Chapter 0
Introduction

A systematic investigation of fracture and fatigue started during the nineteenth century mainly as a consequence of repeating failures of dynamically loaded engineering components and structures. In the first half of the last century, pure empirical and mechanical views on fracture prevailed and this explains the rather empirical understanding of the failure of engineering components and structures under applied static or dynamic loads. Results of experiments were evaluated by using linear–elastic fracture mechanics and the resistance of structural materials to fracture was believed to be predominantly determined by their chemical composition. However, fundamental experience revealed that the fracture resistance of materials is to a large extent influenced by their microstructure. Since about 1950, therefore, the materials science approaches based on physics, chemistry and mechanical engineering became very important in fracture research. Advanced experimental methods such as electron microscopy, atomic-force microscopy, Auger spectroscopy, X-ray methods, electron-beam microstructure analyses and servohydraulic close-loop testing devices started to be utilized in fracture research. At the same time, the employment of numerical methods in materials science and fracture was promoted by the rapidly increasing efficiency of computer systems as well as by growing demands for quantitative predictions in industrial research. Thus, the theoretical models of fracture and fatigue processes started to be developed and experimentally supported on all spatial scales from atomistic to macroscopic approaches.

Phenomenological fracture models beyond the atomic scale are based on constitutive relationships that usually involve many *variables*. These variables can be categorized into independent variables, state variables and parameters [2]. As a rule, time and space coordinates serve as independent variables while state variables represent physical quantities as functions of the independent variables. Quantities such as stress, strain, dislocation density, vacancy concentration, particle size or interphase spacing are typical examples of state variables. A further distinction between *explicit* and *implicit* state variables can often be encountered, especially in microstructure mechanics. The ex-

plicit state variables define *local* microstructural features such as grain size or particle volume. On the other hand, the implicit variables are defined as mesoscopic or even macroscopic *averages*. In kinematic equations describing the evolution of microstructural damage during the fracture process, the state variables are usually weighted, i.e., based on parameters. The parameters should be measurable quantities of well–defined physical meaning.

As a consequence of both advanced experimental and theoretical studies, the fracture of engineering components is, nowadays, commonly grasped as a process of damage accumulation in the materials microstructure. This process consists of four fundamental stages: Localization of plastic deformation, nucleation of cracks, propagation of cracks and final fracture of the component. However, the duration of these stages can substantially differ depending on microstructure, chemical composition, loading, temperature and environment. Some of these stages might be absent as well. The materials microstructure should be understood in terms of a spatial hierarchy ranging from the *nanoscale* (electrons, atoms, individual lattice defects), through the *microscale* (crystallography, lattice defects ensembles and secondary phases below the grain scale) up to the *mesoscale* (defects and phase ensembles at the grain scale). The *macroscopic* level embraces the geometry of samples and components. The state variables that quantify microstructural elements are often called *microstructural characteristics*. In order to illustrate the role of microstructural elements and characteristics in individual stages of the fracture process, the physical background of uniaxial tension tests of metallic materials of the same chemical composition but possessing a different microstructure will be briefly discussed hereafter. The influence of microstructure on fracture characteristics will also be mentioned.

Let us first consider a perfect single crystal as a highly ordered solid possessing the lowest possible internal energy per atom. In this case, the first three stages of the fracture process are absent. Indeed, such a crystal would experience a nonlinear–elastic deformation until it fails either by homogeneous unstable decohesion along the atomic planes perpendicular to the applied load (when reaching the ideal tensile strength) or, much more probably, by a shear instability (when reaching the ideal shear strength). In both cases, however, this stress would significantly depend on the direction of the applied load, i.e., on the crystallography (see Chapter 1 for details). The related uniaxial fracture stress σ_u would lie close to an upper limit of the material strength of the order of 10 GPa, whereas the fracture strain would approach the lower limit of the order of 0.1. The cohesive energy per atom U is another important mechanical characteristic related to this fracture process. This energy is proportional to the fracture (surface) energy γ that refers to the work necessary to create a unit area of an internal free surface (crack), and also depends on the crystallography.

Real single crystals exhibit much lower fracture stresses. This is, however, not a consequence of a lower cohesive (or fracture) energy due to the presence of dislocations. Indeed, the cohesive energy associated with a dislocation core

is only slightly lower than that of the perfect crystal. On the other hand, real crystals exhibit much higher fracture strains due to a long mean free path of dislocation. The reason is that the fracture process involves all four fracture stages, thereby being completely different from that of the perfect crystal. In the first stage, the mobile primary dislocations on selected glide planes move rather long distances thus producing large macroscopic strains under very small applied stresses of the order of 10 MPa. In the second stage, the interaction of dislocations at intersections of primary and secondary slip planes builds long pile-ups associated with very high local internal stresses. When a superposition of internal stresses with the external stress locally approaches the ideal strength, microcracks nucleate in the bulk. Growth and coalescence of these cracks lead to a final fracture at a rather high fracture strain ($\varepsilon_f \gg 1$). In body centred cubic (bcc) metals the interaction of pile-ups creates sessile dislocations that initiate cleavage fracture along (100) crystallographic planes (see Chapter 2 for more details).

Polycrystalline single-phase materials contain grain boundaries that restrict the dislocation motion. Therefore, lower fracture strains ($\varepsilon_f \geq 1$) are usually observed. On the other hand, higher external stresses ($\sigma \approx 100\,\text{MPa}$) are needed to build dislocation pile-ups inside the grains. The high-angle grain boundaries possess a rather low cohesive energy. This energy and the related ideal strength can be further reduced by a diffusion of interstitial atoms like hydrogen or oxygen to the grain boundary sites where high triaxial tensile stresses are built by the superposition of internal and external stresses. This can lead to grain boundary cracking (see Chapter 3 for more details).

Engineering polycrystalline materials contain secondary phase particles (precipitates and inclusions) both inside the grains and at the grain boundaries. This restricts dislocation motion to an even greater extent so that the fracture strain is further reduced ($\varepsilon_f \leq 1$). On the other hand, higher external stresses are needed to build dislocation pile-ups which leads to a higher fracture stress. Incoherent matrix/particle interfaces exhibit a very low cohesive energy and a reduced ideal strength. These characteristics can be further worsened by interstitial diffusion and/or segregation of impurity atoms (see Chapter 2 for more details). Therefore, the microcracks can be initiated at both the particle/matrix interfaces and the grain boundaries. Consequently, the fracture process can be accomplished by diverse micromechanisms: Transgranular cleavage, intergranular decohesion, coalescence of voids or their mixture (see Chapter 2 for more details). In comparison to previously discussed microstructures, the stress-strain diagram of a typical high-strength engineering material ($\sigma_u \approx 1\,\text{GPa}$, $\varepsilon_f \approx 0.3$) is closer to that of the perfect crystal.

The radical engagement of dislocations in the microcrack nucleation might be understood in terms of their negative role in fracture processes. However, this statement is generally not true. When the microcrack is already formed, dislocations start to serve in a very positive way particularly in the case of brittle or quasi-brittle fracture. Indeed, the emission of dislocations from the crack tip (or their absorption at the crack tip) increases the fracture energy

and blunts the crack tip, thus increasing the material resistance to unstable fracture. This favourable effect is appreciated in the case of engineering components containing microdefects that have been produced during their production or nucleated by corrosion and/or fatigue. On the other hand, a repeated emission and absorption of dislocations enables stable crack propagation under fatigue loading. These examples demonstrate a miscellaneous role of lattice defects in fatigue and fracture. Simultaneously, they highlight the importance of recognizing the fracture micromechanism in the research and development of advanced materials with high resistance to fracture and fatigue.

Table 0.1 Space scales and simulation methods

Scale range [m]												
10^{-12}	10^{-11}	10^{-10}	10^{-9}	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{0}
Subnano		Nano			Micro			Meso		Macro		
ab initio, phonon spectra												
		Monte Carlo, cluster variation, molecular dynamics										
			dislocation dynamics, **discrete dislocations**									
				tessellation, **topology**, grain boundary dynamics								
					percolation							
					finite element, **boundary element**, finite difference, rheology, cellular automata							

There are many simulation methods used in modelling deformation and fracture processes on different scales. In Table 0.1, selected methods are collected according to their applicability in subnano-nano-micro-meso-macro regimes. Many of these methods (emphasized in Table 0.1) were also employed by us. Advanced microstructure models of fracture and fatigue processes based on simulation methods should enable us to use, or even derive, path-independent relationships between microstructural parameters and fracture characteristics. They should provide an insight into physical principles that govern the damage accumulation in materials microstructure as well as allow a proper interpretation of experimental results. To fulfil these requirements, the advanced models are increasingly complemented by the concept

of integrated modelling and simulation. This means that computer codes and methods are coupled with the aim of bridging the scale differences between adjacent simulation levels. Such models belong to the *multiscale* category. To our knowledge, there is no generalized rule for how to design the multiscale approach. However, there are two principally different integration methods widely employed in such simulations: *simultaneous* integration and *sequential* integration [2]. The first method means that various interacting simulation codes are utilized simultaneously in one computer experiment. The second principle is based on an adequate transfer of parameters between simulation that are used sequentially. Multiscale models of fracture processes, presented in the works of the authors of this book, are preferentially built on the second approach.

It should be emphasized that partial submodels of the sequential multiscale model should not involve too many state variables serving as *fitting* parameters. Indeed, too complicated mathematical descriptions can lead to a physical nontransparency of the model. Similarly, a deficiency of experimental verification of partial theoretical concepts usually results in a misleading phenomenology of the multiscale model. Nevertheless, without analyzing the fracture micromechanisms in the frame of relevant multiscale approaches, many rather surprising experimental results (or even those standardly accepted) could not be reasonably elucidated. Since these models embrace a wide range of microstructure states, they are able to predict materials behaviour and fracture properties on different scales. Let us briefly mention a few examples of such unique capabilities.

In 1970–1974, numerical simulations of an arrangement of atoms in screw dislocations in bcc metals confirmed that their core is spatially extended into three slip planes that lie in the zone of a common slip direction [3, 4]. Much later, the coupling of codes based on atomistic, crystallographic and finite element approaches revealed that such dislocations exhibit asymmetry in their mobility under tensile and compressive loading [5]. Moreover, they do not follow the Schmid's law at low temperatures. These unique properties could explain an asymmetric mechanical hysteresis observed in bcc single crystals or the anomalous temperature dependence of the yield stress in some intermetallic materials [6]. This multiscale analysis led to the development of a physically based yield criterion with generally asymmetric yield surface that is directly applicable in macroscopic analyses of yielding [7].

In fatigue, the existence of the threshold ΔK_{th} of long crack growth has been well known and widely accepted since nearly 1970. Unfortunately, the theoretical methods based on the macroscopic theory of plasticity did not predict such a threshold behaviour at all. Starting from 1990, however, discrete dislocation concepts could be brushed up and applied to fracture research owing to a massive involvement of new numerical methods (e.g., [8]). One of the most important results that followed from such approaches was the exact theoretical confirmation of the threshold behaviour [9]. Afterwards, the discrete dislocation concept proved to be a very useful tool for elucidation and

quantification of various phenomena near the fatigue threshold, e.g., crack closure effects under plane strain conditions [10, 11]. These concepts were also able to provide a physically clear background of the size effect observed in micro and nanocomponents [12].

During 1975–1985, many experimental results verified an anomalous fracture behaviour of ultra-high-strength low-alloy (UHSLA) steels. The fracture toughness of these steels significantly increased with coarsening of the mean prior austenite grain size (raising austenitizing temperature). On the other hand, the absorbed energy in impact tests revealed the opposite trend. These contradictions could be elucidated by an extreme geometrical shielding of the crack tip that was produced by decohesion of coarse grain boundaries during the fracture toughness tests. A multiscale model that coupled methods based on topology, stereology and metallography with finite element analysis quantitatively predicted fracture behaviour in very good agreement with experimental data. A similar model could quantitatively reproduce a steep increase in fracture toughness of borosilicate glasses with increasing concentration of reinforced particles (see also Chapter 2).

Besides a survey of our work, this book aims to present a rather consistent overview of fracture micromechanisms. Indeed, all the fundamental kinds of fracture processes and related micromechanisms are considered except for high-temperature creep damage. The description of fracture processes ranges from atomistic up to macroscopic levels. Therefore, the multiscale context can be easily found in many models of fracture processes that couple such approaches by means of sequential integration. Although emphasis is given to metallic materials, the fracture behaviour of ceramics and composites is also discussed.

The topic of the first chapter is the deformation and fracture of perfect crystals. Their mechanical behaviour under various kinds of monotonously increasing (static) loading is preferentially investigated by means of *ab initio* (first principles) methods based on electronic structure calculations. It is our strong belief that engineers can also learn a lot from the results of these apparently academic studies. They provide a clear distinction between intrinsic lattice properties and those induced by defects and secondary phases in engineering materials. They also constitute physical benchmarks for engineering multiscale models such as upper and lower limits of fracture and fatigue characteristics (ideal strength and fracture toughness). Three-scale models coupling electronic structure with atomic arrangements and crystallography are applied to calculate the ideal strength of crystals and nanocomposites under various loading conditions. Multiscale models predicting intrinsic ductile/brittle behaviour of crystals are also presented. These models couple atomistic, crystallographic and fracture-mechanics approaches. Finally, a multiscale model of nanoindentation is presented in order to quantify pop-in effects observed in load-penetration diagrams. This model links numerical methods and results embracing all spatial scales from nano to macro.

The second chapter is divided into sections devoted to micromechanisms of brittle, quasi-brittle and ductile fracture under static (low strain rate) and dynamic (high strain rate) loading. The leading theme of the first topic is the geometrically-induced crack tip shielding effect and the related fracture micromechanism. A two-scale analytical model based on quantitative fractography and mixed-mode fracture mechanics is applied to explain the fracture behaviour of borosilicate glasses. In order to quantify the quasi-brittle fracture, the geometrically-induced shielding effect is related to the ratio of a characteristic microstructure dimension and the crack-tip plastic zone size (the size ratio) in a two-scale analytical model based on quantitative fractography and fracture mechanics. This model is employed to describe the anomalous fracture behaviour of UHSLA steels as well as to assess the value of fracture energy of grain boundaries with segregated phosphorus in ferritic alloys. Finally, analytical three-scale models of ductile fracture processes based on dislocation dynamics, microvoids formation kinetics and fracture mechanics are presented. These models are able to predict the fracture strain in the tensile testing of ductile metallic materials and to assess the values of fracture toughness for steels exhibiting the ductile fracture micromechanism.

The last chapter is dedicated to fatigue fracture of metallic materials. The micromechanisms of mechanical hysteresis, crack initiation and crack propagation under all modes of crack-tip loading are described in the multiscale concept from nanoscale to mesoscale levels. An analytical multiscale model of crack closure was developed in order to evaluate individual crack-tip shielding components and to assess the intrinsic fatigue threshold value under the opening loading mode. Micromechanisms of crack propagation under shear and mixed-mode loading are also discussed from the point of view of both theoretical and experimental approaches. For example, a two-scale model connecting three-dimensional topology with linear–elastic fracture mechanics is able to explain a formation of factory-roof morphological patterns on the fracture surfaces generated by cyclic torsion. The initiation and propagation of fish-eye cracks is studied under combined bending-torsion loading in specimens made of nitrided steel. A method enabling a quantitative reconstitution of the fatigue process from the fracture morphology is described in the final part of the chapter. This method of engineering failure analysis was successfully applied in many practical cases.

The book is complemented by three appendices devoted to *ab initio* methods utilized in atomistic models, criteria employed in mixed-mode fracture and derivation of void-induced dislocation dynamics in the model of ductile fracture.