Part I

Introduction and Fundamentals
Chapter 1

Introduction

Modern materials science is based on the fundamental experience that the properties of materials are not unalterably determined by their average chemical composition but they are to a large extent influenced by their microstructure. This applies particularly for their mechanical and electromagnetic properties. Thus, modern "materials research" is often used as a synonym for "microstructure research".

While the evolutionary direction of microstructure is prescribed by thermodynamics, its actual evolution path is selected by kinetics. It is this strong influence of thermodynamic non-equilibrium mechanisms that entails the large variety and complexity of microstructures typically encountered in engineering materials. It is an essential observation that it is not those microstructures that are close to equilibrium, but often those that are in a highly non-equilibrium state that provide particularly advantageous material property profiles.

Microstructure can be defined as the totality of all thermodynamic non-equilibrium lattice defects on a space scale that ranges from Ångströms (e.g. non-equilibrium foreign atoms) to meters (e.g. sample surface) (Haasen 1984). Its temporal evolution ranges from picoseconds (dynamics of atoms) to years (corrosion, creep, fatigue). It is one major aim of materials science to quantitatively relate macroscopic sample behavior to microstructure. This goal imposes the task of identifying and describing those lattice defects, including their collective static and dynamic behavior, that are responsible for specific macroscopic properties. Figures 1.1 and 1.2 show that the characteristic scales which are associated with the various lattice defects establish a certain hierarchy of microstructure.

This sequence, however, merely reflects a spatial rather than a crisp physical classification. Following this length scale hierarchy, the various levels of microstructure modeling can be roughly grouped into the nanoscopic, microscopic, mesoscopic, and macroscopic regimes. In this context the term nanoscopic refers to the atomic level, microscopic to lattice defects ensembles below the grain scale, mesoscopic to lattice defect ensembles at the grain scale, and macroscopic to the sample geometry. Of course, this subdivision is to a certain extent arbitrary. As will be discussed later, various alternative subdivisions are conceivable.

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1 In pure metals, only vacancies or certain foreign atoms provide sufficient entropy to compensate their enthalpy of formation or solution, respectively: \( c_{\text{vac}}(T < T_{\text{mel}}) \approx 10^{-4} \).

2 For instance, small defects, such as dopants, can have a larger influence on strength or conductivity than large defects such as precipitates.
Due to the large spatial and temporal spread of microstructural ingredients and the complexity of possible interaction phenomena among the various lattice defects, a quantitative physical prediction of microstructure evolution and of relevant microstructure-property relations increasingly requires the employment of modeling and simulation (Figures 1.1, 1.2; Tables 1.1, 1.2, and 1.3). This applies particularly when closed analytical expressions cannot be formulated, and when the investigated problem is not easily accessible to experiments. Furthermore, as far as practical engineering aspects are concerned, the use of numerical approaches with predictive power reduces the huge number of experiments typically required in optimizing materials and designing new processes. Progress in the simulation of materials and corresponding manufacturing processes thus facilitates and accelerates the development and optimization of new products.

By using a concept which could be referred to as the "generalized state variable approach", the method of modeling and simulation can be defined in terms of a small number of characteristic steps (see also Section 2.3).

First one defines a set of independent variables and a set of dependent variables. In advanced discrete microstructure models the independent variables typically quantify time and space. The dependent variables are referred to as state variables (Kocks et al. 1975). These must be chosen in a way to allow a sufficiently precise quantification of the material properties under investigation. Subsequently, the mathematical model is formulated. It typically consists of a set of state equations which express certain properties of the material in terms of a given set of state variables, and a set of evolution equations which describe the changes of the values of the state variables as functions of the independent variables. In materials mechanics the state equations typically cover the statics of microstructures, while the evolution equations describe their kinetics. These sets of equations are often accompanied by expressions that reflect the kinematics of the material under the constraints imposed by the manufacturing process or experiment considered.

The selection of adequate state variables, state equations, and evolution equations can be made heuristically, on the basis of theoretical ab-initio concepts, or on the basis of phenomenological observations. This selection represents the most important steps in modeling and reflects the particular physical approach that is made by the researcher to
Figure 1.2: Typical space and time scales and simulation methods in computational materials science.
Figure 1.3: Alternative approaches to simulate crystal plasticity at various scales: (a) two-dimensional finite element simulation; (b) statistical constitutive simulations based on the original kinematical one-parameter model (Kocks, Mecking) and their extensions to more-parameter descriptions (Mughrabi, Estrin, Argon); (c) two-dimensional dislocation dynamics; (d) three-dimensional dislocation dynamics; (e) molecular dynamics.
approximate the problem being addressed. After setting up this framework of variables and equations, which are usually in the form of differential equations, adequate boundary- and initial-value conditions must be formulated which are in accord with the problem under investigation and which turn the initial model into a well-defined mathematical formulation. The final numerical (or analytical) solution of such a well-posed problem can be referred to as simulation or numerical (or analytical) experimentation.

The employment of numerical methods in materials science is promoted by the ever-increasing capability of computer systems in terms of speed and information storage, and by the growing demands for quantitative predictions in industry and research. The scientific branch that has matured within this interdisciplinary field, bringing together approaches from materials science, physics, computer science, mathematics, chemistry, and mechanical engineering, is often referred to as "computational materials science".

Computer simulation nowadays complements most if not all fields of materials science and engineering. For instance, simulations in materials physics aim at predicting microstructural phenomena at the atomic scale using ab-initio molecular dynamics and Monte Carlo methods. Simulations in materials science pertaining to mechanical engineering typically focus on large-scale construction problems using finite element approaches where the microstructure is reduced to the incorporation of averaging constitutive laws.

In contrast to these examples, the original domain of materials science is the investigation of lattice defect ensembles at the mesoscale. The use of simulations in this particular field represents a great challenge, in that it must bridge enormous space and time scales and provide concepts to adequately describe complex many-body interaction phenomena. For this purpose a number of new concepts have been developed which enable one to handle the interaction of many individual lattice defects in a more or less discrete fashion. The latter aspect is of special interest, since most microstructural evolution phenomena are highly nonlinear and entail self-organization on a microstructural scale (Haken 1978; Khachaturyan 1983; Kubin 1988; Martin and Kubin 1992).

In contrast to atomic-scale molecular dynamics and Monte Carlo simulations, most mesoscale approaches are formulated as continuum models, but often with a discrete consideration of lattice defects. The methods include deterministic and probabilistic cellular
Table 1.2: Space scales and methods in materials simulation, micro–meso level.

<table>
<thead>
<tr>
<th>Scale [m]</th>
<th>Simulation method</th>
<th>Typical applications</th>
</tr>
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<tbody>
<tr>
<td>$10^{-10} - 10^0$</td>
<td>cellular automata</td>
<td>recrystallization, grain growth, and phase transformation phenomena, fluid dynamics, crystallaghraphic texture, crystal plasticity</td>
</tr>
<tr>
<td>$10^{-7} - 10^{-2}$</td>
<td>spring models</td>
<td>fracture mechanics</td>
</tr>
<tr>
<td>$10^{-7} - 10^{-2}$</td>
<td>vertex models, network models, grain boundary dynamics</td>
<td>subgrain coarsening, recrystallization, secondary recrystallization, nucleation, recovery, grain growth, fatigue</td>
</tr>
<tr>
<td>$10^{-7} - 10^{-2}$</td>
<td>geometrical, topological, and component models</td>
<td>recrystallization, grain growth, secondary recrystallization, crystallographic textures, solidification, crystal topology</td>
</tr>
<tr>
<td>$10^{-9} - 10^{-4}$</td>
<td>dislocation dynamics</td>
<td>crystal plasticity, recovery, microtexture, dislocation patterning, thermal activation</td>
</tr>
<tr>
<td>$10^{-9} - 10^{-5}$</td>
<td>kinetic Ginzburg–Landau-type phase field models</td>
<td>diffusion, interface motion, precipitation formation and coarsening, polycrystal and polyphase grain coarsening phenomena, isostructural and non-isostructural phase transformation, type II superconductivity</td>
</tr>
<tr>
<td>$10^{-9} - 10^{-5}$</td>
<td>multistate kinetic Potts models</td>
<td>recrystallization, grain growth, phase transformation, crystallographic textures</td>
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Table 1.3: Space scales and methods in materials simulation, meso–macro level.

<table>
<thead>
<tr>
<th>Scale [m]</th>
<th>Simulation method</th>
<th>Typical applications</th>
</tr>
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<tbody>
<tr>
<td>$10^{-5} - 10^0$</td>
<td>large-scale finite element, finite difference, linear iteration, and boundary element methods</td>
<td>averaged solution of differential equations at the macroscopic scale (mechanics, electromagnetic fields, hydrodynamics, temperature fields)</td>
</tr>
<tr>
<td>$10^{-5} - 10^0$</td>
<td>crystal plasticity finite element models, finite elements with advanced constitutive laws considering microstructure</td>
<td>microstructure mechanics of complex alloys, fracture mechanics, textures, crystal slip, solidification</td>
</tr>
<tr>
<td>$10^{-6} - 10^0$</td>
<td>Taylor–Bishop–Hill, relaxed constraints, Sachs, Voigt, and Reuss models, Hashin–Shtrikman model, Eshelby and Kröner-type self-consistent models</td>
<td>polyphase and polycrystal elasticity and plasticity, microstructure homogenization, crystallographic textures, Taylor factors, crystal slip</td>
</tr>
<tr>
<td>$10^{-8} - 10^0$</td>
<td>cluster models</td>
<td>polycrystal elasticity</td>
</tr>
<tr>
<td>$10^{-10} - 10^0$</td>
<td>percolation models</td>
<td>nucleation, fracture mechanics, phase transformation, current transport, plasticity, superconductivity</td>
</tr>
</tbody>
</table>
 automata which may account for both short-range (local) and long-range (global) interactions, Ginzburg–Landau–, Cahn–Hilliard–, and Allen–Cahn-type phase field methods, dislocation dynamics, polycrystal and nonlinear crystal plasticity finite element models, topological network and vertex models, boundary dynamics, and multistate kinetic Potts methods. However, classical techniques such as molecular dynamics, Metropolis Monte Carlo, and conventional finite element simulations are also used extensively.

Advanced microstructure simulations should meet three major requirements. First, they should enable one to use, or even derive, advanced path-independent microstructure–property relations with quantitative validity. Second, they should provide insight into the underlying thermodynamic and path-dependent physical principles that govern the complex nature of microstructure evolution at the various space and time scales. Third, they should allow one, at least in certain cases, to replace and complement experimentation by simulation.

In engineering terms microstructure simulations should thus provide a convenient means of predicting and understanding material properties and microstructure evolution for technical applications under conditions that have not yet been studied or that are not amenable to experiments. To fulfill these requirements and at the same time to optimize the predictive power of models, the various numerical methods are increasingly complemented by the concept of integrated modeling and simulation (Gottstein 1996). This term characterizes the coupling of computer codes with the aim of bridging the scale discrepancies between different simulation levels. This can be achieved by either simultaneous integration (direct integration) or sequential integration (Raabe 1997). The first notion means that various interacting simulation codes, which may use different numerical techniques, are employed simultaneously in one computer experiment. The second term describes the alternative method of an adequate parameter-transfer between simulations that are used sequentially.

Since microstructure evolution is path-dependent, concepts of integrated modeling and simulation should include as many of the microstructurally relevant processing steps and parameters as possible. However, such a procedure requires the incorporation of various space and time scales which can differ by some orders of magnitude. One reasonable approach for combining various scales consists in the incorporation of constitutive laws that have been derived from non-averaged, i.e. space- and time-discretized, simulations on the appropriate smaller scale. In such a concept, the results obtained from simulations on a certain scale are averaged and condensed before being considered at the next scale. This means that the phenomenological character of the model equations used in each step increases with increasing scale.

However, there is also a more direct way of bridging scale discrepancies. Some of the simulation techniques mentioned above were originally confined to particular space and time scales. This applies especially to methods which reveal intrinsic physical scaling parameters, e.g. molecular dynamics and some Monte Carlo methods. In contrast, most mesoscale models are continuum approaches, i.e. they are not intrinsically calibrated and have thus a larger potential for spanning time and length scales. In this context especially the various crystal plasticity finite element, cellular automaton, dislocation dynamics, boundary dynamics, and multistate Potts\(^3\) models are of importance.

For instance, the finite element technique is designed to provide approximate solutions to coupled sets of partial differential equations subject to appropriate boundary- and initial-value conditions. Its application in computational materials science was orig-

\(^3\)Monte Carlo method with a delta-type Hamiltonian for the identification of interfaces.
inally confined to solving elastic and simple plastic problems at the macroscopic level using averaging constitutive laws and the conditions for equilibrium and compatibility. However, through the introduction of improved constitutive laws, i.e. elements of crystal plasticity, finite element methods are nowadays increasingly capable of considering material heterogeneity also at the mesoscopic level. This trend in finite element simulations points from the macroscopic to the mesoscopic scale. For the Potts model, which has its roots in the stochastic Metropolis Monte Carlo method, the reverse applies. By mapping generalized spin numbers to discrete domains which comprise cells with identical spin, it enables one to extend the use of the Monte Carlo algorithm to the description of interfaces. This approach points from the microscopic to the mesoscopic scale.

The material in this book should assist the reader in selecting appropriate simulation methods and critically estimating the plausibility of the predictions. Both aspects are important, since one often encounters different concepts for simulating the same problem. For instance, in the field of plasticity, one can use finite element methods, statistical kinematical simulations, discrete dislocation dynamics, molecular dynamics, or combinations of these (Figure 1.3).

Besides the numerous technical details that will be reviewed in the following chapters, the selection of appropriate simulation techniques should be accompanied by the following more general considerations:

- **Scales**: What are the physical time and length scales of the phenomenon?
- **Microstructure**: Is it necessary to incorporate microstructure?
- **Analytical solution**: Is it possible to solve the problem analytically?
- **Experimental data**: Are experimental data available to check the predictions?
- **Independent variables**: Which variables should serve as independent variables?
- **Dependent variables**: Which variables should serve as dependent variables?
- **Model approach**: Should a first-principles, phenomenological, or empirical model approach be used?
- **Model parameters**: Do the required parameters have any physical meaning and are corresponding experimental or theoretical data available?
- **Boundary conditions**: Which boundary- and initial-value conditions are adequate?
- **Realistic conditions**: Are particular boundary- and initial-value conditions known?
- **Discretization**: What degree of spatial and temporal discretization is required?
- **Simulation scale**: Which simulation method is suited for the scale addressed?
- **Error tolerance**: What degree of precision is required? Which error can be tolerated?
- **Deterministic/stochastic**: Is the phenomenon deterministic or stochastic?
- **Atomistic/continuum**: Should an atomistic or continuum model be used?
- **Combination of scales**: Is it required to combine various space and/or time scales?
- **Integrated simulation**: What is the appropriate integrated simulation method to bridge the various space and/or time scales?
- **Simulation code**: Are existing simulation codes available?
- **Comparison**: Were the chosen simulation methods quantitatively compared with experiments, analytical solutions, and/or competitive numerical approaches?
- **Programming language**: Which programming language, compiler, commercially available solver, etc. should be used?
- **Speed**: Which is the fastest simulation method?
- **Price**: Which is the cheapest simulation method?
- **Computer power**: How much computer power is available for the simulation?
- **Data analysis**: What methods must be used to analyze and present the data?