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Materials Modeling – Challenges and Perspectives

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1.1
Introduction

The development of materials modeling has experienced a huge growth in the last 10 years. New mathematical approaches (formulations, concepts, etc.), numerical techniques (algorithms, solution strategies, etc.), and computing methods (parallel computing, multigrid techniques, etc.), allied to the ever-increasing computational power, have fostered the research growth observed in recent times. Numerical implementation of some modeling concepts, such as multiscale formulations and optimization procedures, were severally restricted two decades ago due to limitation of computing resources. What were once perspectives of new advancements have become a reality in the last few years and longstanding difficulties have been overcome.

It is important to emphasize that materials modeling is not a recent concept or a new research topic. Some material descriptions widely accepted and used these days were actually proposed in the late eighteenth century. For instance, within the framework of modeling inelastic deformation of metals, the French engineer Henri Tresca (1814–1884), professor at the *Conservatoire National des Arts et Métiers* (CNAM) in Paris, was the first to define distinct rules for the onset of plastic flow in ductile solids [1]. Tresca's groundbreaking studies established a material-dependent critical plastic threshold given by the maximum shear stress. The apparently simple concept gave rise to a completely new approach to studying deformation of solid materials, and, today, his principle is known as *Tresca's yield criterion*. It is interesting to mention that, in spite of many years of proposition, numerical implementation of Tresca's criterion is not straightforward because of the sharp corners of the yield locus and its association with the plastic-normality flow rule [2, 3].

The search for alternate modeling descriptions is also not a new endeavor. For similar problems, Maksymilian Tytus Huber (1872–1950), a Polish engineer, postulated that material strength depends upon the spatial state of stresses and not on a single component of the stress tensor [4]. Independently, the Austrian mathematician and engineer, Richard von Mises (1883–1953), indicated that plastic

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deformation of solids is associated with some measure of an equivalent stress state [5]. The assumption indicates that plastic deformation is initiated when the second deviatoric stress invariant reaches a critical value. A few years later, the German engineer, Heinrich Hencky (1885–1952), still within the criterion introduced by Huber and von Mises, suggested that the onset of plastic deformation takes place when the elastic energy of distortion reaches a critical value [6]. An alternate physical interpretation was proposed by Roš and Eichinger, who demonstrated that the critical distortional energy principle is equivalent to defining a critical shear stress on the octahedral plane [7], generally known as *maximum octahedral shear stress criterion*. The aforementioned elastic–plastic modeling assumptions are known today as the *Huber–Mises–Hencky yield criterion*. A brief review of the early works on modeling of plastic deformation of metals illustrates the drive toward understanding the physics of material behavior and its translation into mathematical descriptions.[1)]

Despite the fact that the principles of *plasticity theory* have long been established, application to realistic problems or advanced materials using only mathematical tools is difficult or even impossible. Following the example on deformation of metals, when addressing computational modeling of elastic–plastic deformation at finite strains, the solution requires a physical/material description (e.g., the classical Huber–Mises–Hencky equation), a mathematical formulation able to handle geometrical and material nonlinearity (e.g., multiplicative decomposition of the gradient of deformation tensor into elastic and plastic components), and a computational approximation/discretization of the physical and mathematical problem (e.g., iterative procedures such as the Newton–Raphson and arc-length methods). This class of problems has already been exhaustively investigated in the last 30 years, and the literature shows a wide variety of strategies (see, for instance, Ref. [11] and references therein).

The illustration on the development of physical/mathematical/numerical formulations of elastic–plastic deformation of ductile solids shows that a proper material modeling requires

1) understanding of the physics involved in the problem;
2) comprehensive theoretical and mathematical treatment of the phenomena;
3) sound and consistent numerical approximation/discretization of the governing and constitutive equations; and
4) adequate computing resources.

These principles are extensive to modeling and simulation of any materials-processing operation. In a broader context of materials modeling, the literature has shown an increasing pace in the evolution of each one of the aspects mentioned in items (1–4). Advancements in mathematical and numerical tools have prompted investigation in areas of materials modeling ranging from

1) Further reading on the history and development of yield criteria and concepts of materials behavior can be found in Refs [8–10].

electronic and atomistic level to complex structures within the continuum realm [12]. Despite this considerable progress, there are still pressing challenges to be overcome, mainly those associated with more realistic materials-processing operations or simulation of complex materials structures. This chapter highlights some modeling issues under current and intense scrutiny by researchers and does not intend to be exhaustive. The other chapters of this book present deeper insights into materials modeling and simulation of some class of problems that, in a way, we hope, will serve as a springboard for further realistic applications.

1.2 Modeling Challenges and Perspectives

Materials modeling is as vast as the types of existing materials. For decades, emphasis has been placed on structural (metals, polymers, composites, etc.) and geotechnical (soils and rocks) classical materials. Behavior prediction of such materials subjected to a given load (mechanical or thermal) in process operations or stress–strain/heat transfer analysis has constituted the bulk of numerical approaches available in the literature. The existing solution approaches are comprehensive and provide accurate results for most classical materials subjected to strain paths of reasonable complexity. However, the constant search for technological advances and understanding of some classes of complex materials and processes has posed new challenges, urging scientists to seek new mathematical and computational tools. The following sections discuss general aspects of (i) *the modeling of ductile deformation and mechanical degradation leading to fracture;* (ii) *the modeling of cellular materials;* and (iii) *multiscale approaches*. Many other constitutive modeling issues and material types could have been included in the list; however, the above aspects have attracted substantial attention of academia and industry due to perspectives of realistic applications in a relatively short term.

1.2.1 Mechanical Degradation and Failure of Ductile Materials

In the last few years, numerical simulation of metal-forming operations has been incorporated into the design procedures of many manufacturing processes. Industry is seeking not only to estimate forming loads and energy requirements with higher accuracy but also to predict possible defects and tool life. Forging, extrusion, and deep drawing are some examples of forming processes that are particularly prone to material failure. For instance, a faulty design of extraction angles, tool radius, or workpiece geometry might lead to either external or internal defects. Therefore, aiming at prediction of fracture onset associated with elastic–(visco)plastic deformation, the modeling of mechanical degradation of ductile materials has been extensively studied in the last few years. A brief literature survey shows many research groups engaged in the aspects listed below, which are intrinsically related to ductile failure:

- **Prediction of failure onset**: numerical and experimental investigation of failure criteria for manufacturing processes (e.g., forming limit diagrams for sheet metal forming);
- **Material response to loading**: computation of stress–strain distribution and loads in multistep forming operations (e.g., springback and residual stress evaluation);
- **Multiscale modeling**: approximations for strongly coupled scales, homogenization strategies, and heterogeneous multiscale techniques (e.g., damage modeling, cohesive failure, biomaterials applications, microstructure design, crystal plasticity, and texture evolution);
- **Anisotropic materials**: modeling anisotropic behavior of materials (e.g., complex yield criteria and its interaction with material failure);
- **Nonlocal models**: material modeling including nonlocal effects (e.g., new weighted averages in nonlocal formulations and suitable gradients in gradient approaches. Applications to nonhomogeneous materials);
- **Deformation and failure under complex stress states**: derivation of material models and failure criteria able to describe plastic deformation under complex stress–strain paths (e.g., failure criteria for tensile and compressive-dominant processes);
- **Parameter identification**: identification of material parameters (e.g., identification of elastic–plastic, damage, and fracture parameters using techniques for inverse problems).

The aforementioned topics are not exhaustive and other aspects associated with modeling of the ductile failure process could be added. Furthermore, some topics can (σ_H/σ_{eq}) also be interrelated to each other, for example, deformation and failure under complex stress states using nonlocal damage models. In order to illustrate the challenges faced by researchers and perspectives eagerly awaited by industry, some issues related to deformation and failure under complex stress states are discussed in the following paragraphs.

The literature shows many attempts to describe the mechanical degradation process and failure initiation based on postprocessed criteria owing to the simplicity of modeling. The following summarizes only the most recent advancements in the area. Wierzbicki and coworkers have extensively investigated the failure process for compression, tension, shear, and combined loads [13]. These authors emphasize that the *failure mechanism* plays an important role in failure onset of ductile materials and report that a critical triaxiality factor, given by the ratio between the hydrostatic and von Mises equivalent stresses, defines a limit between shear and void growth fracture modes, as illustrated in Figure 1.1 Furthermore, even restricted to ductile fracture, such differences in the *failure mechanisms* have prevented derivation of a single postprocessed criterion able to successfully predict failure onset for both tensile and compressive-dominant loads [14].

Many other works have attempted to predict ductile failure onset using postprocessed ductile fracture criteria. Most approaches attempt to describe the microscopic phenomena associated with mechanical degradation by either experimental analysis (empirical criteria) or mathematical and/or physical models (e.g., growth of

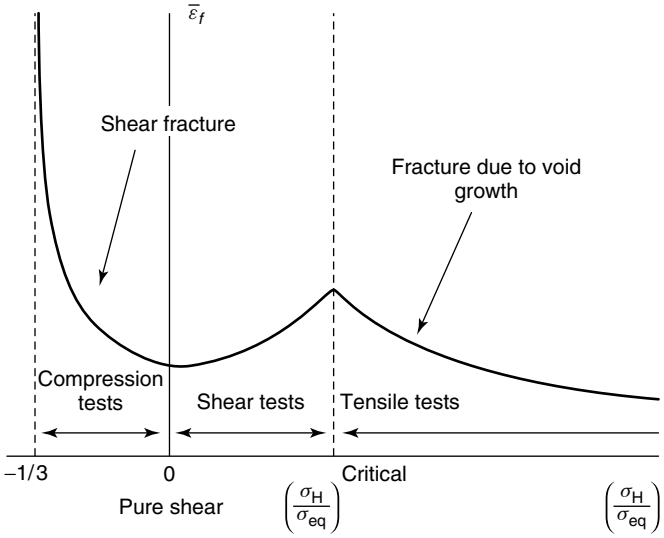

Figure 1.1 Fracture locus in the equivalent strain and stress triaxiality space: Bao and Wierzbicki [10] presented the effect of the stress triaxiality in fracture onset based on three different tests, namely, compression, shear, and tensile tests. The authors also postulate that a change of the fracture mechanism provides a slope discontinuity in the fracture locus. In the range of negative stress triaxiality, the equivalent strain to fracture decreases with the stress triaxiality, reaching a minimum at $\sigma_H/\sigma_{eq} = 0$ (pure shear). The fracture strain increases for low-stress triaxiality factors, reaching a peak at a given (material-dependent) stress triaxiality. For high-stress triaxiality, the shear fracture decreases with the stress triaxiality.

spherical voids, dissipation of plastic energy, etc.). In spite of greater modeling difficulties, a coupled description of elastic–(visco)plastic deformation and mechanical degradation has proved to be the best approach to model the ductile fracture process. In general, such formulations form what is currently known as *continuum damage mechanics* (CDM). However, for years, accurate material degradation and fracture prediction using damage mechanics were restricted to tensile-dominant loading, since the material description was unable to distinguish between tensile and compressive deformation. Its extension to deformation under complex stress–strain paths is one of the most intensively studied topics in recent years. For instance, Vaz *et al.* [15], on the basis of Ladèveze and Lemaitre's [16] and Lemaitre's [17] considerations, proposed a general approach based on the total damage work, W_D,

$$W_D = \int_0^t (-Y)\,\dot{D}\mathrm{d}t = \int_0^{D_c} (-Y)\,\mathrm{d}D \tag{1.1}$$

where D is the damage variable, t is the time, D_c is the critical damage, and $(-Y)$ is the damage strain energy release rate,

$$(-Y) = (-Y)^+ + (-Y)^- - \frac{\nu}{E}\left[\frac{\left(-f'\right)^{1/2}}{f}\mathrm{tr}\left[\boldsymbol{\sigma}^+\right]\right]\left[\frac{\left(-f'\right)^{1/2}}{f}\mathrm{tr}\left[\boldsymbol{\sigma}^-\right]\right] \tag{1.2}$$

where $(-Y)^+$ and $(-Y)^-$ are the individual contribution of tensile and compressive stresses,

$$(-Y)^+ = \frac{(-f')}{f^2}\left[\frac{(1+\nu)}{2E}\boldsymbol{\sigma}^+ : \boldsymbol{\sigma}^+ - \frac{\nu}{2E}\left(\mathrm{tr}\left[\boldsymbol{\sigma}^+\right]\right)^2\right]$$
$$(-Y)^- = \frac{(-f')}{f^2}\left[\frac{(1+\nu)}{2E}\boldsymbol{\sigma}^- : \boldsymbol{\sigma}^- - \frac{\nu}{2E}\left(\mathrm{tr}\left[\boldsymbol{\sigma}^-\right]\right)^2\right] \tag{1.3}$$

$f = f(D)$ is the damage function, and $\boldsymbol{\sigma}^+$ and $\boldsymbol{\sigma}^-$ are the individual contributions of tensile and compressive principal stresses to the loss of material stiffness,

$$\boldsymbol{\sigma}^+ = \sum_{i=1}^{3} \langle\sigma_i\rangle\, \mathbf{e}_i \otimes \mathbf{e}_i \quad \text{and} \quad \boldsymbol{\sigma}^- = \sum_{i=1}^{3} \langle-\sigma_i\rangle\, \mathbf{e}_i \otimes \mathbf{e}_i \tag{1.4}$$

in which, mathematically, $\{\boldsymbol{\sigma}_i\}$ and $\{\mathbf{e}_i\}$ denote the eigenvalues and an orthonormal basis of eigenvectors of $\boldsymbol{\sigma}$.

In spite of the apparent success, *local* damage models suffer from dependence on the finite element mesh. In classical plasticity theories, the state of any point in a body depends only on the state of its infinitesimal neighborhood, thereby excluding the internal characteristic lengths of the material from the local field theory [18]. Therefore, in elastic–plastic formulations based on local approaches, the element size defines the minimum dimension within which the plastic deformation takes place, serving as an internal characteristic length of the material. As a consequence, the subsequent mesh refinement in the critical zones causes the damage process to become more concentrated in ever smaller volumes, leading to physical–numerical inconsistencies (e.g., loss of ellipticity of the differential equations in strain localization problems). In order to overcome such difficulties, *nonlocal* formulations have been proposed. It is relevant to mention that nonlocal approximations are not restricted to damage modeling. In general, nonlocal models are formulated using two approaches: integral models and gradient-based formulations. The former builds the nonlocal variable based on weighted and averaged local variables in areas defined by the internal characteristic length. Gradient-based formulations, divided into explicit and implicit schemes, include the gradient of a collection of field variables linked to the inelastic deformation process (e.g., equivalent plastic strain) into the material constitutive equations.

A survey in the recent published literature on the application of damage models to the assessment of failure process shows increasing interest in the use of nonlocal approaches. For instance, Meinders *et al.* [19] reported that, in the area of damage and fracture behavior, a nonlocal damage model provided better predictions of sheet failure than the conventional forming limit diagram. Velde *et al.* [20] presented a nonlocal damage model for viscoelastic materials aiming at time-dependent inelastic behavior of steel structures up to failure. These authors used a nonlocal implicit gradient-based formulation coupled to a hybrid damage approach (Lemaitre and Gurson type damage models), being verified in 3D-structural analysis of Compact Tension (CT) specimens. Failure analysis of CT-specimens was also discussed by Samal *et al.* [21], who presented a nonlocal damage formulation for

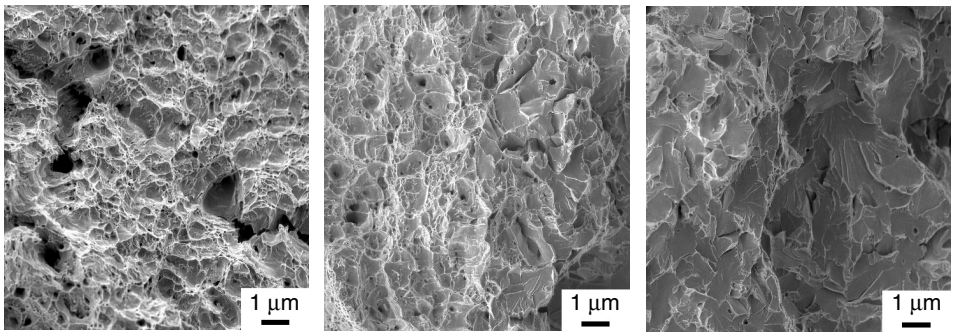

Figure 1.2 Microscopy of the fractured region of a low-carbon V-notched specimen: (a) stress concentration at the root of the V-notch causes failure onset at the external surface of the specimen; the micrography taken at this region shows dimples, which represents the typical texture of ductile fracture. (b) Transitional region: evolution of the stress state caused by a reduction of the resisting area leads to a change in the fracture mechanism from ductile to brittle-type fracture. (c) The end of the failure process exhibits cleavage microplanes, which are typical structures of brittle fracture.

Rousselier's damage model. The model was based on a nonlocal implicit gradient formulation, in which a diffusion-type differential equation correlates the nonlocal damage variable to the local void volume fraction. Finally, it is relevant to emphasize that the considerable potential for model failure analysis in complex materials using nonlocal damage approximations has stimulated research on purely computational issues and modeling approaches, for example, hybrid-displacement finite-element formulations [22], nonhomogeneous elasticity [23], consistent tangent matrix [24], and two-field variational formulation [25].

When addressing the physics of the failure process, using either local or nonlocal formulations as previously mentioned, the *failure mechanism* is fundamentally important when modeling the deformation process leading to failure. For instance, most, if not all, computational models discussed in the literature are not able to properly describe the transition between the initial ductile failure and the brittle-type fracture (catastrophic failure) that takes place at the end of the failure process. Such difficulties are expressed even in the presence of predominantly uniform stress fields. For example, in a tensile test of a low-carbon V-notched specimen, a comprehensive material model should describe the initial ductile failure at the external surface (Figure 1.2a) of the specimen, the transition in the fracture mechanism (Figure 1.2b) as the fracture progresses, and the brittle-type fracture which takes place at the center of the specimen (Figure 1.2c).

1.2.1.1 **Remarks**

Material models able to account for elastic–plastic deformation and change in failure mechanisms are still unavailable even for isotropic materials under one-directional loading. Phenomenological approaches to material degradation

and failure progression based on macroscale models seem to lack essential physical tools to properly describe the phenomena involved. Therefore, the natural research direction points to using physics-based failure modeling based upon multiple scales (nano-, micro-, meso-, and macroscales)/nonlocal approximations coupled to a macroscopic scheme of fracture progression.

1.2.2 Modeling of Cellular Structures

Development of manufacturing technologies has instigated investigation on the use of cellular-type materials in many different areas. The literature shows applications ranging from simple filters, as illustrated in Figure 1.3, to flow straighteners, containment matrices and burn-rate enhancers for solid propellants, pneumatic silencers/sound absorbers, catalytic surfaces for chemical reactions, core structures for high-strength panels, crash energy absorbers, flame arresters, heat sinks, and heat exchangers, in general [26–28]. This section summarizes some aspects of the current discussions on modeling strategies and, more importantly, topology design for some classes of problems.

Cellular topology can be generally classified into (i) regular or stochastic cellular structures and (ii) open or closed cellular materials. Most authors agree that stochastic metal foams with open cells have better thermal, acoustic, and energy-absorption properties; however, their load-bearing capacity is significantly inferior to periodic structures with the same weight [30]. Open cell materials have also been regarded as one of the most promising materials for manufacturing heat exchangers due to the high surface area density and strong mixing capability for the fluid [28]. Ultralight structures, energy-absorption systems, and fuel cell and battery subsystems are applications suited to purpose-tailored extruded metal honeycombs or prismatic/periodical cellular materials [31]. A visual summary of the application of cellular metallic materials was presented by Banhart [27], who plotted *purpose* (functional or structural) against the *recommended foam topology* (open, partially open, or closed), as illustrated in Figure 1.4.

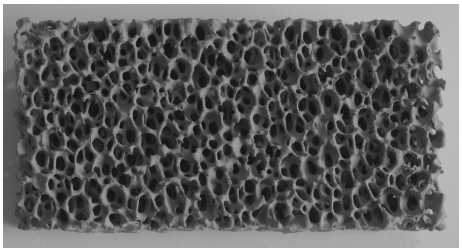

Figure 1.3 Open cell structure: ceramic foam filter used to remove impurities from liquid metals in casting [26]. The materials used in ceramic filters are silicon carbide, alumina, and zirconia. This application requires not only mechanical strength to withstand high-temperature flow but also to yield low pressure loss, erosion resistance, and chemical and thermal stability, to avoid reaction with the molten metal being filtered.

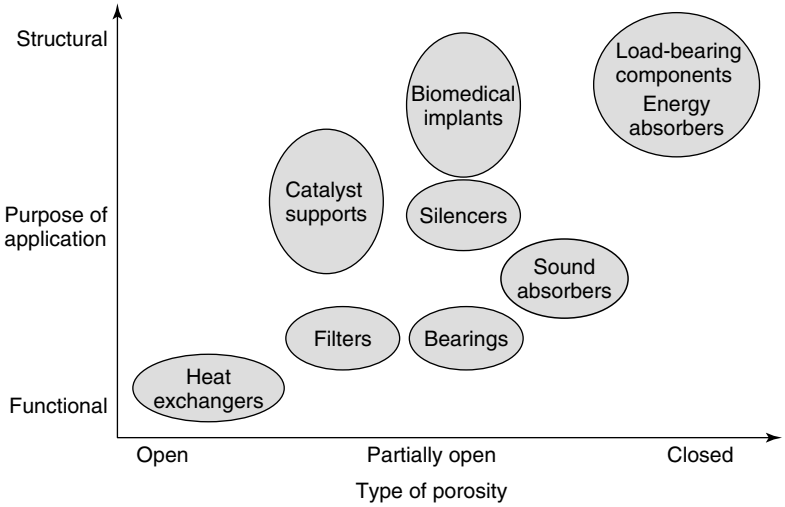

Figure 1.4 Application of porous metals or metal foams [24]. Combination between more than one application poses the greatest challenge when choosing cell topology. For instance, in the automotive industry, the goal is to design components able to combine lightweight, high deformation (plastic) energy absorption, and sound insulation among other desired characteristics. Metal foams, more than other materials, and despite design challenges, have emerged as a possible solution for different types of car parts that require such combinations of functionality.

A brief review on the potential application of cellular materials shows a wide variety of approaches to recommended cellular topology. Furthermore, the modeling strategy also varies according to the analysis of the desired behavior: structural, thermal, or multifunctional formulations. The numerical techniques used to solve the problem are also important when addressing this class of problems. Therefore, modeling and simulation of cellular structures is an enormous research field, still wide open to new developments and modeling strategies. In general, the following aspects have been under intense research in the last few years:

- **Constitutive modeling**: development of global constitutive models for elastic–plastic deformation and failure (e.g., induced anisotropy and yield criteria);
- **Structural and functional behavior**: study of the behavior of a cellular structure under given physical conditions (e.g., deformation and densification and dissipation of thermal energy);
- **Material properties**: material properties of cellular structures (e.g., parameter identification of global mechanical and thermal properties, homogenization, and global properties design);
- **Morphology design**: numerical design of cellular topology (e.g., design optimization, lattice structure modeling, and multiobjective topology design).

The topics listed above represent only the mainstream research on modeling and simulation of cellular materials. One can discern frontline research in each one of those research areas; however, this section is not exhaustive in describing every new approach or modeling technique, but highlights only some issues on topology design of cellular materials using *inverse modeling*.

Cell topology design using *inverse modeling* consists of determining the best configuration of material distribution according to given criteria. Development of techniques using this strategy constitutes one of the greatest challenges in the field of modeling cellular materials. This method, however, does not present solution unicity, making possible to obtain different configurations for the same structural and/or functional requirements. A specific class of *inverse modeling* is concerned with finding the optimum cellular structure from basic known geometries. Note that, in this case, the unit-cell geometrical shape does not change (e.g., triangles and hexagons in 2D configurations), but the individual cell size or other geometrical/material parameters can be determined according to given optimization criteria. Inverse modeling contrasts with *direct approaches*, which are concerned with studying the behavior of cellular structures with known geometrical configuration. Direct strategies can by no means be underestimated, since the target problems and applications may require complex formulations of individual functional characteristics.

Direct approaches are by far the most common strategies used to design cellular structures. The recent work of De Giorgi *et al.* [32] is an example of the use of such modeling techniques to topology design of aluminum foams. The authors aimed at finding the best structural response based on closed-cell configuration using tetrakaidecahedron and ellipsoidal cells of different sizes associated with periodic microstructures. The latter was found to be the best configuration to reproduce the mechanical response of the AlSi10Mg commercial foam produced by Alulight® International GmbH. *Inverse modeling* using cells of predefined geometrical shapes was presented by Kumar and McDowell [33], who used a homogenization-based method to design cellular structures able to maximize heat dissipation and to improve structural performance. Prismatic honeycombs with uniform and graded cell sizes of known topologies (squares, equilateral triangles, and regular hexagons) were used by these authors.

Owing to flexibility and generality, the application of *inverse modeling* techniques to design the unit cell itself has gained increasing attention in the last few years. Sigmund [34] was one of the pioneers in the application of inverse modeling based on *topology optimization* to find the optimum unit-cell configuration. This strategy was subsequently utilized to study different aspects of this class of problems. Recently, application of inverse homogenization for designing two-phase periodic materials under multiple load conditions was introduced by Guedes *et al.* [35]. The technique also used topology optimization to determine the optimum material distribution within a unit cell. The problem considered by the authors corresponded to finding the stiffest microstructure for a minimum compliance problem involving multiple loads (tensile and shear loading conditions). Muñoz-Rojas *et al.* [36], in a general discussion on the application of optimization to heat transfer in cellular

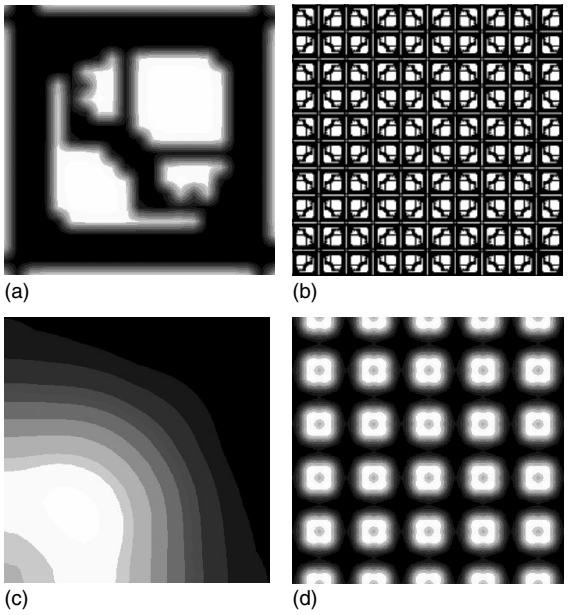

Figure 1.5 One-fourth of a unit-cell pseudodensity distribution and corresponding composite material matrix [33]. The problem consists of achieving the highest possible thermal conductivity for a given volume fraction for an FGM. The figures illustrate results for increasing gradient lengths – from (a)–(b) almost no property gradation to (c)–(d) high gradation. The gradient control makes it possible to address the influence of FGM gradation in the design of purpose-tailored, high-performance materials. Further discussions on this method, including detailed mathematical modeling aiming at structural applications, was presented by Paulino *et al*. [34].

materials, presented some insights into the design of periodic cellular structures using functionally graded materials (FGMs). The strategy uses the concept of the relaxed problem in continuum topology optimization and maximizes the homogenized thermal conductivity for a certain volume fraction. Figure 1.5 illustrates the final material morphology for two different gradation parameters. Paulino *et al*. [37] present a detailed description of the method, in which examples aiming at structural applications are discussed. The great potential of the strategy is illustrated by designing extreme material topologies, such as structures presenting negative Poisson's ratio and near-zero shear modulus. The most recent design techniques use multiscale considerations based upon alternative approaches. For instance, Giusti *et al*. [38] proposed a new numerical strategy that uses the mathematical concept of topological derivative within a variational, multiscale constitutive framework. Application of this method to microstructure design has been recently presented by Giusti *et al*. [39] and Amstutz *et al*. [40], in which the final unit-cell morphology was obtained by reaching the optimality condition defined as the function of a given homogenized property (e.g., Poisson's ratio, bulk modulus, and shear modulus).

A distinct class of cellular materials comprises the lattice/grid structures, which are also known as *lattice-block materials, lattice-truss structures, lattice-block structures, and cellular lattices*. Lattice materials with periodic unit-cell microstructures are trusslike structures mainly conceived to maximize the load-bearing capacity at minimum weight, with potential high energy absorption. Multifunctional applications may also combine heat transfer/thermal dissipation, sound absorption, or other requirements. Industries have shown growing interest in truss microstructures aiming at high-performance applications, motivated by the development of high-precision manufacturing processes, such as rapid prototyping (e.g., selective laser sintering, digital light processing, and microstereolithography [41, 42]). Most research works are concerned with either modeling the global behavior of the lattice materials or determining their homogenized properties, all of which are based on known unit-cell microarchitectures (similar to the *direct approach* discussed in the previous paragraphs). Luxner *et al.* [43], for instance, addressed the macromechanical behavior of six different 3D base-cell geometries presenting cubic material symmetry (simple cubic, Gibson Ashby, reinforced body-centered cubic, body-centered cubic, Kelvin, and Weaire–Phelan structures). The authors' current research is focused on the effect of irregularities on elastic–plastic deformation and localization. A similar approach was also used to address bonelike structures using the simple cubic structure [44]. In all cases, a direct problem was solved, that is, material properties and cell microarchitecture were known in advance.

Conceptually, application of *inverse modeling* to lattice-block materials is similar to that discussed already, that is, (i) use of optimization techniques to design cellular structures based on unit cells of predefined microarchitecture or (ii) designing of the unit-cell lattice microstructure. The former is illustrated by Yan *et al.* [45], who presented an optimization procedure for structural analyses of truss materials. The authors adopted 2D quadrilateral unit cells and used two classes of design variables: relative density and cell-size distribution, under a given total material volume constraint. The technique was able to determine a cell distribution of different sizes and cells with walls of different thickness based only on quadrilateral unit-cell structures. However, the challenge posed to this class of materials is associated with determining the optimum microarchitecture of the unit cell that is capable of achieving maximum performance without predefining its basic geometry.

Studies using homogenization, sensitivity analysis, and optimization are in progress aiming at finding the optimum morphology of lattice materials based on general trusslike unit cells [46]. The combined homogenization–optimization technique has been developed for multifunctional applications, that is, the optimum structure should achieve the best performance for both structural and thermal applications. The method uses homogenization of the elasticity and conductivity tensors, combined with analytical sensitivity analysis based on symbolic computation.

Initially, a general unit cell with arbitrary microarchitecture is defined (which contains an arbitrary number of interlocked struts). The first step corresponds to

computing the homogenized elasticity and conductivity tensors, respectively,

$$\mathbf{E}^{\mathrm{H}}(\mathbf{x}) = \frac{1}{|\mathbf{Y}|}\int_{Y} \mathbf{E}\cdot(\boldsymbol{I} - \boldsymbol{\partial}_{y}\boldsymbol{\chi})\mathrm{d}y \quad \text{and} \quad \mathbf{k}^{\mathrm{H}}(\mathbf{x}) = \frac{1}{|\mathbf{Y}|}\int_{Y} \mathbf{k}\cdot(\mathbf{I} - \boldsymbol{\nabla}_{y}\mathbf{R})\mathrm{d}y \quad (1.5)$$

where $\mathbf{I}$ is the identity tensor, $|\mathbf{Y}|$ is the volume of the unit cell, $\mathbf{E}$ and $\mathbf{k}$ are the elasticity and conductivity tensors, $\boldsymbol{\chi}$ and $\mathbf{R}$ are the characteristic displacements and temperatures of the unit cell, and $\boldsymbol{\partial}_{y}$ and $\boldsymbol{\nabla}_{y}$ are the strain and heat flux operators with respect to the unit cell.

The optimization procedure is based on sequential linear programming (SLP) and uses an *objective function* defined according to the desired structural and functional behavior. The initial studies adopt specific components of the homogenized elasticity and conductivity tensors to handle the structural and thermal

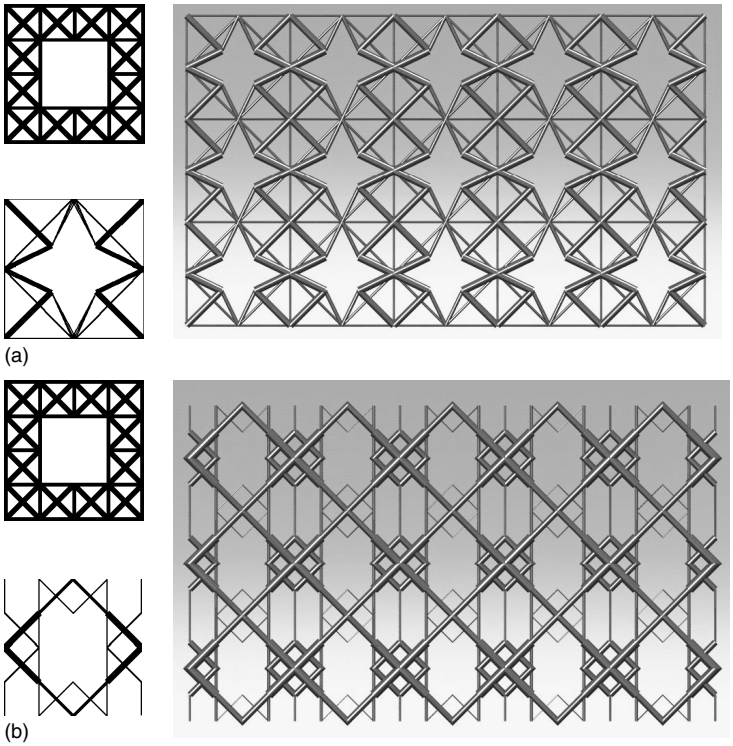

Figure 1.6 Two-dimensional lattice structures: initial and final unit-cell microstructures and the corresponding optimized lattice material. Both examples account for structural and functional (thermal) properties. The lattice microarchitectures were obtained by maximizing the ratio between the homogenized shear component of the elasticity tensor and the normal (vertical in the figure) component of the homogenized conductivity tensor for a constant initial volume of the unit cell. The design variables for each case are (a) strut areas and x and y coordinates of the cell internal nodes and (b) only the strut areas. It should be remarked that these results are not necessarily unique, since the optimization problem does not ensure existence of a global minimum.

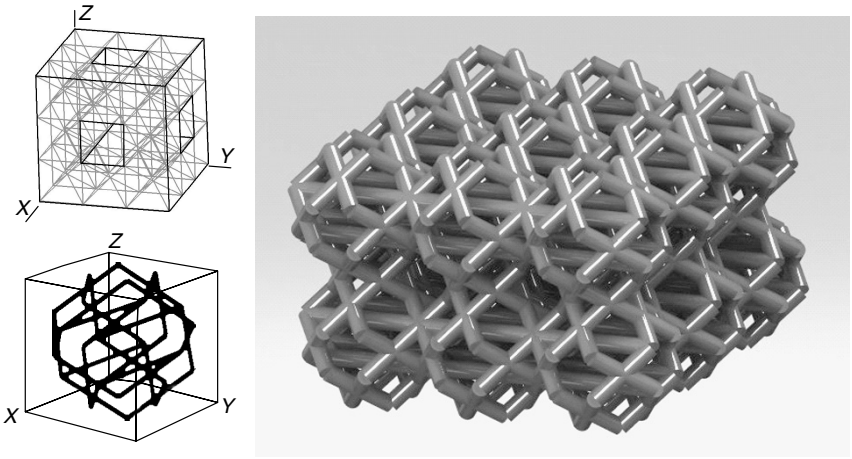

Figure 1.7 Three-dimensional lattice structures: initial and final unit cells and the lattice material. The unit cell is divided into $3 \times 3 \times 3$ subcells so that struts are initially distributed following a pyramidal shape with the vertex located in the center of each subcell. Struts are placed only in the subcells connected to an edge of the unit cell. The design variables are the strut areas. The final lattice material was obtained by maximizing the product between the homogenized shear component, E^{H}_{1212}, of the elasticity tensor, and the homogenized normal component, k^{H}_{11}, of the conductivity tensor.

response, respectively. The multifunctional approach is accounted for an objective function defined as a combination of both homogenized tensors. In the homogenization–optimization process, the strut areas and nodal coordinates inside the unit cell are modified following the direction provided by the structural and thermal requirements. It is interesting to mention that the generality of this strategy makes it possible to recover classical configurations, such as Kagomé and Diamond lattice materials, depending on the structural and functional requirements. The technique was applied to 2D and 3D structures, as illustrated in Figures 1.6 and 1.7. Further aspects of the design technique, including detailed mathematical modeling, is addressed elsewhere in a publication dedicated to lattice materials modeling.

1.2.2.1 **Remarks**

The benefits provided by cellular materials are undisputable. Low specific mass, high energy absorption, and multipurpose thermal behavior are some characteristics of this class of materials. The development of mathematical and numerical tools, allied to the increasing viability of manufacturing complex microstructures, has encouraged investigation on this topic. It is also expected that great advancements in numerical strategies for parameter identification of material properties will be attained in the next few years, especially in the context of hybrid schemes (gradient-based and evolutionary algorithms) and topological derivative-based approaches. Microstructure design using homogenization and optimization techniques, encompassing both topology optimization and lattice-block materials, has also evolved rapidly in the last few years. Although still in the nascent

stages, application of multiscale algorithms (e.g., those aiming at strongly coupled scales) to designing the unit-cell microstructure is a welcome event.

1.2.3 Multiscale Constitutive Modeling

Over the last decade or so, the modeling of the dissipative behavior of solids by means of so-called *multiscale theories* has been attracting increasing interest within the applied and computational mechanics communities. The general concept of multiscale modeling extends from quantum mechanics and particle physics, molecular dynamics, and dislocation theory to macroscopic constitutive relations, as illustrated in Figure 1.8. At present it is well accepted that classical, purely phenomenological theories, in which the constitutive response is defined by a set of ordinary differential equations, possess stringent restrictions on the complexity

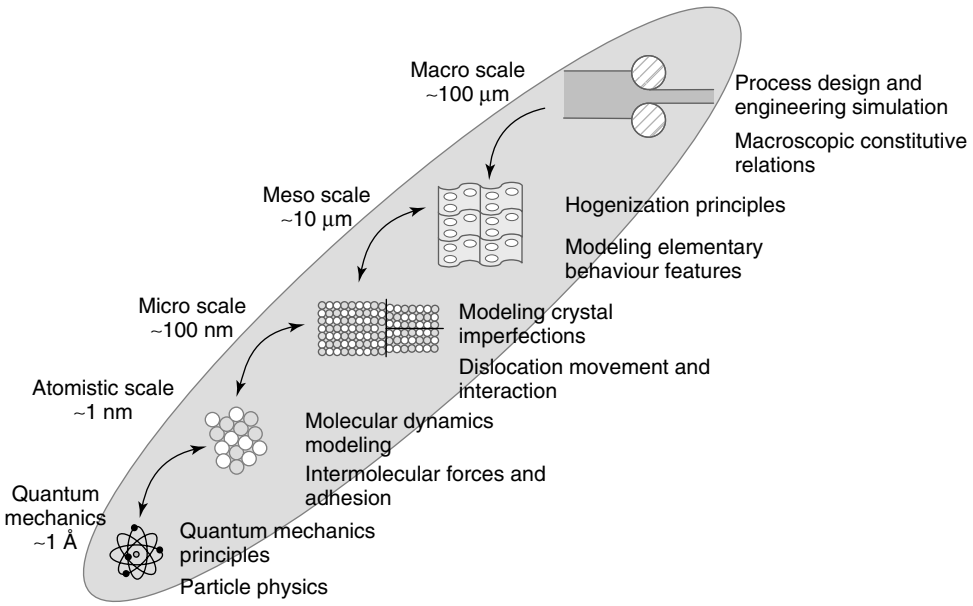

Figure 1.8 Length scales for most metal materials. Classification of physical phenomena in different time and length scales is not an easy task. The concept of scales often differs over the spectrum of nature of materials and microstructures. For instance, biological tissues, such as tendons, frequently present scale classes based upon structural/hierarchical characteristics (from tropocollagen molecules and microfibril structures to the endotendon and tendon itself, the length scale spans from ~1.5 nm to ~3000 μm) [44]. Computational modeling of engineering materials requires also careful considerations owing to different natures and structures: the typical length scales for geotechnical and building materials are significantly different from those characteristic of metal materials, for example, the former can handle macroscales measured in meters, whereas the latter can be modeled using phenomenological approaches with macroscales measured in micrometers.

of strain paths for which reasonable predictions can be obtained. This is particularly true when more intricate micromechanically related phenomena such as damaging, microcracking, or phase debonding are present.

Tackling the problem by the classical approach consists usually in introducing new internal state variables to capture finer details of the phenomenological effects of such mechanisms on the overall response of the material [48]. In many cases, this approach can be very successful but its main side effect is the fact that the greater number of internal variables requires the identification and definition of their corresponding evolution laws with the associated material parameters. Such identification is by no means trivial and may become particularly challenging in situations where phenomena such as, for instance, anisotropy evolution is present.

One possible alternative to address the problem is the adoption of multiscale theories, where the macroscopic stress and strain tensors are defined as volume averages of their microscopic counterparts over a *representative volume element* (RVE) of material. The foundations for this family of constitutive theories in the dissipative range are laid by Germain *et al.* [49]. Owing to their suitability for implementation within nonlinear finite element frameworks, such theories are particularly attractive for the description of complex constitutive response by means of finite element approximations. In such cases, complex macroscopic response can be obtained from the volume averaging of a finite element-discretized RVE containing a relatively accurate representation of the morphology of the microstructure and whose constituents are modeled by simple phenomenological constitutive theories, with possible added nonlinear phase interaction laws. Methodologies of this type are normally used in the following main contexts:

1) determination of the material parameters of an assumed canonical macroscopic constitutive model by fitting the homogenized response produced by finite element solutions of a single RVE under prescribed macroscopic strain paths [50, 51];
2) development of new macroscopic constitutive laws capable of capturing the homogenized response of a finite element-discretized RVE [52–54];
3) fully coupled two-scale finite element analyses where the macroscopic equilibrium problem is solved simultaneously with one RVE equilibrium problem for each Gauss quadrature point of the macroscopic mesh. In this case, the constitutive law at each Gauss point is defined by the homogenized response of the corresponding discretized RVE [55–58].

Items (1) and (2) above are very closely related. In some situations of practical interest, the microstructural features of the material may be such that its macroscopic behavior can be reasonably modeled by means of an existing constitutive law. One such typical situation arises in the modeling of strongly directional fiber-reinforced composites for which macroscopic hyperelastic constitutive models are available to some extent. In Ref. [51], for instance, approach (1) was used to determine the macroscopic material parameters of a suitably chosen hyperelastic model for arterial wall tissue. The idea (generally referred to as *numerical material testing* in Ref. [50]) involves the numerical determination of the homogenized response of

the RVE (whose topology and material properties are assumed known) followed by a curve-fitting exercise whereby the material parameters are chosen so as to minimize, in some sense, the error between the homogenized response and the response predicted by the macroscopic model for the range of strains under consideration. The main advantage of such procedures lies in the computing times required for the solution of macroscopic boundary value problems involving only conventional (macroscopic) constitutive models are bound to be far lower than those of similar simulations based on the fully coupled approach of item (3). Hence, whenever it is possible to describe the homogenized behavior of the microstructure by means of an existing macroscopic model with acceptable accuracy, preference should be given to such models. Potential drawbacks of this approach, however, are as follows:

- The set of macroscopic parameters that minimize the errors may not be unique and the selection procedure (based on optimization in Ref. [51]) needs to be sufficiently robust.
- The behavior of the constituents of the RVE needs to be known and appropriate models need to be selected together with their corresponding material parameters. This can often be a problem as, in many realistic situations, it is not possible or practical to test the behavior of the individual constituents of a composite material. Note that this particular issue affects approach (3) equally.

Another important fact here is that, in the presence of dissipative phenomena, the issue of parameter identification in the present context appears to remain largely open, as the fitting of the macroscopic response for a range of strain *paths* is by no means trivial. Experience shows, however, that observations made during *numerical materials testing* often lead to significant insights into the (possibly dissipative) behavior of the tested material. Such insights, in turn, may point to improvements to existing constitutive laws and/or definition of completely new ones – item (2) above. In Refs [52–54], for example, macroscopic yield surfaces are obtained as a result of numerical material testing of elastic, perfectly plastic RVEs. In Ref. [54], macroscopic functional forms of macroscopic yield surfaces are proposed as an alternative to the classical Gurson model [59]. We believe that further studies of the dissipative and nondissipative behavior of materials with a microstructure within the present multiscale framework should lead to the much needed development of new macroscopic models with an ability to capture the material behavior more accurately over a wider range of strain histories of greater complexity. In our view, this is a very interesting research topic with a potential to bring substantial benefits to the field of constitutive modeling of solids.

Finally, in spite of the physical appeal of item (3), this approach remains of relatively limited use in large-scale simulations of industrial problems mainly due to the massive computing costs associated with the fully coupled two-scale analysis. Needless to say, in the case of dissipative RVEs undergoing finite straining, for instance, the solution of one RVE equilibrium problem per macroscopic Gauss quadrature point is a formidable task even for reasonably small macroscopic problems running in high-performance machines. The use of parallel algorithms

appears then to be a natural course of action and is discussed by Matsui *et al.* [57] and Kuramae *et al.* [60]. Algorithmic techniques aiming the improvement of solution times [61] are also welcome in this context and should be further pursued in order to make fully coupled analyses a realistic option in the future.

1.3 Concluding Remarks

The role and importance of materials modeling has long been established by the seminal works of Tresca [1], Huber [4], von Mises [5], and Hencky [6], among others, who developed the modern theoretical basis of stress and strain analysis. In the last two decades, *computational* materials modeling has consolidated its importance and has become one of the fastest-growing research areas.

Materials modeling encompasses developments associated with materials as diverse as biological tissues, composite materials for aeronautical and aerospace applications, polymeric materials for technical components and ordinary household objects, and heterogeneous geotechnical materials. Furthermore, physical aspects are also as vast as the nature of the materials: structural and thermal behavior under different physical loading, material degradation and failure, and microstructure design, are some examples of applications under intense investigation. Computational issues have been equally relevant and advancements in a wide range of modeling strategies have been introduced in recent years, among which solution techniques for multiphysics problems, strongly coupled multiscale (or multiple scales) and stable cross-scale formulations, and homogenization and optimization techniques have experienced extraordinary growth. Such variety of materials, physical aspects, and computational issues render the task of reviewing the recent advances almost impossible. However, despite the almost boundless research field, it is possible to discern common directions and challenges faced by scientists across research domains:

- derivation of strong physically based constitutive models;
- numerical and experimental procedures to determine the corresponding material parameters;
- multiphysics and multiple scale formulations, ranging from nano- to meso- and macroscales;
- development of robust solution algorithms able to handle complex materials descriptions;
- Application of homogenization and optimization to new materials design.
- Development of new numerical methods aiming at improving handling of discontinuities and heterogeneities typical of some class of materials.

Most modeling issues are strongly related to one or more of the aforementioned aspects. The brief reviews discussed in Sections 1.2.1–1.2.3 highlight the multidisciplinary character of materials modeling: (i) the failure process under general stress–strain paths requires a multiphysics degradation model based on

nonlocal formulation, in which multiscale approximations coupled to macrofracture algorithms are the expected advancements; (ii) modeling of multifunctional cellular materials require cross-scale formulations based on homogenization of local properties and microstructure design using optimization procedures; and (iii) multiscale computational modeling techniques. In particular, advancements are expected in multiple scale formulations coupled to multiphysics approaches able to model individual requirements (structural, plastic energy absorption, thermal dissipation, etc.). Finally, it has been observed that an increasing move toward the application of complex material models in industry or, in cases such as geotechnical and civil materials, more realistic analyses have been used by building companies to improve construction design.

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