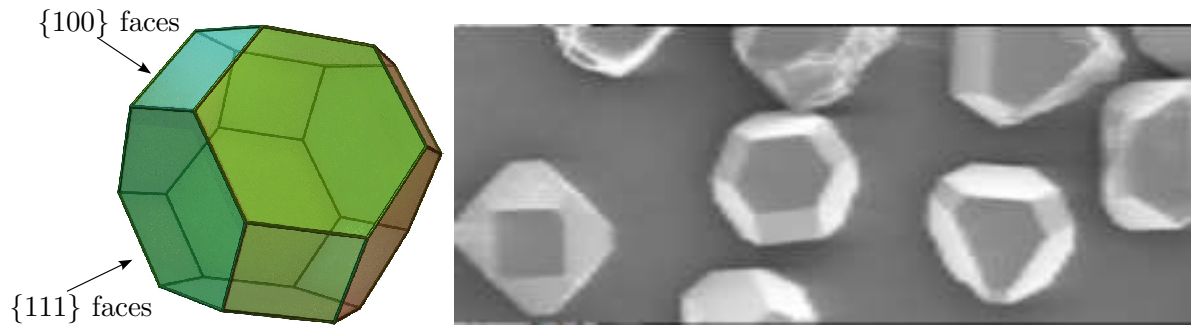


Figure 4.1: Cubo-octahedral geometry of the diamond particles used in the numerical models (left) and actual shapes of diamond particles (right) (courtesy EMPA).

4.3.1 Analytical/Semianalytical methods

DRMMCs are complex materials to model. They are reinforced by non-ellipsoidal and non-aligned particles with inhomogeneously distributed interfacial conductance. Due to

Table 4.2: Estimates for the thermal conductances of the diamond-aluminum interfaces, [137].

$h_{\beta_{\{100\}}}$ [MW/Km ²]	$h_{\beta_{\{111\}}}$ [MW/Km ²]
100	20

the complex shapes of the reinforcements, it is easier to study the effects of the interfacial conductance via models using an interface of zero thickness rather than by methods based on coatings of finite thickness that are more restricted to ellipsoidal and cylindrical reinforcement shapes. Within the “interface of zero thickness” methods only MFMs allow to simultaneously study all of the factors described above [43]. Among the MFMs a MTM-scheme was selected because of its simplicity and efficiency. In the following, the MTM replacement inclusion (RMTM) method of Duschlbauer [48] is extended to studying DRMMCs.

4.3.1.1 Extension of Duschlbauer’s method

The main idea behind the method, see section 3.2.2.2 for a detailed description, is the replacement of a particle with an imperfect interface by a less conducting particle having a perfect interface, so that the effective conductivity of a dilute composite reinforced by a single inclusion is not affected by this change. The approach can also account for non-spheroidal particle shapes. For ellipsoidal particles with isotropic conductivity and a homogeneous distribution of the interfacial conductance analytical solutions can be found for the dilute thermal gradient concentration tensor of the inclusion, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, and the replacement conductivity of the inclusion, $\mathcal{K}^{(i,r)}$, see [47]. However, for the present case this is not possible and numerical procedures are needed for extracting $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$.

In order to obtain $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$, dilute models consisting of a single reinforcement embedded in large matrix regions are employed, see figure 4.2 (left). These volume elements are subjected to three linearly independent applied temperature gradients. The averaged heat fluxes in the phases and the effective heat flux are then evaluated from the phase averaged fields in the inhomogeneity, see section 3.3.2.2.3. The dilute heat flux concentration tensor, $\bar{\mathcal{B}}_{\text{dil}}^{(i,r)}$, follows directly from the phase averaged heat fluxes and the effective heat flux, equations (3.17). The effective conductivity of the dilute unit cell, $\mathcal{K}_{\text{dil}}^*$, can be evaluated from the effective heat flux and the effective thermal gradient which is known a priori. Using equation (4.2) for the dilute case, and the consistency condition, equation (3.44), $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$ are obtained.

Once the replacement tensors, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$, are known they are inserted into the Mori-Tanaka scheme, eqns. (3.31)–(3.33), in lieu of the “standard ones”, $\bar{\mathcal{A}}_{\text{dil}}^{(i)}$ and $\mathcal{K}^{(i)}$. It is worth noting that this procedure can be applied to any particle shape. Furthermore, this procedure is valid for any MFM.

Alternatively, one can directly extract $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, see [47], in this case three independent heat fluxes must be applied. The volume integrals of the thermal gradient over the volume of the cube or the diamond can be calculated by transforming them into surface integrals, see section 3.3.2.2.3. Note, that the surface integral over the diamond surface must contain the interface so that the interfacial temperature jumps are accounted for. The unit cells used for the dilute models are, usually, meshed very finely in the neighborhood of the inclusion and rather coarsely at the boundaries of the cube, see figure 4.2 (right). This may lead to numerical errors when approximating the surface integral on the boundaries of the cube. For dilute unit cells, the fields on the boundary are nearly homogeneous and the problem is avoided, but if the unit cell is not dilute the fields on the boundaries may be rather inhomogeneous leading to non trivial numerical errors.

It is worth noting that both methods for extracting the dilute concentration tensors are equivalent. Recall that in the direct evaluation of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ the temperature jumps at the interface are taken into account and therefore equations (3.18) hold. Furthermore, equations (3.23) always hold for the matrix of the composite with imperfect interfaces. Therefore, it follows that the concentration tensors, as calculated above, of the composite with imperfect interfaces, are not independent, and the results obtained with both methodologies are equivalent.

In a dilute composite, an inclusion is embedded in an infinite matrix. How to approximate this with numerical models, or in other words, how small must be the volume fraction so that the composite can be considered dilute, is an open question. Therefore it must be studied how the “diluteness” of the composite affects the estimations of the method. Furthermore, the FE mesh may play a role, too. In the following both aspects are studied in detail.

For studying the influence of dilute volume fraction, the $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$ tensors obtained from different volume elements, such as the one shown in figure 4.2 (left), are compared. Recall that the reinforcement is a cubo-octahedral particle. The volume elements studied follow the material parameters in tables 4.1 and 4.2, and they differ in the reinforcement volume fraction, the boundary conditions used, and the radius of the particle. The volume fractions used are 0.00001, 0.0001, 0.001, 0.01, 0.1, and 0.2. Three types of boundary conditions are considered, Uniform Thermal Gradient boundary conditions (UTGBC), Periodicity boundary conditions (PBC), and Uniform Heat Flux boundary conditions (UHFBC), that correspond to essential, periodicity, and natural boundary conditions respectively, see section 3.3.3. Three different particle radii, $1\mu\text{m}$, $10\mu\text{m}$ and $1000\mu\text{m}$, are studied, which

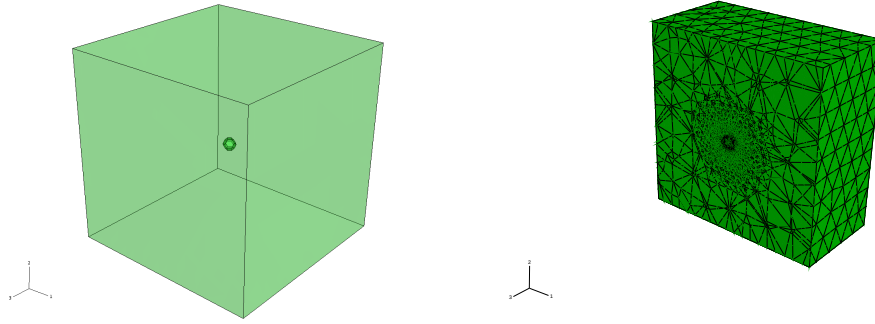


Figure 4.2: Geometry (left) and mesh (right) of a dilute volume element used for obtaining the replacement concentration and conduction tensors.

are smaller than, comparable to, and larger than, respectively, the critical radius, r_c , pertinent to the chosen material parameters. The critical radius is the radius below which even highly conductive particles fail to increase the overall conductivity of the composite. This size effect is due to the presence of the interfacial resistances between reinforcements and matrix, and it is a well known phenomenon, see e.g. [53; 96]. The critical radius depends not only on the constituent's properties and the interfaces between them, but also on the shapes of the particles, see figures 4.11 and 4.12. In this case (cubo-octahedral particles which inhomogeneous distribution of the interfacial conductance) the critical radius is $8.335\mu\text{m}$, see figure 4.10. It was obtained numerically by interpolation, in some cases, e.g, spherical particles with homogeneous distribution of the conductance, it can be obtained analytically, see equation (3.43). In the following the results obtained are compiled.

As DRMMCs are reinforced by equiaxed particles and the assumed distribution of the interfacial conductance does not break the cubic symmetry of the material, dilute concentration tensors, effective conductivities, ... are diagonal tensors with diagonal elements of equal value, and they can be described by one of these elements.

The behaviour of the replacement conductivity and the dilute replacement concentration tensor can be divided into 5 cases: $r \ll r_c$, $r < r_c$, $r \approx r_c$, $r > r_c$ and $r \gg r_c$. When $r \ll r_c$, the inclusion behaves as a void, the replacement conductivity is zero and the diagonal elements of the replacement dilute inclusion concentration tensor are greater than unity. When $r < r_c$, see table 4.3, the replacement conductivity is smaller than the conductivity of the matrix, and the diagonal elements of the replacement dilute inclusion concentration tensor are higher than unity, i.e., the particle does not succeed in increasing

the effective thermal conductivity of the composite. When $r \approx r_c$, see table 4.4, the diagonal elements of the replacement dilute inclusion concentration tensor are approximately 1, and the replacement conductivity approaches the value of the conductivity of the matrix, in other words the composite behaves like a homogeneous material. If $r > r_c$, see table 4.5, the replacement conductivity is higher than that of the matrix, and the diagonal terms of the replacement dilute inclusion concentration tensor are lower than unity, i.e., the reinforcements do increase the effective conductivity of the composite. If $r \gg r_c$ the replacement conductivity approaches the conductivity of the inclusion and the diagonal terms of the replacement dilute inclusion concentration tensor approach the dilute concentration tensor, i.e., the composite behaves as a composite with perfect interfaces.

This behaviour of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ is similar to the one obtained for the same material properties but spherical reinforcements. For this case the $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ obtained are diagonal tensors, recall that the conductivities are isotropic. Therefore, equation (3.29) can be decomposed into three uncoupled scalar equations:

$$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) = \frac{1}{1 + \mathcal{S}(i, i) \left(\frac{\mathcal{K}^{(i,r)}(i, i)}{\mathcal{K}^{(m)}(i, i)} - 1 \right)} \quad (4.1)$$

which are monotonously decreasing functions of the conductivity contrast, which tends to zero when $\mathcal{K}^{(i,r)}(i, i) \rightarrow \infty$, and which equals 1 when $\mathcal{K}^{(i,r)}(i, i) = \mathcal{K}^{(m)}(i, i)$. Furthermore $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) \rightarrow 1.5$ when $\mathcal{K}^{(i,r)}(i, i) \rightarrow 0$, and $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) \rightarrow \frac{3\mathcal{K}^{(m)}(i, i)}{2\mathcal{K}^{(m)}(i, i) + \mathcal{K}^{(i)}(i, i)} \approx 0.31266$ when $\mathcal{K}^{(i,r)}(i, i) \rightarrow \mathcal{K}^{(i)}(i, i)$. These values approach the correspondent values, 1.44 and 0.34, obtained for cubo-octahedral reinforcements, see tables 4.3 and 4.5. Nevertheless, the shape effect can be observed.

The behaviour of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ with the volume fraction and the boundary conditions follows, almost, a clear pattern. In the following, the boundary conditions are arranged in a natural order: UHFBC $\leq$ PBC $\leq$ UTGBC. Let's call this order boundary condition ordering. A variable increases its value with the boundary condition ordering, when the value of this variable is higher for the UTGBC than for the PBC, and higher for the PBC than for the UHFBC. For $r < r_c$, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ decreases with the volume fraction and with the boundary condition ordering. For $r > r_c$, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ increases with the volume fraction and the boundary condition ordering, as observed in tables 4.3–4.5. However, some exceptions to this pattern can be observed, mainly in the UTGBC case. Because surface integrals at the boundaries of the cube are needed for extracting the replacement tensors in this case, this behaviour may be due to small numerical errors as explained above.

To explain the above trends, the following equation which is analogous to equation (3.23):

$$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)} = \mathcal{R}^{(i,r)} \bar{\mathcal{B}}_{\text{dil}}^{(i,r)} \mathcal{K}_{\text{dil}}^* \quad (4.2)$$

is needed. For the material studied all matrices are diagonal with equal components, therefore, equations (3.17), (3.7) and (4.2) can be reduced to scalars. If we let all the variables vary, the following equations are obtained:

$$\begin{aligned} \Delta \bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) &= \mathcal{R}^{(i,r)}(i, i) [\bar{\mathcal{B}}^{(i,r)}(i, i) \Delta \mathcal{K}_{\text{dil}}^*(i, i) + \dots \\ &\dots + \Delta \bar{\mathcal{B}}^{(i,r)}(i, i) \mathcal{K}_{\text{dil}}^*(i, i) + \Delta \bar{\mathcal{B}}^{(i,r)}(i, i) \Delta \mathcal{K}^{*, \text{dil}}(i, i)] \\ \Delta \mathbf{q}_{\text{dil}}^*(i, i) &= \Delta \mathcal{K}_{\text{dil}}^*(i, i) \mathbf{d}_{\text{dil}}^*(i, i) \\ \Delta \bar{\mathcal{B}}^{(i,r)}(i, i) &= \frac{\Delta \mathbf{q}^{(i)} - \bar{\mathcal{B}}^{(i,r)}(i, i) \Delta \mathbf{q}_{\text{dil}}^*(i, i)}{\mathbf{q}_{\text{dil}}^*(i, i) + \Delta \mathbf{q}_{\text{dil}}^*(i, i)} \end{aligned} \quad (4.3)$$

where $\bar{\mathcal{A}}^{(i)}(i, i)$, $\mathcal{R}^{(i)}(i, i)$, $\bar{\mathcal{B}}^{(i)}(i, i), \dots$ are the initial values, and $\Delta \bar{\mathcal{A}}^{(i)}(i, i)$, $\Delta \mathcal{R}^{(i)}(i, i)$, $\Delta \bar{\mathcal{B}}^{(i)}(i, i), \dots$ are the values of the increment of the variables. Recall, that the effective thermal gradient has been considered constant in all the unit cells, and therefore its increment is always zero. Note that the effective thermal gradient can be kept constant without loss of generality because of the isotropy of the material studied. Combining equations (4.3), the following result can be obtained:

$$\Delta \bar{\mathcal{A}}^{(i,r)}(i, i) = \frac{\Delta \mathbf{q}^{(i)}}{\mathbf{q}_{\text{dil}}^*(i, i) + \Delta \mathbf{q}_{\text{dil}}^*(i, i)} \Delta \mathcal{K}_{\text{dil}}^*(i, i) \quad (4.4)$$

which will be used in the following for studying the influence of the boundary conditions and the volume fraction. Note that for very small volume fractions, the increment of the heat flux in the inclusion and the effective conductivity may be very small, which may produce an increment of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ that is very small and comparable to numerical fluctuations.

The influence of the volume fraction depends on the radius of the particle:

- For $r < r_c$: As the replacement conductivity of the particle is smaller than the conductivity of the matrix, if the volume fraction increases, the dilute effective conductivity decreases. The higher the volume fraction, the higher the averaged flux in the inclusion. Obviously, the effective heat flux won't change sign. Therefore $\bar{\mathcal{A}}^{(i,r)}$ decreases with the volume fraction.
- for $r = r_c$: the material behaves as a homogeneous material and the replacement tensors are not affected by the volume fraction.

- For $r > r_c$: In this case, the replacement conductivity of the inclusion is bigger than the conductivity of the matrix and therefore the dilute effective conductivity increases with the volume fraction. As the effective heat flux and the average heat flux in the inclusion increase as well, it is clear that $\bar{\mathcal{A}}^{(i,r)}$ increases with the volume fraction.

The behaviour of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ for the different boundary conditions depends, too, on the radius of the particle. The dilute conductivity increases with the boundary condition, see section 3.3.3. The increment of the effective heat flux does not change the sign of the effective heat flux. The increment of the average heat flux in the inclusion depends on the radius of the inclusion. The higher the boundary condition ordering, the higher the effective heat flux, recall that the effective thermal gradient is considered a constant. If $r > r_c$ it is clear that the average heat flux in the inclusion increases and therefore $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ increases with the boundary condition ordering. If $r < r_c$ the behaviour of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ depends on the sign of the increment of the average heat flux.

Whilst the behaviour of the $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ can be more or less predicted, the behaviour of $\mathcal{K}^{(i,r)}$ is more complex and there is no clear pattern. This may be due to the complex form of the consistency condition, equation (3.44). Furthermore, it can be noted that the replacement conductivity does not necessarily obtain its minimum and maximum values for natural and essential boundary conditions, respectively.

For a dilute composite, the same results must be obtained independently of the boundary conditions used. As observed in tables 4.3–4.5, up to volume fractions of 0.01 the results obtained are very similar for both the replacement conductivity and the replacement gradient concentration tensor. For volume fraction smaller than 0.01, the particle does not “feel” the boundary conditions and the values of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$ and $\mathcal{K}^{(i,r)}$ remain constants. In other words, the microfields in the particle and the surrounding matrix are not affected by the boundary conditions for volume fraction smaller than 0.01, as can be seen in figures 4.3–4.5.

In figures 4.3–4.5 fringe plots of the heat flux magnitude in dilute volume elements exposed to thermal loadings in horizontal direction are plotted, the boundary conditions applied being UTGBC, PBC, and UHFBC respectively. In each row, fringe plots for UC reinforced with particles of the same radius are represented for $r < r_c$, $r \approx r_c$, and $r > r_c$ (from top to bottom). All the volume elements in a row are exposed to the same thermal loading so that they can be compared. The columns represent different volume fractions, 0.0001, 0.001, 0.01 and 0.1 (from left to right). In all the pictures it can be observed how

Table 4.3: Dilute replacement thermal gradient concentration tensor, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, and replacement conductivity tensor, $\mathcal{K}^{(i,r)}$, of dilute volume elements (see figure 4.2 (left)) as a function of the reinforcement volume fraction (VF), and the boundary conditions used to calculate it: Periodic boundary conditions (PBC), uniform heat flux boundary conditions (UHFBC), and uniform thermal gradient boundary conditions (UTGBC). The isotropic tensors are represented by 1 term. Material parameters follow tables 4.1 and 4.2. Case: $r < r_c$.

$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) []$						
VF []	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	1.43950	1.43945	1.43874	1.43219	1.36924	1.30588
PBC	1.43951	1.43947	1.43891	1.43388	1.38829	1.34799
UHFBC	1.43159	1.43691	1.43624	1.43377	1.40240	1.37050

$\mathcal{K}^{(i,r)}(i, i) [\text{W/Km}]$						
VF []	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	35.7340	35.7335	35.7342	35.7293	35.6665	35.5170
PBC	35.7340	35.7335	35.7341	35.7266	35.5421	35.1348
UHFBC	35.9316	35.7977	35.8051	35.7765	35.6825	35.5872

Table 4.4: Dilute replacement thermal gradient concentration tensor, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, and replacement conductivity tensor, $\mathcal{K}^{(i,r)}$, of dilute volume elements (see figure 4.2 (left)) as a function of the reinforcement volume fraction (VF), and the boundary conditions used to calculate it: Periodic boundary conditions (PBC), uniform heat flux boundary conditions (UHFBC), and uniform thermal gradient boundary conditions (UTGBC). The isotropic tensors are represented by 1 term. Material parameters follow tables 4.1 and table 4.2. Case: $r \approx r_c$.

$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) []$						
VF	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	0.98976	0.98976	0.98991	0.99036	0.99759	1.00838
PBC	0.98973	0.98976	0.98990	0.99028	0.99905	1.01414
UHFBC	0.98959	0.98986	0.99022	0.99016	0.99323	0.99860

$\mathcal{K}^{(i,r)}(i, i) [\text{W/Km}]$						
VF	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	273.193	273.200	273.156	273.240	273.882	275.950
PBC	273.205	273.200	273.156	273.241	273.782	275.378
UHFBC	273.242	273.171	273.063	273.205	273.262	271.654

Table 4.5: Dilute replacement thermal gradient concentration tensor, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, and replacement conductivity tensor $\mathcal{K}^{(i,r)}$ of dilute volume elements (see figure 4.2 (left)) as a function of the reinforcement volume fraction (VF), and the boundary conditions used to calculate it: Periodic boundary conditions (PBC), uniform heat flux boundary conditions (UHFBC), and uniform thermal gradient boundary conditions (UTGBC). The isotropic tensors are represented by 1 term. Material parameters follow tables 4.1 and table 4.2. Case: $r > r_c$.

$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) []$						
VF	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	0.34120	0.34124	0.34153	0.34429	0.37513	0.41879
PBC	0.34121	0.34124	0.34146	0.34363	0.36774	0.40160
UHFBC	0.34077	0.34486	0.34401	0.34500	0.35800	0.37790

$\mathcal{K}^{(i,r)}(i, i) [\text{W/Km}]$						
VF	0.00001	0.0001	0.001	0.01	0.1	0.2
UTGBC	1676.23	1676.23	1676.20	1676.22	1677.18	1679.59
PBC	1676.23	1676.23	1676.20	1676.24	1678.12	1682.25
UHFBC	1678.52	1658.76	1663.45	1665.84	1677.45	1668.52

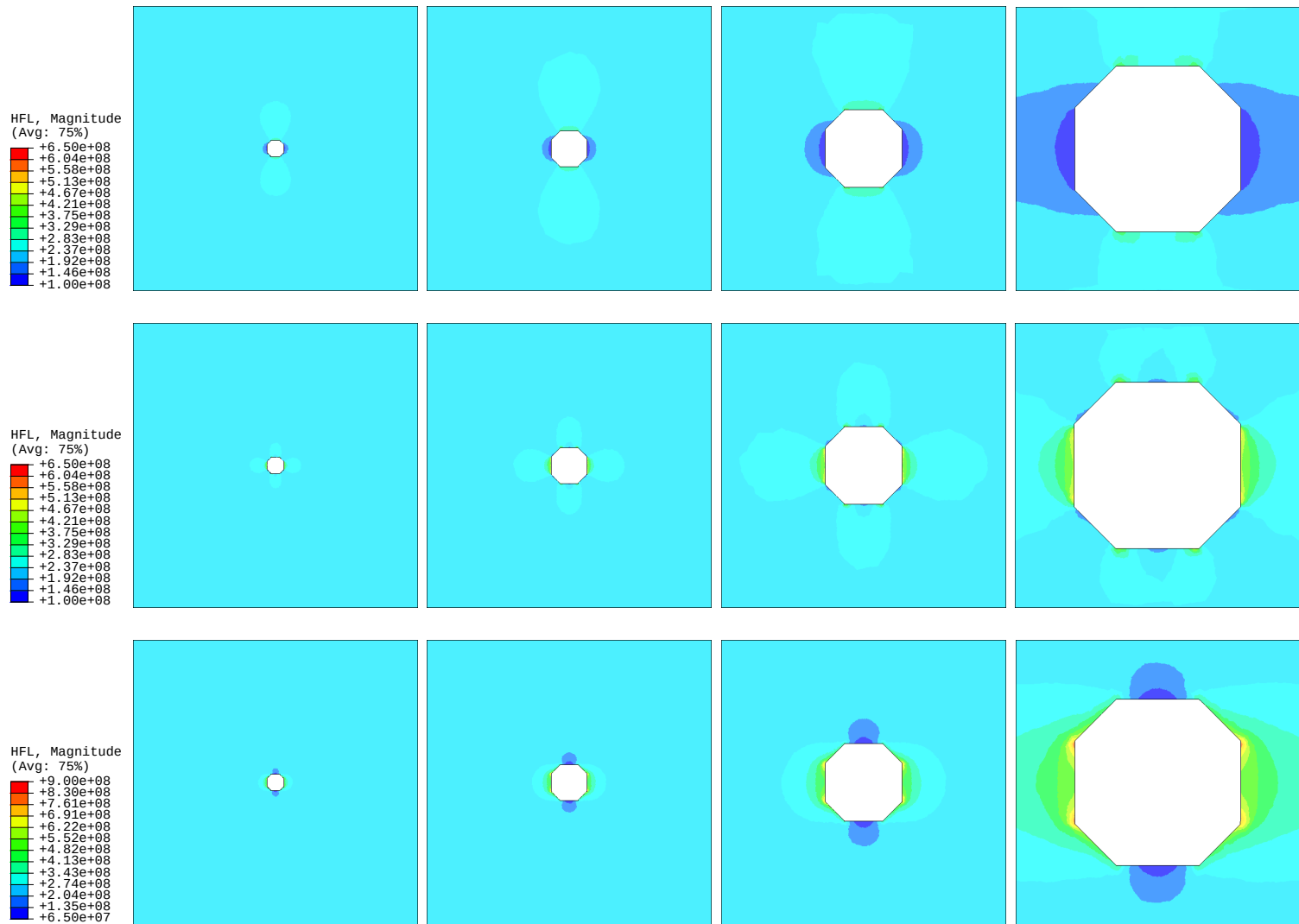


Figure 4.3: Fringe plots of the heat flux magnitude in the matrix of DRMMCs in a central section of volume elements exposed to a unit thermal gradient in horizontal direction. Material parameters follow tables 4.1 and table 4.2. Volume fractions: 0.0001, 0.001, 0.01 and 0.1 (from left to right), and particle radii: $r < r_c$, $r \approx r_c$, and $r > r_c$ (from top to bottom), all the UCs in the same row have the same particle radius. TGUBC are applied to all the volume elements.

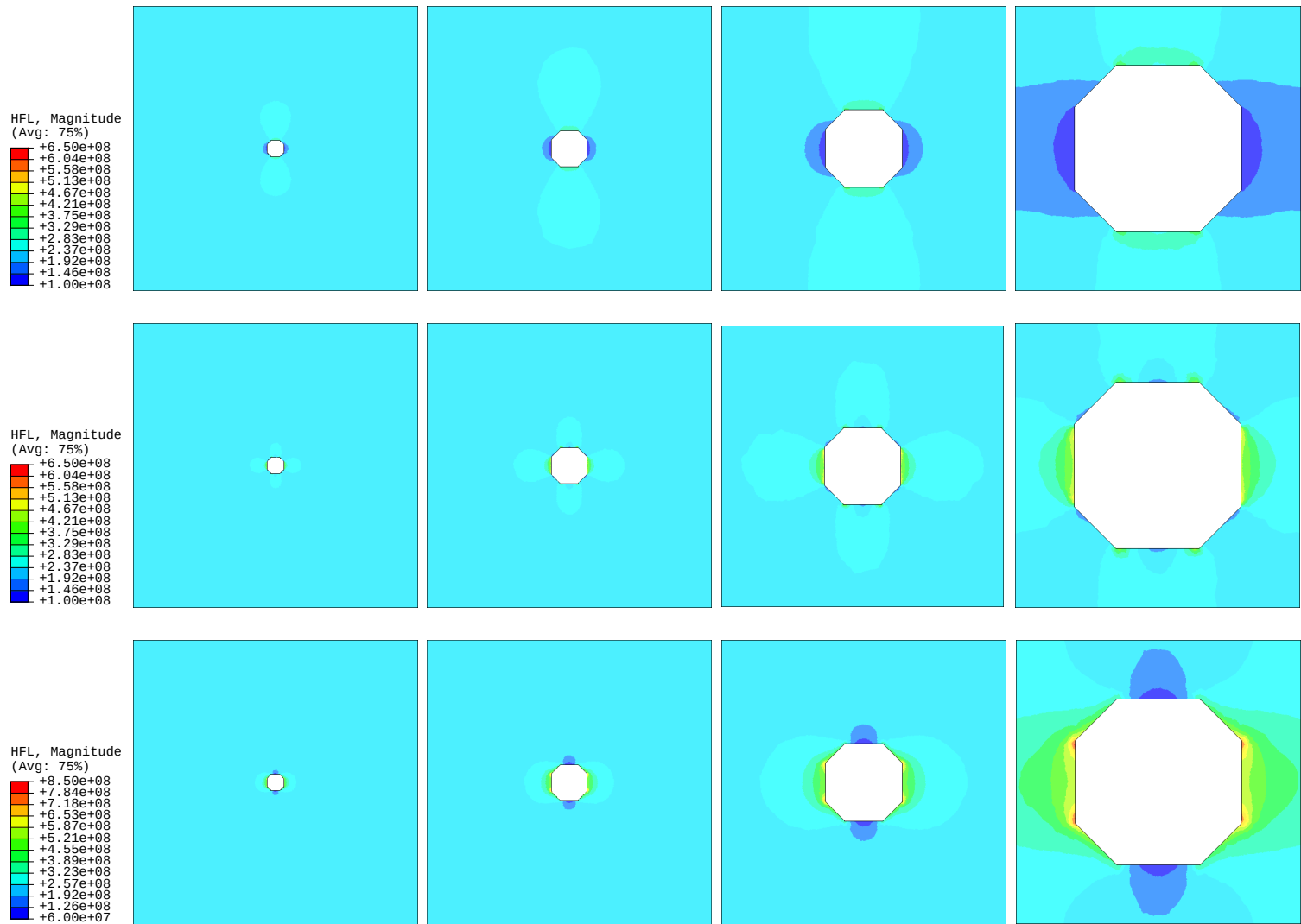


Figure 4.4: Fringe plots of the heat flux magnitude in the matrix of DRMMCs in a central section of UCs exposed to a unit thermal gradient in horizontal direction. Material parameters follow tables 4.1 and table 4.2. Volume fractions: 0.0001, 0.001, 0.01 and 0.1 (from left to right), and particle radii: $r < r_c$, $r \approx r_c$, and $r > r_c$ (from top to bottom), all the UCs in the same row have the same particle radius. PBC are applied to all the UCs.

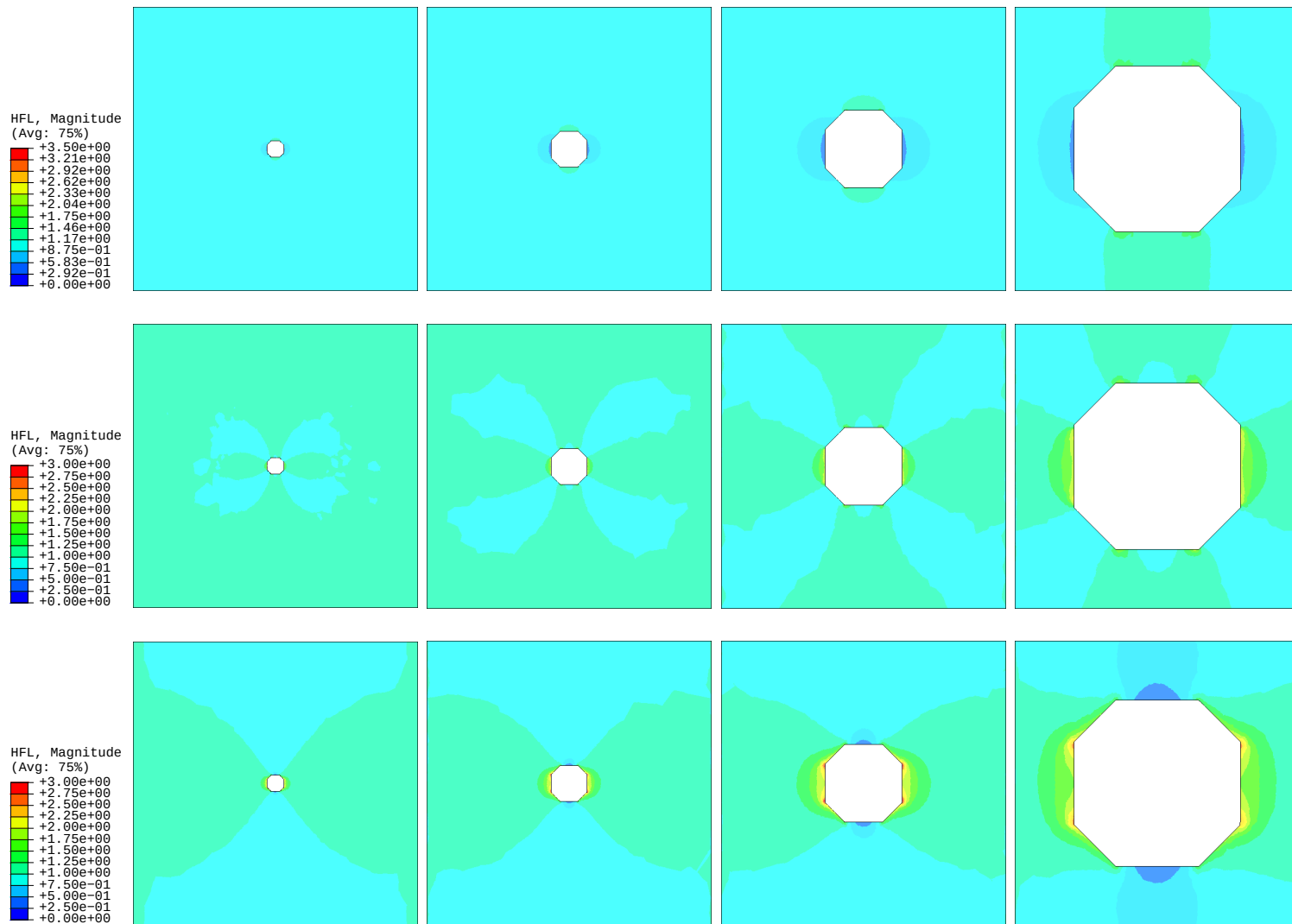


Figure 4.5: Fringe plots of the heat flux magnitude in the matrix of DRMMCs in a central section of volume elements exposed to a unit heat flux in horizontal direction. Material parameters follow tables 4.1 and table 4.2. Volume fractions: 0.0001, 0.001, 0.01 and 0.1 (from left to right), and particle radii: $r < r_c$, $r \approx r_c$, and $r > r_c$ (from top to bottom), all the UCs in the same row have the same particle radius. HFUBC are applied to all the volume elements.

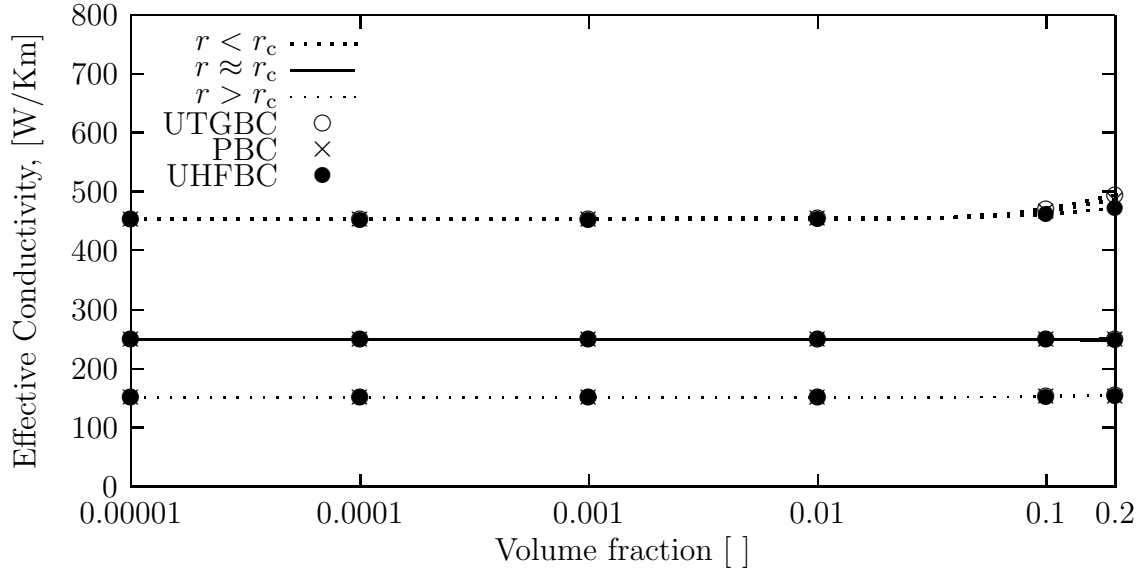


Figure 4.6: Estimates of the effective conductivity of a DRMMC with a volume fraction of 0.34 using a RTM with material parameters following tables 4.1 and 4.2, as a function of the volume fraction and the boundary conditions of the numerical models used for obtaining the replacement tensors.

the microfields in the inclusion are affected by the boundary conditions, the “worst” case being $r > r_c$ because the microfields are most inhomogeneous. The PBC case, figure 4.4, has a clear physical meaning. As the volume fraction increases, the particle “feels” the presence of the neighboring particles, and the field in its surroundings is clearly perturbed. Below a volume fraction of 0.01, the influence of the boundary conditions is negligible.

The replacement tensors obtained from the dilute volume elements were used to estimate the effective conductivity of the material studied with a reinforcement volume fraction of 0.34, see figure 4.6. As can be observed the estimated effective conductivity does not change for volume fractions of the volume elements below 0.01. For volume fractions higher than 0.01 the influence becomes noticeable for $r > r_c$. This indicates that the $\frac{1}{f_{\text{dil}}}$ term in the consistency relations, eqn. (3.44), can account for volume fraction effects only in the dilute range. For all volume fractions the effective conductivities using the replacement tensors obtained with essential and natural boundary conditions bound the corresponding effective conductivities using the replacement tensor obtained with PBC.

Therefore, it can be concluded, that the “diluteness” of the volume element used to calculate the replacement tensors does not play an important role on the effective conductivity of the composite, provided the value of the dilute volume fraction is below certain limits. For the material tested UCs with a volume fraction smaller than 0.01 can be considered dilute for linear heat conduction.

The discontinuity of the normal vector at edges on the surface of the diamond may lead to some numerical problems when implementing the interfacial conductance into FE models. Recall that the nodes at the edges do not have a clearly defined normal. To study this effect, a mesh refinement study was done.

The same dilute volume elements, see figure 4.2 (left), with a dilute volume fraction of approximately 0.001, as in the previous study are used. Note that for the volume fraction used, the results are independent of the applied boundary conditions. The dilute volume elements were meshed using different mesh densities, described by the number of elements per edge of the cubo-octahedral particles. In table 4.6, the dilute concentration tensors of DRMMCs are presented as functions of the mesh density. Whilst $\mathcal{K}^{(i,r)}$ decreases with the mesh density, there is no clear pattern of the evolution of $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$. For the values studied, the influence is smaller than for changes of the volume fractions of the dilute volume elements.

In figure 4.7, the effective conductivity of the material was estimated using the replacement tensors obtained for the different mesh densities. The influence in the results is negligible, even for low mesh densities.

It can then be concluded that the mesh densities do not have a major influence on the estimates obtained with the method, provided the meshes are sufficiently fine to capture the geometry of the particle.

In order to check the numerical evaluation of the replacement tensors, the RMTM and the Hasselman–Johnson method were applied to a material reinforced with spherical particles and with an homogeneous distribution of the interfacial conductance, using the thermal conductivities listed in table 4.1, and an isotropic thermal conductance of 27.7 MW/Km². Recall that for this case both methods should lead to exactly the same results, because the only difference between them is that for the RMTM the replacement tensors are calculated numerically, and for the other method they are calculated analytically, see section 3.2.2.1. Evidently, the replacement concentration tensors could be obtained analytically for this case. In figure 4.8 both methods are compared for different reinforcement volume fractions and three different particle radii: $r < r_c^s$, $r = r_c^s$, and $r > r_c^s$, where $r_c^s = 9.85\mu\text{m}$ is the critical radius for spherical particles, which can be obtained using

Table 4.6: Dilute replacement thermal gradient concentration tensor, $\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}$, and replacement conductivity tensor, $\mathcal{K}^{(i,r)}$, of dilute volume elements (see figure 4.2 (left)) as a function of the number of elements per edge of the cubo-octahedral particles used to mesh it. Material parameters follow tables 4.1 and 4.2. The isotropic tensors are represented by 1 term.

$\bar{\mathcal{A}}_{\text{dil}}^{(i,r)}(i, i) []$							
Edge elements	2	4	6	7	8	10	20
$r < r_c$	1.42952	1.43714	1.43888	1.43934	1.43992	1.44022	1.44075
$r \approx r_c$	0.98232	0.98753	0.98944	0.98951	0.99001	0.99033	0.99084
$r > r_c$	0.34123	0.34129	0.34122	0.34124	0.34120	0.34122	0.34127

$\mathcal{K}^{(i,r)}(i, i) [\text{W/Km}]$							
Edge elements	2	4	6	7	8	10	20
$r < r_c$	35.9503	35.7865	35.7463	35.7353	35.7215	35.7144	35.7017
$r \approx r_c$	277.282	274.389	273.362	273.326	273.070	272.909	272.655
$r > r_c$	1681.23	1677.81	1676.57	1676.26	1675.94	1675.63	1675.01

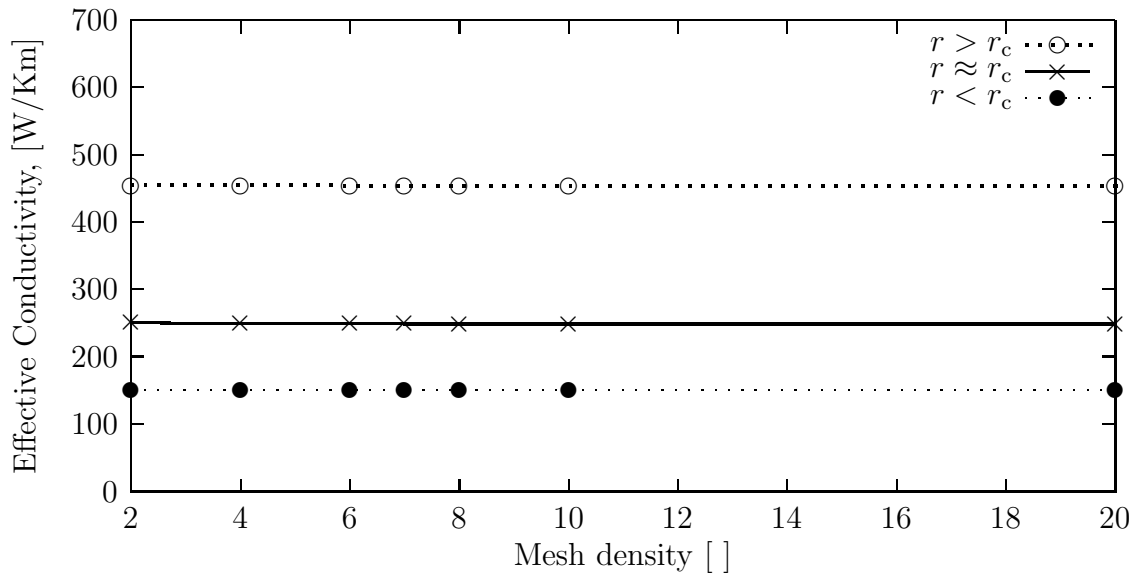


Figure 4.7: RMTM estimates of the effective conductivity of a DRMMC with a volume fraction of 0.34, material parameters follow tables 4.1 and 4.2, as a function of the number of elements per edge used for calculating the replacement tensors and the size of the particles. The volume elements used for obtaining the replacement tensors have a volume fraction of 0.001.

equation (3.43). For $r < r_c^s$ the replacement conductivity is smaller than the conductivity of the matrix, and, therefore, as the volume fraction increases the effective conductivity decreases, the opposite effect can be observed for $r > r_c^s$. When $r = r_c^s$, the replacement conductivity of the particle equals the conductivity of the matrix, the composite behaves as a homogeneous material and the effective conductivity does not change with the volume fraction. As observed in the figure, both methods give rise to the same results for all the scenarios studied. There are only small differences, not resolved in figure 4.8, for high volume fractions, which can be explained because of small numerical errors, i.e., the spheres are meshed using quadratic tetrahedra. It is worth noting that this method makes physical sense only left of the vertical line plotted in the graphic. Recall that although the Mori–Tanaka methods do not have an intrinsic length scale and they fill the space with inclusion of different size, see figure 3.3, in this case an intrinsic length scale has been introduced when calculating the replacement tensors and the limiting volume fraction for spheres of equal size holds.

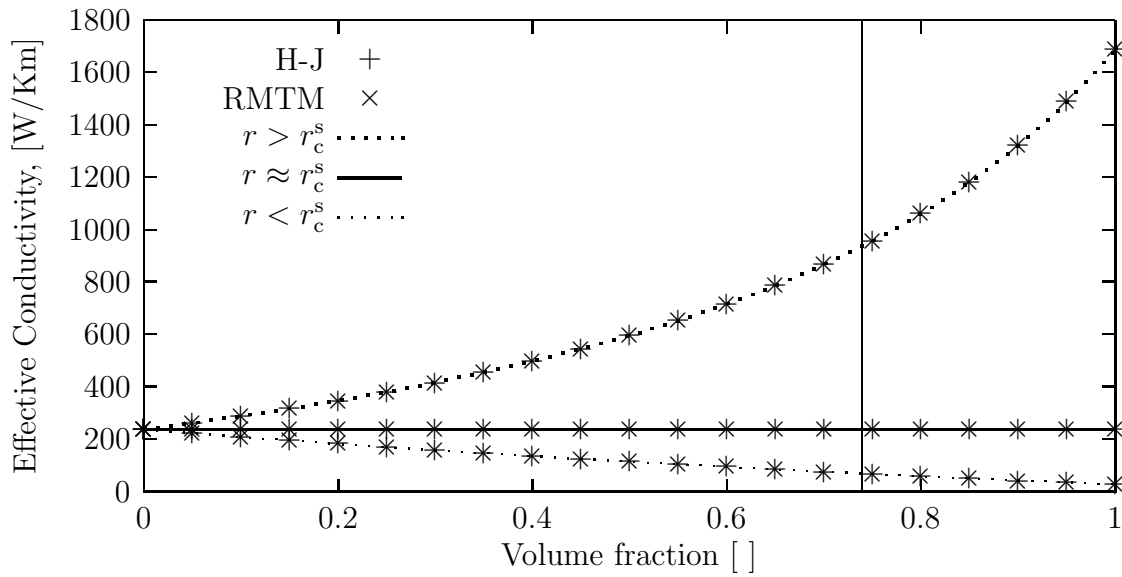


Figure 4.8: Estimates of the effective conductivity of a sphere reinforced composite with material parameters following tables 4.1 and a homogeneous interfacial conductance of 27.7 MW/Km², using the RMTM with numerical evaluation of the replacement tensors and the Hasselman–Johnson models.

For further checking, the model is applied to spheres and compared with some other well-established micromechanical approaches such as the differential scheme and the Torquato/Rintoul 3-point bounds, compare section 3.2.1.3. The results are presented in figure 4.9. The RMTM (which is equivalent to the Hasselman–Johnson model) clearly captures the size effect of the material. When $r = r_c^s$ the material behaves as a homogeneous material and all the micromechanical approaches give rise to the same results. For $r > r_c^s$ the RMTM does not fall within the Torquato/Rintoul-Bounds. This is not surprising because the Torquato/Rintoul-Bounds are 3-point bounds, whilst the RMTM is a Mori–Tanaka method, and Mori–Tanaka methods coincide with the lower Hashin–Shtrikman bound (which is not within the Torquato/Rintoul-Bounds) for two-phase composites with ideal interphases, see section 3.2.1.3, when the conductivity of the reinforcement is higher than the conductivity of the matrix. In contrast, the differential scheme falls within the bounds for the case considered, but it is closer to the upper one, which is not the behaviour expected for composites with matrix topology [151]. For $r < r_c^s$ the RMTM falls within the bounds. The differential scheme estimates are lower than the RMTM in this case, but

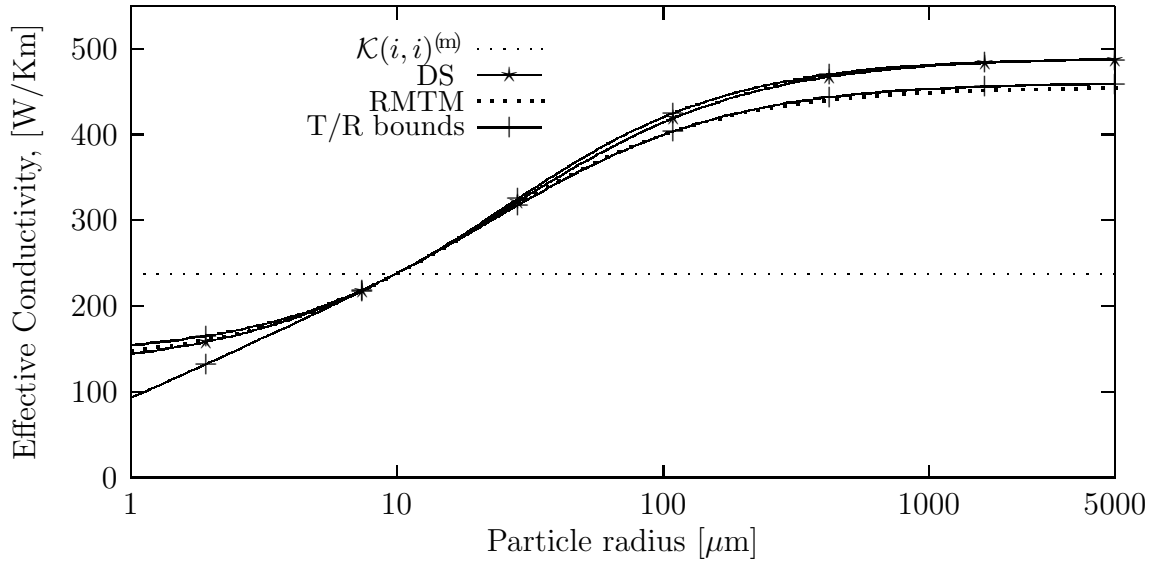


Figure 4.9: Comparison of the estimates of the effective conductivity of a sphere reinforced composite with material parameters following table 4.1 and a homogeneous interfacial conductance of 27.7 MW/Km^2 , obtained using a differential scheme (DS), the Torquato/Rintoul 3-point Bounds (T/R bounds) and a RMTM, as a function of the particle radius.

the difference is small.

It can be concluded that the RMTM is in good agreement with the most commonly used micromechanical approaches, but tends to give somewhat low estimates for $r > r_c^s$.

4.3.1.2 Examples and discussion

The RMTM allows quick estimates of the effective conductivity of particle reinforced composites with inhomogeneous distribution of the interfacial conductance. It can be used in advance to study the effects of the size and the shape of the particles as well as any interfacial conductance scenario. In the following, some interface conductance scenarios and shape studies are presented.

In figure 4.10, different interfacial scenarios are studied for a DRMMC with properties following table 4.1 and a reinforcement volume fraction of 0.34. The case “RMTM, Perfect” represents perfect interfacial conductances, “RMTM, Voids” vanishing interfacial conductances, “RMTM, Inho $\{100\}$ ” finite conductances for the $\{100\}$ faces and perfect

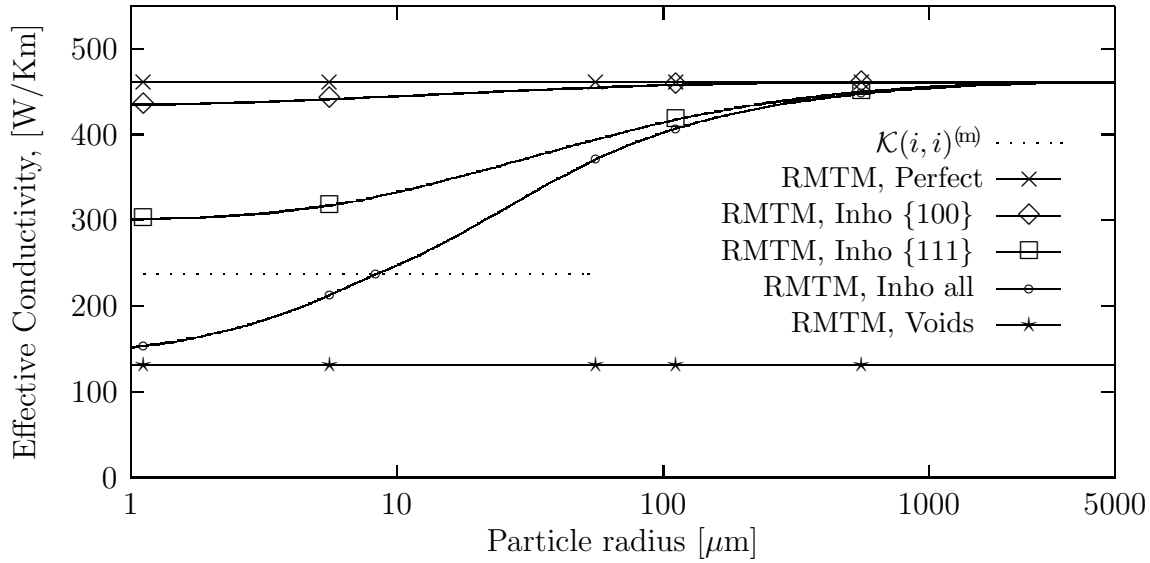


Figure 4.10: Estimates of the effective conductivity for different interfacial conductance scenarios of a DRMMC with material parameters following table 4.1, as a function of the particle radius.

conductances for the $\{111\}$ faces, “RMTM, Inho $\{111\}$ ” finite conductances for the $\{111\}$ faces and perfect conductances for the $\{100\}$ faces, and “RMTM, Inho all” finite conductances for the $\{100\}$ and $\{111\}$ faces, with all of the conductance values following table 4.2. Note that the conductance scenarios chosen do not break the cubic symmetry of the dilute volume elements and, therefore, orientational averaging is not needed. The “RMTM, Perfect” and “RMTM, Voids” cases do not show a size dependence. The rest of the curves show a sigmoid dependence on the radius of the particle. Each case has a different critical radius. As the finite conductance on the $\{100\}$ faces is higher than the finite conductance in the $\{111\}$ faces, and the area fraction of the $\{100\}$ faces is considerably smaller than that of the $\{111\}$ faces, the estimates for the effective conductivity are correspondingly higher.

For a specific size of a diamond with an inhomogeneous distribution of the interfacial conductance, it is possible to find a diamond with the same dilute effective conductivity but with a homogeneous distribution of the conductance. This can be done only if the inhomogeneous distribution of the conductance has at least cubic symmetry. The equivalent homogeneous conductance, $h_{\beta_{\text{Equi, homo}}}^{r=}$, can be obtained by interpolation between suitably chosen test values for which the dilute effective conductivity is evaluated. For the mate-

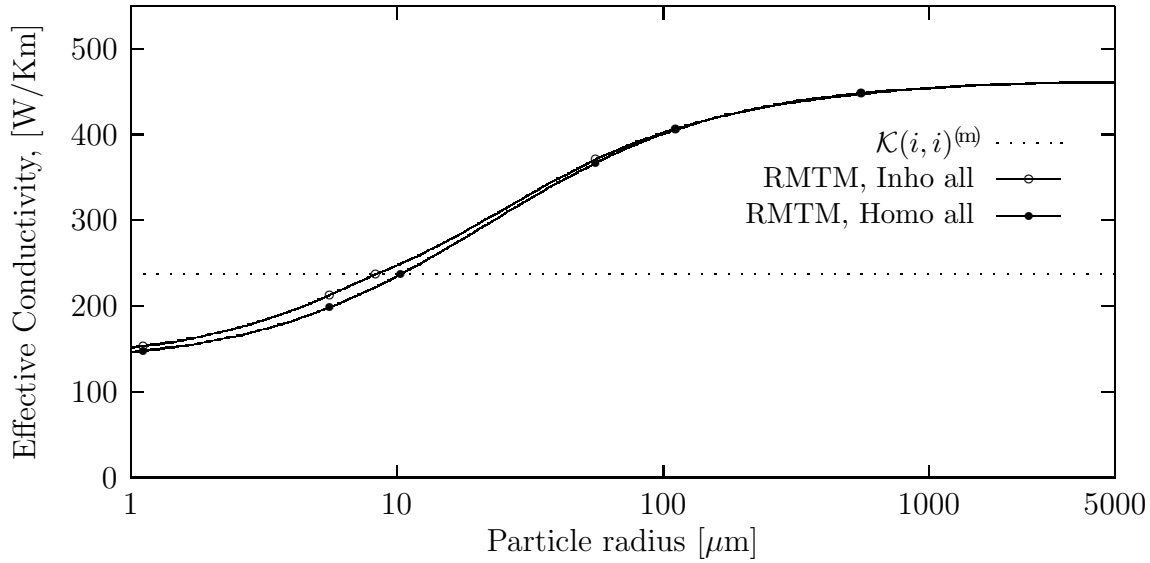


Figure 4.11: Comparison of the effective conductivity of a DRMMC with material parameters following table 4.1 for homogeneous and inhomogeneous distributions of the interfacial conductances for different particle radius. “RMTM, Inho all” refers to an inhomogeneous distribution of the interfacial conductance following table 4.2, and “RMTM, Homo all” refers to a homogeneous distribution of the interfacial conductance with value of $h_{\beta_{\text{Equi, homo}}}^{r=100\mu\text{m}} = 27.7 \text{ MW/Km}^2$.

rial studied, a DRMMC with cubo-octahedral particles and material properties following tables 4.1 and 4.2, the equivalent homogeneous conductance at $r = 100\mu\text{m}$ was found to be 27.7 MW/Km^2 . Note that the equivalent conductance depends on the radius of the particle. In figure 4.11 the estimates of the RMTM for a material with an inhomogeneous distribution of the conductance, denoted as “Inho all”, are compared with the estimates for the same material but with a homogeneous conductance of $h_{\beta_{\text{Equi, homo}}}^{r=100\mu\text{m}}$, denoted as “Homo all”. The estimates are very similar, but there are some differences for radii in the range from $1\mu\text{m}$ to $100\mu\text{m}$, where the estimates of the “Homo all” case are slightly lower than the estimates of the “Inho all” case. Therefore the critical radius is slightly different for the “Homo all” case, $r_c^{\text{Homo}} = 10.34\mu\text{m}$. Nevertheless, the “Homo all” case can be considered as a good approximation for the whole range of radii.

The homogeneous equivalent interfacial conductance allows to directly compare spheres and diamonds. In figure 4.12 DRMMCs with the same material parameters but different shapes are compared. The results are very similar, there are only some small differences

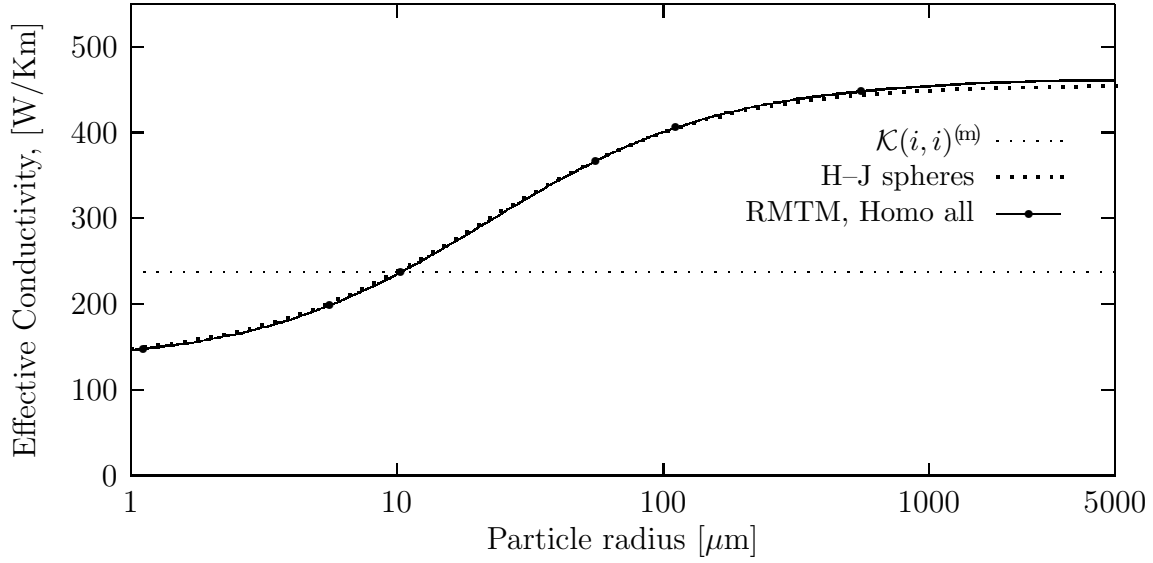


Figure 4.12: Comparison of the effective conductivity of spherical and cubo-octahedral reinforced composites with material parameters following table 4.1 and an interfacial conductance of 27.7 MW/Km²

for $r \gg r_c^{\text{Homo}}$ and $r \ll r_c^{\text{Homo}}$. For the radius range where the estimates for the “Homo all” case differ noticeably from the estimates of the “Inho all” case, the estimates of spheres do not increase this difference.

Therefore, it can be concluded that for the material studied, DRMMC with material properties following tables 4.1 and 4.2, spheres with a conductance equal to the equivalent conductance of the diamond at $r = 100\mu\text{m}$ are a very good approximation. This can be used to study distributions of particles, see section 4.4. The same procedure can be applied to more general particle shapes such as truncated octahedra.

4.3.2 Numerical Methods

In this section, PMAs and Windowing methods, see section 3.3, are used to study the thermal conduction behaviour of DRMMCs. These methods are not only intended for checking the semianalytical models in section 4.3.1, they also offer the possibility of studying the microscopic behaviour of these materials in detail.

4.3.2.1 Generation of the arrangements

For the present work periodic and non-periodic volume elements containing randomly oriented positioned particles of equal size and shape were used.

Periodic arrangements of equally sized spheres were generated by the two-step algorithm of Segurado [139], which involves random sequential insertion followed by a Monte-Carlo compaction procedure. Randomly oriented identical regular cubo-octahedra as shown in fig. 4.1(left) were then inscribed into the spheres, which allowed particle volume fractions of some 0.34 to be attained. This strategy provides for the generation of unit cells that contain cubo-octahedral particles at different positions and orientations, such as cell UCDA. The cell UCDB contains regular cubo-octahedra at the same positions as UCDA, but with different orientations. Volume UCS contains spheres at the same positions as the above, see fig. 4.13. Together with the capability of prescribing different or equal conductances at the $\{100\}$ and $\{111\}$ faces of the diamond particles, the resulting family of models allows various aspects of the phase geometry to be studied in detail at both the micro- and macro-scales. The ideal geometry of UCS has a nominal volume fraction of 0.34, but due to meshing effects the particle volume fraction of the actual cell was 0.339.

The main limitation to the models described above lie in the relatively low particle volume fraction that can be attained, which is little more than half of the diamond volume fractions reported for actual samples [111]. Alternatively, algorithms for generating densely packed cubo-octahedral particles, see [57], were used for studying non-periodic volume elements with volume fractions of up to 0.445, such as cell UCNP in figure 4.14. It is worth noting that the algorithm can generate volume elements with particle volume fractions of up to 0.65, but the meshing of these phase arrangements is challenging.

A further difficulty lies in the limited number of particles that could be handled within the constraints of available computer resources, an issue that is exacerbated in PMAs by the large number of multi-point constraints required for implementing periodicity boundary conditions, which tend to degrade the efficiency of Finite Element solvers. As discussed in

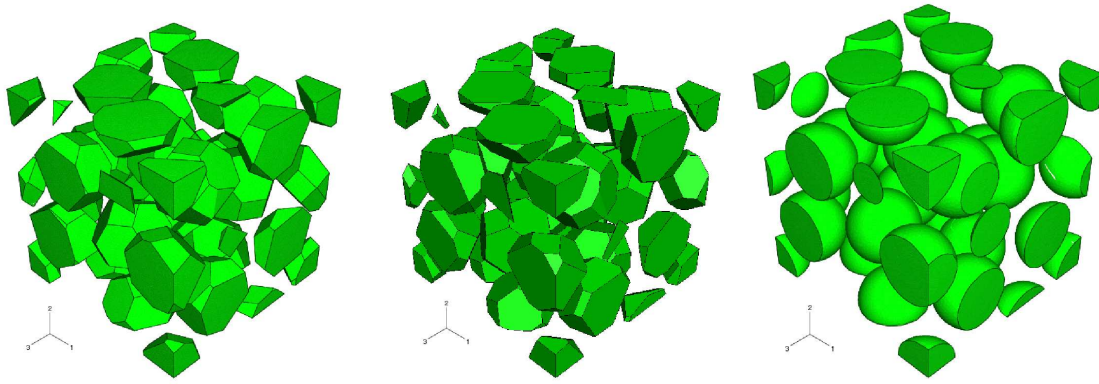


Figure 4.13: Periodic multi-particle unit cells, UCDA (left), UCDB (middle) and UCS (right), used in the analysis. The three unit cells have, approximately, the same reinforcement volume fraction of $f = 0.34$ and use the same particle centers.

sections 4.3.2.2 and 4.3.2.3 some anisotropy is present in the overall conductivities predicted for the three configurations shown in fig. 4.13, which indicates that the unit cells are too small for being proper reference volume elements for linear heat conduction. The same applies to elasticity problems, see section 5.2. Even though ensemble averaging over different configurations can be employed for improving the predictions of the macroscopic properties, unit cells containing a higher number of particles are clearly desirable.

4.3.2.2 Periodic Microfield Approaches

The unit cells UCDA, UCDB and UCS, see figure 4.13, together with the appropriate periodicity boundary conditions were used for studying details of the microgeometry such as orientation, size and shape of the reinforcements or distributions of the interfacial conductances. Sizes of the diamonds studied were 1, 10 and 1000 μm , $r < r_c$, $r \approx r_c$ and $r > r_c$, respectively. Additionally 100 μm size particles were used because the equivalent homogeneous conductance was evaluated for this particle size. Recall, that as all the UCs used have the same volume fraction, the corresponding radii of the spheres are 0.88, 8.8, 888.8 and 88.8 μm . The scenarios studied were “Perfect”, which refers to perfect interfacial conductances, “Inho all” that refers to finite conductances following table 4.2, and “Homo all” which refers to a homogeneous distribution of the conductance with a value of $h_{\beta\text{Equi, homo}}^{r=100\mu\text{m}} = 27.7 \text{ MW/Km}^2$.

The isotropy of the unit cells is studied in tables 4.7–4.10. In these tables, estimates of

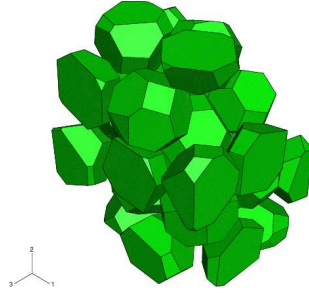


Figure 4.14: Non-periodic volume element, UCNP, used in the analysis. The volume element has a reinforcement volume fraction of $f = 0.445$.

the effective conductivity of the material for temperature gradients in 1-, 2- and 3- directions are compared for different interfacial conductance scenarios and particle radii. The largest differences are found for the scenario of perfect interfaces, for which the conductivity contrast is highest. The anisotropy of the results for the inhomogeneous distribution of the interfacial conductance is slightly higher than the anisotropy of the results for the homogeneous distribution of the interfacial conductance, the difference being smaller for bigger radii. This behaviour is similar to the behaviour of the replacement conductivity, see figure 4.11. For the scenarios with imperfect interfaces, the higher the radius the bigger the anisotropy. This is because the replacement conductivity is bigger and therefore the conductivity contrast is bigger. The predictions obtained for unit cells UCDA and UCDB differ only by a small amount, indicating that the orientation of the particles and consequent local changes in the flux distributions have little influence in the macroscopic anisotropy. The estimates in 1-direction give the highest values in almost all the cases, which shows the importance of the positions and that the unit cell is not a proper representative volume element. The differences in the effective conductivity are slightly higher for the diamond unit cells than for UCS, which indicates that UCS is slightly more isotropic than the unit cells with polyhedral particles, as expected because of the additional local perturbations due to vertices and edges. For all the cases considered the differences in the effective conductivities are below 1%, and therefore these conductivities can be considered as valid estimates.

Table 4.7: Effective conductivities, $\mathcal{K}^*$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to the unit cells UCDA, UCDB, and UCS (see fig.4.13) for different conductance scenarios, a diamond volume fraction of $f = 0.34$, and $r < r_c$ ($r=1 \mu\text{m}$ for diamonds and $r=0.88 \mu\text{m}$ for spheres).

		$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UCDA	Perfect	471.9	467.3	467.9	469.0
	Homo all	145.0	144.3	144.4	144.6
	Inho all	150.0	149.3	149.4	149.6
UCDB	Perfect	472.7	468.7	467.9	469.8
	Homo all	144.8	144.2	144.5	144.5
	Inho all	149.8	149.2	149.5	149.5
UCS	Perfect	459.7	457.2	456	457.6
	Homo all	146.6	146.2	146.1	146.3

Table 4.8: Effective conductivities, $\mathcal{K}^*$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to the unit cells UCDA, UCDB, and UCS (see fig.4.13) for different conductance scenarios, a diamond volume fraction of $f = 0.34$, and $r \approx r_c$ ($r=10 \mu\text{m}$ for diamonds and $r=8.8 \mu\text{m}$ for spheres).

		$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UCDA	Perfect	471.9	467.3	467.9	469.0
	Homo all	234.6	234.5	234.6	234.6
	Inho all	249.4	249.1	249.2	249.2
UCDB	Perfect	472.7	468.7	467.9	469.8
	Homo all	234.5	234.6	234.6	234.6
	Inho all	249.1	249.1	249.1	249.1
UCS	Perfect	459.7	457.2	456.0	457.6
	Homo all	229.2	229.2	229.2	229.2

Table 4.9: Effective conductivities, $\mathcal{K}^*$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to the unit cells UCDA, UCDB, and UCS (see fig.4.13) for different conductance scenarios, a diamond volume fraction of $f = 0.34$, and $r > r_c$ ($r=100 \mu\text{m}$ for diamonds and $r=88 \mu\text{m}$ for spheres).

		$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UCDA	Perfect	471.9	467.3	467.9	469.0
	Homo all	405.4	403.0	403.4	404.0
	Inho all	406.5	404.1	404.6	405.1
UCDB	Perfect	472.7	468.7	467.9	469.8
	Homo all	405.7	403.6	403.3	404.2
	Inho all	406.7	404.8	404.2	405.2
UCS	Perfect	459.8	457.2	456.0	457.7
	Homo all	394.7	393.5	393.0	393.7

Table 4.10: Effective conductivities, $\mathcal{K}^*$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to the unit cells UCDA, UCDB, and UCS (see fig.4.13) for different conductance scenarios, a diamond volume fraction of $f = 0.34$, and $r > r_c$ ($r=1000 \mu\text{m}$ for diamonds and $r=880 \mu\text{m}$ for spheres).

		$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UCDA	Perfect	471.9	467.3	467.9	469.0
	Homo all	463.4	459.1	459.7	460.8
	Inho all	463.1	458.8	459.4	460.4
UCDB	Perfect	472.7	468.7	467.9	469.8
	Homo all	464.1	460.3	459.7	461.4
	Inho all	463.7	460.0	459.3	461.0
UCS	Perfect	459.7	457.2	456.0	457.7
	Homo all	451.6	449.4	448.2	449.7

In tables 4.11–4.14, the average effective conductivities of the unit cells are compared with the analytical methods described in section 4.3.1. If $r < r_c$ the replacement conductivity of the inclusion is lower than the conductivity of the matrix, and therefore the MTM-based methods are upper estimates of the solution. This does not hold for the scenario with perfect interfacial conductances, because in this case the replacement conductivity equals the conductivity of the inclusion and thus is higher than the conductivity of the matrix, so that the MTM-based methods are a lower estimate. If $r \approx r_c$ the behaviour is more complex. Recall that the critical radius of the spheres and the diamonds for the homogeneous conductance scenario is higher than the radius used, whilst r_c for the inhomogeneous interfacial conductance scenario is below the radius used. Therefore, the MTM-based methods are an upper estimate for all UCs for the homogeneous conductance scenario, whilst they are a lower estimate for all UCs for the perfect and inhomogeneous interfacial conductance scenarios. If $r > r_c$ the MTM-based methods are a lower estimate for all UCs and interfacial conductance scenarios.

For all the radii and interfacial conductance scenarios studied, the difference between the RMTM and PMAs are very small. The maximum deviation is 2% for the perfect interfacial conductance scenario for the diamonds. As observed, the higher the conductivity contrast the higher the deviation between the estimates of the RMTM and the unit cells. The inhomogeneous distribution of the conductance causes a slight increase of the deviation for all the radii studied except for $r > r_c$.

The deviations between the RMTM and unit cells are smaller for UCS than for the unit cells containing polyhedra. This is explained by the more homogeneous fields that occur within and around the sphere. Recall that the RMTM are based on phase averages. The orientation of the particles does not play a major role for the effective conductivity of the composite.

Figures 4.15 – 4.18 concentrate on the distribution of microscopic heat fluxes in the particles. In figure 4.15 and 4.16 the three unit cells shown in figure 4.13 are subjected to thermal gradients acting in 3-direction, for the “Homo all” and “Inho all” scenarios, respectively. The resulting intra-particle fluctuations of the fluxes are represented in terms of averages and standard deviations. The spherical particles consistently show slightly smaller particle averages and significantly smaller standard deviations of the fluxes than do the cubo-octahedra. This behaviour is related to the fact that in dilute spheres the microfields are homogeneous, whereas in polyhedra they are not. For all the unit cells the averages and the standard deviations of the fluxes decrease with the radius, which is due

Table 4.11: Comparison of effective conductivities, $\mathcal{K}^*$ [W/Km], predicted by the unit cells UCDA, UCDB and UCS (see fig.4.13), by the semi-analytical Mori–Tanaka model (RMTM, cubo-octahedral particles), and by the Hasselman–Johnson model (HJ, spherical particles) for different interfacial conductance scenarios for a diamond volume fraction of $= 0.34$ and $r < r_c$ ($r = 1 \mu\text{m}$ for diamonds and $r = 0.88 \mu\text{m}$ spheres).

	$\mathcal{K}_{\text{UCDA}}^*(i, i)$	$\mathcal{K}_{\text{UCDB}}^*(i, i)$	$\mathcal{K}_{\text{RMTM}}^*(i, i)$	$\mathcal{K}_{\text{UCS}}^*(i, i)$	$\mathcal{K}_{\text{HJ}}^*(i, i)$
Perfect	469.0	469.8	461.4	457.6	453.0
Homo all	144.6	144.5	146.1	146.3	146.9
Inho all	149.6	149.5	151.3	—	—

Table 4.12: Comparison of effective conductivities, $\mathcal{K}^*$ [W/Km], predicted by the unit cells UCDA, UCDB and UCS (see fig.4.13), by the semi-analytical Mori–Tanaka model (RMTM, cubo-octahedral particles), and by the Hasselman–Johnson model (HJ, spherical particles) for different interfacial conductance scenarios for a diamond volume fraction of $f = 0.34$ and $r \approx r_c$ ($r = 10 \mu\text{m}$ for diamonds and $r = 8.8 \mu\text{m}$ for spheres).

	$\mathcal{K}_{\text{UCDA}}^*(i, i)$	$\mathcal{K}_{\text{UCDB}}^*(i, i)$	$\mathcal{K}_{\text{RMTM}}^*(i, i)$	$\mathcal{K}_{\text{UCS}}^*(i, i)$	$\mathcal{K}_{\text{HJ}}^*(i, i)$
Perfect	469.0	469.8	461.4	457.64	453.0
Homo all	234.6	234.6	234.6	229.24	229.86
Inho all	249.2	249.1	249.2	—	—

Table 4.13: Comparison of effective conductivities, $\mathcal{K}^*$ [W/Km], predicted by the unit cells UCDA, UCDB and UCS (see fig.4.13), by the semi-analytical Mori–Tanaka model (RMTM, cubo-octahedral particles), and by the Hasselman–Johnson model (HJ, spherical particles) for different interfacial conductance scenarios for a diamond volume fraction of $f = 0.34$ and $r > r_c$ ($r = 100 \mu\text{m}$ for diamonds and $r = 88 \mu\text{m}$ for spheres).

	$\mathcal{K}_{\text{UCDA}}^*(i, i)$	$\mathcal{K}_{\text{UCDB}}^*(i, i)$	$\mathcal{K}_{\text{RMTM}}^*(i, i)$	$\mathcal{K}_{\text{UCS}}^*(i, i)$	$\mathcal{K}_{\text{HJ}}^*(i, i)$
Perfect	469.0	469.8	461.4	457.7	453.0
Homo all	404.0	404.2	400.5	393.7	392.5
Inho all	405.1	405.2	401.0	—	—

Table 4.14: Comparison of effective conductivities, $\mathcal{K}^*$ [W/Km], predicted by the unit cells UCDA, UCDB and UCS (see fig.4.13), by the semi-analytical Mori–Tanaka model (RMTM, cubo-octahedral particles), and by the Hasselman–Johnson model (HJ, spherical particles) for different interfacial conductance scenarios for a diamond volume fraction of $f = 0.34$ and $r > r_c$ ($r = 1000 \mu\text{m}$ for diamonds and $r = 880 \mu\text{m}$ for spheres).

	$\mathcal{K}_{\text{UCDA}}^*(i, i)$	$\mathcal{K}_{\text{UCDB}}^*(i, i)$	$\mathcal{K}_{\text{RMTM}}^*(i, i)$	$\mathcal{K}_{\text{UCS}}^*(i, i)$	$\mathcal{K}_{\text{HJ}}^*(i, i)$
Perfect	469.0	469.8	461.4	457.7	453.0
Homo all	460.8	461.4	453.3	449.7	445.9
Inho all	460.4	461.0	453.6	—	—

to the conductivity contrast. The orientation of the particles does not seem to play an important role either for the average values or for the standard deviations.

In figure 4.17 the unit cell UCDA is subjected to thermal gradients acting in 3-direction, different interfacial conductance scenarios being studied. The perfect scenario, which is size-independent, shows the biggest standard deviations because of the high conductivity contrast. The inhomogeneous distribution of the interfacial conductance does not seem to have an important effect for the cases studied except for $r \approx r_c$. For this case, the differences in the average value are due to the different critical radii of the scenarios studied some of which are below and some above the radius studied. The standard deviation for the inhomogeneous distribution case is bigger because for this case there are two sets of interfaces in different regimes. In 4.18 the same results for a radius of $100 \mu m$ are shown. Recall that the conductance used in the “Homo all” scenario, $h_{\beta \text{Equi, homo}}^{r=100\mu m}$, was calculated for this radius. In this case, slightly higher averages and standard deviations are evident in the inhomogeneous distribution of the interfacial conductance.

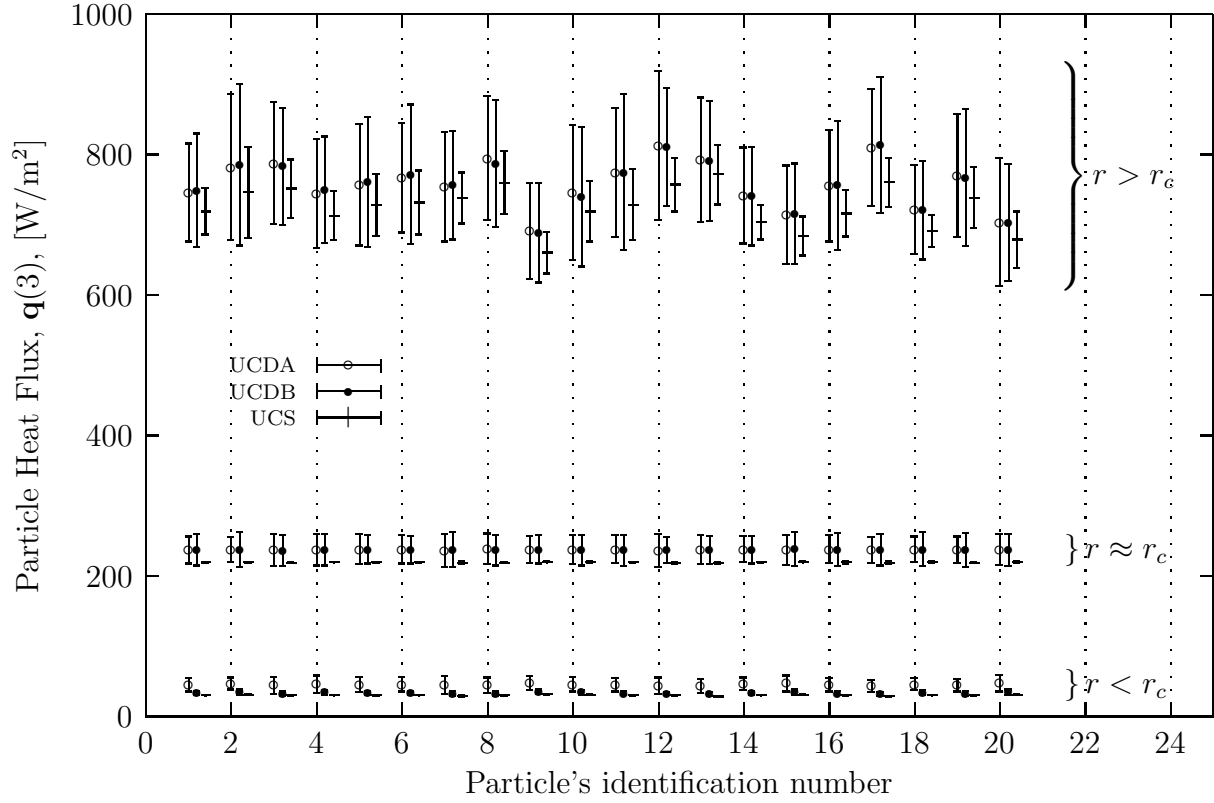


Figure 4.15: Heat fluxes in the particles (means and standard deviations) predicted by unit cells UCDA, UCDB and UCS (compare fig. 4.13) for different particle radii, for a homogeneous interfacial conductance of 27.7 MW/Km^2 and loading by a thermal unit gradient acting in 3-direction.

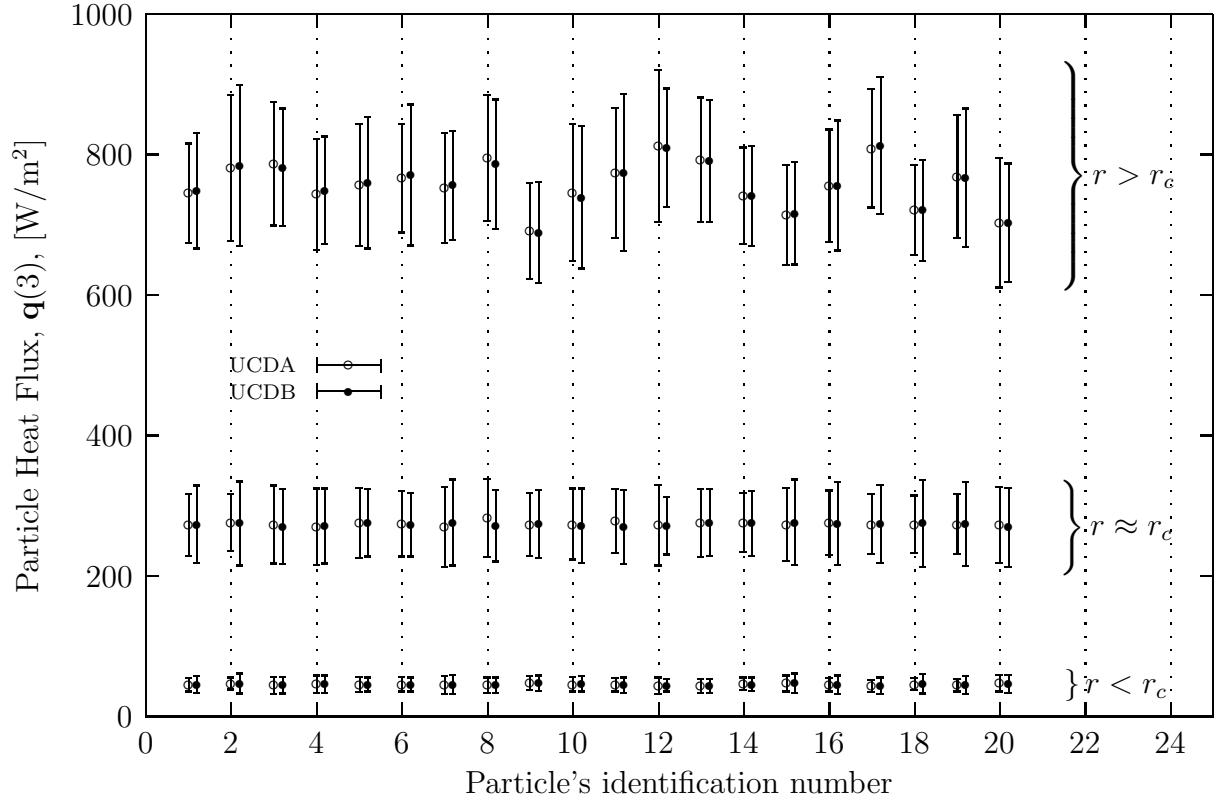


Figure 4.16: Heat fluxes in the particles (means and standard deviations) predicted by unit cells UCDA and UCDB (compare fig. 4.13) for different particle radii and loading by a thermal unit gradient acting in 3-direction. Material properties following tables 4.1 and 4.2 (Inho all case).

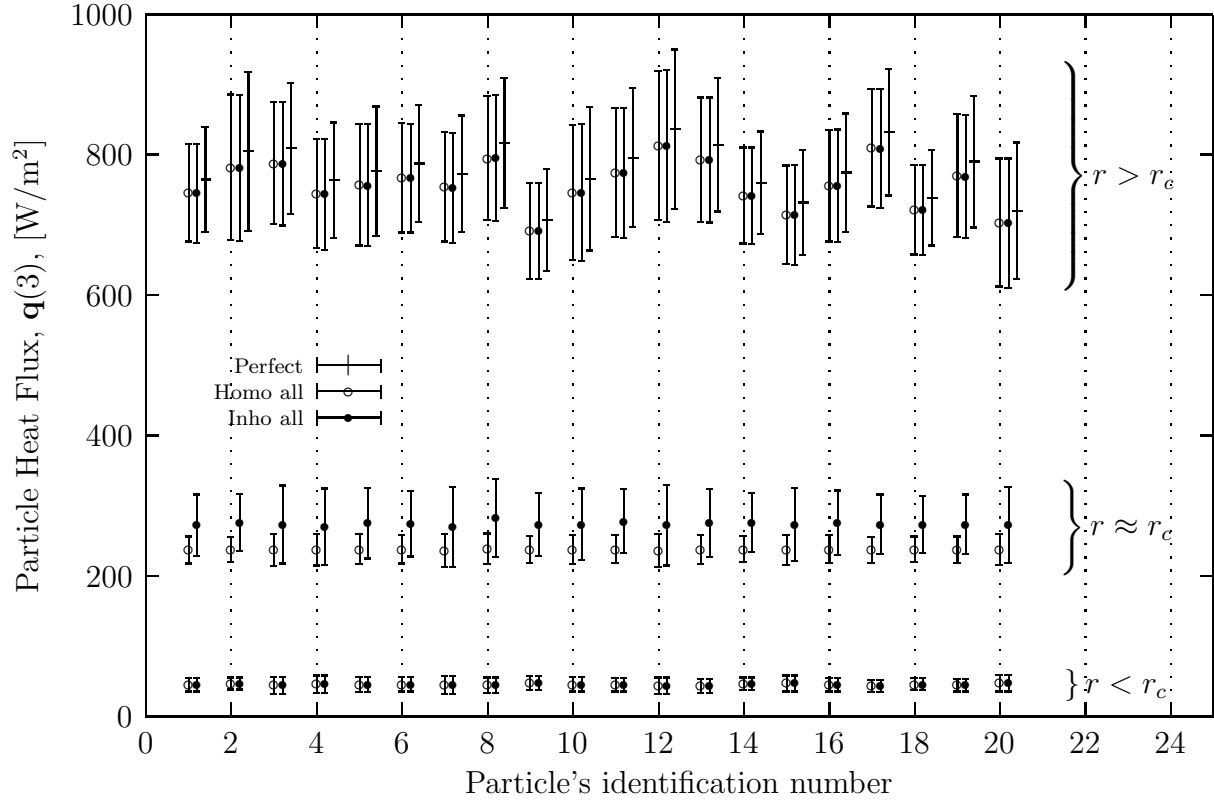


Figure 4.17: Heat fluxes in the particles (means and standard deviations) predicted by unit cell UCDA (compare fig. 4.13) for different particle radii and interfacial conductance scenarios and loading by a thermal unit gradient acting in 3-direction.

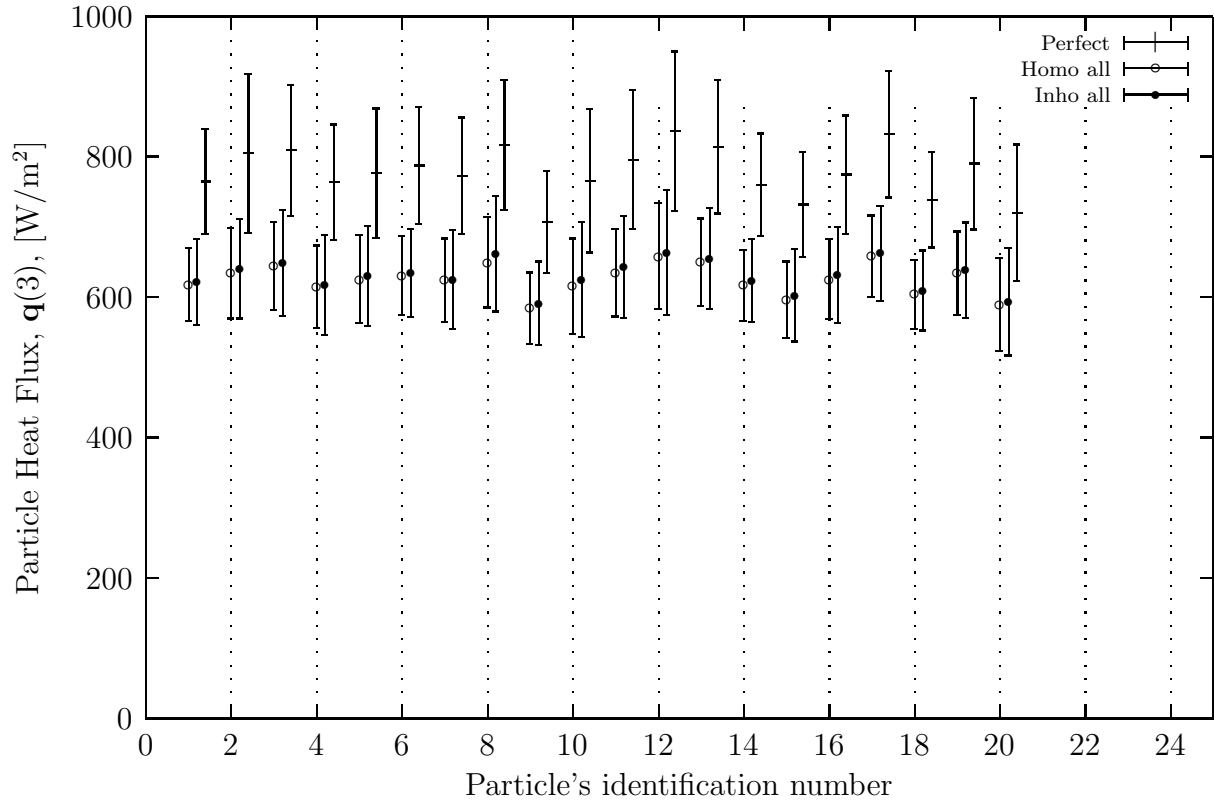


Figure 4.18: Heat fluxes in the particles (means and standard deviations) predicted by unit cell UCDA (compare fig. 4.13) for different interfacial conductance scenarios and loading by a thermal unit gradient acting in 3-direction (particle radius $r = 100\mu\text{m}$).

4.3.2.3 Windowing methods

Actual DRMMCs for heat–sink applications are produced with high reinforcement volume fractions, up to 80% [165], in order to achieve a high thermal conductivity. The generation of periodic arrangements at these volume fractions is challenging. Tomographic techniques can be used to obtain particle arrangements from the actual composites, but they are, evidently, not periodic. Windowing methods do not need periodic arrangements for estimating the conductivity of these materials, and, therefore, they are excellent candidates for studying their behaviour at high volume fractions. Furthermore, windowing methods can estimate the apparent conductivity of periodic arrangements at a slightly lower cost than PMAs. In the following, windowing methods are applied to a periodic unit cell, UCDA, to compare the results with those of periodic homogenization, and to a non–periodic volume element, UCNP, with a higher volume fraction. The boundary conditions are denoted as UTGBC for uniform temperature gradient boundary conditions (uniform essential BCs, eqn. (3.82)), UHFBC for uniform normal heat flux boundary conditions (uniform natural BCs, eqn. (3.83)), and MUBC for mixed uniform BCs. The MUBC conditions used in this section correspond to essential boundary conditions on two parallel faces of the volume element, and natural conditions on the other four faces, in other words the temperature is kept constant on two parallel faces, the values of which are different, and the normal heat flux in the other faces is set to zero, see [87; 123].

In tables 4.15–4.18, the estimates obtained for different loading directions and different particle radii for cell UCDA are collected. The anisotropy of the results is higher than for the periodic cases studied above.

In table 4.19 the averaged results are collected and compared with the estimates of PMAs and RMTM. It can be observed that the full equivalence between PBC and MUBC reported in [87] only holds for orthotropic or higher symmetry. There is a tendency for the conductivities obtained with MUBC to be slightly higher than those generated with PBC. The present results show that MUBC give valid results also for volume elements that have some sub–orthotropic contributions to their geometry. The difference between the lower and upper estimates decrease with decreasing radius. Such a behaviour, however, is not observed for higher volume fraction of cell UCNP, see table 4.24.

In tables 4.20–4.23, the estimates obtained for different loading directions and different particle radii for cell UCNP are presented. Due to numerical problems, the estimates could not be calculated for all cases. The anisotropy of the results is, in general, smaller than for UCDA.

In table 4.24 the averaged results are collected and compared with the estimates of the RMTM. For all the radii studied the Mori–Tanaka estimates are within the lower and upper estimates obtained by windowing. For $r > r_c$ the windowing estimates using MUBCs are closer to the upper than the lower estimate. The higher the conductivity contrast, the higher the difference between the lower and upper estimates. For $r \approx r_c$, the upper and lower estimates are not identical, but the differences between them are the smallest of all the cases studied. For $r < r_c$, the RMTM is closer to the lower estimate than for $r \approx r_c$, but it is higher than the windowing estimate using MBCs. The upper estimate exceeds the conductivity of the matrix. The fact that MUBC predictions, as expected, show somewhat higher effective conductivity than RMTM for $r > r_c$ and the opposite behaviour for $r < r_c$ indicates the validity of both methods at elevated reinforcement volume fractions.

Table 4.15: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1–, 2– and 3-directions to cell UCDA (see fig. 4.13) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=1 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	294.5	276.4	292.5	287.8
MUBC	153.5	150.0	150.4	151.3
UHFBC	131.0	127.8	132.5	130.4

Table 4.16: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1–, 2– and 3-directions to cell UCDA (see fig. 4.13) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=10 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	371.2	353.6	368.0	364.3
MUBC	260.4	254.7	254.8	256.6
UHFBC	245.9	245.4	248.2	246.5

Table 4.17: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCDA (see fig. 4.13) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=100 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	489.6	475.7	487.0	484.1
MUBC	416.3	409.5	409.8	411.9
UHFBC	391.7	387.2	393.3	390.7

Table 4.18: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCDA (see fig. 4.13) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=1000 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	534.5	521.4	531.6	529.2
MUBC	471.2	463.2	464.0	466.1
UHFBC	443.4	436.4	443.1	441.0

Table 4.19: Comparison of apparent and effective conductivities, $\mathcal{K}$ [W/Km], predicted with cell UCDA (see fig. 4.13) for different boundary conditions and by the semianalytical Mori–Tanaka model (RMTM, cubo–octahedral particles), for different radii. Material properties follow tables 4.1 and 4.2.

	UTGBC	MUBC	PBC	UHFBC	RMTM
$r = 1\mu\text{m} < r_c$	287.8	151.3	149.6	130.4	151.3
$r = 10\mu\text{m} \approx r_c$	364.3	256.6	249.2	246.5	249.2
$r = 100\mu\text{m} > r_c$	484.1	411.9	405.1	390.7	401
$r = 1000\mu\text{m} > r_c$	529.2	466.1	460.4	441.0	453.6

Table 4.20: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCNP (see fig. 4.14) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=1 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	287.6	273.9	271.0	277.5
MUBC	126.7	—	130.7	128.7
UHFBC	87.0	85.7	88.8	87.2

Table 4.21: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCNP (see fig. 4.14) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=10 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	384.0	377.9	374.3	378.7
MUBC	265.7	266.3	268.1	266.7
UHFBC	189.3	189.9	190.5	189.9

Table 4.22: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCNP (see fig. 4.14) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=100 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	570.0	571.9	573.7	571.9
MUBC	494.1	489.8	—	492.0
UHFBC	336.9	336.1	338.1	337.0

Table 4.23: Apparent conductivities, $\mathcal{K}$ [W/Km], obtained by applying thermal gradients in 1-, 2- and 3-directions to cell UCNP (see fig. 4.14) for different boundary conditions with material properties following tables 4.1 and 4.2. Particle radius $r=1000 \mu\text{m}$.

	$\mathcal{K}_1^*(i, i)$	$\mathcal{K}_2^*(i, i)$	$\mathcal{K}_3^*(i, i)$	$\mathcal{K}_{\text{avg}}^*(i, i)$
UTGBC	664.1	669.0	674.6	669.2
MUBC	596.58	588.9	621.7	602.4
UHFBC	397.1	395.4	399.2	397.2

Table 4.24: Comparison of apparent and effective conductivities, $\mathcal{K}$ [W/Km], predicted with cell UCNP (see fig. 4.14) for different boundary conditions and by the semianalytical Mori–Tanaka model (RMTM, cubo–octahedral particles), for different radii. Material properties follow tables 4.1 and 4.2.

	UTGBC	MUBC	UHFBC	RMTM
$r = 1\mu\text{m} < r_c$	277.5	128.7	87.2	129.2
$r = 10\mu\text{m} \approx r_c$	378.7	266.7	189.9	253.1
$r = 100\mu\text{m} > r_c$	571.9	492.0	337.0	466.8
$r = 1000\mu\text{m} > r_c$	669.2	602.4	397.2	546.2

4.4 Polydisperse particle size distributions

Actual “monodisperse” composites do not have particles of exactly the same size, but the particle sizes follow narrow statistical distributions. Furthermore, in order to obtain higher volume fractions, different particles of sizes are commonly mixed, see [110]. In this section, the effect of particle size distributions is studied in detail via a multiphase RMTM.

4.4.1 Methods

Among micromechanical methods, analytical or semianalytical methods are more suitable for the problem at hand than numerical methods. Numerical methods are based on discrete microgeometries which need a high number of particles to describe particle size distributions that are not very sharp. The meshing of arrangements with particles of different size is not trivial and can lead to meshes with extremely high numbers of nodes. Furthermore, the generation of particle arrangements at high volume fractions is not trivial, either.

Within the semianalytical methods the RMTM can, in principle, be a solution, because it can take into account several descriptors of the material such as particle sizes and shapes as well as interfaces. Furthermore, Mori–Tanaka methods can be easily extended to studying multi-phase materials, see section 3.2.1.2.3. Nevertheless, for studying size distributions of particles of general shape they may be quite expensive because three numerical analyses are required per radius studied.

In section 4.3, it was shown that, for the material studied, a sphere with a homogeneous interfacial conductance of suitable value is an excellent approximation for diamonds at all particle radii. Furthermore, the RMTM for spheres with a homogeneous distribution of the interfacial conductance embedded in an isotropic matrix is fully analytic, being equivalent to the Hasselman–Johnson method in the monodisperse case. In the following, these results are used for studying distributions of spherical particles with inhomogeneous distribution of the interfacial conductance.

4.4.1.1 Multiphase MTM for spherical composites with interfacial resistance

In this method, the particles with different radii are considered as different classes of reinforcements. First the distribution of radii is divided into n classes, and then a multiphase MTM (see section 3.2.1.2.3) is applied to the $(n + 1)$ -phase material.

For spherical particles of isotropic conductivity, $\mathcal{K}^{(\text{p})}$, interfacial conductance, h_β , and radius, r , the replacement conductivity, $\mathcal{K}^{(\text{p},r)}(i, i)$, takes the form [10; 47]:

$$\mathcal{K}^{(\text{p},r)}(i, i) = \mathcal{K}^{(\text{p})}(i, i) \frac{r h_\beta}{r h_\beta + 2\mathcal{K}^{(\text{p})}(i, i)} \quad (4.5)$$

and the replacement dilute concentration tensor, $\bar{\mathcal{A}}_{\text{dil}}^{(\text{p},r)}$, follows from equation (3.28) as:

$$\bar{\mathcal{A}}_{\text{dil}}^{(\text{p},r)}(i, i) = \frac{3\mathcal{K}^{(\text{m})}(i, i)}{2\mathcal{K}^{(\text{m})}(i, i) + \mathcal{K}^{(\text{p},r)}(i, i)} \quad (4.6)$$

Combining equations (3.34), (3.35), (4.5) and (4.6), the effective conductivity follows as:

$$\mathcal{K}_{\text{M}}^*(i, i) = \mathcal{K}^{(\text{m})}(i, i) + \frac{\sum_{j=1}^N f^{(\text{j})} (\mathcal{K}^{(\text{j},r)}(i, i) - \mathcal{K}^{(\text{m})}(i, i)) \bar{\mathcal{A}}_{\text{dil}}^{(\text{j},r)}(i, i)}{f^{(\text{m})} \sum_{j=1}^N f^{(\text{j})} \bar{\mathcal{A}}_{\text{dil}}^{(\text{j},r)}(i, i)} \quad (4.7)$$

Analogous explicit scalar equations can be derived for the transverse macroscopic conductivity of composites reinforced by unidirectional continuous fibers that show non-uniform diameters and interfacial resistances, see [20]. An analogous scheme for studying the thermal conduction properties of composites with aligned reinforcements having interfacial conductances can be formulated in terms of replacement flux concentration tensors.

4.4.2 Examples and discussion

In this section the Mori–Tanaka expressions for composites reinforced by equiaxed particles that show an interfacial resistance and follow prescribed size distributions, equations (4.5), (4.6), and (4.7), are applied to modelling a material the properties of which follow tables 4.1 and 4.2. The effect of the statistical distributions used to model the particle size distribution is studied.

Independently of the distribution used to model the particles size, the RMTM needs as input a set of radii and the reinforcement volume fraction corresponding to the particles associated with each radius within this set. This function can be derived from any statistical distribution. In this section monomodal log-normal distributions of the particle radii and a “cropped” distribution of the particle radii are studied.

For monomodal log-normal distributions of the particle radii, the probability density function, c^{df} , reads:

$$c^{\text{df}}(r) = \frac{1}{rc^\sigma \sqrt{2\pi}} e^{-\left(\frac{\ln(r) - c^\mu}{\sqrt{2}c^\sigma}\right)^2} \quad (4.8)$$

where c^σ and c^μ are the standard deviation and the mean of the variables' logarithm. Alternatively $c^{\text{df}}(r)$ can be defined in terms of the span, c^S , and the median, c^M . The span is defined as the value of the random variable below which 90% of the cases are found minus the value of the random variable below which 10% of the cases are found, divided by the median. In the present study results are parameterized in terms of medians and spans. For log-normal distributions the relationships:

$$\begin{aligned} c^\mu &= \ln(c^M) \\ c^\sigma &= \frac{1}{1.2816} \ln \left(\frac{c^S + \sqrt{(c^S)^2 + 4}}{2} \right) \end{aligned} \quad (4.9)$$

hold.

For this distribution, two different meanings for the probability functions were considered:

- Radius probability: The probability associated with each radius, r , gives the probability of finding a particle in the composite which radius is r . Its density function is called c^{df}, r .
- Relative volume fraction probability: The probability associated with each radius, r , is the relative volume fraction of particles of radius r . The relative volume fraction is the ratio between the volume of the reinforcement phase of radius r and the volume occupied by all the reinforcements. Its density function is c^{df}, v .

The probability density function of the “cropped” uniform distribution is:

$$c^{\text{df}, v\text{-CROP}}(r) = \begin{cases} \frac{0.8}{c^M c^S} & \text{for } c^M (1 - 0.625c^S) \leq r \leq c^M (1 + 0.625c^S) \\ 0 & \text{otherwise} \end{cases} \quad (4.10)$$

The meaning of the probability function is the same as for c^{df}, v .

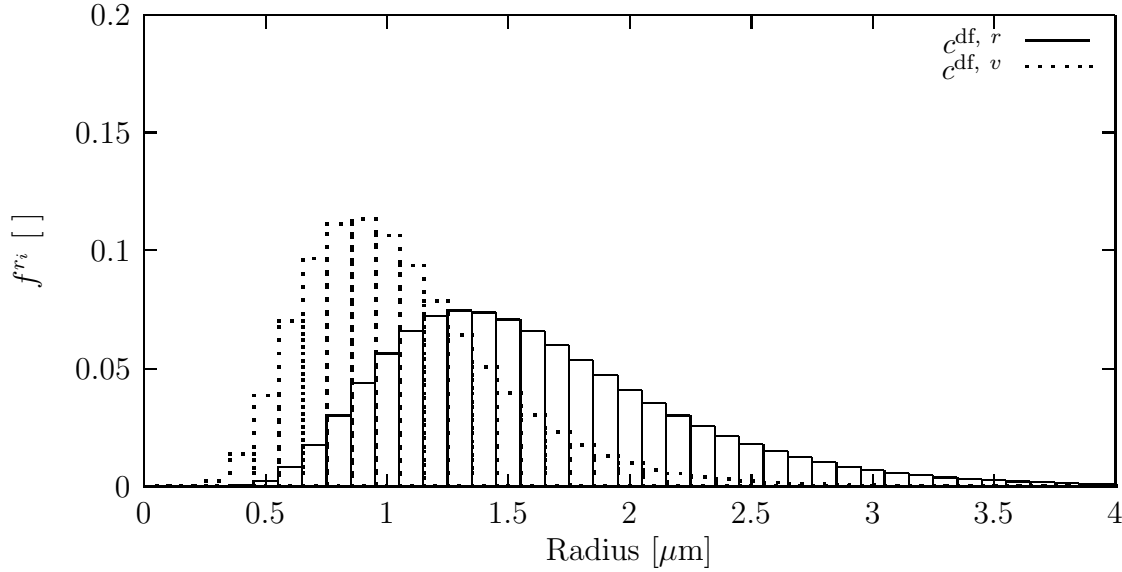


Figure 4.19: Input for the Mori–Tanaka method, f^{r_i} , obtained from log-normal distributions of the radii for a span of 1 and a median radius of 1 μm . In $c^{\text{df}, r}$ the probability function gives the probability of finding a particle of radius r and in $c^{\text{df}, v}$ the probability function gives the relative volume fraction associated with the radius r .

The three distributions can be discretized into different, logarithmically or equally spaced classes. The volume fractions corresponding to each class are:

$$\begin{aligned} f^{r_i} &= \frac{(c^{\text{df}, r}(r_i))r_i^3}{\sum_j (c^{\text{df}, r}(r_j))r_j^3} (1 - f^{(\text{m})}) \\ f^{r_i} &= c^{\text{df}, v}(r) (1 - f^{(\text{m})}) \\ f^{r_i} &= \frac{0.8}{c^{\text{M}}c^{\text{S}}} (1 - f^{(\text{m})}) \end{aligned} \quad (4.11)$$

for $c^{\text{df}, r}$, $c^{\text{df}, v}$, and $c^{\text{df}, v-\text{CROP}}$, respectively.

In figures 4.20 and 4.21 estimates of the effective conductivities of composites having log-normal distributions of the radii, $c^{\text{df}, r}$ and $c^{\text{df}, v}$, are compared. The span in the “relative volume fraction” distribution does not qualitatively change the conductivity vs. size curves, but makes the transition between the large and small radius regimes more gradual. $c^{\text{df}, r}$ is much more sensitive to its span, especially for the small radius regime. This can be observed better in figure 4.19. In this figure, the normalized f^{r_i} are plotted. Note that the f^{r_i} of $c^{\text{df}, v}$ coincides with the probability density function of both log-normals divided by a constant. For $c^{\text{df}, r}$ particle radii with a very low probability to be

found, can produce a relative volume fraction that is significant. This is because a given size difference in the radius implies a much larger difference in the volumes and viceversa.

A somewhat larger sensitivity to the span of volume of particles distributions can be found for “cropped” uniform monomodal distributions. As can be seen in figure 4.22 these distributions lead to a qualitatively different behaviour than log-normal ones. A decrease in the overall conductivity is predicted for all median radii.

In the following, a multiphase RMTM is used to study composites with bimodal distributions of particles. The partial distribution with the small radius is denoted by S, and the partial distribution with the bigger diameter with L. Particle mixes containing different contributions of both populations are described by a “mixing parameter”, f^{MIX} , describing the percentage of the total volume fraction that corresponds to the distribution with the biggest median radius.

In figure 4.23 predictions of the effective conductivity as functions of the “mixing parameter” evaluated for log-normal partial distributions of equal span, and for median radii that differ by a factor of 10 are presented. Two different cases are studied, in the first one, figure 4.23 (top), the radii of the partial distributions, 50 and 500 μm , are chosen so that they are close to the right-hand “shoulder” of the overall conductivities as shown in figure 4.9. In the second one, figure 4.23 (bottom), the median radii, 1.6 and 16 μm , are chosen so that they straddle the critical radius. The results are compared with the ones obtained by applying a rule of mixtures:

$$\mathcal{K}_{\text{ROM}}^*(i, i) = f^{\text{MIX}} \mathcal{K}_{\text{ROM}}^*(r = r^{\text{L}})(i, i) + (1 - f^{\text{MIX}}) \mathcal{K}_{\text{ROM}}^*(r = r^{\text{S}})(i, i) \quad (4.12)$$

where the effective conductivities are calculated by using equation (4.5).

For small spans the Rule of Mixtures is an excellent approximation for the distributions studied. The difference between the RMTM and the ROM are appreciable only for big spans, and when the radii studied straddle the critical radius.

Predictions pertaining to monomodal log-normal distributions, $c^{\text{df}, v}$, with a median equal to the median of the highest median radius, span equal to one and a particle volume fraction of 0.17 are also plotted in figure 4.23. As expected the use of bimodal distributions can considerably improve the the effective conductivity of the composite if the median radii of both populations are sufficiently large, compare figure 4.23 (top). Adding particles smaller than the critical radius produces limited gains at best and may actually degrade the macroscopic conductivity of the composite, see figure 4.23 (bottom).

Summarizing, the multiphase RMTM has been used to study the effective behaviour of DRMMCs with polydisperse size distributions. The estimates obtained are highly dependent on the distribution function used to model the particle size distribution. Therefore, special care must be taken when choosing it, and this should be as close as possible to the real one.

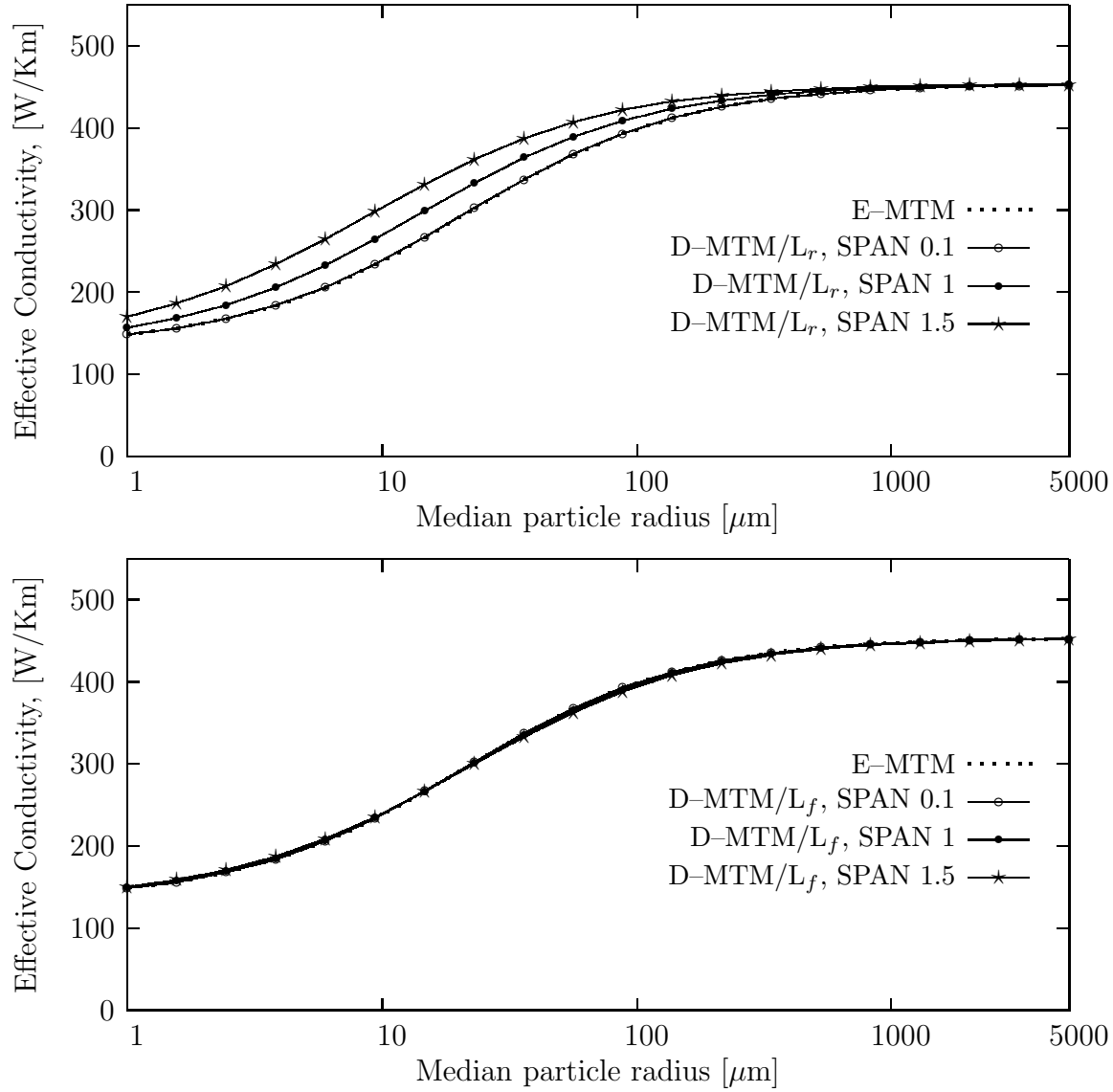


Figure 4.20: Mori–Tanaka predictions for the effective conductivity of DRMMCs with material properties following tables 4.1 and 4.2 and a total particle volume fraction of 0.34. E-MTM denotes predictions for equal-sized particles composites and D-MTM/L predictions for distribution of particles having log-normal size distributions for different spans. L_r (Top) denotes a log normal distribution of the radii, c^{df}, r , and L_f (Bottom) denotes a log normal distribution of the radii, c^{df}, v .

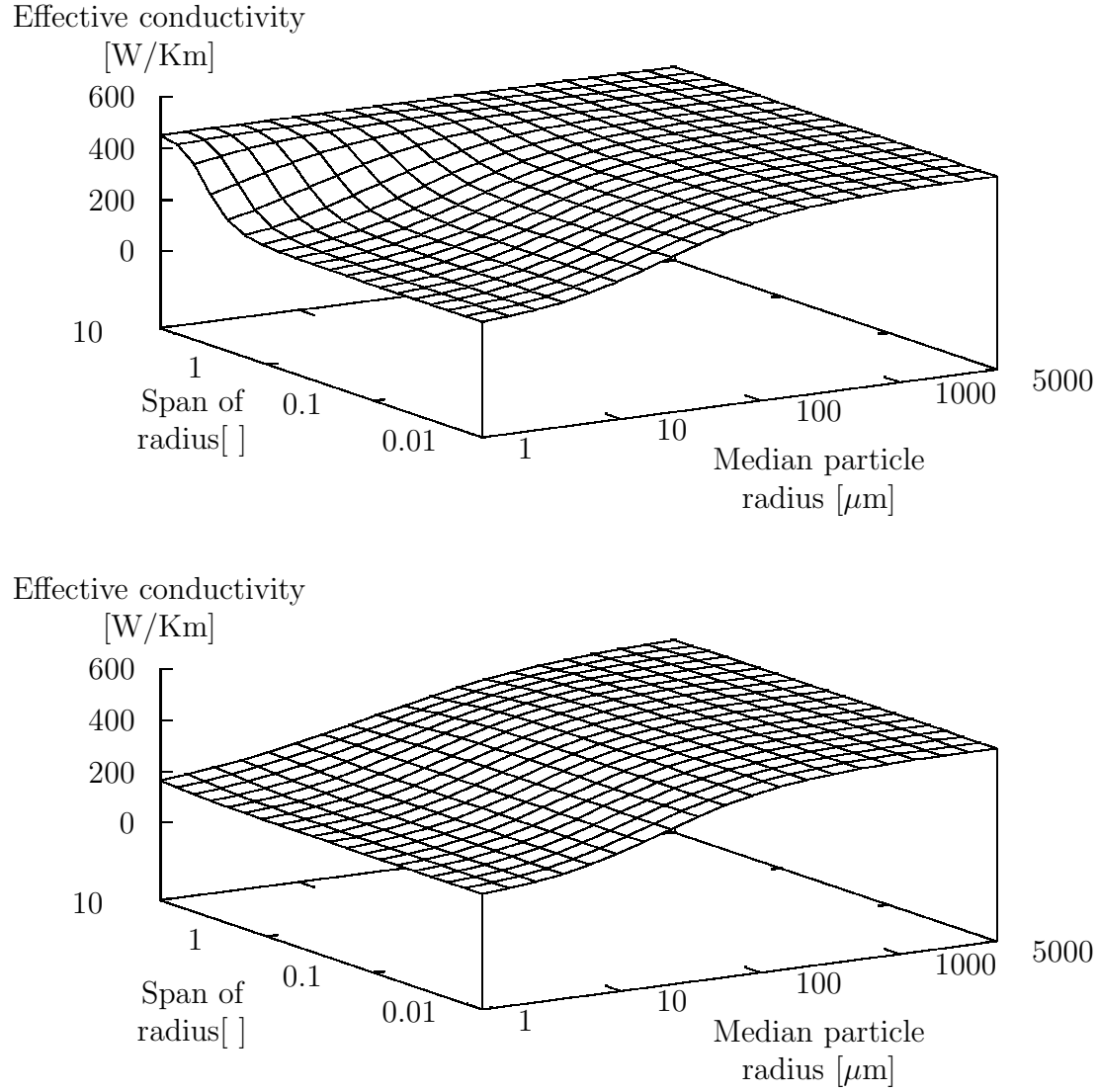


Figure 4.21: Mori–Tanaka predictions for the effective conductivity of DRMMCs with material properties following tables 4.1 and 4.2 and a total particle volume fraction of 0.34. The top plot pertains to a log normal distribution of the radii, c^{df}, r , and the bottom plot pertains to a log normal distribution of the radii, c^{df}, v .

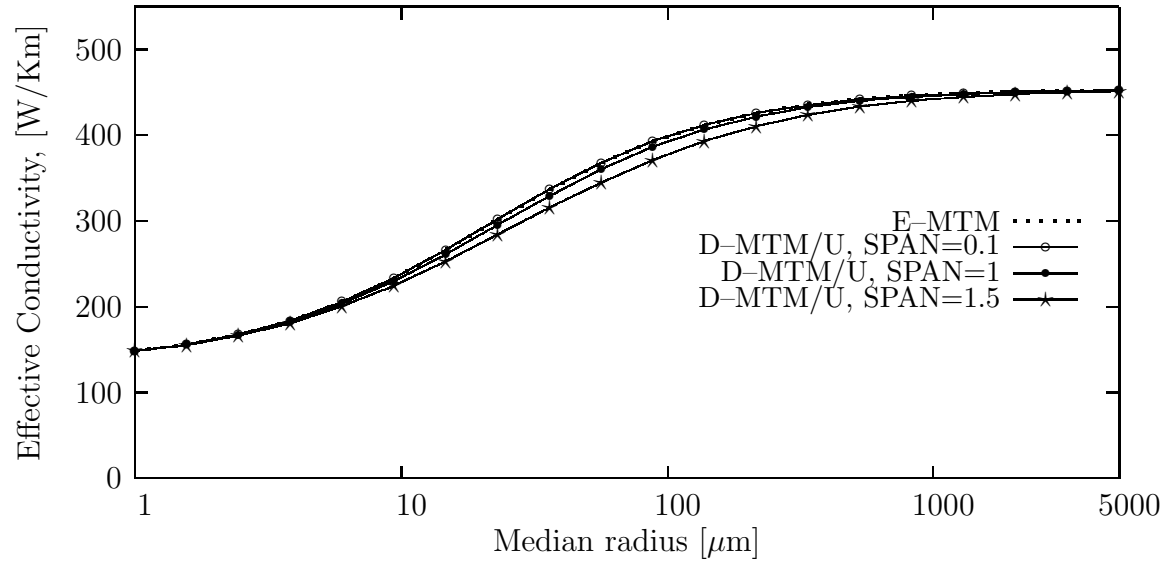


Figure 4.22: Mori–Tanaka predictions for the effective conductivity of DRMMCs with material properties following tables 4.1 and 4.2 and a total particle volume fraction of 0.34. E-MTM denotes predictions for composites reinforced by particles of equal size and D–MTM/U predictions for distribution of particles having a “cropped” uniform distribution of the radius for different spans.

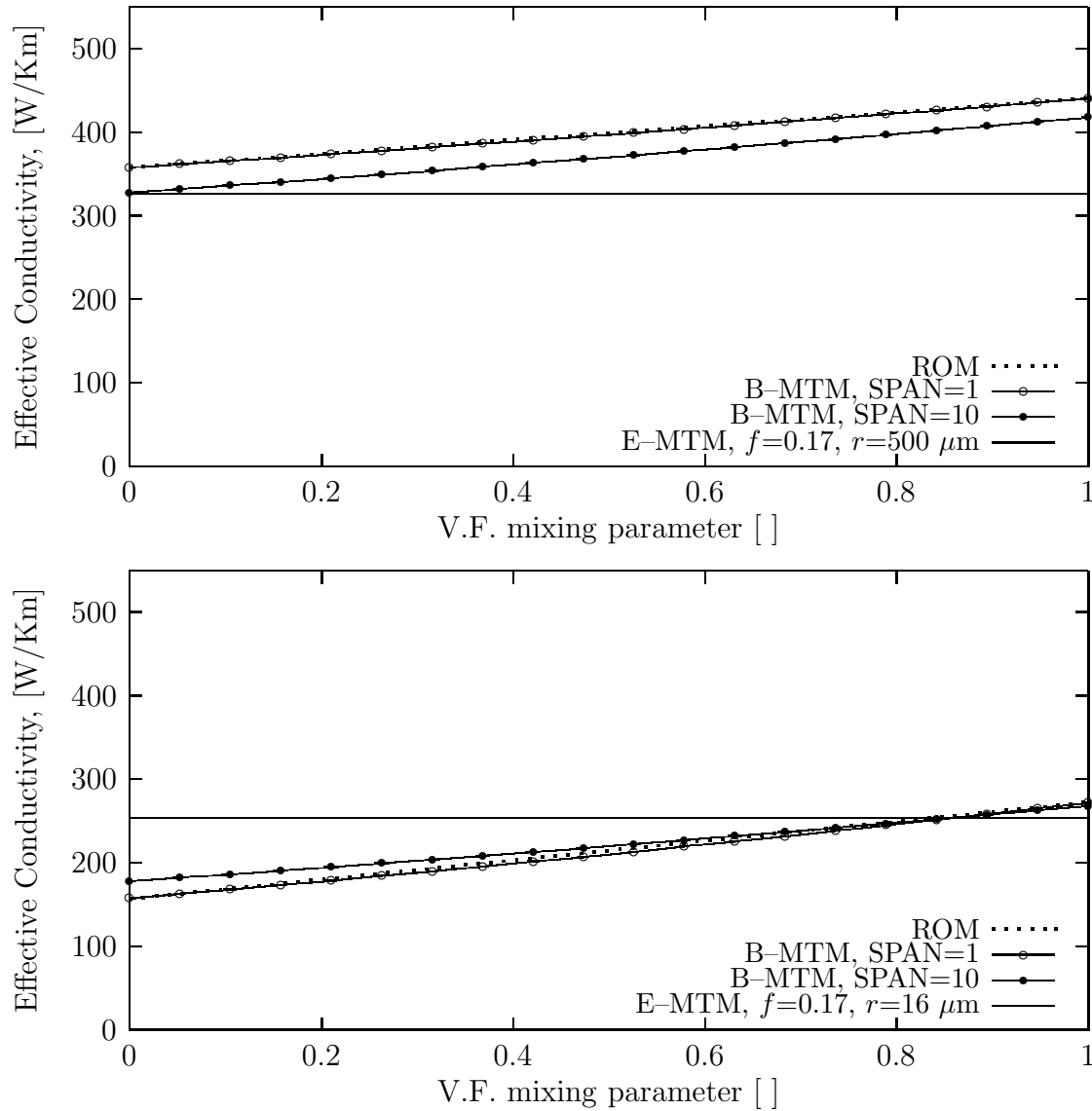


Figure 4.23: Comparison of “rule of mixture” (ROM) and Mori–Tanaka predictions (B–MTM) for the effective conductivities of composites reinforced by particles having bimodal size distributions of different spans, the total volume fraction being 0.34. In the upper plot, the partial distributions have the same span and median radii of 50 and 500 μm . In the lower plot, the partial distributions have the same span and median radii of 1.6 and 16 μm . The critical particle radius is 9.85 μm .

Chapter 5

Study of the thermomechanical behaviour of Diamond Reinforced Metal Matrix Composites using Continuum Micromechanics of Materials

In this chapter some micromechanical methods are applied to studying the mechanical behaviour of Metal Matrix Composites. The discussion is centered on the thermo-elastic and thermoelasto-plastic behaviour of DRMMCs. Additionally, some micromechanically-based models for describing the thermoelastoplastic behaviour of components made of inhomogeneous materials are discussed.

5.1 Material Parameters

Two different sets of material parameters were used for the simulations discussed in this chapter. The first one corresponds to diamond particles and aluminium matrix, and the second one to particle reinforced steel. The latter set was used only for some cyclic load cases at the end of the chapter.

5.1.1 Diamond/Aluminium composites

In table 5.1 the isotropic Young's moduli, E , the shear moduli, g , and the bulk moduli, k , used for Diamond and Aluminium, are listed. Diamond is approximated as an isotropic material although single crystal diamonds show cubic elasticity.

Whereas temperature independent elastic constants were employed in all studies of the thermomechanical behaviour of DRMMCs, temperature dependent hardening curves were obtained from the results given for aluminium 99.99 by Chinh et al. [31]. Table 5.2 list the corresponding initial yield stresses, $s^{y,0}$, for a number of temperatures. The coefficients of thermal expansion of the constituents were prescribed as functions of temperature following [153], see table 5.3.

5.1.2 Particle reinforced steel

The steel considered is AISI 1010. In table 5.1 the elastic moduli of the material are collected. The isotropic hardening of the material is described using a Voce law, see section 2.5.1, the correspondent material parameters are listed in table 5.4. The non-linear kinematic hardening is described by a Frederick–Armstrong model, see equation (2.56). The parameters of the non linear kinematic hardening are listed in table 5.5.

5.2 Thermo–elastic behaviour

In this section, numerical and semianalytical methods are used for extracting the effective elasticity tensor and coefficient of thermal expansion tensor of DRMMCs.

Table 5.1: Elastic material parameters (Young's modulus, E , shear modulus, g , and bulk modulus, k) of the constituents.

	E [GPa]	g [GPa]	k [GPa]
Diamond	1050	477	438
Aluminum	70	26	69
Steel	210	81	175

Table 5.2: Initial yield stress, $s^{y,0}$, of Al 99.99 as function of the temperature, t (data estimated from curves given in [31]).

	$t=293$ K	$t=353$ K	$t=433$ K	$t=623$ K	$t=673$ K	$t=738$ K
$s^{y,0}$ [MPa]	20.8	17.5	12.0	7.5	5.8	4.3

Table 5.3: Total coefficients of thermal expansion, α , of aluminum and diamonds as functions of the temperature t [153]. Reference temperature 200 K.

t [K]	α^{Al} [1/K]	α^{Diam} [1/K]
200	20.3×10^{-6}	1.50×10^{-6}
300	21.7×10^{-6}	1.50×10^{-6}
400	22.9×10^{-6}	1.57×10^{-6}
500	23.8×10^{-6}	1.80×10^{-6}
600	24.7×10^{-6}	2.08×10^{-6}
800	26.9×10^{-6}	2.55×10^{-6}

Table 5.4: Coefficients of the Voce law, see section 2.5.1, for an AISI 1010 steel, see Doghri [38].

	$c^{(1),\text{Voce}}$ [GPa]	$c^{(2),\text{Voce}}$ [GPa]	$c^{(3),\text{Voce}}$ []	$s^{y,0}$ [MPa]
Steel	2	2	-0.26	200MPa

Table 5.5: Coefficients of the Frederick Armstrong law, equation (2.56), for an AISI 1010 steel, see Doghri [38].

	$c^{(1),\text{C-M}}$ [GPa]	$c^{(2),\text{C-M}}$ []
Steel	17	21

Unit cells UCDA, UCDB and UCS, see figure 4.13, together with the appropriate periodicity boundary conditions, were subjected to six linearly independent mechanical loadings for obtaining the elasticity tensors, and one temperature excursion for obtaining the CTE tensor. Constituent material properties follow the data for diamond and aluminium in tables 5.1 and 5.3.

The elasticity tensors obtained with UCDA, $\mathbf{E}^{\text{UCDA}}$ [GPa], UCDB, $\mathbf{E}^{\text{UCDB}}$ [GPa], and UCS, $\mathbf{E}^{\text{UCS}}$ [GPa], are:

$$\begin{aligned}
 \mathbf{E}^{\text{UCDA}} &= \begin{pmatrix} 182.0 & 71.9 & 71.5 & 0 & 0 & 0 \\ 71.9 & 180.0 & 71.5 & 0 & 0 & 0 \\ 71.5 & 71.5 & 180.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 55.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 55.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 56.1 \end{pmatrix} \\
 \mathbf{E}^{\text{UCDB}} &= \begin{pmatrix} 182.0 & 71.7 & 72.0 & 0 & 0 & 0 \\ 71.7 & 180.6 & 71.7 & 0 & 0 & 0 \\ 72.0 & 71.7 & 180.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 55.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 56.3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 55.9 \end{pmatrix} \\
 \mathbf{E}^{\text{UCS}} &= \begin{pmatrix} 176.9 & 71.9 & 71.8 & 0 & 0 & 0 \\ 71.9 & 176.0 & 71.7 & 0 & 0 & 0 \\ 71.8 & 71.7 & 175.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 52.9 & 0 & 0 \\ 0 & 0 & 0 & 0 & 53.2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 53.2 \end{pmatrix}
 \end{aligned} \tag{5.1}$$

where the zero components of the elasticity matrices were “numerical zeros”. Because the unit cells were too small to be representative volume elements some anisotropy was present in their responses, however the differences between corresponding diagonal terms of the elasticity tensor being less than 1.5%. In table 5.6, the Zener factors of the above elasticity tensors are listed. The Zener factors are a measure for the anisotropy of orthotropic materials. As can be observed, the symmetry of the unit cells is clearly anisotropic. UCS, as expected, is less anisotropic because of the symmetry of its particles.

Analogously, Mori–Tanaka based methods were used to estimate the elasticity tensor and CTE vector. Whilst for spherical reinforcements, analytical solutions, i.e. Mori–

Tanaka method, can be found, see section 3.2.1.2.3, for cubo–octahedral particles semi-analytical solutions are needed, e.g. RMTM. For the latter case, dilute unit cells, see figure 3.2.2.2 were subjected to six linearly independent mechanical loads for extracting the replacement dilute strain concentration tensor and the replacement inclusion elasticity tensor. Note, that due to the symmetry of the particles, the dilute strain concentration tensors obtained by this procedure, which pertains to particles having identical orientation, are cubic and not isotropic. A quasi-isotropic overall elastic behaviour corresponding to randomly oriented diamond particles can be approximated by “isotropizing” the elasticity tensors, e.g. by using the Hershey–Kröner–Eshelby (HKE) method [94], which was developed to evaluate the macroscopically isotropic elastic response of polycrystals consisting of randomly oriented cubic grains. Note that the method can be applied at the microscale (at the dilute level) or at the macroscale level, leading to different results.

Predictions for the macroscopic elastic moduli and coefficients of thermal expansion for a reinforcement volume fraction of 0.34 at room temperature (293 K) are collected in table 5.7. Here “MTM, sph” stands for the classical Mori–Tanaka estimates employing spherical particles [10] and “RMTM, diam” for the Mori–Tanaka method using replacement tensors evaluated for cubo–octahedral particles. For the latter case isotropic effective elasticity tensors were obtained by applying the HKE method at the macroscopic level. Torquato’s three-point estimates [150] evaluated for spherical particles of uniform size are listed under the heading “3PE, sph”, and results from the unit cell models shown in fig. 4.13 are marked as “UCS”, “UCDA” and “UCDB”. The unit cell results pertain to macroscopic tensors made quasi-isotropic by the HKE algorithm. In contrast to the effective thermal conductivities, the predicted elastic tensors do not have an intrinsic length scale.

Table 5.6: Zener factors of the orthotropic material behaviour obtained from the elasticity tensors of UCDA, UCDB and UCS, eqn. (5.1).

	UCDA	UCDB	RMTM
$\frac{2\mathbf{E}(4,4)}{\mathbf{E}(1,1) - \mathbf{E}(1,2)}$	1.0064	1.0100	1.0076
$\frac{2\mathbf{E}(5,5)}{\mathbf{E}(2,2) - \mathbf{E}(2,3)}$	1.0267	1.0340	1.0201
$\frac{2\mathbf{E}(6,6)}{\mathbf{E}(3,3) - \mathbf{E}(3,1)}$	1.0284	1.0352	1.0250

Table 5.7: Predictions for the effective elastic moduli and the CTE at 293 K of diamond reinforced aluminum at a diamond volume fraction of $\xi = 0.34$ obtained by Mori–Tanaka methods (MTM and RMTM), Torquato’s three-point estimates (3PE), and unit cells UCS, UCDA and UCDB.

	E^* [GPa]	g^* [GPa]	k^* [GPa]	α^* @ 293 K
MTM, sph	131.2	50.7	106.1	1.394×10^{-5}
RMTM, diam	134.0	51.9	106.7	1.258×10^{-5}
3PE, sph	137.2	53.3	107.3	1.376×10^{-5}
UCS	135.7	52.7	106.6	1.397×10^{-5}
UCDA	141.7	55.3	108.0	1.376×10^{-5}
UCDB	142.0	55.4	108.2	1.358×10^{-5}

Both the Mori–Tanaka methods and the multi-particle unit cells predict a stiffer macroscopic behaviour for cubo-octahedral particles compared to spheres, the effect being more pronounced in the unit cell models. The overall elastic behaviour obtained from the Mori–Tanaka methods is more compliant than the predictions of the three-point estimates and the unit cells. This is due to the fact that Mori–Tanaka approaches provide lower estimates for the stiffness of composites in which the reinforcements are stiffer than the matrix; for the spherical particles the MTM results correspond to the Hashin–Shtrikman lower bounds. A higher CTE is predicted for the spheres than for the diamonds for both numerical and analytical methods. The MTM for spheres is closer to the estimates of UCS than the Torquato estimates. The orientation of the particles plays a bigger role in the CTEs tensors than in the elasticity tensors.

Inspection of the stress distributions obtained with the numerical models using cubo-octahedral particles indicates that at the interfaces singularities may be present in the elastic stress and strain fields in the matrix at reentrant edges and corners, see figure 5.1. Even though such singularities cannot be resolved with the Finite Elements models employed in the present study, their presence does not compromise the evaluation of the reduced elastic concentration tensors, for which the volume averaged strains in the inhomogeneities are required. They lead to difficulties, however, in using criteria for macroscopic yielding that are based on the maximum of the equivalent stress in the matrix as predicted by multi-particle unit cells.

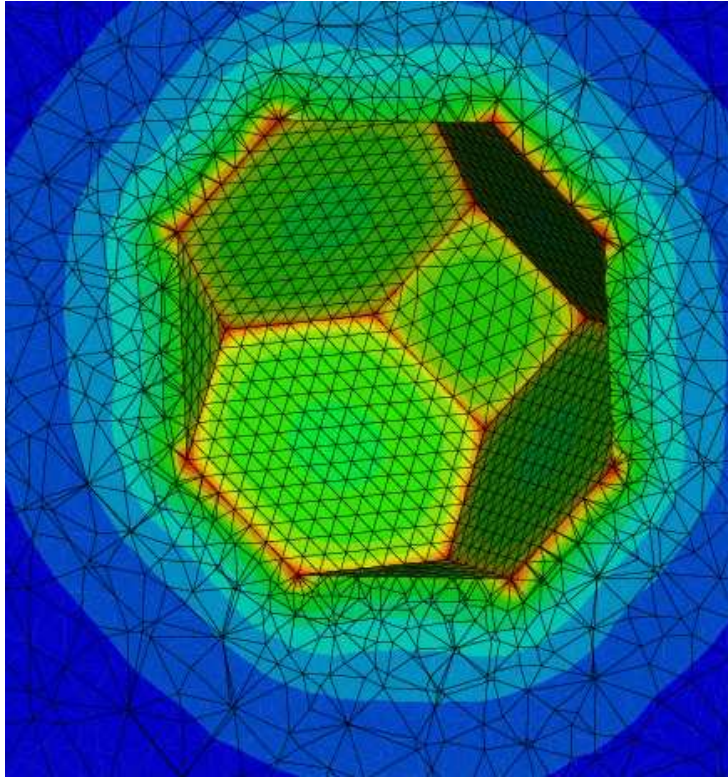


Figure 5.1: Fringe plot of the Von-Mises stress distribution in the matrix of a DRMMCS subjected to an elastic loading.

5.3 Thermo Elasto-Plastic behaviour

In this section numerical and analytical methods are used for studying the thermo-elasto-plastic behaviour of Metal Matrix Composites. In the first part, PMAs are used for studying in detail the local behaviour of DRMMCs under fabrication and service conditions. The second part is devoted to the thermo-elasto-plastic analysis of components made of inhomogeneous material, such as the divertor of a nuclear reactor.

5.3.1 Local Behaviour

Due to the marked thermal expansion contrast between the constituents, aluminum and diamond, and the low initial yield stress of the matrix, compare tables 5.2 and 5.3, a strong tendency of DRMMCs toward matrix yielding under thermal loading must be expected. Plastic yielding of macroscopically isotropic composites under pure thermal loading cannot

be described by Mori–Tanaka methods, which always predict hydrostatic matrix stress states under such conditions. Unit cell methods, however, are well suited to the task. Thermoelastic modeling with unit cell UCS (20 spherical particles) indicated that the temperature change required for initiating local plastic yielding is more than an order of magnitude smaller in a DRMMC with a matrix of Al99.99 compared to a high strength aluminum alloy reinforced by SiC particles of the same volume fraction.

Thermoelastoplastic analysis employing the multi-particle unit cells shown in fig. 4.13 and the temperature dependent constituent properties listed in tables 5.2 and 5.3 can be used to study the macroscopic thermomechanical responses as well as the effects of local thermal stresses and strains in DRMMCs. Figure 5.2 (left) shows the distribution of the accumulated equivalent plastic strains, p , predicted for the matrix domain of unit cell UCDA after cooling down from a stress-free temperature of 450 K to room temperature. The plastic strains can be seen to be highly inhomogeneous and to exceed a value of 0.01 over a considerable part of the volume element. Because hardly any elastic matrix regions remain, the matrix may be viewed as fully yielded in this state. Heating up to 373 K from this state leads to further plastic yielding as displayed in fig. 5.2 (right), where especially the increased extent of regions with accumulated equivalent plastic strains in excess of 0.01 is noteworthy. To further illustrate this behaviour, the evolution of the equivalent accumulated plastic strain in the matrix is shown in fig. 5.3, where the phase averages and standard deviations of p are plotted for selected temperatures during the heating-up process. Temperature changes of up to 20 K give rise to some local yielding, but have little influence on the distribution of the plastic strains in the matrix. Temperature excursions in excess of 40 K, however, lead to an increase in the averages of p , which indicates bulk yielding of the matrix, and to a marked rise in the standard deviations, the latter indicating an intensifying inhomogeneity of the plastic strains.

Figure 5.4 compares the macroscopic responses of initially stress-free (virgin) and cooled-down diamond–aluminum (from 450 K to room temperature) composites to uniaxial tensile loading as predicted with unit cell UCDA. Up to an applied stress of approximately 20 MPa there is little difference between the two curves, but for tensile stresses exceeding 25 MPa the residual stresses in the cooled-down material lead to a markedly stronger hardening behaviour.

In figure 5.5 the ratchetting behaviour of the material is studied. UCDA was exposed to thermal cycling from 293 K to 393 K. For a thermal cycling of 100 degrees the material shows an accumulation of residual strains from cycle 2 to 3.

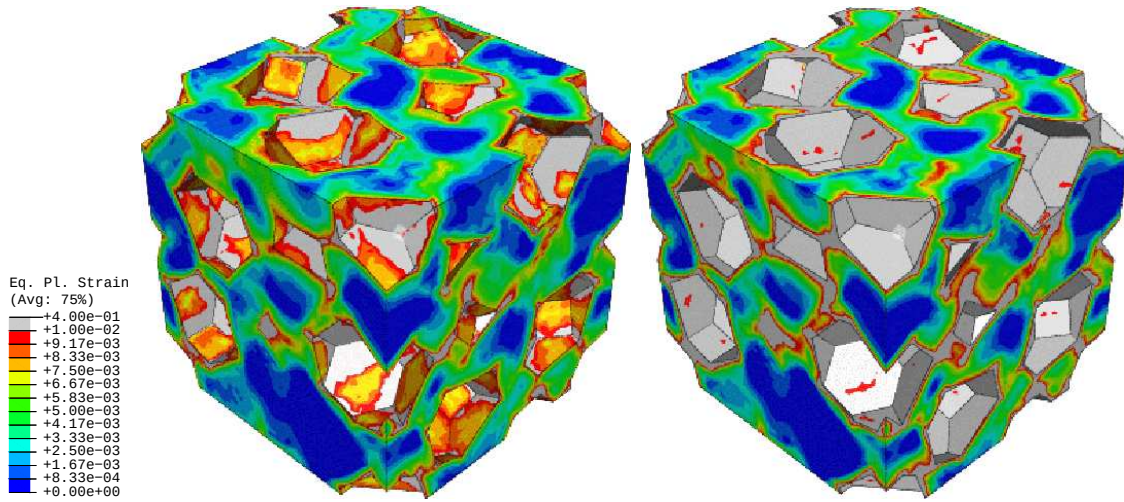


Figure 5.2: Predicted distributions of equivalent plastic strain in the matrix of UCDA following cool-down from a stress-free temperature of 450 K to room temperature (left) and after subsequent heating up by 80 K (right).

The above modeling results clearly indicate that DRMMCs tend to be subject to marked matrix plasticity effects under thermal loading. The resulting residual stress states may also strongly influence the mechanical responses. This behaviour must be accounted for in the development, production and use of such materials for heat sink applications.

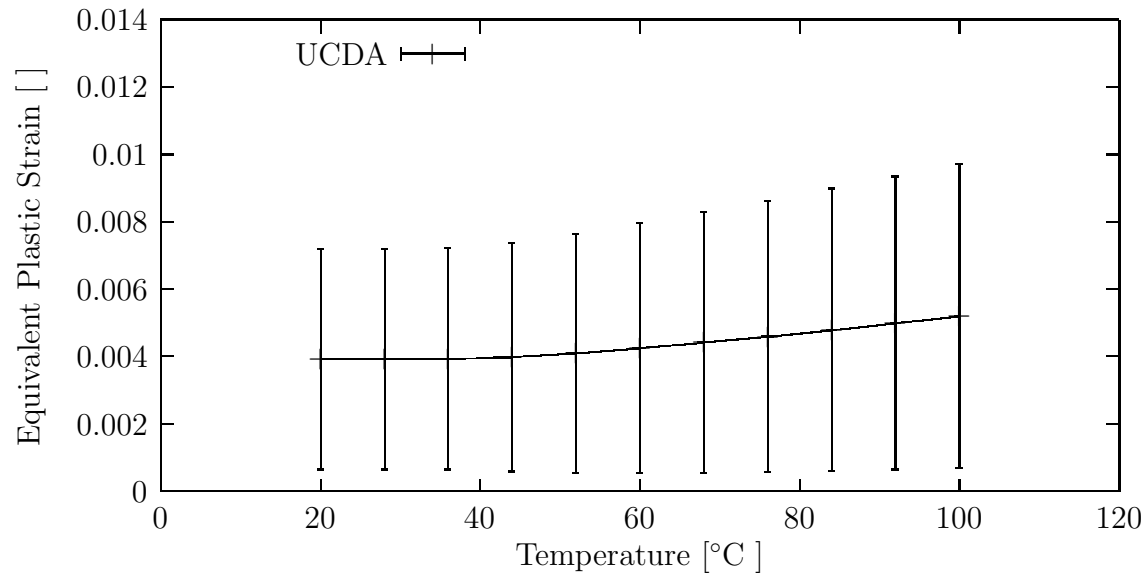


Figure 5.3: Evolution of the average and the standard deviation of the accumulated equivalent plastic strain in the matrix, p , during heating up from the cooled-down state to 100 °C as predicted by unit cell UCDA ($f = 0.34$).

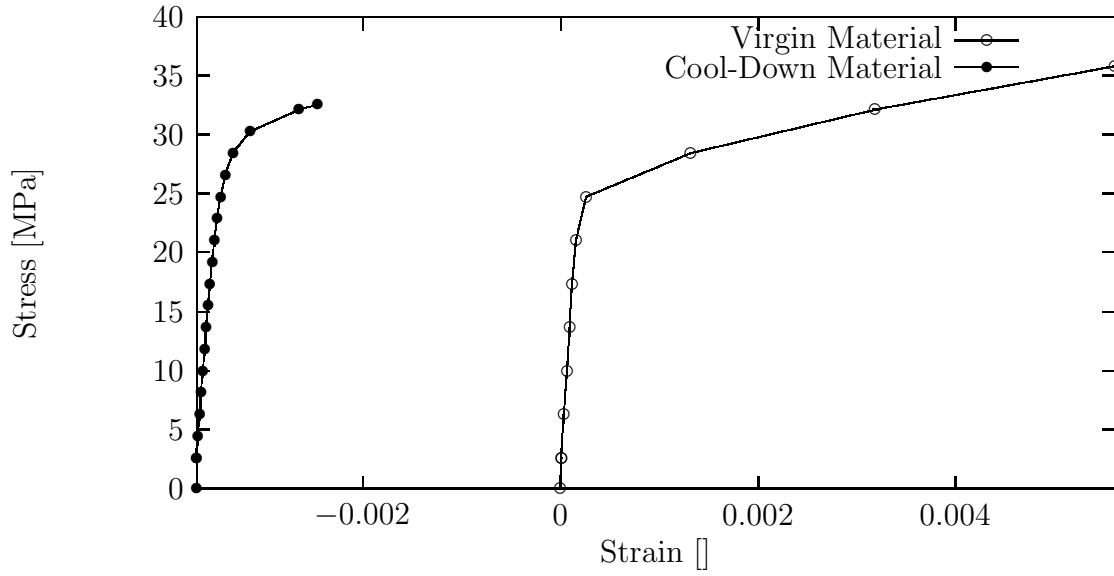


Figure 5.4: Macroscopic stress-strain responses of DRMMC subjected to uniaxial tensile loading predicted for virgin and cooled-down conditions with unit cell UCDA ($f = 0.34$).

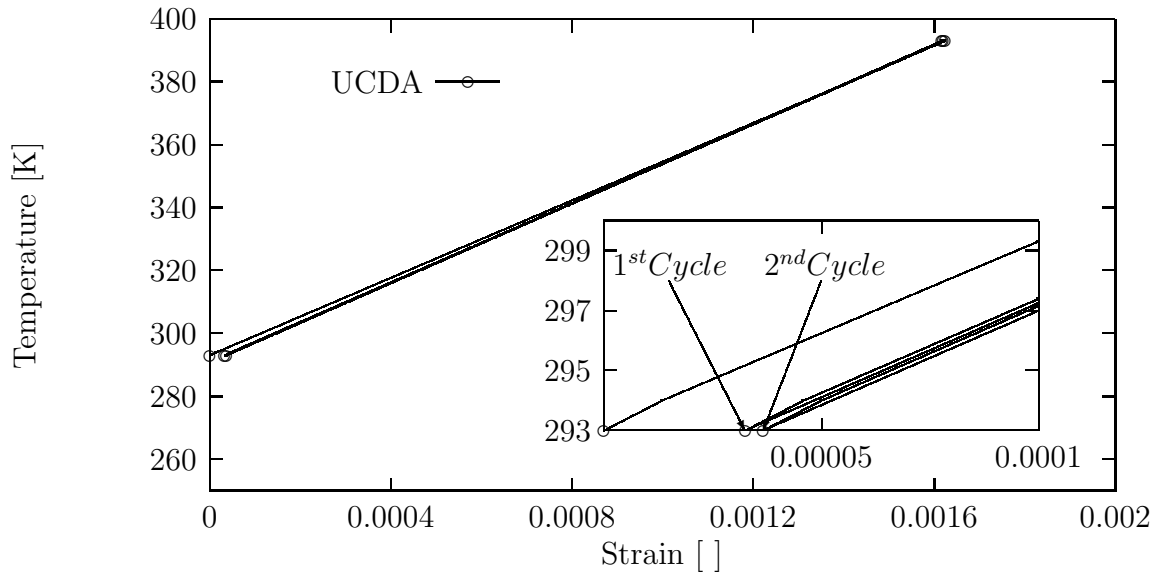


Figure 5.5: Macroscopic stress-strain responses of DRMMC subjected to cyclic uniaxial tensile loading predicted with unit cell UCDA ($f = 0.34$).

5.3.2 Effective Behaviour

A component made of an inhomogeneous material cannot be fully modelled via numerical micromechanical methods, i.e., all the fibers of the divertor of a nuclear reactor cannot be taken into account in a model because of the computational power needed. Therefore simplifications are needed. One possibility is to treat the inhomogeneous material as an homogeneous material the properties of which are obtained from experiments. This approach does not allow for zooming into the local behaviour of the phases of the inhomogeneous materials, and requires numerous experiments, which make it inappropriate for parametric studies. Another possibility is the use of Incremental Mori–Tanaka methods, see section 3.2.1.2.3. The IMT-methods need as input the material properties of the constituents and not of the actual composite. They are capable of handling complex loading conditions and arbitrary load paths.

In this thesis, the IMT of Pettermann was extended for studying the cyclic thermoe-elastoplastic behaviour of particle reinforced composites. For this purpose the Chaboche–Marquis model was implemented into it. The IMT is implemented in the finite element code ABAQUS through a user subroutine UMAT. For testing purposes, a single element test was carried out. The element was exposed to a uniaxial cyclic load. In figure 5.6, stress–strain curves obtained using the IMT-UMAT material model for vanishing reinforcement volume fraction are compared with the results obtained with Chaboche–Marquis material model of ABAQUS. Material parameters follow tables 5.1, 5.4 and 5.5 for steel.

In figure 5.7 the stress–strain curves obtained using the IMT for a single element exposed to a uniaxial cyclic load for different volume fractions are presented. As observed, even for high reinforcement volume fraction the ratchetting effect is not avoided for this material.

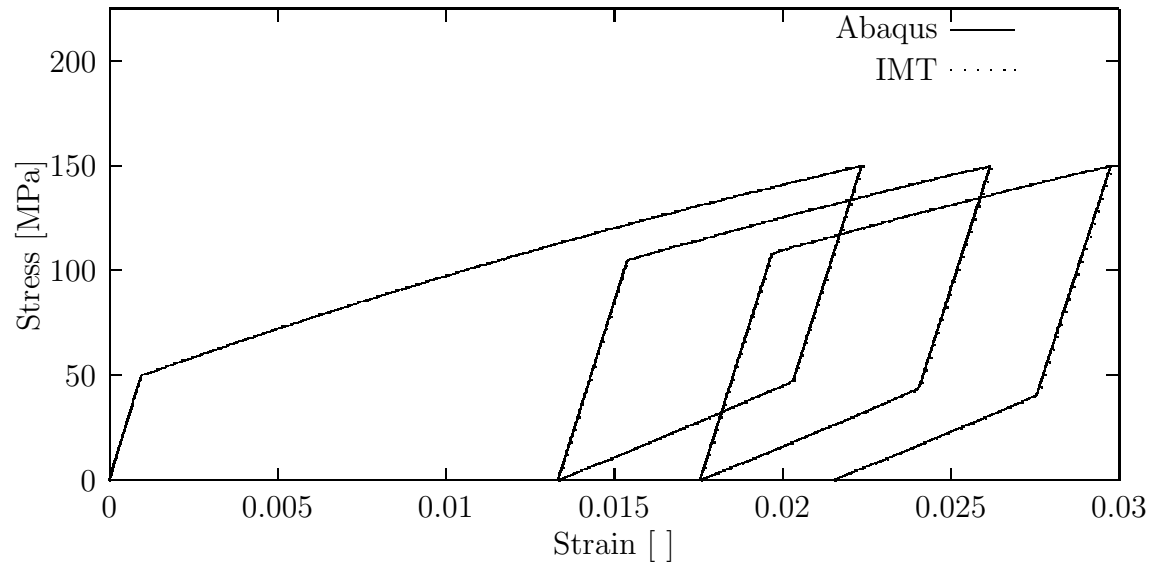


Figure 5.6: Comparison of the stress–strain curves obtained for a single element exposed to a uniaxial cyclic load using the Chaboche–Marquis model of Abaqus, and the Chaboche–Marquis model of the IMT of Pettermann at vanishing reinforcement volume fraction. Material properties follow tables 5.1, 5.4 and 5.5 for steel.

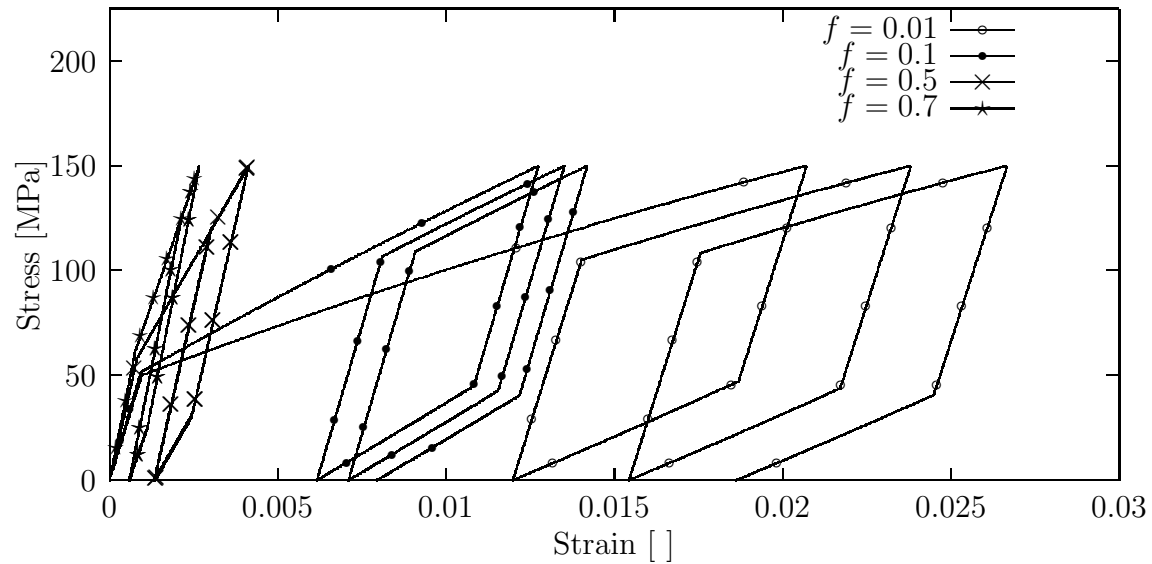


Figure 5.7: Stress strain curves obtained in a single element test exposed to a uniaxial cyclic loading for different reinforcement volume fractions. Material properties following tables 5.1, 5.4 and 5.5 for steel. The plasticity model was implemented using the IMT-UMAT of Pettermann.

Chapter 6

Conclusions

Micromechanical methods for studying the thermophysical and thermomechanical behaviour of particle reinforced metal matrix composites were reviewed. Special emphasis was placed on diamond reinforced metal matrix composites.

Replacement tensor Mori–Tanaka approaches, unit cells and windowing methods were extended/used for investigating the thermal conduction behaviour of DRMMCs with interfacial conductances. The predictions of unit cells and the R–MTM at a moderate volume fraction of $f = 0.34$ were found to be in good agreement. At higher volume fractions windowing methods and R–MTM were found to be in agreement, too. For cubo–octahedral particles, spheres with an equivalent homogeneous distribution of the interfacial conductance were found to give good results. This concept was used for studying monomodal and bimodal distributions of particle sizes. The equivalent sphere concept may be extended to more complex shapes by using ellipsoids instead of spheres. However, orientational averaging may be needed.

The thermomechanical behaviour of DRMMCs was studied by unit cells, and the results were compared with some analytical methods.

The results of the previous studies support the viability of the concept of using DRMMCs as high–conductivity heat sink materials. The main problem are the thermomechanical behaviour of these composites due to the high contrast of the coefficients of thermal expansion of the constituents. Therefore, special care must be taken during the manufacturing process and the service conditions must be chosen to reduce cyclic plastic yielding.

Additionally incremental Mori–Tanaka methods were extended to studying the cyclic thermoelastoplastic behaviour of particle reinforced composites. The method allows ther-

moelastoplastic FEM analysis of components made of inhomogeneous materials.

Appendix A

Tensorial and engineering notation

Tensorial notation is elegant and useful for theoretical derivations. However, when implementing a model into a finite element code, the conventional approach is to use engineering notation. This conversion is a common source of errors when implementing a plasticity model. In this thesis only tensors of second and fourth rank are used.

Any second rank tensor has 9 components. If the tensor is symmetric, $\beta_{ij} = \beta_{ji}$, the number of independent components is reduced to six and can be represented as a quasi-vector. There is no standard way to arrange these components, but, usually, the normal components are given first and arranged in “natural” order, and then the shear components, or a modification of them, follow:

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_{11} \\ \beta_{22} \\ \beta_{33} \\ \beta_{12}^* \\ \beta_{13}^* \\ \beta_{23}^* \end{pmatrix} \quad (\text{A.1})$$

In the present work $\beta_{ij}^* = 2\beta_{ij}$ if $\boldsymbol{\beta}$ is a strain quasi-vector, otherwise $\beta_{ij}^* = \beta_{ij}$.

Any fourth order tensor, A_{ijkl} , has 81 components. If the tensor possesses major symmetry, $A_{ijkl} = A_{klij}$, the number of components is reduced to 45. If the tensor has minor symmetry, $A_{ijkl} = A_{jikl} = A_{ijlk}$, the tensor has 36 independent constants and it can be represented as a quasi-matrix:

$$\mathbf{A} = \begin{pmatrix} A_{1111} & A_{1122} & A_{1133} & A_{1112} & A_{1113} & A_{1123} \\ A_{2211} & A_{2222} & A_{2233} & A_{2212} & A_{2213} & A_{2223} \\ A_{3311} & A_{3322} & A_{3333} & A_{3312} & A_{3313} & A_{3323} \\ A_{1211} & A_{1222} & A_{1233} & A_{1212} & A_{1213} & A_{1223} \\ A_{1311} & A_{1322} & A_{1333} & A_{1312} & A_{1313} & A_{1323} \\ A_{2311} & A_{2322} & A_{2333} & A_{2312} & A_{2313} & A_{2323} \end{pmatrix} \quad (\text{A.2})$$

It is worth noting that if the tensor possesses major and minor symmetry, the number of independent constants reduces to 21, and the tensor can be represented as a symmetric quasi-matrix. In this notation, the decomposition of the fourth order symmetric unit tensor into its deviatoric and its volumetric parts reads:

$$\mathbf{1}^s = \mathbf{1}^{\text{dev},s} + \mathbf{1}^{\text{vol}}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (\text{A.3})$$

Note that the fourth order unit tensor cannot be written in this notation because it does not have minor symmetry. For different notations see e.g. [35; 116].

The main reasons for using this notation are that when every second order tensor is represented using (A.1) and every fourth order tensor is represented using equation (A.2):

- The energy product, $\sigma_{ij}\varepsilon_{ji}$, is replaced in the engineering notation by a simple scalar product of column matrices $\boldsymbol{\sigma}^T \boldsymbol{\varepsilon}$
- The equation $\sigma_{ij} = E_{ijkl}\varepsilon_{lk}$ is replaced by a simple product of a matrix and a column vector, $\boldsymbol{\sigma} = \mathbf{E}\boldsymbol{\varepsilon}$

This is the convention used by ABAQUS [2] for the stress and strain quasi-vectors and for the elasticity quasi-matrix. However, ABAQUS uses a slightly different notation for

the compliance matrix, in order to avoid the use of the correction terms discussed in the following.

The above simple transcription of tensors, however, does not always work and some terms must be modified so that correct results are obtained in general cases. It is worth to review briefly the main operations. It is obvious that addition, subtraction, and multiplication by a scalar do not need any corrections.

In the following second order tensors are assumed to be symmetric and they are represented in engineering notation using equation (A.1). Furthermore, all fourth order tensors are assumed to have minor symmetry and are represented in engineering notation using equation (A.2).

The double contraction, a , of two second order tensors, β_{ij} and ζ_{ji} , is:

$$a = \beta_{ij}\zeta_{ji} = \beta_{11}\zeta_{11} + \beta_{22}\zeta_{22} + \beta_{33}\zeta_{33} + 2(\beta_{12}\zeta_{12} + \beta_{13}\zeta_{13} + \beta_{23}\zeta_{23}) \quad (\text{A.4})$$

whilst:

$$\boldsymbol{\beta}^T \boldsymbol{\zeta} = \beta_{11}\zeta_{11} + \beta_{22}\zeta_{22} + \beta_{33}\zeta_{33} + \beta_{12}^*\zeta_{12}^* + \beta_{13}^*\zeta_{13}^* + \beta_{23}^*\zeta_{23}^* \quad (\text{A.5})$$

To obtain the correct result a correction term c^{M_1} must be introduced. The modified product, $[\boldsymbol{\beta}^T \boldsymbol{\zeta}]^M$, reads:

$$a = [\boldsymbol{\beta}^T \boldsymbol{\zeta}]^M = \beta_{11}\zeta_{11} + \beta_{22}\zeta_{22} + \beta_{33}\zeta_{33} + c^{M_1}(\beta_{12}^*\zeta_{12}^* + \beta_{13}^*\zeta_{13}^* + \beta_{23}^*\zeta_{23}^*) \quad (\text{A.6})$$

where $c^{M_1} = 2$, if none of the participating quasi-vectors is the strain quasi-vector, $c^{M_1} = 1$ if one of them is a strain quasi-vector, and $c^{M_1} = \frac{1}{2}$ if both are strain quasi-vectors.

The tensorial product, A_{ijkl} , of two second order tensors, β_{ij} and ζ_{ij} is:

$$A_{ijkl} = \beta_{ij}\zeta_{kl} \quad (\text{A.7})$$

As β_{ij} and ζ_{ij} are symmetric, A_{ijkl} has minor symmetry and it can be represented as:

$$\mathbf{A} = \begin{pmatrix} \beta_{11}\zeta_{11} & \beta_{11}\zeta_{22} & \beta_{11}\zeta_{33} & \beta_{11}\zeta_{12} & \beta_{11}\zeta_{13} & \beta_{11}\zeta_{23} \\ \beta_{22}\zeta_{11} & \beta_{22}\zeta_{22} & \beta_{22}\zeta_{33} & \beta_{22}\zeta_{12} & \beta_{22}\zeta_{13} & \beta_{22}\zeta_{23} \\ \beta_{33}\zeta_{11} & \beta_{33}\zeta_{22} & \beta_{33}\zeta_{33} & \beta_{33}\zeta_{12} & \beta_{33}\zeta_{13} & \beta_{33}\zeta_{23} \\ \beta_{12}\zeta_{11} & \beta_{12}\zeta_{22} & \beta_{12}\zeta_{33} & \beta_{12}\zeta_{12} & \beta_{12}\zeta_{13} & \beta_{12}\zeta_{23} \\ \beta_{13}\zeta_{11} & \beta_{13}\zeta_{22} & \beta_{13}\zeta_{33} & \beta_{13}\zeta_{12} & \beta_{13}\zeta_{13} & \beta_{13}\zeta_{23} \\ \beta_{23}\zeta_{11} & \beta_{23}\zeta_{22} & \beta_{23}\zeta_{33} & \beta_{23}\zeta_{12} & \beta_{23}\zeta_{13} & \beta_{23}\zeta_{23} \end{pmatrix} \quad (\text{A.8})$$

which is very similar to the product of the quasi-vectors:

$$\boldsymbol{\beta}\boldsymbol{\zeta}^T = \begin{pmatrix} \beta_{11}\zeta_{11} & \beta_{11}\zeta_{22} & \beta_{11}\zeta_{33} & \beta_{11}\zeta_{12}^* & \beta_{11}\zeta_{13}^* & \beta_{11}\zeta_{23}^* \\ \beta_{22}\zeta_{11} & \beta_{22}\zeta_{22} & \beta_{22}\zeta_{33} & \beta_{22}\zeta_{12}^* & \beta_{22}\zeta_{13}^* & \beta_{22}\zeta_{23}^* \\ \beta_{33}\zeta_{11} & \beta_{33}\zeta_{22} & \beta_{33}\zeta_{33} & \beta_{33}\zeta_{12}^* & \beta_{33}\zeta_{13}^* & \beta_{33}\zeta_{23}^* \\ \beta_{12}^*\zeta_{11} & \beta_{12}^*\zeta_{22} & \beta_{12}^*\zeta_{33} & \beta_{12}^*\zeta_{12}^* & \beta_{12}^*\zeta_{13}^* & \beta_{12}^*\zeta_{23}^* \\ \beta_{13}^*\zeta_{11} & \beta_{13}^*\zeta_{22} & \beta_{13}^*\zeta_{33} & \beta_{13}^*\zeta_{12}^* & \beta_{13}^*\zeta_{13}^* & \beta_{13}^*\zeta_{23}^* \\ \beta_{23}^*\zeta_{11} & \beta_{23}^*\zeta_{22} & \beta_{23}^*\zeta_{33} & \beta_{23}^*\zeta_{12}^* & \beta_{23}^*\zeta_{13}^* & \beta_{23}^*\zeta_{23}^* \end{pmatrix} \quad (\text{A.9})$$

Nevertheless, some correction terms must be introduced when at least one of the participating quasi-vectors is a strain quasi-vector:

$$\mathbf{A} = [\boldsymbol{\beta}\boldsymbol{\zeta}^T]^M = \begin{pmatrix} \beta_{11}\zeta_{11} & \beta_{11}\zeta_{22} & \beta_{11}\zeta_{33} & c^{M_1}\beta_{11}\zeta_{12}^* & c^{M_1}\beta_{11}\zeta_{13}^* & c^{M_1}\beta_{11}\zeta_{23}^* \\ \beta_{22}\zeta_{11} & \beta_{22}\zeta_{22} & \beta_{22}\zeta_{33} & c^{M_1}\beta_{22}\zeta_{12}^* & c^{M_1}\beta_{22}\zeta_{13}^* & c^{M_1}\beta_{22}\zeta_{23}^* \\ \beta_{33}\zeta_{11} & \beta_{33}\zeta_{22} & \beta_{33}\zeta_{33} & c^{M_1}\beta_{33}\zeta_{12}^* & c^{M_1}\beta_{33}\zeta_{13}^* & c^{M_1}\beta_{33}\zeta_{23}^* \\ c^{M_2}\beta_{12}^*\zeta_{11} & c^{M_2}\beta_{12}^*\zeta_{22} & c^{M_2}\beta_{12}^*\zeta_{33} & c^{M_2}c^{M_1}\beta_{12}^*\zeta_{12}^* & c^{M_2}c^{M_1}\beta_{12}^*\zeta_{13}^* & c^{M_2}c^{M_1}\beta_{12}^*\zeta_{23}^* \\ c^{M_2}\beta_{13}^*\zeta_{11} & c^{M_2}\beta_{13}^*\zeta_{22} & c^{M_2}\beta_{13}^*\zeta_{33} & c^{M_2}c^{M_1}\beta_{13}^*\zeta_{12}^* & c^{M_2}c^{M_1}\beta_{13}^*\zeta_{13}^* & c^{M_2}c^{M_1}\beta_{13}^*\zeta_{23}^* \\ c^{M_2}\beta_{23}^*\zeta_{11} & c^{M_2}\beta_{23}^*\zeta_{22} & c^{M_2}\beta_{23}^*\zeta_{33} & c^{M_2}c^{M_1}\beta_{23}^*\zeta_{12}^* & c^{M_2}c^{M_1}\beta_{23}^*\zeta_{13}^* & c^{M_2}c^{M_1}\beta_{23}^*\zeta_{23}^* \end{pmatrix} \quad (\text{A.10})$$

where $c^{M_2} = c^{M_1} = 1$ if none of the participating quasi-vectors is a strain quasi-vector, $c^{M_1} = \frac{1}{2}$ if $\boldsymbol{\zeta}$ is a strain quasi-vector, and $c^{M_2} = \frac{1}{2}$ if $\boldsymbol{\beta}$ is a strain quasi-vector.

The double contraction, β_{ij} , of a fourth order tensor, A_{ijkl} , and a second order tensor, ζ_{ij} , is:

$$\beta_{ij} = A_{ijkl}\zeta_{lk} \quad (\text{A.11})$$

As the fourth order tensor has minor symmetry, the result can be written as a quasi-vector:

$$\boldsymbol{\beta} = \begin{pmatrix} A_{1111}\zeta_{11} + A_{1122}\zeta_{22} + A_{1133}\zeta_{33} + 2(A_{1112}\zeta_{12} + A_{1113}\zeta_{13} + A_{1123}\zeta_{23}) \\ A_{2211}\zeta_{11} + A_{2222}\zeta_{22} + A_{2233}\zeta_{33} + 2(A_{2212}\zeta_{12} + A_{2213}\zeta_{13} + A_{2223}\zeta_{23}) \\ A_{3311}\zeta_{11} + A_{3322}\zeta_{22} + A_{3333}\zeta_{33} + 2(A_{3312}\zeta_{12} + A_{3313}\zeta_{13} + A_{3323}\zeta_{23}) \\ A_{1211}\zeta_{11} + A_{1222}\zeta_{22} + A_{1233}\zeta_{33} + 2(A_{1212}\zeta_{12} + A_{1213}\zeta_{13} + A_{1223}\zeta_{23}) \\ A_{1311}\zeta_{11} + A_{1322}\zeta_{22} + A_{1333}\zeta_{33} + 2(A_{1312}\zeta_{12} + A_{1313}\zeta_{13} + A_{1323}\zeta_{23}) \\ A_{2311}\zeta_{11} + A_{2322}\zeta_{22} + A_{2333}\zeta_{33} + 2(A_{2312}\zeta_{12} + A_{2313}\zeta_{13} + A_{2323}\zeta_{23}) \end{pmatrix} \quad (\text{A.12})$$

whilst:

$$\mathbf{A}\boldsymbol{\zeta} = \begin{pmatrix} A_{1111}\zeta_{11} + A_{1122}\zeta_{22} + A_{1133}\zeta_{33} + A_{1112}\zeta_{12}^* + A_{1113}\zeta_{13}^* + A_{1123}\zeta_{23}^* \\ A_{2211}\zeta_{11} + A_{2222}\zeta_{22} + A_{2233}\zeta_{33} + A_{2212}\zeta_{12}^* + A_{2213}\zeta_{13}^* + A_{2223}\zeta_{23}^* \\ A_{3311}\zeta_{11} + A_{3322}\zeta_{22} + A_{3333}\zeta_{33} + A_{3312}\zeta_{12}^* + A_{3313}\zeta_{13}^* + A_{3323}\zeta_{23}^* \\ A_{1211}\zeta_{11} + A_{1222}\zeta_{22} + A_{1233}\zeta_{33} + A_{1212}\zeta_{12}^* + A_{1213}\zeta_{13}^* + A_{1223}\zeta_{23}^* \\ A_{1311}\zeta_{11} + A_{1322}\zeta_{22} + A_{1333}\zeta_{33} + A_{1312}\zeta_{12}^* + A_{1313}\zeta_{13}^* + A_{1323}\zeta_{23}^* \\ A_{2311}\zeta_{11} + A_{2322}\zeta_{22} + A_{2333}\zeta_{33} + A_{2312}\zeta_{12}^* + A_{2313}\zeta_{13}^* + A_{2323}\zeta_{23}^* \end{pmatrix} \quad (\text{A.13})$$

the following corrections terms may be used:

$$\boldsymbol{\beta} = [\mathbf{A}\boldsymbol{\zeta}]^{\mathbf{M}} = \begin{pmatrix} A_{1111}\zeta_{11} + A_{1122}\zeta_{22} + A_{1133}\zeta_{33} + c^{\mathbf{M}_1}(A_{1112}\zeta_{12}^* + A_{1113}\zeta_{13}^* + A_{1123}\zeta_{23}^*) \\ A_{2211}\zeta_{11} + A_{2222}\zeta_{22} + A_{2233}\zeta_{33} + c^{\mathbf{M}_1}(A_{2212}\zeta_{12}^* + A_{2213}\zeta_{13}^* + A_{2223}\zeta_{23}^*) \\ A_{3311}\zeta_{11} + A_{3322}\zeta_{22} + A_{3333}\zeta_{33} + c^{\mathbf{M}_1}(A_{3312}\zeta_{12}^* + A_{3313}\zeta_{13}^* + A_{3323}\zeta_{23}^*) \\ c^{\mathbf{M}_2}(A_{1211}\zeta_{11} + A_{1222}\zeta_{22} + A_{1233}\zeta_{33} + c^{\mathbf{M}_1}(A_{1212}\zeta_{12}^* + A_{1213}\zeta_{13}^* + A_{1223}\zeta_{23}^*)) \\ c^{\mathbf{M}_2}(A_{1311}\zeta_{11} + A_{1322}\zeta_{22} + A_{1333}\zeta_{33} + c^{\mathbf{M}_1}(A_{1312}\zeta_{12}^* + A_{1313}\zeta_{13}^* + A_{1323}\zeta_{23}^*)) \\ c^{\mathbf{M}_2}(A_{2311}\zeta_{11} + A_{2322}\zeta_{22} + A_{2333}\zeta_{33} + c^{\mathbf{M}_1}(A_{2312}\zeta_{12}^* + A_{2313}\zeta_{13}^* + A_{2323}\zeta_{23}^*)) \end{pmatrix} \quad (\text{A.14})$$

where $c^{\mathbf{M}_1} = 2$ if $\boldsymbol{\zeta}$ is not a strain quasi-vector, or $c^{\mathbf{M}_1} = 1$, if it is, and $c^{\mathbf{M}_2} = 2$ if $\boldsymbol{\beta}$ is a strain quasi-vector, otherwise $c^{\mathbf{M}_2} = 1$.

The double contraction, A_{ijkl} , of two fourth order tensors, B_{ijkl} and C_{ijkl} , is:

$$A_{ijkl} = B_{ijmn}C_{nmkl} \quad (\text{A.15})$$

As both fourth order tensors have minor symmetry, the result, too, has minor symmetry. In the following a component of the tensor A_{ijkl} in engineering notation is compared with the same component of the matrix $\mathbf{D}$ obtained by multiplying the matrices $\mathbf{B}$ and $\mathbf{C}$:

$$\begin{aligned}
A(i, j) &= B_{mm11}C_{11nn} + B_{mm22}C_{22nn} + B_{mm33}C_{33nn} + \dots \\
&\quad \dots + 2(B_{mm12}C_{12nn} + B_{mm13}C_{13nn} + B_{mm23}C_{23nn}) \\
D(i, j) &= B_{mm11}C_{11nn} + B_{mm22}C_{22nn} + B_{mm33}C_{33nn} + \dots \\
&\quad \dots + (B_{mm12}C_{12nn} + B_{mm13}C_{13nn} + B_{mm23}C_{23nn})
\end{aligned}$$

where:

$$mm = \begin{cases} ii & \text{if } i = \{1, 2, 3\} \\ 12 & \text{if } i = 4 \\ 13 & \text{if } i = 5 \\ 23 & \text{if } i = 6 \end{cases} \quad nn = \begin{cases} jj & \text{if } j = \{1, 2, 3\} \\ 12 & \text{if } j = 4 \\ 13 & \text{if } j = 5 \\ 23 & \text{if } j = 6 \end{cases} \quad (\text{A.16})$$

Note that Einstein summation is not followed. It is obvious that some correction terms must be introduced. The following operations with some modifications of one of the matrices give the same results:

$$\mathbf{A} = \mathbf{B} [\mathbf{C}]^{\mathbf{M}_1} = [\mathbf{B}]^{\mathbf{M}_2} \mathbf{C} \quad (\text{A.17})$$

where:

$$\begin{aligned}
[\mathbf{B}]^{\mathbf{M}_1} &= \begin{pmatrix} B_{1111} & B_{1122} & B_{1133} & 2B_{1112} & 2B_{1113} & 2B_{1123} \\ B_{2211} & B_{2222} & B_{2233} & 2B_{2212} & 2B_{2213} & 2B_{2223} \\ B_{3311} & B_{3322} & B_{3333} & 2B_{3312} & 2B_{3313} & 2B_{3323} \\ B_{1211} & B_{1222} & B_{1233} & 2B_{1212} & 2B_{1213} & 2B_{1223} \\ B_{1311} & B_{1322} & B_{1333} & 2B_{1312} & 2B_{1313} & 2B_{1323} \\ B_{2311} & B_{2322} & B_{2333} & 2B_{2312} & 2B_{2313} & 2B_{2323} \end{pmatrix} \\
[\mathbf{C}]^{\mathbf{M}_2} &= \begin{pmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1112} & C_{1113} & C_{1123} \\ C_{2211} & C_{2222} & C_{2233} & C_{2212} & C_{2213} & C_{2223} \\ C_{3311} & C_{3322} & C_{3333} & C_{3312} & C_{3313} & C_{3323} \\ 2C_{1211} & 2C_{1222} & 2C_{1233} & 2C_{1212} & 2C_{1213} & 2C_{1223} \\ 2C_{1311} & 2C_{1322} & 2C_{1333} & 2C_{1312} & 2C_{1313} & 2C_{1323} \\ 2C_{2311} & 2C_{2322} & 2C_{2333} & 2C_{2312} & 2C_{2313} & 2C_{2323} \end{pmatrix}
\end{aligned}$$

This last result can be used in advance to obtain the inverse of a fourth order tensor that exhibits minor symmetry. Let $[\mathbf{A}]^{-1}$ be the inverse of a fourth order tensor, $[\mathbf{A}]$, that exhibits minor symmetry and $[\mathbf{A}]^{\#}$ the inverse of the matrix that represents $[\mathbf{A}]$ in

engineering notation, in other words using equation (A.17) :

$$\begin{aligned} \mathbf{A} [\mathbf{A}]^{-1}{}^{M_2} &= [\mathbf{A}]^{-1}{}^{M_1} \mathbf{A} = \mathbf{1}^s \\ \mathbf{A} [\mathbf{A}]^\# &= [\mathbf{A}]^\# \mathbf{A} = \mathbf{I} \end{aligned} \quad (\text{A.18})$$

where $\mathbf{I}$ is the unit matrix of fourth order. Equation (A.18) can be modified into the equation:

$$[\mathbf{A}]^{-1}{}^{M_2} = [\mathbf{A}]^\# \mathbf{1}^s \quad (\text{A.19})$$

and then it follows:

$$[\mathbf{A}]^{-1} = \begin{pmatrix} B(1,1) & B(1,2) & B(1,3) & 1/2B(1,4) & 1/2B(1,5) & 1/2B(1,6) \\ B(2,1) & B(2,2) & B(2,3) & 1/2B(2,4) & 1/2B(2,5) & 1/2B(2,6) \\ B(3,1) & B(3,2) & B(3,3) & 1/2B(3,4) & 1/2B(3,5) & 1/2B(3,6) \\ 1/2B(4,1) & 1/2B(4,2) & 1/2B(4,3) & 1/4B(4,4) & 1/4B(4,5) & 1/4B(4,6) \\ 1/2B(5,1) & 1/2B(5,2) & 1/2B(5,3) & 1/4B(5,4) & 1/4B(5,5) & 1/4B(5,6) \\ 1/2B(6,1) & 1/2B(6,2) & 1/2B(6,3) & 1/4B(6,4) & 1/4B(6,5) & 1/4B(6,6) \end{pmatrix} \quad (\text{A.20})$$

where $\mathbf{B} = [\mathbf{A}]^\#$.

Appendix B

Thermal conduction Eshelby tensor for ellipsoidal particles embedded in an isotropic matrix

Following Hatta and Taya [76], and Khare [91], the non-zero components of the Eshelby tensor for thermal conduction are:

- For a prolate spheroid:

$$\begin{aligned}\mathcal{S}(1,1) &= \mathcal{S}(2,2) = \frac{1}{4} \frac{2c^{\text{ar}}}{((c^{\text{ar}})^2 - 1)^{\frac{3}{2}}} \left(c^{\text{ar}} ((c^{\text{ar}})^2 - 1)^{\frac{1}{2}} - \cosh^{-1} c^{\text{ar}} \right) \\ \mathcal{S}(3,3) &= 1 - 2\mathcal{S}(1,1)\end{aligned}\tag{B.1}$$

where c^{ar} is the aspect ratio of the ellipsoid, and the 3-axis is the axis of rotation.

- For a long fiber:

$$\mathcal{S}(1,1) = \mathcal{S}(2,2) = \frac{1}{2}\tag{B.2}$$

- For a sphere:

$$\mathcal{S}(1,1) = \mathcal{S}(2,2) = \mathcal{S}(3,3) = \frac{1}{3}\tag{B.3}$$

- For a plate:

$$\mathcal{S}(3,3) = 1\tag{B.4}$$

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