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Pattern Formation and Fracture in Brittle and Polymer-like Failure of Disordered Materials

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de Rector Magnificus, prof.dr.ir. C.J. van Duijn, voor een commissie aangewezen door het College voor Promoties in het openbaar te verdedigen op dinsdag 26 juni 2007 om 16.00 uur

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Chapter 1

Introduction

Failure of materials is an important, extremely interesting and challenging subject. It is important because understanding of how materials break is vital for material science, engineering applications and for the design of new materials. It is so interesting and challenging because breakdown is not easy to describe within known theories. The heterogeneity of materials microstructure and formation of cracks and cavities during failure are main pitfalls which stand in the way of any theoretical study trying to describe breakdown.

Ways in which materials deform and fail can be very different. The initial phase of the deformation of common solids is usually linearly elastic and all differences come afterwards. So-called "brittle" materials break abruptly almost immediately after the elastic regime. "Ductile" or "plastic" ones yield at some point to large inelastic deformations and break only after that. Materials with even more complex behavior can have the plastic regime followed by strain hardening. It is possible as well to observe softening - a stress drop immediately after the yield peak. Although not all known experimental results are well understood, most of them are very well described by rheological constitutive laws. This allows to model the behavior of materials within the methods of continuum mechanics. However, this is not enough to understand the underlying physics of the process, especially those physical aspects that are related to disorder. Such understanding can help to explain phenomena which do not have a good explanation yet, it can also provide a new view on things that were thought to be understood sufficiently. Metals are an example of the latter: although they have been investigated very thoroughly and for a very long time, new views on plasticity based of statistical analysis of defects have appeared quite recently. There are many materials that are investigated much less than metals and new ones are constantly being designed. Polymers, for example, have often stood aside the mainstream of material research due to their unique microscopic architecture and very distinctive macroscopic behavior.
1. Introduction

Clearly, the role of disorder in materials failure should be revealed, carefully studied and become an established part of strength theories and engineering procedures.

1.1 Historical overview

Material science and continuum mechanics have a rather long history. People became interested in materials behavior and strength since they started to make things like houses, tools and weapons. A systematic knowledge in this area, though mostly empirical, started to appear already in antiquity. Aristotle and Archimedes described complex structures and principles of mechanics in their works. Galileo and Leonardo Da Vinci continued this quest during the Renaissance in a more formal and systematic way.

The first task related to materials behavior was to describe the initial and the most simple phase of materials deformation - linear elasticity. That was done in 1660 by Robert Hooke, who suggested a linear dependence between the force acting on a spring and the relative elongation of this spring, the so-called Hooke’s law. This law was generalized as a dependence between stress and strain in deforming bodies within the theory of stress which was introduced by Augustin Louis Cauchy more than a century later. After describing linear elasticity, the next problem was to understand somewhat more complex types of behavior, such as plasticity. The first steps in understanding plasticity were taken by Tresca and Maxwell in the 19th century and later, in the beginning of the 20th century, by von Mises, who advanced and argued physically the concept of Maxwell. The criteria of plasticity introduced by Tresca and von Mises are still the most frequently used by engineers and scientists.

Elasticity and plasticity are just two of many branches that form the tree of continuum solid mechanics, which by now has developed into a distinct, well established and mathematically precise discipline owing to efforts of such brilliant scientists as Cauchy, Bernoulli, Euler, Lagrange and many others mostly during the 18th century. Continuum solid mechanics described strain and stress fields in deformable bodies but not the process of failure. This had to wait until the beginning of the 20th century when Inglis and Griffith first considered the influence of microcracks and the conditions under which they start growing. This was the beginning of fracture mechanics - another branch of the tree, one of the most recent. Griffith himself focused on the behavior of a single defect under certain loading conditions. Already this problem, simple at first glance, was rather hard to handle analytically. Classical fracture mechanics did not take into account statistics of defects, which of course was very important. That was done later by Weibull, who invented a statistical theory of breakdown and introduced a special distribution for it. Now a statistical treatment in describing the strength of materials is accepted in science quite widely. Nevertheless, engineering textbooks and regulations pay little attention to this problem,
apparently because there is no universal and simple method to handle it.

The presence of experimentally observable power-law scaling in fracture (for example, in the distribution of fracture events and the crack roughness) made it tempting to consider breakdown as a critical phenomenon, like a phase transition, or at least to look for similarities with such phenomena. This attracted statistical physicists to the problems of fracture and made them try to describe the observed scaling laws using the ideas of random percolation and self-organized criticality (SOC).

Recently, computer simulations have become widely utilized to model breakdown. The most frequently used methods are: atomistic simulations, finite-element modelling, lattice models or hybrid methods combining some of the three. In the next chapter we will describe more in detail those of theoretical and numerical techniques that are related to our work.

1.2 Experimental observations on fracture of heterogeneous materials

Most materials are heterogeneous to some extent. For the present study those experimental observations are the most important that can provide an evidence of critical behavior, like scaling or power-law distributions in any property. Scaling is experimentally found in fracture in at least two forms. The first one is known already for a long time; it is the size effect in materials strength. It was observed as early as in the 1500’s by Leonardo da Vinci, who noticed that a short truss is stronger than a long one [12]. Later on one has found experimentally for many materials that their strength decreases when the size of a sample is getting larger.

Estimating a strength scaling law is itself a difficult task due to large sample-to-sample fluctuations, influence of surface defects and necessity to test a wide range of sample sizes. Another difficulty is in the fact that a statistically induced size effect should be distinguished from a deterministic one. In other words, the size effect from the extreme statistics of a weakest link, or the random statistics of disorder, should be distinguished from the one caused by stress gradients that originate from fracture process zones and that interfere with the sample size. Experimentally found distributions of material strength are usually described rather well by so-called Weibull or Gumbel laws. As we will show later there are also some theoretical arguments leading to these two special distributions.

Universal scaling of crack roughness is another observation of scaling that has been discovered rather recently. It is an interesting and truly intriguing experimental observation in fracture [13]. This reflects the dependence between the roughness (average height variation) \( \Delta h \) of a crack surface and the size \( d \) of the window over which it is measured (Fig. 1.1). Initially the power-law scal-
1. Introduction

Figure 1.1: Crack-roughness definition via the minimum-maximum method: the average height variation $\Delta h$ depends on the window size $d$

ing of surface roughness was found in metals [49, 50]. Then experiments were performed for other materials and, surprisingly, for an extremely broad range of materials, with different properties and microstructure, the same scaling dependence in the general form of $\Delta h \propto d^\zeta$ was found for the lengthscales up to a certain characteristic correlation length $\Xi$, after which the dependence saturates [51, 13]. Moreover, the precise value of the exponent $\zeta$ was found to be nearly the same (about 0.8 in three-dimensional experiments) and for almost all investigated materials, while $\Xi$ changes from one material to another. Later the roughness scaling was found to be anisotropic [51], i.e. to have different scaling exponents in the direction along and across the direction of crack propagation. Some late studies [1] describe the existence of two scaling regimes: short- and long-range roughness scaling, with different exponents. Authors of very recent works [60, 59] claim that the scaling of crack roughness can be most generally described by an anisotropic scaling law that uses three exponents which, however, are still supposed to be universal. Although many studies have been performed, there is no general satisfactory explanation of this phenomenon so far.

There is one more important observation on statistical aspects of fracture, namely the energy of fracture bursts, which can be measured in experiments via acoustic emission. The energy released in bursts is often found to follow a power-law distribution, which is a fingerprint of critical behavior. A similar behavior is observed in the statistics of earthquakes and is called the Gutenberg-Richter law in seismology. This law states that the distribution of earthquakes of Richter magnitude $R$ has the form $10^{a-bR}$. 
1.3 Theoretical approaches to disorder

Local heterogeneity is inevitable in any material except, maybe, ideal monocrystals, and the role of such disorder is crucial for deformation and fracture. Ideally homogeneous materials would have a fracture stress many times larger than real ones, would not have any size effect and there would be no reason for quasistatic-crack surfaces to be rough. Furthermore, microscopic disorder has a very strong influence on the nature of the macroscopic response of a material and can change it completely, from brittle to ductile, from elastic to plastic. Therefore, disorder should be taken into account by a theory intended to capture any of the aforementioned effects.

Continuum solid mechanics (without fracture mechanics yet) is based on the average representation of materials, which makes it difficult to introduce disorder explicitly. It is only possible to model the average effect of disorder rather than disorder itself. The fracture-mechanics approach describes the behavior of a single defect incorporated in an elastic body. In the case of many non-interacting cracks it is possible to use the approach of extreme statistics. This is finding the most dangerous defect in the system and relating the strength of the whole system to it. The approach leads, depending on initial assumptions, to the well-known Gumbel or Weibull distributions of the macroscopic strength [70]. The case of interacting cracks is very complicated to handle, unless it is treated at a coarse-grained scale by decreasing the stiffness in the Hooke’s law locally. This method which is called “damage mechanics” is applicable when the interactions between microcracks are still moderate and fracturing happens in a stable way without strong fluctuations of damage.

As mentioned already, there is a possibility to consider breakdown as a phase transition. It is then natural to involve random percolation theory, which is a tool that has been successfully used to describe connectivity and transport problems in disordered media. However, the ability of random percolation theory to describe fracture is debatable due to the presence of long-range correlations and localization in the latter. This is one of the main issues we focus our research on.

Breakdown can also be analyzed from the point of view of self-organized criticality. This is a concept to describe how a system dynamically steers itself towards a critical point, going from one intermediate state to a similarly unstable following one, until the final critical point is reached. We will discuss further the arguments allowing to consider failure in terms of SOC.

Describing failure of heterogeneous materials theoretically is a very involved task whatever the chosen methodology is. Simulations are of course very helpful in the analysis of such a complex phenomenon, but choosing the right model is not trivial at all. Those models which are based on continuum mechanics can hardly take into account microscopic disorder, especially if the latter is strong. Atomistic simulations, being another extreme, are computationally expensive and usually do not allow modelling at a scale large enough for ana-
lyzing failure. Thus, something in between should provide a nice compromise. Lattice (or network) models are a very natural choice for two main reasons. First, they allow to explicitly introduce disorder, even a strong one. Secondly, they give a possibility to compare simulation results with theories applicable to lattices, e.g. random percolation of damage. The importance of such a comparison for our study will be clarified further. We will provide an overview of what has been done in the field of lattice models in the next chapter, where we describe the methodology of lattice models as well.

1.4 Aim of the research and outline of the thesis

As becomes clear from the title of this work, we are interested in two different types of materials failure: "brittle" and "polymer-like". The former, as described earlier, is characterized by yield and immediate breakdown after the (quasi-) elastic regime. The latter consists of a few successive phases: the (quasi-) elastic one, start of yielding, softening, plastic flow, hardening and, eventually, final breakdown. This sequence is very general, but some of the phases can be absent at certain conditions. The main difference for the present purpose is in the failure behavior following the yield point: "brittle" breakdown vs "polymer-like" softening and plastic flow. In real materials both are generally related to the disruption of local cohesive bonds. We will not enter into the final breakdown after strain hardening, which in polymers is related to the rupture of covalent bonds and chain entanglements. For the two types of failure to be considered, we want to reveal the role of disorder. We follow neither the approach of continuum mechanics nor the one of statistical physics to full extent. Instead, we try to combine them in a reasonable way. We represent disordered media by means of a central-force lattice model, which is close, in spirit, to continuum solid mechanics. Then we analyze the results following the ideas of statistical physics, in particular of random percolation theory.

The thesis is structured in the following way. In Chapter 2 we present the theoretical background of our work, including basics of continuum solid mechanics, fracture mechanics and lattice-model simulations. There we also give a review of scaling phenomena and self-organized criticality and present the basic ideas and results of random percolation theory. In Chapter 3 we give a detailed description of our modelling techniques. In Chapter 4 we address the question to what extent the damage evolution in brittle fracture can be understood as random damage percolation. To that end we first introduce the methods that we use to identify the presence of a percolation-like regime in the simulated damage pattern. Considering the extreme case of strong disorder is important, since it allows to make the effect of disorder really pronounced and also helps to understand to what extent the disorder is able to suppress typical features of materials deformation: localization and long-range interactions between local stress fields around single defects. We extend our analysis in Chap-
1.4. Aim of the research and outline of the thesis

In Chapter 4 we perform an analysis of crack profiles obtained in brittle-fracture simulations with different disorder strengths. We quantify roughness via the power-law scaling of self-affine surfaces. In Chapter 6 we perform an analysis of crack profiles obtained in brittle-fracture simulations with different disorder strengths. We quantify roughness via the power-law scaling of self-affine surfaces. In Chapter 7 we present the results of 3D simulation of brittle fracture and repeat some elements of analysis performed in Chapters 4 and 5. In Chapter 8 we investigate polymer-like behavior, modelled by a 2D lattice model with a certain fraction of unbreakable springs to represent the covalent and entanglement bonds. We show the effect of disorder in the weak cohesive bonds on the macroscopic response of the lattices. In particular we study the relation between this disorder and the existence and shape of the yield peak. We finish our work with a summary and conclusions in Chapter 9.

Chapter 4 of the thesis mostly follows two of our publications [44, 45] while the major part of Chapter 5 follows the third paper [46]. Chapter 6 combines the results related to crack roughness of all three publications [44, 45, 46]. Publications on Chapters 7 and 8 are in preparation.
1. Introduction
Chapter 2

Theoretical background

In this chapter we present theoretical considerations which are most relevant for our study. We depart with a very brief description of linear elasticity, then introduce the fracture-mechanics approach and a review of relevant numerical methods. Next, we introduce scaling phenomena, starting with a general description and arriving at a particular example related to fracture. We extend the description of scaling by introducing fractals, together with the concept of self-affinity. Then we present basic concepts and results of random percolation theory, which we will use intensively throughout our work. After that, the framework of self-organized criticality is introduced in order to prepare a background for our analysis of fracture-avalanche statistics. We finish the chapter with an overview of modelling fracture with lattice models, presenting main ideas and results as a retrospective.

This chapter contains very brief information on every touched topic. A lot more on continuum solid mechanics can be found in [43, 23, 26]. For additional information on fracture mechanics we refer a reader to [4]. Random percolation theory is described in detail in [73, 28, 40]. The monographs of Bak [6] and Sornette [72] can serve as a general introduction to self-organized criticality. The latter is also a good introduction to fractals. An explicit review on statistical models of fracture and, in particular, on lattice models, can be found in [2].

2.1 Continuum solid mechanics

2.1.1 Linear elasticity

Behavior of deformable solids under the action of external forces and applied displacements is described by continuum solid mechanics. Linear elasticity is the most simple case where constitutive equations are linear and deformations
are small enough to allow first-order approximations.

Consider a deformable solid which is described by a coordinate vector \( \mathbf{r} \) in its rest state. Let \( \mathbf{r}' \) describe the geometry of the solid when it is deformed. Then we can define the displacement field as \( \mathbf{u} = \mathbf{r}' - \mathbf{r} \). The strain (or deformation) tensor \( \mathbf{\epsilon} \) can be defined as the symmetric part of the displacement gradient: 

\[
\mathbf{\epsilon} = \frac{1}{2} ( \nabla \mathbf{u} + (\nabla \mathbf{u})^T ).
\]

The Cauchy stress tensor \( \sigma \) describes surface traction \( \mathbf{t} \) acting on an arbitrary surface \( dS \) with the unit normal \( \mathbf{n} \) within the body according to Cauchy's formula:

\[
\mathbf{t} = \mathbf{n} \cdot \sigma.
\]

In linear elasticity the relation between \( \sigma \) and \( \mathbf{\epsilon} \) is linear and can be written as

\[
\sigma = \frac{\partial \Pi}{\partial \mathbf{\epsilon}} = C : \mathbf{\epsilon},
\]

where \( \Pi \) is the deformation energy per unit volume and \( C \) is the fourth-rank stiffness tensor. This relation can be written in a much simpler form (known as Hooke's law) for isotropic materials:

\[
\sigma = K \text{tr}(\mathbf{\epsilon}) \mathbf{I} + 2\mu (\mathbf{\epsilon} - \frac{1}{3} \text{tr}(\mathbf{\epsilon}) \mathbf{I}),
\]

where \( K \) is the bulk modulus, \( \mu \) is the shear modulus, \( \mathbf{I} \) is the unity tensor and \( \text{tr}(\mathbf{\epsilon}) \) denotes the trace of \( \mathbf{\epsilon} \). It can be rewritten in a form more popular in engineering as

\[
\sigma = \frac{E}{1 + \nu} (\mathbf{\epsilon} - \frac{\nu}{1 - 2\nu} \text{tr}(\mathbf{\epsilon})),
\]

where \( E \) is Young's modulus and \( \nu \) is the Poisson ratio of the material.

The solid (Fig. 2.1) is loaded by external body forces \( \mathbf{f} \) (per unit volume) and surface forces \( \mathbf{p} \) (per unit area). Both body forces and surface forces are assumed to be "dead" loads, i.e. they do not depend on deformation. The latter ones are acting on a part of the external surface denoted as \( S' \). Displacements are prescribed in the form of \( \mathbf{u} \mid_{S''} = \mathbf{u}^* \) for the remaining part of the external surface \( S'' \).

According to the principle of minimum total potential energy, the following functional should be minimal

\[
A = \int_V (\Pi(\mathbf{\epsilon}) - \mathbf{f} \cdot \mathbf{u}) \, dV - \int_{S'} \mathbf{p} \cdot \mathbf{u} \, dS \rightarrow \min,
\]

still following the kinematic boundary condition:

\[
\mathbf{u} \mid_{S''} = \mathbf{u}^*.
\]

Using the divergence theorem, the extremum condition for \( A \) can be written as follows

\[
\delta A = \int_V (\sigma : \delta \mathbf{\epsilon} - \mathbf{f} \cdot \delta \mathbf{u}) \, dV - \int_{S'} \mathbf{p} \cdot \delta \mathbf{u} \, dS =
- \int_V (\nabla \cdot \mathbf{\sigma} + \mathbf{f}) \cdot \delta \mathbf{u} \, dV + \int_{S''} (\mathbf{n} \cdot \mathbf{\sigma} - \mathbf{p}) \cdot \delta \mathbf{u} \, dS = 0,
\]
2.1. Continuum solid mechanics

Figure 2.1: Loaded elastic body

where $n$ stands for the unit outward normal to the surface of the body. This leads to the equation of balance

$$\nabla \cdot \sigma + f = 0, \quad (2.8)$$

and the natural boundary condition on $S'$

$$n \cdot \sigma - p = 0. \quad (2.9)$$

Equations (2.4) and (2.8) can be combined into one differential equation for displacements:

$$(K + \frac{1}{3} \mu) \nabla (\nabla \cdot u) + \mu \nabla^2 u = 0. \quad (2.10)$$

Equations (2.10), (2.9) and (2.6) form a closed system uniquely defining the displacements corresponding to equilibrium.

2.1.2 Fracture mechanics

Linear elasticity allows to define, within the mentioned assumptions, strain and stress fields in a body but it does not tell when and how the body will break or how it will behave outside the accepted assumptions. If the deformations become large, it is necessary to use the deformation gradient tensor $F = r' \otimes r$ ($\otimes$ denotes a dyadic product) for describing finite deformations and to use another measure of deformation (Cauchy-Green deformation tensor or Finger deformation tensor) instead of $\epsilon$. In the case of finite deformations the Piola-Kirchhoff stress tensor is sometimes used instead of the Cauchy stress.
Theoretical background

Figure 2.2: An infinite plate with an elliptic opening loaded by a tensile stress tensor. The mathematics gets much more difficult in this case compared to the classical linear elasticity even if the constitutive relation (the relation between stress and strain) remains linear. If the latter becomes non-linear as well, the mathematical description gets even more involved. Even this complex description still does not take into consideration physical disintegration of materials, whether it happens via cracking, void formation or via some other mechanism.

There is a class of materials that are called "brittle", in which failure immediately follows the elastic regime and happens abruptly. This type of failure is described by linear elastic fracture mechanics. Fracture mechanics originated from continuum mechanics of solids in the beginning of the 20's century. The stress occurring in an elastic plate in the presence of an elliptic opening (Fig. 2.2) was first described by Inglis in 1913 [36]. He found that the stress in the concentration point is

\[ \sigma_c = \sigma (1 + \frac{2a}{b}) \]  

(2.11)

where \( a \) and \( b \) are defined as shown in Fig. 2.2 and \( \sigma \) is a stress applied to the boundary infinitely far away from the opening. An exact solution for the stress field in a plate with an elliptic opening loaded by an arbitrary (but uniform) stresses acting on infinitely distant boundaries can be obtained by using Kolosov-Muskhelishvili's potentials [43]. The stress concentration in this case consists of two decaying terms of the order of \( \frac{1}{r^2} \) and \( \frac{1}{r^4} \), where \( r \) is the distance from the opening center. In other words the opening acts as a long-range disturbance of the uniform stress field. If the curvature radius \( \rho = \frac{b^2}{a} \) is used
Instead of \( b \) and under the condition that \( a \gg b \), the expression (2.11) takes the following form

\[
\sigma_c = 2\sigma \frac{a}{\rho}.
\]  

(2.12)

This formula gives an infinite stress for a sharp crack (when \( \rho = 0 \)). This result is unrealistic, but one should keep in mind that in reality materials consist of atoms and the minimum \( \rho \) is comparable to the atomic radius rather than equal to zero. This paradox motivated Griffith, a British engineer, to base his theoretical findings on energy instead of local stress. In 1920 he developed and published [27] a theory which described propagation of an elliptic crack inside a stressed elastic plate with thickness \( h \) (Fig. 2.3). His idea was clear and simple. A brittle body fails if defects (cracks) start to grow. They can grow only if the energy which is released due to crack extension, is sufficient to form new surface. Griffith considered a two-dimensional problem with an elliptical crack loaded by normal stress. He found that the strain energy released due to crack opening was directly proportional to the square of the crack length. The surface energy required to open a crack obviously was proportional to its doubled length. Therefore crack growth was only energetically favorable if the length of the crack was larger than some critical value.

For the considered problem of an elliptic crack the energy balance looks as follows

\[
\frac{d\Pi}{ds} + \frac{dA}{ds} = 0,
\]

(2.13)

where \( \Pi \) is the potential energy of deformation and external forces, \( A \) is the energy required to create a new surface and \( ds \) stands for an infinitely small
increase of the crack surface. Using the results of Inglis [36] it is possible to show that the potential energy can be written as

$$\Pi = \Pi_0 - \frac{\pi ha^2 \sigma^2}{E},$$  \hspace{1cm} (2.14)

where \(\Pi_0\) is the potential energy of the plate without a crack and \(E\) is Young’s modulus. The surface energy \(A\) can be written as

$$A = 4ah\gamma_s,$$  \hspace{1cm} (2.15)

where \(\gamma_s\) stands for surface energy of the material. Equations (2.13 - 2.15) result in

$$\frac{d\Pi}{ds} + \frac{dA}{ds} = -\frac{\pi a^2 \sigma^2}{E} + 2\gamma_s = 0,$$  \hspace{1cm} (2.16)

which allows to write an expression for fracture stress in the following form

$$\sigma_f = \left(\frac{2E\gamma_s}{\pi a}\right)^{1/2}.$$  \hspace{1cm} (2.17)

Before Griffith’s work there was no clear understanding how differently prepared samples of one and the same material could have very different strengths. Engineers of that time usually employed Young’s modulus divided by ten in order to estimate failure stress, which was often far from reality. Griffith suggested that material strength was defined by defects, inevitably present in any sample. As it follows from (2.17), for a given material and given defect size, there is a critical tensile stress at which the defect starts to grow catastrophically. The criterion can be formulated in the opposite way: for a given material and given stress, there is a critical defect size that makes the material break.

The same approach can be applied to other crack shapes. The so-called “penny-shaped” crack (Fig. 2.4) will lead to the following expression for the fracture stress:

$$\sigma_f = \left(\frac{\pi E\gamma_s}{2(1-\nu^2)a}\right)^{1/2},$$  \hspace{1cm} (2.18)

where \(\nu\) is Poisson’s ratio of the material.

Griffith’s invention immediately changed engineers’ and scientists’ views on strength. Its effect increased even more after the works of Irwin [37], who extended the crack-growth criterion to plastic materials by introducing the so-called fracture process zone and taking the energy of plastic deformation \(\gamma_p\) into account:

$$\sigma_f = \left(\frac{\pi E(\gamma_s + \gamma_p)}{2(1-\nu^2)a}\right)^{1/2}.$$  \hspace{1cm} (2.19)

The same modification was independently proposed by Orowan [57].
Nearly at the same time Irwin [38] and other scientists [76, 71] came to one of the most important results of fracture mechanics which states that irrespective of loading type the components of the stress field around a crack tip have the following form

$$\sigma_{ij} = \frac{K}{\sqrt{2\pi}r} f_{ij}(\theta),$$

(2.20)

where $K$ is the stress intensity factor (SIF), $f_{ij}$ is a crack-tip function, $r$ and $\theta$ are polar coordinates with the origin at the crack tip. SIF and the crack-tip function depend on loading and crack topology.

The case of many non-interacting defects is described by the extreme-statistics approach [2, 75]. According to it, the strength of the whole sample equals the strength of its weakest defect. So if one of the defects fails under a certain load, the entire sample fails. Consider a body that has $n$ defects each of which having a failure strength $s_i$ according to the same distribution $p(s)$. If the defects are independent, the distribution $P(s)$ of the total failure strength will obey the following dependence:

$$1 - P(s) = (1 - p(s))^n \approx \exp(-np(s)) = \exp(-\rho V p(s)),$$

(2.21)

where $V$ is the volume of the sample and $\rho$ is the defect density. Thus, the strength distribution of the sample is defined by the strength distribution of its defects. In particular, narrow (thin-tailed) distributions of defect strengths

---

**Figure 2.4:** A penny-shaped crack inside a body loaded by a remote tensile stress
give a Gumbel-type of sample-strength distribution [29]:

$$P_G(s) \sim 1 - \exp \left( -V \exp \left( \frac{s - \alpha}{\beta} \right) \right). \tag{2.22}$$

Wide (thick-tailed) distributions of defect strength result in a Weibull-type of sample strength distribution:

$$P_W(s) \sim 1 - \exp \left( -V \left( \frac{s}{\beta} \right)^\alpha \right). \tag{2.23}$$

All the analytical approaches described above have their limits, and in a situation when all (or even a few) complications like complex loading, local heterogeneity, dynamic effects, crack interaction and coalescence are put together, analytical approaches typically retreat and numerical simulations become unavoidable.

We would like to note again that a lot of information on theoretical fracture mechanics, its applications and experimental techniques can be found in a comprehensive monograph of Anderson [4]. A nice and recent review on statistical modelling of fracture can be found in [2].

### 2.1.3 Numerical methods

Complex problems in science and engineering often require numerical methods to be used. In principle, any numerical technique of solving partial differential equations can be used to solve problems of continuum mechanics, but not all of them are equally convenient. The finite-element method occupies a well-deserved leading place in this area. It is based on the energy-minimization principle (2.5). The displacements are approximated by means of special shape functions which have non-zero values only in finite regions around discretization points (nodes). This results in a system of equations with a diluted matrix that can be solved numerically together with appropriate boundary conditions. We will not describe the method here in view of many detailed and comprehensive handbooks available [81, 20, 26].

With regard to fracture, common finite elements are capable of modelling damage evolution of homogeneous or nearly-homogeneous materials in the mentioned manner of damage mechanics. Presence and growth of large cracks or voids makes the analysis much more difficult. It becomes necessary to use adaptive meshing and special finite elements: crack-surface elements and crack-tip elements. The finite-element method, being based on a continuum (or mean-field) representation of materials, can not easily deal with disordered materials unless only the average effect of disorder is to be modelled. Nevertheless significant progress has been made over recent years in the area of continuum-based models of fracture [56, 77, 74].
Another alternative is in using discrete lattice models. In this case the medium is represented by number of elastic bonds connected at nodal points. Similar to the finite-element representation, a lattice model can be considered as a discretization of a continuum [17, 18], though the properties of this discretization are different from ones of finite elements. The main distinction is in the fact that topological and orientational details of the lattice influence the properties of the corresponding continuum and, therefore, the result of the calculation. Opposite to that, the finite-element discretization is known to be mesh-independent. This feature of lattice models, which can be an issue for modelling homogeneous materials, becomes helpful when the material is heterogeneous or has an internal lattice-like microstructure like, for example, concrete. A comparison of using finite-element modelling vs lattice models is done in [2] and [39].

Central-force springs or bending beams can be used as elastic bonds in lattice models. The former corresponds to the conventional momentum-free continuum while the latter is related to a Cosserat-like continuum with independent rotation degrees of freedom [17]. Contrary to finite elements, lattice models provide a direct and natural way to introduce disorder. Another advantage is that damage evolution modelled by removing bonds from a lattice or by dramatically degrading their stiffness does not lead to computational problems.

Technically there is no difference at the stage of solution between lattice models and finite-element models in a sense that both formulations lead to a system of linear equations (not identical for the two) representing mechanical equilibrium and of boundary conditions representing constraints.

2.2 Scaling, fractals and self-affinity

2.2.1 Scaling phenomena

Scaling, as a term, usually means a relationship between two physical quantities in the form of a power law. Sometimes it is also used as a synonym of size effect, whether that can be expressed as a power law or not. Both of the two meanings are important for our study.

Size dependence is of a great importance for any physical theory or experimental study. First of all, it reflects fundamental laws of the theory or real phenomena. Secondly, it has a direct practical meaning, showing how the behavior changes with system size. Scaling laws can be very different, but in the most simple and pure case, for theories and experimental observations with no characteristic length, scaling should have a form

\[ S(L_2) \propto S(L_1) \left( \frac{L_2}{L_1} \right)^m, \]  

(2.24)
where $m$ is a scaling exponent [12]. This dependence represents how values of the physical quantity $S$ for two different system sizes $L_1$ and $L_2$ are related.

Power laws are met in physics rather often. In theory, many of them can be obtained by dimensional analysis and by finding the right asymptotics of the physical problem [9]. Power laws are very typical for critical phenomena, and phase transitions in particular. It can be shown [6, 21, 22] that self-organized criticality (SOC), which is a property of dynamical systems that have a critical point as an attractor, can give rise to power-law dependencies in critical phenomena. SOC is of course not the only possible cause of the appearance of scaling laws in nature, but studying scaling laws is always important because, as G.I. Barenblatt says in his remarkable monograph [9], they never appear by accident. They may e.g. appear when the ratio $l/L$ of two dominant length scales $l$ and $L$ of a problem vanishes, so that any variation of properties of the problem at an intermediate scale $x (l << x << L)$ can only be of power-law form in $x$.

The size effect in fracture is in decreasing of the sample strength with increasing sample size. The simplest explanation for this phenomenon would be: the larger the sample, the larger the probability of finding a defect, and therefore the smaller the critical strain. This explanation is related to what nowadays is called the "statistical size effect". In 1939 Weibull was the first to apply statistics in order to give this type of size effect a formal description [12, 75]. He discovered the importance of having a correct representation for the distribution of strengths of small material elements, in particular in the range of very low strength. Weibull introduced a function especially for this purpose, which is now known as the Weibull distribution (already mentioned in Section 2.1.2 of the present chapter). Most statistical theories of size effects that appeared later on were based on Weibull’s concept.

There is also a size effect (often called "deterministic") caused by strong gradients of the stress field near defects [12, 11]. It is not easy to clearly distinguish between the two size effects both in experiments and simulations.

We have already mentioned in Chapter 1 another example of an experimental observation of scaling in fracture - the scaling of crack roughness. This is the dependence between the roughness $\Delta h$ of a crack surface and the size $d$ of the window over which it is calculated:

$$\Delta h \propto d^\zeta. \quad (2.25)$$

The roughness itself is defined as the averaged maximum height variation according to the following formula:

$$\Delta h = \langle \max(h(y_1) - h(y_2); \ y_1, y_2 \in [y_0, y_0 + d]) \rangle_{y_0}. \quad (2.26)$$

where $y$ is the coordinate along the average crack-propagation direction and $h(y)$ is the height of the crack profile (Fig. 1.1). The definition (2.26) of roughness via height variation is only one of a few existing ways, among which the
2.2. Scaling, fractals and self-affinity

Figure 2.5: Three division steps of generating the Sierpinski gasket

"box-counting method", "divider method", "method of return probability" and "power-spectrum method" can be named as frequently used ones (see [69] for the definitions of these methods).

2.2.2 Fractals and self-affinity

The concept of space dimension was introduced by Euclid as the number of independent directions, which can take only positive integer values. A line (or curve) has dimension 1, a plane (or surface) has dimension 2 and our space has dimension 3. The formal definition was only formulated in 1913 by the Dutch mathematician L. Brouwer [16, 3]. This definition is constructed inductively as follows. The empty set is assigned dimension $-1$. Assuming that the spaces of dimension $\leq n$, and hence their subsets, have been defined, one says that a space $X$ has dimension $\leq n + 1$ if between any two disjoint closed sets $A$ and $B$ of $X$ there is a partition $P$ of dimension $\leq n$. Here a partition between two sets $A$ and $B$ in a space $X$ is a closed subset $P$ of this space such that the complement $X \setminus P$ is the sum of two disjoint open sets $C$ and $D$, one of which contains $A$ and the other one $B$.

Dimension can be generalized in such a way that it can also take fractional values and describe non-Euclidean shapes. Such shapes received a special name “fractal” owing to Mandelbrot [47, 72]. Initially the concept “fractal” was defined to describe a geometrical object with a complex shape that can be subdivided into parts, each of which is a replica in shape (exactly or approximately) of the whole. The Sierpinski gasket (Fig. 2.5) is a very popular example of an exact fractal. It is obtained from an equilateral triangle. At the first division step the initial triangle is halved in size and reproduced twice in such a way that all three obtained triangles touch each other and form one triangle equal to the very initial one. At the second step the process is repeated for every triangle of the step one, and so on. This process is unlimited in the sense that it continues down to any arbitrarily small scale.

Scaling of the weight-measure $M$ with the resolution $\epsilon$ at which it is estimated and with its length $L$ can for any geometrical object be written in the
form of
\[ M \propto \epsilon^D \left( \frac{L}{\epsilon} \right)^{D_f}, \]  
(2.27)

where \( D \) is the topological dimension and \( D_f \) is the so-called fractal dimension. For Euclidean shapes \( D \) equals \( D_f \) and the scale dependence of the weight measure disappears. A fractal object, in contrast to Euclidean shapes, has a fractional value of \( D_f \). The fractal dimension can be defined in a somewhat distinct way as

\[ D_f = \frac{\log \text{[number of self-similar pieces]}}{\log \text{[linear size magnification factor]}}. \]  
(2.28)

The fractal dimension \( D_f \) of the Sierpinski gasket will be \( \frac{\log 3}{\log 2} \approx 1.58 \) because at every step the number of triangles is multiplied by 3 while the length is changed by factor 2. Physically, the fractal dimension shows how densely a fractal object fills space.

A fractal is geometrically similar to itself at different scales. This self-similarity can be defined not only for a geometrical shape but also for any quantity, function or functional \( F \) in the following way

\[ F(kx) = k^{1/\alpha} F(x), \]  
(2.29)

where \( x \) is length (distance), \( k \) defines the scale change and \( \alpha \) is a scaling exponent. This expression (2.29) can be generalized to the one which defines self-affinity if the scaling relation is direction-dependent:

\[ F(k_x x, k_y y) = k_x^{1/\alpha_x} k_y^{1/\alpha_y} F(x, y), \]  
(2.30)

where \( x \) and \( y \) stand for coordinates in different directions [48]. The self-affinity of a fracture surface implies therefore that

\[ \Delta h(k_x x, k_y y) = k_x^{1/\zeta_x} k_y^{1/\zeta_y} \Delta h(x, y), \]  
(2.31)

where \( \Delta h \) is the height variation and \( x, y \) stand for coordinates along and across the crack-propagation direction respectively. In applications to real phenomena, and very often in theories, self-similarity (2.29) as well as self-affinity (2.30) are followed not exactly but statistically. A statistical definition of self-similarity via the concept of a singularity strength can be found in [30].

### 2.3 Random-percolation theory

Random percolation is one of the simplest models of a disordered medium. Consider a square lattice (Fig. 2.6-a) in which each site is occupied with probability \( p \) or otherwise empty (with probability \( 1 - p \)). Neighboring occupied sites
are supposed to be connected. If $p = 0$, there will be no occupied and therefore no connected sites in the lattice. Thus, two opposite sides of the lattice will be isolated from each other. Another extreme with $p = 1$ will ensure that every site is occupied and the opposite sides will be connected. In any situation in between the two extremes, connected occupied sites will form clusters, i.e. isolated aggregations. The main concept of random percolation theory is the existence of a so-called percolation threshold. The percolation threshold (usually denoted as $p_c$) is the value of the occupation probability $p$ at which a cluster of connected sites spanning from one side of the lattice to another, first appears. This means that below $p_c$ there is no spanning cluster in an infinite lattice and there is at least one spanning cluster above $p_c$. This description refers to "site percolation". "Bond percolation" is conceptually the same, with the one exception that bonds (occupied or empty, connected or disconnected) are considered instead of sites (Fig. 2.6-b).

Random percolation can be interpreted physically in many ways. If each bond represents a simple conductor, the lattice will be an isolator below $p_c$ and conductor above $p_c$. Generally speaking, the percolation concept is applicable for the description of various transport problems in disordered media. However its applicability for describing fracture as the appearance of a sample-spanning damage cluster is not clear due to the presence of long-range interactions typical for materials deformation and failure. The most important result of random percolation theory is the universal scaling of certain quantities related to cluster statistical properties in the vicinity of the percolation threshold.

In the remaining part of this paragraph we will briefly describe the main concepts and results of percolation theory, mostly following [73], which is a very nice introductory book on the topic. More detailed and mathematical de-
Let $s$ denote the cluster size, i.e. the number of sites in a cluster (single occupied sites are also clusters, of size 1). Note that from here on we will consider the case of site percolation without any loss of generality since the logic and results remain the same for bond percolation. We can define then the distribution $n_s$ of cluster size as the number of $s$-clusters (clusters of size $s$) divided by the total number of sites in a lattice. For the simplest case, which is percolation in one dimension (Fig. 2.7), exact formulas can be easily obtained. The probability for one arbitrary site to be occupied is $p$, for two arbitrary sites it is $p^2$, it is $p^3$ for three and so on. Apparently it is $p^s$ for $s$ sites. Each of the two ends of a cluster should face an empty site, and a site is empty with probability $(1 - p)$. Thus, the expression for $n_s$ can be obtained as the probability of a site to be the left end of a $s$-cluster:

$$n_s = p^s(1 - p)^2.$$  

The probability that a site (occupied or not) belongs to an $s$-cluster is then

$$P_s = n_s s.$$  

A site cannot be occupied without being a part of some cluster. Therefore the probability for an arbitrary site to be a part of a cluster is equal to the occupation probability $p$:

$$\sum_{s=1}^{\infty} n_s s = p.$$  

This sum is exactly the first moment $M_1$ of the cluster-size distribution. Here and further “infinite” clusters are excluded from the statistics in order to avoid the situation when (2.34) becomes undefined. We will also omit explicit summation limits, always assuming that sums are from 1 to $\infty$. The probability $\tilde{P}$ that an arbitrary occupied site belongs to a cluster of size $s$ can be expressed as

$$\tilde{P} = \frac{n_s s}{\sum_s n_s s}.$$  

The average size $S$ of the cluster to which an arbitrary occupied site belongs is defined as

$$S = \sum_s \tilde{P} s = \frac{\sum_s n_s s^2}{\sum_s n_s s} = \frac{M_2}{M_1}.$$
2.3. Random-percolation theory

where $M_2 = \sum s_n s^2$ is the second moment of the cluster-size distribution. It can be shown for the 1D case that

$$S = \frac{1 + p}{1 - p}, \quad (p < p_c).$$

(2.37)

This means that the average cluster size together with the second moment $M_2$ algebraically diverges on approaching $p_c$, with $p_c = 1$ in one dimension. Similar results (average cluster size diverging as $1/(p_c - p)$) can be obtained exactly for another special case - percolation on a Bethe lattice (or Cayley tree). Unfortunately there is no exact solution for the cluster-size distribution in other cases. Nevertheless, it is possible to obtain some interesting results using reasonable assumptions and generalizations.

The main assumption is in a universal scaling of the cluster-size distribution for large clusters ($s \to \infty$) for $p$ approaching $p_c$ from below. The scaling is assumed to have the following form

$$n_s(p) = s^{-\tau} f(s^\sigma (p - p_c)),$$

(2.38)

where $f$ is a scaling function which is not universal and needs to be defined numerically. This scaling law leads to the following formula for the asymptotic (for $p \to p_c, p < p_c$) behavior of the average cluster size

$$S \propto M_2 \propto |p - p_c|^{-\gamma},$$

(2.39)

where $\gamma = \frac{3 - \tau}{\sigma}$. In general, the scaling for any $n$-th moment of the cluster-size distribution ($n \geq 2$) becomes

$$M_n = \sum_s s^n n_s \propto |p - p_c|^{(\tau - n - 1)/\sigma}.$$  

(2.40)

The probability $P$ for a site to belong to an infinite cluster above $p_c$ also scales with $|p - p_c|$ in a similar way:

$$P \propto |p - p_c|^\beta, \quad p > p_c, \quad \beta = \frac{\tau - 2}{\sigma}. $$

(2.41)

So far we have been describing clusters in terms of their numbers of sites but studying their spatial extent and topology are no less important. The geometry of a cluster can be defined via the so-called "gyration radius" - a quantity inherited from polymer physics where it is used for description the geometry of polymer chains. For a cluster of size $s$ the gyration radius is defined as

$$\rho_s = \sum_{i=1}^s \frac{(r_i - r_{cm})^2}{s},$$

(2.42)
where \( \mathbf{r}_i \) is a vector defining the position of the \( i \)-th site and \( \mathbf{r}_{cm} \) defines the position of the center of mass of the cluster:

\[
\mathbf{r}_{cm} = \frac{1}{s} \sum_{i=1}^{s} \mathbf{r}_i. \tag{2.43}
\]

The average squared gyration radius \( R_s^2 \), shows the average spatial extent of clusters of one particular size \( s \):

\[
R_s^2 = \left\langle \frac{1}{s} \sum_{i=1}^{s} |\mathbf{r}_i - \mathbf{r}_{cm}|^2 \right\rangle_{\text{(all } s\text{-clusters)}}. \tag{2.44}
\]

This average gyration radius can be easily related to the average distance between two sites of a cluster:

\[
2R_s^2 = \left\langle \frac{1}{s} \sum_{ij} (\mathbf{r}_i - \mathbf{r}_j)^2 \right\rangle_{\text{(all } s\text{-clusters)}}. \tag{2.45}
\]

The correlation length \( \xi \) is the average distance between two sites of the same cluster calculated over clusters of all sizes \( s \). Since the probability for a site to belong to an \( s \)-cluster is \( n_s/s \) and this site is connected to \( s \) sites including itself within this cluster, the distances should be averaged with weight \( n_s/s^2 \) and normalized by \( \sum_s n_s/s^2 \):

\[
\xi^2 = \frac{2 \sum_s R_s^2 n_s s^2}{\sum_s n_s s^2}. \tag{2.46}
\]

The correlation length also diverges algebraically approaching the percolation threshold \( p_c \) from below, similar to the average cluster size

\[
\xi \propto |p - p_c|^{-\nu}. \tag{2.47}
\]

It is this divergence of the average cluster size (\( \propto M_2 \), compared to the primary particle) and cluster extent (\( \propto \xi \), compared to the lattice-cell dimension) which leads to scaling laws near \( p_c \). The maximum cluster at the percolation threshold is expected to behave as a fractal, i.e. to have a power-law relation between its "weight" which is \( s \) and its spatial size which is \( R_s \):

\[
s \propto R_s^{D_f}, \tag{2.48}
\]

where \( D_f \) is obviously called "fractal dimension". Substituting (2.48) into (2.46) leads to

\[
\xi^2 \propto \frac{\sum_s n_s s^{2+2/D_f}}{\sum_s n_s s^2} \propto \frac{M_2 s^{2+2/D_f}}{M_2}. \tag{2.49}
\]
Recalling the scaling expressions (2.40) for the moments of the cluster-size distribution and the one for the correlation length (2.47) one can obtain the relation between $D_f$ and the other exponents:

$$D_f = \frac{1}{\sigma \nu}.$$ (2.50)

The scaling relations (2.39-2.41) and (2.47), and the corresponding exponents are "universal" in the sense that they do not depend on the topological details of the lattice. For two dimensions ($D = 2$) one exactly has $\gamma = 43/18$, $\nu = 4/3$, $D_f = 91/48$, $\tau = 187/91$; for $D = 3$ the numerical values are $\gamma = 1.80$, $\nu = 0.88$, $D_f = 2.53$, $\tau = 2.18$. Contrary to the scaling exponents, the percolation threshold $p_c$ is not a universal quantity.

All the above results are obtained with the assumption that the lattice is infinite, i.e. has no boundaries. The results are still valid for lattices with finite size if the correlation length $\xi$ remains significantly smaller than the lattice size $L$. If not, a finite-size correction in the form of an extra proportionality factor should be added to all scaling expressions. In other words, if some quantity $A$ is found to scale as $|p - p_c|^{-\alpha}$ for an infinite lattice (or for $\xi << L$), for a finite-size lattice the scaling expression changes to

$$A \propto |p - p_c|^{-\alpha} \theta\left(\frac{L}{\xi}\right).$$ (2.51)

As a result of the finite-size effect, the effective percolation threshold $p_{\text{eff}}$, i.e. the one of a finite lattice, differs from $p_c$ for an infinite lattice. By identifying $p_c$ and $p_{\text{eff}}$ when $L = \xi$ it follows that $p_{\text{eff}}$ approaches $p_c$ according to the following law

$$p_c - p_{\text{eff}} \propto L^{-1/\nu}.$$ (2.52)

We must mention here that there is another type of percolation problem, namely "rigidity percolation", that is sometimes used in the context of fracture modelling [52]. In this problem simple connectivity is not enough for a site (or bond) to be a part of a cluster. Instead, the property of rigidity is used. This means that only rigid clusters are taken into consideration. Consequently, the rigidity-percolation problem belongs to a different universality class than the ordinary percolation.

### 2.4 Self-organized criticality

"Self-organized criticality" is a rather broad term which is not defined very precisely. Generally speaking, this term is applicable to almost any complex dynamical system that experiences critical behavior and shows some self-organization. In the broadest sense SOC can be defined as spontaneous organization of a complex system consisting of many interacting parts that is driven to a
2. Theoretical background

Figure 2.8: SOC example of a one-dimensional (axially symmetric) sandpile model according to [7] with the critical slope $Z_c = 3$

critical point. The latter may be dynamical but must be a stationary state [72]. This phenomenon is typically accompanied by self-similar statistics of event sizes and self-similar geometrical patterns.

The term "critical point" refers to such a state at which the correlation length becomes infinite in the infinite-size limit. The term "spontaneous organization" means that the organization process is uncontrolled, although it does not need to be totally uncorrelated.

SOC was first introduced by Bak, Tang and Wiesenfeld [6, 7] in their works on so-called $1/f$ noise. They used a very illustrative example of a sandpile. A one-dimensional (axially symmetric) sandpile is formed on a horizontal circular plate (Fig. 2.8). The initial distribution of sand grains can be arbitrary. The boundary of the plate (right boundary in Fig. 2.8) can be open (sand can leave the plate) or closed (it can not). Columns of sand are characterized by number $n$, height $h_n$, and ensuing slope (height difference) $z_n = h_n - h_{n+1}$. At each step a sand grain is added to a randomly chosen column. If the height difference $z_n$ of some column reaches the critical value $Z_c$ this column drops a grain to the following column. Each grain added to the system can trigger zero, one or a few toppling events, i.e. avalanches. This model can be easily generalized to arbitrary dimensions and other underlying physics. The authors of [6, 7] show by simulations and argued theoretically that the sand-pile system has a power-law scaling of the distribution of avalanche sizes and avalanche lifetimes, which means that the process has no characteristic length or time scale.

The concept of self-organized criticality was defined as a general framework for explanation of the frequently observed power laws in physical phenomena. Many systems can be described or attempted to be described by SOC. To be a good candidate a system should contain many interacting units, be capable of ordered pattern formation, have a critical point, and be able to drive itself to
the critical point and maintain this state. SOC has been successful in describing such phenomena as $1/f$ noise, earthquakes, fluctuations in economic systems, forest fires, epidemics. It can possibly be used in the description of fracture, which in principle satisfies the mentioned criteria.

Fracture can be studied in terms of SOC in various ways. An approach based on the so-called fiber-bundle model (FBM) [32, 79] is a serious simplification of fracture since it represents a material by a set of parallel bonds; however, it allows to establish basic ideas which can be elaborated further. Random-fuse models (RFM) are more realistic and allow to study fracture by means of simulation, or analytically in the mean-field limit [80, 79].

In order to apply SOC to fracture we need to define an order parameter and a driving variable. In the present study the former is damage ($\rho$ in our notation) while the latter can be stress $\sigma$ or strain $\varepsilon$. It is more convenient to use stress as a driving parameter for a description of a fracturing system in terms of SOC even if the system is strain-driven. The point where stress reaches its maximum is a critical point for such systems. For systems with a brittle response this is the point when stress starts to decrease rapidly due to a catastrophic overall failure. It can be named yield point for systems with a plastic type of response following the (quasi-) elastic regime, though this is not how yield stress is defined in structural mechanics.

On approach of the critical point $\sigma_c$ the damage growth accelerates, i.e. $\frac{d\rho}{d\sigma}$ becomes a diverging function of $|\sigma - \sigma_c|$. Microscopically the failure process can be studied via the statistics of avalanches. An avalanche is then a sequence of breaking events that happen at the same value of strain (if a system is strain-driven) or stress (in the case of a stress-driven system).

Since the essence of self-similarity in SOC is the absence of scale, we can assume that within a given small stress increment $(\sigma, \sigma + \Delta\sigma)$ the induced avalanches will have a power-law distribution of sizes (by size we mean the number of single fracture events) $a$; however, this will only hold up to an upper cut-off size $a^{*}$ that depends on $\sigma$ and that diverges in the limit $\sigma \to \sigma_c$. As $a^{*}$ is itself the only relevant scale beyond a primary scale $a_0$, this divergence should follow a power-law in $|\sigma - \sigma_c|$. For convenience, we will describe the statistics of avalanches in a continuum approximation (pretending that $a$ as well as the number of avalanches are not integer but continuous quantities).

Let $\Phi(\sigma)$ be the total number of avalanches up to a certain stress $\sigma$. An infinitely small stress increment $d\sigma$ will then correspond to an increment of the number of avalanches $d\Phi$. Due to the absence of scale all avalanches within $d\sigma$ are distributed according to the following size distribution:

$$n_a(\sigma) = \left( \frac{a}{a_0} \right)^{-\gamma} f\left( \frac{a}{a^*(\sigma)} \right).$$  \hspace{1cm} (2.53)

This means that the number of avalanches of size $a$ within the interval $d\sigma$ equals $n_a(\sigma)d\Phi(\sigma)$. In equation (2.53) $a$ is the avalanche size, $f(x)$ is a cut-off function
and \( a^*(\sigma) \) is the cut-off which algebraically diverges on approach of \( \sigma_c \):

\[
a^*(\sigma) = a_0|\sigma - \sigma_c|^{-1/\delta} .
\]

The exponents \( \gamma \) and \( \delta \) in equations (2.53, 2.54) are critical exponents. The cut-off function \( f(x) \) satisfies:

\[
f(x) = \text{const, } x \ll 1, \\
f(x) \to 0, x \gg 1.
\]

Note the similarity with the scaling (2.38) of percolation theory, which is alike in logic. However, the variable \( a \) and the critical exponents \( \gamma, \delta \) should not be confused with the corresponding ones of percolation theory.

A few relevant results following from the form of the avalanche-size distribution can be derived analytically. The \( m \)-th moment of distribution (2.53) can be calculated as follows:

\[
< a^m > = \int a^m f(a/a^*) da = a^* m - \gamma + 1 \int x^{m-\gamma} f(x) dx \propto a^* m - \gamma + 1 .
\]

For the existence of all moments of the distribution starting from order 1 the convergence of the integral in (2.56) would be required. Then, the scaling exponent of the distribution should satisfy \( \gamma < 2 \). The boundedness of the integrand at \( x = \infty \) is also required.

Equations (2.54) and (2.56) result in the following scaling expression for the \( m \)-th moment of the avalanche-size distributions:

\[
< a^m > \propto a^* m + 1 - \gamma \propto |\sigma - \sigma_c|^{-m+1-\gamma} .
\]

Since the number of avalanches of size \( a \) within \( d\sigma \) is \( n_a(\sigma) d\Phi(\sigma) \), the unnormalized cumulative avalanche-size distribution (the total number of avalanches of a certain size \( a \)) over the range from zero to a certain stress \( \sigma \) is obviously calculated as

\[
C_a(\sigma) = \int_0^\sigma n_a(\tilde{\sigma}) \frac{d\Phi(\tilde{\sigma})}{d\tilde{\sigma}} d\tilde{\sigma} = \int_0^\sigma n_a(\tilde{\sigma}) \phi(\tilde{\sigma}) d\tilde{\sigma} ,
\]

where \( \phi(\sigma) \equiv d\Phi(\sigma)/d\sigma \). As follows from (2.53), \( C_a(\sigma) \) can be further expressed as:

\[
C_a(\sigma) = \left( \frac{a}{a_0} \right)^{-\gamma} \int_0^\sigma f(a/a^*(\tilde{\sigma})) \phi(\tilde{\sigma}) d\tilde{\sigma} .
\]

By introducing the new variable \( y = a/a^* \) and using equation (2.54) the expression for the cumulative distribution can be rewritten as

\[
C_a(\sigma) = \delta \sigma_c \left( \frac{a}{a_0} \right)^{-\gamma - \delta} \int_{a/a^*(\sigma)}^{a/a_0} f(y) \phi(\sigma(y)) y^{\delta-1} dy .
\]
If $a_0 \ll a \ll a^*(\sigma)$, the cumulative distribution will behave as a pure power law. If $a \gg a^*(\sigma)$, then $y$ lies in the range $\gg 1$ which is exactly the range where the cut-off function $f$ operates. Consequently, the integral in (2.60) vanishes for $a \gg a^*(\sigma)$. Hence, the cumulative distribution can be written in the following general form:

\[ C_a(\sigma) = \left( \frac{a}{a_0} \right)^{-\tau} G(a/a^*(\sigma)) \]  

(2.61)

where $\tau = \gamma + \delta$ and $G$ is a cut-off function for the cumulative distribution. Here an assumption is made that the integral in (2.60) with function $f$ leads to a function $G$ with similar properties. The normalized cumulative distribution will have the following form:

\[ c_a(\sigma) = C_a(\sigma)/\Phi(\sigma), \]  

(2.62)

Now we need to make a connection between the avalanche statistics and the damage. The damage $dp$ developed per infinitely small stress interval $d\sigma$ is

\[ dp = d\Phi(\sigma) \int an_a(\sigma)da = \phi(\sigma)d\sigma < a >. \]  

(2.63)

Consequently, the damage rate $dp/d\sigma$ can be related to the avalanche statistics in the following form:

\[ \frac{dp}{d\sigma} = \phi(\sigma) < a > \propto \phi(\sigma)|\sigma - \sigma_c|^{-\frac{2-\gamma}{\delta}}, \]  

(2.64)

with $\gamma < 2$ as mentioned earlier. If $\phi(\sigma)$ is assumed to be constant, the expression for the damage rate simplifies to

\[ \frac{dp}{d\sigma} \propto |\sigma - \sigma_c|^{-\frac{2-\gamma}{\delta}}. \]  

(2.65)

Generally speaking, the above formulas are derived for infinite systems. As commonly proposed in literature and used in [79], the finite-size effect manifests itself via the following modification of equation (2.54):

\[ a^*(\sigma) = \frac{a_0}{|\sigma - \sigma_c|^{1/\delta} + C L^{-D_f}}, \]  

(2.66)

where $L$ is the system size, $D_f$ is the avalanche fractal dimension and $C$ is an arbitrary constant. The interpretation is that on approach of the critical point the increasing avalanches will ultimately be limited by the sample size, rather than by an internal mechanism. The scaling expression (2.66) for $a^*$ with a finite-size correction will also influence the equations (2.64, 2.65) for the damage rate.
2. Theoretical background

2.5 Lattice models

Over the last decades rather significant efforts have been made in the field of simulating fracture with lattice models [5, 17, 18, 31, 33, 53, 54, 63, 64, 65, 66, 67]. Initially this approach has been applied much to "fuse networks" - networks of resistors that are able to burn out at a certain critical load. This implies that the vectorial problem (solving a displacement field) has been replaced by a scalar one (solving a potential field). The main focus of this research has been on such phenomena as: threshold scaling, influence of the distribution of local failure properties on macroscopic behavior, and scaling of the damage-profile roughness. In most of the works fracture has been interpreted in terms of damage percolation. This approach has been based on a few important commonalities between the two phenomena. First of all, fracture of fuse networks and random percolation have one common object - the lattice. Secondly, disorder plays an important role for both, being an essential ingredient of fracture and the only driving force in random percolation. Scaling is the third common feature. In fracture experiments size scaling is observed for material strength and crack roughness. Percolation theory also reveals an intrinsic size effect. The internal structure of a large but finite cluster on a larger lattice shows self-similarity, and will become a percolating cluster when the lattice size decreases.

The fracture of lattices with moderate disorder or uniformly distributed properties is of course a highly correlated process, different from random percolation. However, the process of damage accumulation becomes less correlated with increasing disorder, and in the limit of infinite disorder the scalar problem can be mapped onto a percolation problem [62]. Still it is not clear to what extent strong, but finite disorder is able to make fracture statistically similar to percolation. It is equally unclear to what extent the arguments of [62] can be extended to damage percolation in the vectorial problem. If the answers are "yes", it opens a way for percolation-theory arguments to be applied to fracture. If it is not the case, then another understanding of the underlying physics is needed.

When the extension is made from local fuses to local mechanical elements, a number of options arise. A few studies have considered central-force spring networks [5, 54], while others have included angular or bond-bending forces as well [33, 66]. Results may differ, certainly in detail, and no consistent overall picture is available. In this thesis we limit ourselves to central-force spring networks.

One option that definitely leads to different results is whether or not to describe the fracture process in terms of loss of rigidity rather than percolation of damage. It has in particular been shown that rigidity percolation is in a different universality class than random percolation, and that the rigid part of a cluster (and even more so the stress-bearing part) is widely different from the cluster itself [52]. In this thesis we always consider damage patterns, not rigidity patterns.
A comparison between random percolation and fracture was already made in [65] on random 2D triangular lattices with central- and bond-bending forces and power-law disorder (see also [66, 5] for more details). Based on a graphical representation of the force distributions in the network it was concluded that only the initial damage development compared well with random percolation; the range over which this extended was observed to be significant only for strong disorder (a strong tail of very weak bonds), but to end well before the maximum in the curve of macroscopic stress vs strain.

A detailed study for 2D central-force lattices [31] has led to the view that for a very strong, but finite, power-law disorder, fuse networks behave similar to percolating systems. For this special case fracture was found to belong to the same universality class as random percolation, and the exponent for threshold scaling coincided with percolation-theory predictions. However, the trend of the threshold scaling observed in [31] is different from random percolation: the rupture threshold decreases as the lattice size grows. In [31], even the exponent \( \zeta \) for the scaling of crack roughness has been calculated, on the basis of percolation in a gradient, and was found to agree well with limited data on 2D systems.

The point of view of [31] has met rather serious opposition in [53]. In that work authors have also investigated fuse networks, but for a much larger size range, and significant deviations from the results of [31] and therefore from random-percolation theory, have been found. At the last fracture stage the authors have found localization in a form different from the observations of [31]; they analyzed it in terms unrelated to percolation theory and demonstrated an accurate size scaling of the avalanche-like final breakdown event. The similarity to percolation was observed in [53] only at the early stage of the fracture process, but was not studied at the microscopic level or quantitatively confirmed. The two stages were believed to be separated by the maximum-stress point in the stress-strain curve and treated as unrelated.

As stated, mechanical deformation and therefore fracture of materials has a vectorial nature (it is described by a vectorial displacement field), while fuse-network simulations are based on conduction of current, which is described by a scalar potential field. In terms of lattice models it implies that each node (i.e. discretization point) has (in 2D) two degrees of freedom in the case of mechanical deformation and only one degree of freedom in the case of current conduction. Related to this, the central-force spring lattice allows for changes of its geometry during the deformation process, while in fuse-network simulations the geometry remains fixed. All mentioned features of the 2D central-force spring lattice imply that it should be a better model for deformation and fracture.

Very recently, the authors of [53] repeated their study also for 2D spring networks [54], although this time only for uniform disorder in the threshold distribution. Their conclusion is that with regard to the pattern of damage evolution and final fracture there are no essential differences between fuse- and spring
networks. But again, as in [53], no microscopic analysis of the percolation-like damage up to the point of maximum stress was attempted.

There is an ongoing discussion in literature on the comparison of finite element methods and lattice models [39, 68, 17, 18]. The main observed disadvantages of lattice models are mesh dependence and problems with modelling uniform stress. They indeed can be of concern if a homogeneous continuum is represented by a lattice, but in the case of a highly heterogeneous medium they are not an issue. We would like to note a conclusion which can be drawn from this discussion: finite elements are preferable if a continuum, with whatever properties, is modelled; lattice models should be preferred if heterogeneous microstructure is to be taken into account.


Chapter 3

Computational models

The simulation scheme which we follow in the present research is the following. We first generate a spring network with a random geometry and locally varying properties, then run two types of simulation. The first one is an iterative simulation of deformation and failure under tension. The second one is a simulation of random percolation of increasing damage, without external load.

3.1 Lattice model for deformation and failure

In our study we consider 2D and 3D lattices of central-force springs. The geometry of the lattice is random and is built as a Delaunay tessellation of a square region with randomly distributed nodes (Fig. 3.1). This tessellation is a set of lines connecting each node to its natural neighbors in such a way that no point is inside the circumcircle (circumsphere) of any triangle (simplex), see e.g. [61]. Note that the average coordination number of an infinite two-dimensional Delaunay tessellation is always 6, while the local number may vary from 3 to infinity; due to the boundaries our average coordination number (in 2D) is not exactly equal but is very close to 6, ensuring mechanical rigidity of the intact network. Although there is no exact result for the average coordination number of a Delaunay tessellation in three dimensions, it is known that it should be close to 14. Indeed, we obtain a coordination number very close to 14 for the 3D lattices that we use.

Equations of mechanical equilibrium for the lattice can be obtained from the minimization of the total potential energy of the system similar to the continuum case (2.5) and the way it is done in the finite-element method [26, 81, 20]. The energy of elastic deformation of the lattice is

\[ E = \frac{1}{2} \sum_{v[i,j]} (K_{ij}(u_j - u_i) \cdot e_{ij})^2 - \sum_{v_i} u_i \cdot f_i, \]
3. Computational models

Figure 3.1: Example of a two-dimensional (a) and three-dimensional (b) Delaunay-tessellation lattice as used in the simulations

where \( i, j \) are nodes, \( u_j, u_i \) are corresponding nodal displacements, \( e_{ij} \) is the unit vector directed from \( i \) to \( j \), \([i, j]\) denotes pairs of nodes connected by bonds, \( \kappa_{ij} \) is the stiffness of the bond connecting nodes \( i \) and \( j \), and \( f \) represents all external loads translated into nodal body forces. Expression (3.1) can be rewritten in a matrix form following the finite-element methodology:

\[
E = \frac{1}{2} U^T \kappa U - U^T F, \tag{3.2}
\]

where \( U = [u_1, u_2, ..., u_n]^T \) is the displacement vector (1 × \( n \) matrix) containing all degrees of freedom, \( \kappa \) is the stiffness matrix with \( n \times n \) elements and \( F \) is the vector (1 × \( n \) matrix) of nodal forces. Minimization of \( E \) leads to a system of linear equations

\[
\kappa U = F, \tag{3.3}
\]

which should, together with appropriate boundary conditions, lead to a unique solution. In this work we use two types of boundary conditions: "busbars" and periodic. In the first case a uniaxial tensile strain is imposed by means of two rigid busbars at the left and right sides of the lattice, while the upper and lower boundaries remain free. For the two-dimensional case the boundary conditions are formulated as

\[
u_x(0, y) = 0, \ u_x(1, y) = U_x, \ u_x(0, 0) = u_y(0, 0) = 0, \tag{3.4}\]

where \( u_x, u_y \) are the displacements along \( x \) and \( y \) axes respectively, with coordinates \( x, y \) each in the unit interval \( (0,1) \), and where \( U_x \) is the prescribed
displacement. In three dimensions the conditions look similar:

\begin{align}
&u_x(0, y, z) = 0, \quad u_x(1, y, z) = U_x, \\
&u_y(0, 0, 0) = u_y(0, 0, 1) = u_y(1, 0, 1) = u_y(1, 0, 0) = 0, \\
&u_z(0, 0, 0) = u_z(1, 0, 0) = 0.
\end{align}

The busbars constraints are incorporated into (3.3) by standard elimination of the prescribed degrees of freedom.

In the second (periodic) case the strain is applied to the lattice via imposing equal relative displacement to the opposite nodes at the left and right sides of the lattice. The opposite nodes of the upper and lower sides are also restricted to have equal relative displacement, which is defined by the solution as an independent degree of freedom. For a 2D lattice these boundary conditions look as follows:

\begin{align}
&u_x(1, y) - u_x(0, y) = U_x, \quad u_y(x, 1) - u_y(x, 0) = U_y, \quad u_x(x, 1) = u_x(x, 0), \\
&u_y(0, 0) = u_y(0, 0) = 0,
\end{align}

where \(u_x, u_y\) are again the displacements along \(x\) and \(y\) axes, \(U_x\) is the prescribed horizontal displacement and \(U_y\) is the vertical displacement, which remains an independent degree of freedom. In this case the shape of the deformed opposite sides (both in \(x\) and \(y\) directions) always stays identical, as if the lattice were wrapped around a torus. For the three-dimensional case the conditions are formulated similar to 2D:

\begin{align}
&u_x(1, y, z) - u_x(0, y, z) = U_x, \\
&u_y(x, 1, z) - u_y(x, 0, z) = U_y, \\
&u_z(x, y, 1) - u_z(x, y, 0) = U_z,
\end{align}

here \(U_x\) is prescribed while \(U_y\) and \(U_z\) are independent degrees of freedom. The most convenient way of implementing periodic constraints is the use of Lagrange multipliers. If the constraints are written in a matrix form:

\begin{equation}
CU - Q = 0,
\end{equation}

the minimized expression (3.2) can be modified in the following way:

\begin{equation}
E^* = \frac{1}{2}U^T KU - U^T F + L^T (CU - Q),
\end{equation}
This will result in the following system of linear equations:

\[
\begin{bmatrix}
    K & C^T \\
    C & 0
\end{bmatrix}
\begin{bmatrix}
    U \\
    L
\end{bmatrix}
=
\begin{bmatrix}
    F \\
    Q
\end{bmatrix}.
\]  

(3.10)

This type of loading (with periodic conditions) is used to eliminate the influence of boundaries.

Upon loading, each bond behaves first as an elastic spring and as a threshold strain is reached the bond breaks; it is then irreversibly removed from the lattice. The thresholds are random and are generated according to a certain distribution. We consider cases with different disorder in the local thresholds. The no-disorder case is the one in which all breakable bonds have equal thresholds. Other cases are described by the same threshold distribution

\[
P(t) = (1 - \alpha)w^{\alpha-1}t^{-\alpha}, \quad t \in [0, w],
\]

(3.11)

but with different values of disorder strength \(\alpha\). In the present work we take \(\alpha\) in the range from 0 to 0.75 (Fig. 3.2). Young's modulus is kept the same for all bonds. The case \(\alpha = 0\) corresponds to a uniform threshold distribution and represents so called "weak disorder". Positive values of \(\alpha\) give distributions with an algebraically diverging tail of very weak bonds. The disorder becomes stronger as \(\alpha\) comes closer to 1. The case of \(\alpha = 1\) provides infinite disorder or, in other words, a nonintegrable threshold distribution. We use the term
"strong disorder" for the 2D cases with $\alpha = 0.7$ and 0.75. Although the disorder would be stronger for $\alpha$ closer to 1, values around 0.7 provide a reasonable compromise whereby the disorder is strong enough, but the problem is still not computationally too demanding.

For simulating polymer-like behavior, which is presented in Chapter 8, we introduce into the model a certain fraction of bonds, denoted $1 - \beta$, that remain unbreakable, i.e. they have infinitely high thresholds. The existence of unbreakable bonds can be interpreted as an additional peak of threshold distribution at infinity.

A finite-element problem is formulated and solved for a given applied strain, i.e. a given set of boundary conditions, in order to determine the spring with the highest ratio of actual strain to threshold. If the highest ratio is larger than or equal to 1, the corresponding spring is removed from the lattice, the actual strain is adjusted according to the breaking event and the finite-element problem is solved again for the modified lattice, until no break events occur for the given boundary conditions. In this process the stiffness matrix is modified and the equations are resolved every time a spring breaks. Bonds are allowed to be broken only one by one. Removing the broken bond is done for calculational reasons by putting its stiffness equal to a very small positive value, i.e. to almost zero.

Technically the fracture part of our model is an iterative finite-element model, consisting of breakable central-force springs with random properties. The stiffness matrix is fully assembled and constrained according to boundary conditions only once (in the beginning) and after that it is only modified when any bond breaks. The obtained system of linear algebraic equations is solved as many times as breaking events occur until the boundary conditions are satisfied or the system falls apart.

Calculations are performed for a range of lattice sizes from $L = 12$ to $L = 200$ in 2D and from $L = 4$ to $L = 24$ in 3D. A set of samples is used for each lattice size (from 500 to 1, depending on size) in order to get sufficient statistical information. By lattice size we always mean the number of bonds per linear lattice side, while the actual width and height of the lattices remain equal to 1.

### 3.2 Lattice model for random percolation of damage

The lattices used for the simulation of random percolation are geometrically the same as the ones used for failure simulation. In the case of RP simulation, lattice bonds are randomly removed from the lattice one by one irrespective of thresholds they have in the case of failure. Thus only a reliable random-number generator is necessary. The result of this simulation is nothing more than a random sequence of removed bonds, without any correlation or under-
lying physics - except the hypothesis that under certain parameter choices local damage under load develops as a random process, due to very strong disorder.

3.3 Simulation output

As an input, our model uses the lattice geometry, properties of bonds (stiffness and threshold) and boundary conditions. The output of the model consists of the sequence of bonds as they break and nodal displacements at each iteration step. From these data the reaction forces (forces on constrained nodes) can be easily obtained. This, in turn, allows to obtain stress at each iteration step and to build a stress-strain relationship. However, not all points of this relationship have physical meaning. Consider the schematic representation of the original, "raw" stress-strain dependence (Fig. 3.3). The green line going through points 1, 2, 3, 4 contains all iterations. Apparently, the overall stiffness of the system (slopes of the dashed green lines) decreases at each iteration. It is possible to have a situation when a certain breaking event (like points 2, 3 of Fig. 3.3) correspond to less strain than the one of previous events. This is physically impossible since we model a displacement-driven deformation, which means that we apply and control displacement and the displacement is increased monotonically. To resolve this contradiction we assume that the macroscopic strain never decreases and "wrong" breaking events (like points 2, 3 of Fig. 3.3) happen at the same strain as has been already achieved due to those breaking events that occurred previously. This is a logical assumption if the system is modelled in
3.3. Simulation output

the quasi-static limit, i.e. if relaxation happens sooner than a new breaking event occurs. The original curve then needs to be modified in such a way that points 2 and 3 are ignored. That can be done in two ways: with or without a stress drop. In the former case a new point (point II) should be added and the resulting curve will go through the points I, II and III. In the latter case, the curve will go through the points I and III without the drop. The difference between the two options is not principal especially if stress-strain dependencies are averaged over many samples.
3. Computational models
Chapter 4

Pattern development in brittle fracture and random damage percolation

The main goal of the present chapter is to explore the origin of scaling in the brittle fracture of disordered materials with high disorder, and in particular the possible connection with, and deviations from, percolation theory. A connection with random percolation has been claimed [33, 31], but also disputed [53, 54, 45] in literature. In such a comparison, only theoretical predictions of percolation theory are usually involved [31, 53]. We performed numerical simulation of random percolation on the same lattices as used for fracture simulations, in order to see the detailed differences at all stages, so not only in the vicinity of the percolation threshold, where the behavior of percolating lattices can also be assumed from scaling theory.

The simulation scheme which we follow here is the following. We first generate a spring network with a random geometry and locally varying properties as described in Chapter 3, then run two types of simulation: the one of fracture and the one of random percolation (RP). After that the statistical analysis of results is performed. In Table 4.1 the statistics of the simulation runs is presented.

4.1 Methods for identifying random-percolation patterns

We obtain two types of results in our simulation: mechanical and statistical ones. The mechanical responses of the lattices (or stress-strain relationships)
are calculated directly and rather easily from the reaction forces. This is the analogue of data that would result from real fracture experiments. Statistical results of course require some processing. The methods we use in this paper to analyze them are mostly taken over from percolation theory [73, 28] and simulation.

From the macroscopic stress-strain curves we calculate two important properties: the survival probability $P_{\text{surv}}$ - the probability that a lattice survives (remains unbroken) at a certain density $p$ of broken (removed) bonds, and the critical strain $\varepsilon$ - the strain at which the stress reaches its maximum and the lattice starts breaking macroscopically. An effective threshold $p_{50}$ - the density at which 50% of lattices survive, can be obtained from $P_{\text{surv}}$.

By analyzing the damage patterns we identify clusters of connected broken (removed) bonds and calculate the following set of microscopic cluster properties as functions of $p$; we therein utilize the same notation as in Chapter 2 for the description of random-percolation ideas, but we will repeat a few formulas in order to have everything in one place.

The cluster-size distribution $n_s$ (the number of clusters of weight $s$ divided by the total number of sites in the lattice) describes the statistics of damage clusters. The average cluster size

$$S = \frac{M_2}{M_1} = \frac{\sum_s n_s s^2}{\sum_s n_s s},$$

shows how damage clusters grow ($M_1 = p$ and $M_2$ are the first and the second moment of the cluster-size distribution respectively).

The correlation length $\xi$, which is an average distance between two sites of the same cluster, is defined as

$$\xi^2 = \frac{2 \sum_s R_s^2 s^2 n_s}{\sum_s s^2 n_s},$$

<table>
<thead>
<tr>
<th>Linear lattice size $L$ (2D)</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>500</td>
</tr>
<tr>
<td>17</td>
<td>500</td>
</tr>
<tr>
<td>25</td>
<td>500</td>
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<td>35</td>
<td>150</td>
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<td>50</td>
<td>100</td>
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<td>70</td>
<td>30</td>
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<td>100</td>
<td>20</td>
</tr>
<tr>
<td>150</td>
<td>10</td>
</tr>
<tr>
<td>200</td>
<td>5</td>
</tr>
</tbody>
</table>
where $R_s$ is the average gyration radius defined by (2.44). Its dependence on $p$ demonstrates the spatial evolution of clusters. In order to identify possible anisotropy of the developing fracture pattern we also calculate longitudinal and transversal correlation lengths:

$$
\xi_\parallel^2 = \frac{2 \sum_s X_s^2 s^2 n_s}{\sum_s s^2 n_s}, \quad \xi_\perp^2 = \frac{2 \sum_s Y_s^2 s^2 n_s}{\sum_s s^2 n_s},
$$

(4.3)

where $X_s, Y_s$ are defined similar to the gyration radius as

$$
X_s^2 = \langle \sum_{i=1}^s |x_i - x_{cm}|^2 \rangle_{(all\ s-clusters)},
$$

$$
Y_s^2 = \langle \sum_{i=1}^s |y_i - y_{cm}|^2 \rangle_{(all\ s-clusters)},
$$

(4.4)

with $x_{cm}, y_{cm}$ denoting the coordinates of the cluster center of mass and $x_i, y_i$ being the coordinates of cluster nodes. From (4.3) a shape factor can be defined as

$$
\Phi = \frac{\xi_\perp - \xi_\parallel}{\xi_\perp + \xi_\parallel},
$$

(4.5)

quantifying the damage anisotropy. For calculating this measure we always use fixed axes which are linked to the direction of load and then average the axial components of the correlation length separately. Therefore the shape factor should be equal to zero for random percolation of damage. This is different from the non-zero anisotropy measure found in [25] for RP. The authors of this work used principal axes of clusters to detect their anisotropy. Then the averaging over all clusters was done with every cluster taken in its own principal coordinates.

**Figure 4.1:** A cluster of connected bonds (a) is split into four rigid clusters (red, blue, green and yellow in (b)) and dangling bonds (black in (b)) connecting them
In the case of random damage, percolation theory describes the large-scale statistics of the developing cluster distribution and cluster pattern, when local details in the underlying lattice become irrelevant. In particular it predicts then the following universal scaling laws for an infinite lattice in the vicinity of the percolation threshold $p_c$ [73, 28]:

\[ S \propto M_2 \propto |p - p_c|^{-\gamma}, \quad (4.6) \]

\[ \xi \propto |p - p_c|^{-\nu}, \quad (4.7) \]

\[ n_s \propto p s^{-\tau} f(s^{3-\tau}/S), \quad (4.8) \]

\[ R_s \propto s^{D_f}, \quad (4.9) \]

where $f$ is a scaling function and where the exponents take universal values depending only on dimension $D$. Due to the scaling the exponents obey the following relations:

\[ \frac{D_f}{D} = \frac{1}{\tau - 1}; \quad \frac{\gamma}{\nu D} = \frac{3 - \tau}{\tau - 1}. \quad (4.10) \]

For $D = 2$ one has $\gamma = 43/18$, $\nu = 4/3$, $D_f = 91/48$, $\tau = 187/91$, while $p_c$ and all the proportionality factors depend on lattice details. The scaling function $f(z)$ should approach a constant for $z << 1$ and decrease to zero for $z >> 1$, expressing that $n_s(p)$ for large $p$ obeys power-law scaling up to a certain cut-off cluster size that diverges towards $p_c$.

In practice, of course, only finite-size lattices are considered. For a finite system size $L$, $\xi$ approaches the lattice size at an effective threshold $p_c(L) < p_c$ when a spanning cluster appears. For a series of finite-size samples $p_{50}$ is a natural estimate of the average threshold. Substituting $\xi = L, p = p_{50}$ into (4.7) results in the finite-size scaling relationship for the percolation threshold

\[ p_{50} = p_c - \frac{c}{L^{1/\nu}}, \quad (4.11) \]

where $c$ is a constant. Finite-size scaling also adds an extra proportionality factor in the form of $\theta(\xi)$ to the expressions (4.6)-(4.9).

By checking the validity of the above expressions for our simulation results we can find out to what extent the simulated fracture process resembles random percolation of damage.

### 4.2 Random percolation of damage vs rigidity percolation

In our research we consider the percolation (random or not) of damage. This is different from rigidity percolation studies similar to that described in the work
4.2. Random percolation of damage vs rigidity percolation

Figure 4.2: Stress-strain relationship (dots represent breaking events) for a single fracture simulation ($L = 200$)

Figure 4.3: Stress-strain relationship averaged over five samples ($L = 200$)

of Moukarzel and Duxbury [52]. Since we know that a reader may confuse the two distinct topics with each other, we explain the difference explicitly.

Consider a cluster of "connected" bonds (Fig. 4.1-a). Obviously it is not "rigid" and according to [52] can be split into rigid clusters and dangling bonds (Fig. 4.1-b). In studies on rigidity percolation typically the process of growth of such rigid clusters is considered. In this case bonds are randomly added to the
initially depleted lattice one by one, until at the rigidity-percolation threshold an infinite rigid cluster is obtained. Contrary to that, we consider the process of removing bonds from an initially complete lattice, until at the connectivity-percolation threshold an infinite damage cluster has been grown. Hence, by damage clusters we mean empty space formed in the latter process. Consequently, the damage clusters should not necessarily be rigid and the two percolation thresholds are not equal. A cluster of broken bonds is a cavity in the material, but not an object that could transmit forces. If we, in our study, would consider the clusters of intact (or rigid) material, then a parallel could be drawn between our work and [52]. The similarity between our study and the paper of Moukarzel and Duxbury still can be drawn in the following sense. If we estimated (which we did not) the exponent \( \nu \) from the finite-size scaling of the failure point, then the estimate of the exponent would have to coincide with \( \nu \approx 1/0.85 \) from [52]. In our work we define \( \nu \) as a scaling exponent of the correlation length of clusters that are defined according to the connectivity rule like in Fig. 4.1-a. Therefore, the exponent should be the same as for connectivity percolation assuming of course that damage indeed develops randomly.

### 4.3 Qualitative features of simulated 2D brittle fracture

Macroscopically the fracture process in our model has some features very typical for highly disordered systems. With the chosen strong disorder there is no linear-elastic part in the stress-strain dependence; the stress-strain curve for one particular lattice with size \( L = 200 \) is shown in Fig. 4.2. Weak springs start breaking from the very beginning, decreasing the overall stiffness and bending the stress-strain curve downwards. This is very much different from the well-known "weakest link" concept, according to which global failure develops like an avalanche right after the failure of a few weakest bonds. In our case the lattice starts breaking apart after a rather long quasi-elastic regime. The averaged stress-strain relationship (Fig. 4.3) of course looks smoother than each single one.

In our simulations we use two types of boundary conditions: busbars and periodic ones, that have been described in Chapter 3. They give qualitatively identical results with very close values of fit parameters. The only significant numerical difference was observed for the values of the macroscopic critical stress and strain, which appear to be higher for busbars boundary conditions. Therefore, only results for periodic boundary conditions are presented graphically in the present section, while the numbers are given for both.

For RP the criterion for identifying when the lattice is broken is obvious: at the point of the first spanning-cluster formation. On the contrary, in fracture simulation we can identify at least two characteristic points on a stress-strain
4.3. Qualitative features of simulated 2D brittle fracture

Figure 4.4: Developing damage pattern in a single fracture simulation with lattice linear size $L = 50$ (broken bonds are printed in red): short-range localization at $p = 0.01$ (a), distributed damage at $p = 0.11$ (b), onset of macroscopic localization (c)

curve: the point of maximum stress and the point where stress drops down to zero or almost zero. The first point precedes fracture, the second one is the mechanical breakdown itself. On top of that there is a final point at which the first spanning cluster is formed - the percolation threshold in the ordinary sense. So note that the percolation threshold and the mechanical breakdown are not
necessarily identical: the former is defined according to topological connectivity, while the latter has to do with rigidity of the lattice as a whole.

When the microscopic damage is considered, our simulations show that during the initial phase of fracture short-range localization takes place (Fig. 4.4-a). However, this is rather soon suppressed by disorder (Fig. 4.4-b). Then
4.4. Size scaling in the macroscopic mechanical response

4.4.1 Size dependence of the survival probability and the effective percolation threshold

As has been already mentioned, random percolation on a 2D lattice must reveal finite-size scaling in the form (4.11), with a proper threshold and a scaling exponent \( \nu = 4/3 \). For our simulation of RP we have checked this scaling law by collapsing the survival-probability plots for different lattice sizes (Fig. 4.6). Scaling in the form \( p_{50} - p_c \propto L^{-\nu} \), with \( \nu = 4/3 \) as predicted by theory, and \( p_c = 0.3333 \) as given in [35] for random lattices, matches our results very well.

![Figure 4.6](image)

(a) (b)

Figure 4.6: Collapse of the survival-probability plots for different lattice sizes for RP simulation, confirming finite-size scaling in RP. The data represent averages over all samples of each particular size \( L \).
4. Pattern development in brittle fracture...

Figure 4.7: Size dependence of the effective threshold $p_{50}$ of RP simulation and of fracture simulation with periodic boundary conditions; the data are scaled with the theoretical exponent $\nu = 4/3$ of RP, which clearly does not apply to fracture.

The survival probability can be defined for fracture simulation in a similar way as for RP. If, for a given $p$, a lattice has not yet reached its maximum-stress point, it is said to be "not broken" or survived. Alternatively, the stress-drop point can be used as a delimiter between survival and failure. Whatever criterion is used (maximum-stress or stress-drop) the data for fracture cannot be fitted to (4.11) with the theoretical values. It is clearly seen (Fig. 4.7) that the graph corresponding to the stress-drop criterion has a significant curvature when scaled with the exponent of $4/3$. The graph following from the criterion of maximum stress does not look straight either, although the deviations are not as dramatic. Furthermore, the data corresponding to fracture simulation show a decrease of $p_{50}$ with increasing lattice size, while RP simulation gives an opposite dependence. A similar contradiction for fuse networks, although not noticed, can be found in the results of [31], while the scaling exponent is found there to coincide with percolation theory.

4.4.2 Size dependence of critical stress and strain

The macroscopic critical stress $\sigma$ and critical strain $\varepsilon$ are defined for each sample as the maximum stress and the corresponding strain respectively. The values of $\sigma$ and $\varepsilon$ are averaged over a set of samples for each system size. Similar to experimental observations, the critical stress and strain decrease as the size of the lattice becomes larger, due to disorder. The size dependence of the macroscopic critical stress can be fitted as a power law $\sigma - \sigma_{\infty} \propto L^{-\kappa}$ for both types of boundary conditions, with $\kappa = 1.04$, $\sigma_{\infty} = 4.9 \times 10^{-3}$ for periodic BC’s (Fig. 4.8).
and \( \kappa = 0.97, \sigma_\infty = 1.3 \times 10^{-2} \) for busbars. The critical strain follows the same behavior \( \varepsilon - \varepsilon_\infty \propto L^{-\lambda} \), but with different numbers: \( \lambda = 0.60, \varepsilon_\infty = 1.3 \times 10^{-4} \) for periodic BC's (Fig. 4.8) and \( \lambda = 0.59, \varepsilon_\infty = 2.2 \times 10^{-4} \) for busbars. Apparently the exponents are independent of boundary conditions within the considered data accuracy: \( \lambda \approx 0.6, \kappa \approx 1 \), while the absolute values of \( \varepsilon \) and \( \sigma \) are significantly higher for the busbars case. The busbars make all nodes on the edge of the lattice have equal displacements, which leads to a more uniform stress distribution across the lattice and, consequently, to higher strength.

The fitting of the size dependence of maximum stress and strain shows that for fracture simulation power laws are followed at least approximately, but with parameters much different from those valid for percolation thresholds of RP and found in [31]. The maximum stress is, as we show later, a cross-over between the percolation-like regime and the regime of macroscopic localization. The very nature of the survival distribution for fracture (in particular with the stress-drop point taken as the point of failure, but probably also with the maximum-stress point) implies that here data without and with a strong macroscopic localization have been combined in one analysis; without further study of the localization regime no conclusions should be attempted from such power-law scaling, except that there is a clear difference with earlier results for fuse-network models that suggest a quantitative agreement with RP up to the final failure point [31].
4.5 Statistics of the damage clusters

We have taken lattices of one particular size $L = 50$ and analyzed the average behavior of the distribution $n_s$ of damage-cluster sizes. This particular lattice size has been chosen as the one providing enough samples for reasonably good statistics and being still not too small. Fig. 4.9 gives the full distribution for RP (upper part) and fracture (lower part), plotted in such a form that power-law scaling may be easily recognized. For RP this power-law scaling at the approach of $p_c$ is indeed seen, with the correct value of the Fisher exponent $\tau = 187/91$. The regime where scaling can be recognized is broad; it starts from half-way to the percolation threshold (about $p = 0.14$) and ends right before $p_c$ at $p = 0.3$. A
4.5. Statistics of the damage clusters

Figure 4.10: Scaling function of the cluster-size distribution for RP (upper graph) and fracture (lower graph) simulation within the scaling regime, showing a plateau at low small arguments. The data represent averages over all samples of size $L = 50$; scattered data for large $s$ are excluded; curves are levelled vertically to match one another (cf. equation (4.8))

qualitatively similar scaling is suggested for fracture, though in a smaller range of $p$ (from $p = 0.1$ to $p = 0.18$). To accurately plot the scaling according to percolation theory, we have replotted the data in the form of equation (4.8), see Fig. 4.10. According to percolation theory, the scaling function $f(z)$ does not need to be universal but needs to be within the scaling assumptions of the cluster-size distribution. The requirement that $f(z)$ has a plateau for $z \to 0$ then proves a fairly sensitive test to the value of $\tau$. Although a slight shape difference exists between the scaling functions for RP and fracture, it has to be concluded that in the considered interval of $p$ (i.e. before the macroscopic localization occurs) the fracture data are consistent with the scaling law (4.8) and the exponent value
\( \tau = 187/91 \) of random damage percolation. This test of scaling-function mapping results in somewhat narrower scaling ranges both for RP \((p \in [0.14, 0.26])\) and fracture \((p \in [0.1, 0.16])\).

Attempts to build a scaling function for fracture by using \( \tau \) different from the theoretical value of RP do not lead to satisfactory results (Fig. 4.11). A scaling function still seems to be plausible for \( \tau \) twenty percent lower than the theoretical value (Fig. 4.11-a) but this function does not have a plateau at low arguments. For \( \tau \) twenty percent higher than \(187/91\) (Fig. 4.11-b) the attempt to build the scaling function is unsuccessful.

Analogous to equation (4.8), the scaling relation for \( n_s \) can be based on \( \xi \) instead of \( M_2 \) and written in a form consistent with the fractal dimension \( D_f \):

\[
n_s \propto g\left(\frac{s}{\xi^{2/D_f}}\right).
\]

(4.12)

Again the scaling function should have a plateau at low arguments. Validation of this relation allows to test how consistent the scaling of the cluster size distribution is with the behavior of \( \xi \). In particular, it allows to examine whether the proper choice of \( \tau \) leads to the proper RP value of \( D_f = 91/48 \) (see equation (4.10)). As seen from Fig. 4.12-a, an attempt to confirm the scaling relation (4.12) for the same range of \( p \) as used in Fig. 4.10 is not really successful. This suggests that \( \xi \) might have a different scaling regime than \( M_2 \). Indeed, if another range of \( p \) is chosen, the scaling relation (4.12) is confirmed (Fig. 4.12-b). Moreover, if we try to use other values of \( D_f \) (again, twenty percent lower or higher than the theoretical value) the scaling becomes worse (Fig. 4.13), though this test appears not as sensitive as the one for \( \tau \). These results
4.5. Statistics of the damage clusters

Figure 4.12: A test of the scaling relation (4.12) for the fracture simulation, using the RP values $\tau = 187/91$ and $D_f = 91/48$ in the scaling regime where (4.8) was satisfied (Fig. 4.10) (a), and in the scaling regime where the relation (4.12) indeed holds (b).

Figure 4.13: Attempts to build a scaling function in the form of (4.12) from the cluster-size distribution for fracture simulation with the fractal dimension 20% different from its RP value: $D_f = 1.52$ (a) and $D_f = 2.28$ (b), and using the same data and procedure as for Fig. 4.12 support the validity of the theoretical value $D_f = 91/48$. The fractal dimension $D_f$ can be estimated directly from the fitting of the power-law relationship between cluster size (weight) $s$ and the cluster spatial extent $R_s$ for big clusters. Fig. 4.14 shows for a damage concentration $p = 0.12$, which is inside both scal-
Figure 4.14: Relationship between the cluster weight $s$ and the cluster gyration radius $R_s$ at the density of broken bonds $p = 0.12$ for $L = 50$. The data for fracture are shifted one unit up. Solid lines show the theoretical RP value of the fractal dimension $D_f = 91/48$.

Following this conclusion we can also verify the additional scaling laws (4.6) and (4.7) vs distance to $p_c$, for the second moment $M_2$ of the mass distribution and for the spatial correlation length $\xi$, respectively. The scaling of $M_2$ follows directly from the scaling of the cluster-size distribution (4.8) and, therefore, should be valid in approximately the same region. Similar to that, the scaling regime of $\xi$ should coincide with the regime where relation (4.12) holds. As follows from percolation theory, the scaling range for the correlation length can, in principle, differ from the one of $M_2$, since the scaling of $\xi$ is based not just on mass, but also on geometrical arguments; also finite-size effects may influence $M_2$ and $\xi$ differently. As shown before, we observe different scaling ranges (though overlapping) in the analysis of the scaling functions, one of which is based on $M_2$ and the other one on $\xi$. This difference is followed by the behavior of $M_2$ and $\xi$. As seen from the graphs (Fig. 4.15) the second moment $M_2$ of the cluster-size distribution as well as the correlation length $\xi$ do not develop in the same way for RP and for fracture simulation. In the case of fracture the cluster mass and cluster extent on average progress faster with damage concentration $p$. This is not surprising since the final damage pattern in the case of fracture simulation is a crack dividing a lattice into two pieces rather than uniformly distributed damage. There is also a difference in the initial regime, especially well-observed for $\xi$; snapshots of the damage suggest that this is re-
4.6. Damage anisotropy and macroscopic localization

lated to an initial enhanced fracture of springs oriented parallel to the loading direction, and to short-range localized growth of the initial fractures. Also the anisotropy and macroscopic localization that in fracture set in around the maximum-stress point, cause visible difference from RP behavior. However, in the intermediate regime, at concentrations corresponding to the scaling in Fig. 4.10, the fracture data for \( M^2 \) and \( \xi \) can be consistently fitted to the RP scaling laws and exponents. The effective fracture percolation threshold can be estimated by plotting \( M^2 \) and \( \xi \) as functions of \( |p_c - p| \) and finding that value of \( p_c \) which gives a linear scaling range (Fig. 4.16). The estimated value of the fracture percolation threshold \( p_c = 0.27 \) is well below that of RP (\( p_c = 0.33 \)).

The difference in the shapes of curves between RP and fracture is more pronounced for \( \xi \) than for \( M^2 \), which suggests that the role of cluster spatial size and shape may be most crucial. Note that the fracture data in which scaling can be observed are in relative terms still farther from \( p_c \) than those for RP; this is again consistent with the cluster-size statistics of Fig. 4.9, in which the range of algebraic scaling remains smaller for fracture.

The scaling of \( \xi \) and \( M^2 \) can be validated without presuming a certain value of \( p_c \) by plotting them (scaled with the exponents of RP) against each other (Fig. 4.17), since they both should (if the random-percolation scaling is valid) behave as powers of \( |p_c - p| \). The scaling regime is identified then by fitting the dependence by a straight line going through the origin. It can be seen that a regime exists where \( \xi \) and \( M^2 \) scale properly against each other, although it is rather narrow. We emphasize that we do not estimate scaling exponents from the simulation data; that would require a much more massive statistics than we have. Instead, we validate the scaling laws of random percolation with the corresponding exponents and identify the limits of the scaling regime.

The above picture of three regimes, with accelerated cluster growth in the initial and final stages, and with intermediate RP statistics, is supported by Fig. 4.18; here we have plotted as a function of increasing damage the joining probability - the probability for an individual newly broken bond to be joined to an already existing damage cluster instead of nucleating a new cluster of one bond. The curve corresponding to fracture raises above the one of RP in those regions where the damage pattern tends to localize. The localization is again seen in the initial and final regimes of the fracture simulation.

### 4.6 Damage anisotropy and macroscopic localization

In the previous section we have shown the existence of a percolation-like regime in our fracture simulations. The end of the regime is signalled by differences from RP in the behavior of \( M^2 \) and \( \xi \). The geometry of damage clusters not only starts to deviate from RP on average, which is described by \( \xi \), but also...
becomes anisotropic. This feature can be easily noticed by the naked eye in a final damage pattern (Fig. 4.5-c; see also Fig. 6.1-c).

Anisotropy can be observed quantitatively by monitoring the shape factor $\Phi$ constructed from the two components $\xi_\parallel$, $\xi_\perp$ of the correlation length, and defined by equation (4.5). The shape factor corresponding to fracture has a stable non-zero level from the very beginning, likely due to the initial localization in the first regime of damage development. However, it starts to deviate from zero significantly only slightly before the point of maximum stress and grows dramatically beyond the maximum stress (Fig. 4.20). This results in a final ratio of the components of the correlation length of about three. Hence, the fracture process gains two clear principal features just before the maximum-stress
4.7 Summary and conclusions

In the present chapter an attempt is made to understand similarities and distinctions between damage development in the brittle fracture of strongly disordered central-force spring lattices on the one hand, and random percolation point: damage anisotropy and localization. This announces the final failure by growth of a localized macroscopic crack. The statistics of this process will be described in Chapter 8.

4.7 Summary and conclusions

Figure 4.16: Scaling of the second moment $M_2$ of the cluster-size distribution (upper graph) and scaling of the correlation length $\xi$ (lower graph) as functions of $|p_c - p|$ for simulations with linear lattice size $L = 50$. Limits of the scaling regime (the same as in Fig. 4.15) are denoted by solid markers; the black solid lines show the theoretical RP slopes.
4. Pattern development in brittle fracture...

Figure 4.17: Correlation length $\xi$ versus second moment $M_2$ of the cluster-size distribution, both scaled with proper RP exponents, for simulations with linear lattice size $L = 50$. Limits of the regime where both $\xi$ and $M_2$ scale, are denoted by solid markers; in the case of fracture the scaling regime is $p \in [0.1, 0.14]$. The solid lines represent least-squares fits through the origin.

Figure 4.18: Joining probability (the probability for an individual newly broken bond to be joined to an already existing damage cluster) for simulations with linear lattice size $L = 50$ for RP (red) and fracture simulation (green). The curves, smoothed by a moving average over 10 subsequent points, overlap in the regime where RP-scaling in the cluster statistics is observed.
4.7. Summary and conclusions

Figure 4.19: Clusters of broken bonds for a single lattice with linear size $L = 100$; (a) for RP simulation at the threshold, (b) for fracture simulation at the maximum-stress point and (c) for fracture simulation at the stress-drop point

on the other hand. The comparison is made both on macroscopic and microscopic levels, by elaborating the statistical and scaling features of the two phenomena.

The fracture scenario of our model is very typical for highly disordered systems: break events start to occur from the earliest stage of deformation, but do
not lead to macroscopic failure until, after progressive distributed damage, the system reaches its critical state. This behavior is different from the way fracture happens in non- or weakly disordered systems, where failure develops like an avalanche already after only few break events. The precise dependence on disorder strength is studied in Chapters 5 and 6.

For the case of strong disorder considered here damage develops in three different stages. Initially some short-range localized growth of small fractures occurs, but this damage nucleates throughout the sample, due to the disorder. In the second stage the effect of disorder takes over and progression of the distributed damage follows a percolation-like picture, with random coalescence of different damage clusters. Already before the point of maximum stress macroscopic localization sets in, with a rough final crack preferentially growing in the direction perpendicular to the loading.

Numerical analysis shows that the macroscopic break-up mechanics and survival-probability statistics allow a power-law fitting of their size dependence; however, the power-law exponents are clearly different from those of random percolation. Such a macroscopic break-up analysis ignores the different mechanisms of damage development in the different stages before break-up, so no further interpretation on the deviating power-law fits can yet be drawn in terms of scaling; the latter may also be approximate and accidental. However, the microscopic data from the intermediate stage, with distributed development of damage, can clearly be fitted consistent with the theory of random percolation and with the theoretical values of its scaling exponents. This applies both to the damage-cluster mass statistics and to the spatial cluster extent.
Our results may be compared with earlier simulation studies which consider fracture vs percolation. The results partially confirm those of Arbabi and Sahimi [65], who used 2D triangular networks with the same type of power-law disorder, however, with bond-bending forces included and with disorder exponents $\alpha = 0.8$ and $0$; they identified the percolation-like regime as the first regime of damage development, but based their conclusions on a graphical comparison of the force distribution in the network only, and did not give a more detailed quantitative analysis. When compared with the burning of fuse networks [31, 53] our investigation provides a more realistic model for the mechanics of fracture, as does the analysis of spring networks in [54]. The percolation-like picture advocated in [31] is microscopically recognized in the present work, although only in a middle regime between the initial short-range and final long-range localization. Our data are not inconsistent with [53] and [54] either, but those studies do not analyze microscopic percolation-like behavior before the maximum stress, and concentrate on the final-stage scaling of the avalanche-like breakdown.
4. Pattern development in brittle fracture...
Chapter 5

The effect of disorder strength on damage-pattern development in brittle fracture

In the previous chapter we have shown the presence of a percolation-like regime of damage development in the case of fracturing lattices with strong disorder, with a disorder exponent $\alpha = 0.7$. This research has left an obvious question: how do the main features (the existence of three regimes and the similarity between the second regime and RP) depend on the disorder strength? In this chapter we present a systematic investigation of these dependencies. In particular we check and confirm our earlier results for even higher disorder strength. Then we systematically decrease the disorder and analyze the behavior of the fracturing lattices. Attention is paid to macroscopic properties of the process like stress-strain dependencies, damage localization and macroscopic features of the damage clusters (weight, spatial size and possible anisotropy), as well as to the microscopic damage-clusters statistics and short-range localization. The disorder strength $\alpha$ that we consider here varies from 0 (uniform disorder) to 0.75 (high disorder). Again we run the simulation for a set of lattice sizes and for a set of samples for each considered lattice size. The set of lattice sizes is more limited than previously while the sets of samples per lattice size are larger than before (see Table 5.1).
5. The effect of disorder strength...

Table 5.1: Statistics of simulation runs

<table>
<thead>
<tr>
<th>Linear lattice size $L$</th>
<th>Number of runs</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>500</td>
</tr>
<tr>
<td>50</td>
<td>500</td>
</tr>
<tr>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>200</td>
<td>25</td>
</tr>
</tbody>
</table>

Note: in all cases the calculations are done for $\alpha \in \{0, 0.3, 0.5, 0.6, 0.7, 0.75\}$

5.1 Macroscopic stress and strain vs disorder strength and sample size

Similar to the results presented in Chapter 4 the stress-strain dependence found when varying the disorder exponent $\alpha$ in the threshold distribution (3.11) remains typical for heterogeneous materials: bonds start to break from the very beginning and when the critical state is reached, macroscopic failure occurs (Figs 5.1-5.3). The critical (maximum) stress and the corresponding critical strain decrease with increasing disorder strength. This fact is logical since we increase disorder at constant value of $w$ in the distribution (3.11), i.e., we introduce more weak bonds in the lattice. Nevertheless, increasing disorder does not affect the initial stiffness of lattices, i.e. the initial slope of a stress-strain curve remains the same for all values of $\alpha$.

The shape of the stress-strain curve also changes with $\alpha$. For uniform disorder ($\alpha = 0$), the dependence (both vs strain and vs damage density $\rho$) slightly curves downwards until the maximum and then rapidly drops (Fig. 5.1). For

figure 5.1: Stress-strain and stress-damage dependencies for a single fracture simulation with uniform disorder ($\alpha = 0$) and lattice linear size $L = 200$
higher disorder (Figs 5.2, 5.3) the stress-strain curve becomes more concave while the stress-damage curve gets more convex. The former can be explained by the fact that at constant strain more bonds are broken for strong disorder than for weak one, simply because stronger disorder implies a more heavy tail of weak bonds in the distribution. This in turn leads to a more significant decrease of the overall stress. The concave shape of the stress-damage curve shows that for larger \( p \) breaking becomes more difficult because relatively stronger bonds remain. For strong disorder with \( \alpha = 0.75 \) (Fig. 5.3) the pre-failure ranges of both the stress-strain and stress-damage dependencies are separated into two parts with different curvatures, and the final drop is smoother. It indicates that the pre-failure phase consists of two qualitatively different regimes: a
very short initial regime where stress builds up quasi-Elastically without much damage, followed by a regime with damage increase and softening like for lower disorder. In the very early stage a fully elastic response (with no break events) is present in the simulation data for $\alpha = 0.75$ (up to a stress of about $0.3 \cdot 10^{-4}$ in Fig. 5.3). This is an artefact at high disorder strength because when randomly generating thresholds we artificially shift all obtained thresholds collectively from zero towards higher values by a very small number. This is done in order to avoid the situation when some bonds need to be removed from the lattice already at zero strain, which is unphysical. It is seen from Figs 5.1-5.3 that contrary to the critical strain, the critical damage density (density of broken bonds
5.1. Macroscopic stress and strain...

\[ \sigma(\alpha) = 0.00, \kappa = 0.63 \]
\[ \alpha = 0.30, \kappa = 0.79 \]
\[ \alpha = 0.50, \kappa = 0.89 \]
\[ \alpha = 0.70, \kappa = 1.04 \]
\[ \alpha = 0.75, \kappa = 1.07 \]

Figure 5.6: Scaling of the critical stress for various disorder strengths, least-squares fitting

\[ \varepsilon(\alpha) = 0.00, \lambda = 0.58 \]
\[ \alpha = 0.30, \lambda = 0.58 \]
\[ \alpha = 0.50, \lambda = 0.59 \]
\[ \alpha = 0.70, \lambda = 0.60 \]
\[ \alpha = 0.75, \lambda = 0.60 \]

Figure 5.7: Scaling of the critical strain for various disorder strengths, least-squares fitting

at the point of maximum stress) increases when \( \alpha \) becomes larger. This means that for higher disorder more damage is allowed before failure, which is a consequence of the fact that well-distributed weak bonds can be relatively harmlessly removed from the lattice without inducing a macroscopic breakdown.

The effect of the disorder strength \( \alpha \) on the averaged stress-strain and stress-damage dependencies is presented in Fig. 5.4. While the initial slope (stiffness)
Table 5.2: Scaling exponents for critical stress and strain for varying disorder

<table>
<thead>
<tr>
<th>α</th>
<th>Critical-strain exponent λ</th>
<th>Critical-stress exponent κ</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.58</td>
<td>0.63</td>
</tr>
<tr>
<td>0.3</td>
<td>0.58</td>
<td>0.79</td>
</tr>
<tr>
<td>0.5</td>
<td>0.59</td>
<td>0.89</td>
</tr>
<tr>
<td>0.7</td>
<td>0.60</td>
<td>1.04</td>
</tr>
<tr>
<td>0.75</td>
<td>0.60</td>
<td>1.07</td>
</tr>
</tbody>
</table>

of the stress-strain curve is the same for all values of α, the curves representing the dependence vs \( p \) change with \( α \) from the very beginning, which once again points at the subtle role of disorder in the damage development towards fracture. Note that the averaging procedure obviously makes the average curves smoother than the ones of single simulations.

We have also studied the size effect in the stress-strain and stress-damage dependencies. As is clear from Fig. 5.5, such an effect is only present in the region around the maximum-stress point and beyond. The maximum stress and the corresponding critical strain and damage are shifted towards smaller values for bigger lattices. The size dependence of the maximum-stress point can be successfully fitted by a power law \( \sigma - \sigma_\infty \propto L^{-\kappa} \) (Fig. 5.6). The corresponding scaling exponent \( \kappa \) changes from 0.63 for \( \alpha = 0 \) up to 1.07 for \( \alpha = 0.75 \); so in terms of critical stress the size effect becomes stronger for stronger disorder.

The critical strain can be fitted quite well by \( \varepsilon - \varepsilon_\infty \propto L^{-\lambda} \) (Fig. 5.7). The exponent \( \lambda \) in this case does not change significantly: it slightly increases (from 0.58 to 0.6) with increasing \( \alpha \). All numbers together are given in Table 5.2. We warn here again (this warning is also given in Chapter 4) that the region around the critical strain is probably a transition between two regimes dominated by different mechanisms, random damage percolation and more avalanche-like behavior. Therefore not much can be concluded fundamentally from the scaling in Figs 5.6 and 5.7 until also the post-yield regime has been understood in more detail. In fact, the observed power-law scaling of the critical stress and strain may be accidental.

5.2 Cluster statistics: high vs low disorder

As in Chapter 4 we have analyzed for various \( \alpha \) the statistics of the damage clusters, and attempted an interpretation in terms of random damage percolation. Simulation results for the second moment \( M_2 \) of the cluster-size distribution and for the correlation length \( \xi \) are given as functions of the damage density \( p \) in Figs 5.8 and 5.9, respectively. The second moment shows a gradual trend with decreasing \( \alpha \), away from the RP behavior. The correlation length qualitatively
5.2. Cluster statistics: high vs low disorder

Figure 5.8: Second moment $M_2$ of the cluster size distribution for lattice linear size $L = 50$; data represent fracture simulations with different values of $\alpha$ and the simulation of random percolation

Figure 5.9: Correlation length $\xi$ of damage clusters for lattice linear size $L = 50$; data represent fracture simulations with different values of $\alpha$ and the simulation of random percolation

deviates from RP behavior for all $\alpha$’s, with a marked crossover in the behavior at low damage when going from high disorder ($\alpha = 0.75, 0.7$) to lower disorder. We therefore will analyze these two disorder regimes separately, and first consider to what extent our previous conclusions for strong disorder ($\alpha = 0.7$, see
5. The effect of disorder strength...

Figure 5.10: Scaling of the second moment $M_2$ of the cluster-size distribution and of the correlation length $\xi$ as functions of $|p_c - p|$ for simulations with linear lattice size $L = 50$ and for $\alpha = 0.75$. Limits of the scaling regime are denoted by solid markers; in the case of fracture the limits are $p \in [0.09, 0.18]$ both for $M_2$ and $\xi$. The black solid lines show the theoretical RP slopes; curves are shifted from each other for clarity.

Chapter 4) are maintained for $\alpha = 0.75$.

5.2.1 Percolation behavior for high disorder

We have already shown in the previous chapter the existence of a percolation-like regime for the case of strong disorder with $\alpha = 0.7$. We confirm now the presence of this regime for $\alpha = 0.75$ by plotting $M_2$ and $\xi$ vs $|p - p_c|$ (Fig. 5.10). Linear parts of the graphs have slopes matching the ones of percolation theory. As in the case $\alpha = 0.7$ (see Chapter 4) the percolation thresholds obtained from the two functions $M_2(p)$ and $\xi(p)$ are the same, and are marginally larger than
5.2. Cluster statistics: high vs low disorder

Figure 5.11: Correlation length $\xi$ versus second moment $M_2$ of the cluster-size distribution, both scaled with proper exponents, for simulations with linear lattice size $L = 50$ and for $\alpha = 0.75$. Limits of the scaling regime are denoted by solid markers; in the case of fracture the scaling regime is $p \in [0.09, 0.18]$. The solid lines represent least-squares fits through the origin.

Figure 5.12: Evolution of the cluster-size distribution; $\alpha = 0.75, L = 50$

In that case: $p_c = 0.28$ ($\alpha = 0.75$) vs $p_c = 0.27$ ($\alpha = 0.7$). Contrary to the results for $\alpha = 0.7$ the scaling ranges of $M_2$ and $\xi$ approximately coincide in the case of $\alpha = 0.75$. The existence of a percolation-like regime can be shown without
Figure 5.13: Scaling function (based on $M_2$) of the cluster-size distribution for fracture simulation within the scaling regime ($p \in [0.09, 0.18]; \alpha = 0.75$). The data represent averages over all samples of size $L = 50$; scattered data for large $s$ are excluded; curves are levelled vertically to match one another (cf. equation (4.8))

Figure 5.14: Scaling function (based on $\xi$) of the cluster-size distribution for fracture simulation within the scaling regime ($p \in [0.09, 0.18]; \alpha = 0.75$). The data represent averages over all samples of size $L = 50$; scattered data for large $s$ are excluded; curves are levelled vertically to match one another (cf. equation (4.12))

assuming a certain value of $p_c$, by plotting $M_2^{-18/43}$ versus $\xi^{-3/4}$ and checking the possibility to fit the dependency by a straight line through the origin. The
5.2. Cluster statistics: high vs low disorder

Figure 5.15: Anisotropy factor $\Phi$ of damage clusters for lattice linear size $L = 50$; data represent fracture simulations with different values of the disorder exponent $\alpha$, and the simulation of random percolation.

result (Fig. 5.11) is fully consistent with Fig. 5.10, where we try to match the proper slopes. Similarity with random percolation is also confirmed by scaling of the cluster-size distribution (equation (4.8) and Figs 5.12, 5.13): for the theoretical RP Fisher exponent ($\tau = 187/91$) the data allow the construction of a scaling function with a plateau at low arguments. As mentioned in Chapter 4, the scaling relation for $n_s$ can be also based on $\xi$, and two exponents $\tau$ and $D_f$, see equation (4.12). Similar to the previous chapter we validate the theoretical values of $\tau$ and $D_f$ and check their consistency with the behavior of the correlation length and with the scaling of the cluster-size distribution. The result based on $\xi$ (Fig. 5.14) is very similar to the one based on $M_2$ (Fig. 5.13) though a small deviation starts to be noticeable at the highest concentration of the assumed scaling regime, $p = 0.18$.

As is seen from Figs 4.17 and 5.11 the percolation-like regime is wider for $\alpha = 0.75$ than for $\alpha = 0.7$. It gets significantly smaller for lower values of disorder strength. It is still possible to claim the presence of an extremely narrow percolation-like phase for $\alpha = 0.65$ and for $\alpha = 0.6$ (not shown). The regime is not observed at all for lower values of the disorder strength. Theoretically, RP behavior is claimed up to the (scalar) fracture point in the infinite-disorder limit $\alpha \rightarrow 1$ [62].

For low damage density $p$, a qualitative deviation of the cluster correlation length $\xi$ from the random-percolation behavior is observed. The deviation is more pronounced in the case of the highest values of $\alpha$ (Fig. 5.9). Contrary to that, the second moment of the cluster-size distribution is quite close to the random-percolation data in the range of low $p$. A localization process with a
characteristic length scale comparable with a bond length can be the cause for the deviation: if the disorder is strong, the probability of two very weak bonds to be close to each other is high. This, in turn, makes these neighboring weak bonds break next to each other, causing short-range localization.

### 5.2.2 Cluster anisotropy for low disorder

The gradual change with $\alpha$ of the second moment $M_2$ certainly does not disprove the presence of a percolation-like regime for weak disorder; on the basis of this graph one still can think that there is a short linear part of the graph corresponding to scaling. Qualitative changes in $\xi$ suggest, however, that different processes are going on in the cases of strong and weak disorder. This can be made clear by considering the anisotropy factor $\Phi$ (equation (4.5)). It is plotted in Fig. 5.15 for different values of $\alpha$. The anisotropy factor is obviously zero for RP (a note on another, non-zero measure of cluster anisotropy has been given in Chapter 4 on page 43). For fracture $\Phi$ has a plateau close to zero in the region of isotropic damage development. The plateau and, correspondingly, the region of possible similarity between fracture and RP is only present in fracture simulations with $\alpha \geq 0.6$. For lower values of $\alpha$ there is apparently no similarity between fracture and random percolation: the range of damage density with an isotropic cluster development is absent, and, as stated above, we observed that a scaling regime like present in Fig. 5.10 vanishes below $\alpha = 0.6$.

For low $\alpha$ the short-range localization at low $p$ is not observed because weak bonds are not likely located close. However, there is another feature typical for low disorder but not observed for high $\alpha$: the anisotropy factor has negative values during the very early deformation stage. This suggests that in the beginning of the fracture process, mostly isolated single bonds oriented parallel to the load are being broken. This fact is rather logical: since the difference in thresholds is not huge, orientation influences the choice of a bond to be broken much more than it does for high disorder strength.

In summary, only for $\alpha$ around 0.6 and higher there is a regime in which damage develops in an isotropic way and in which both $M_2$ and $\xi$ numerically follow random-percolation scaling laws, with classical exponents $\gamma = 43/18$, $\nu = 4/3$.

### 5.3 Damage patterns and profiles: percolation, localization and anisotropy

Both for high and low $\alpha$ the regime of damage development with low to moderate anisotropy is limited from above by the onset of strong anisotropy in the
5.3. Damage patterns and profiles...

Figure 5.16: Snapshots for a single fracture simulation with uniform disorder (\(\alpha = 0\)) (a, b, and c) and with strong disorder (\(\alpha = 0.75\)) (d, e, and f) for lattice linear size \(L = 200\); the corresponding damage densities are: \(p = 0.7 \times p_{\text{max.stress}}\) for (a) and (d), \(p = 1.0 \times p_{\text{max.stress}}\) for (b) and (e), and \(p = 1.2 \times p_{\text{max.stress}}\) for (c) and (f).

damage clusters, which signals the macroscopic localization of damage (Fig. 5.15). It is clearly seen that the curve corresponding to the highest \(\alpha\) shows a noticeable increase of anisotropy at \(p = 0.18\). This is most likely the cause of the small deviation of the scaling function \(g(s^{2/D}/\xi^2)\) at \(p = 0.18\) that was men-
5. The effect of disorder strength... 

Figure 5.17: Centered averaged damage-density profiles for simulations with uniform disorder ($\alpha = 0$) (a) and strong disorder ($\alpha = 0.75$) (b) and with lattice linear size $L = 200$; curves represent (from bottom upward) damage densities $p_1 = 0.7 \times p_{\text{max.stress}}, p_2 = 0.95 \times p_{\text{max.stress}}, p_3 = 1.0 \times p_{\text{max.stress}}, p_4 = 1.1 \times p_{\text{max.stress}}, p_5 = 1.2 \times p_{\text{max.stress}}$

As seen from the damage-development snapshots (Fig. 5.16), the macroscopic localization comes into play at (or very close to) the point of maximum stress both for uniform ($\alpha = 0$) and high disorder ($\alpha = 0.75$). To support this finding we plot the average damage-density profiles along the loading direction (Fig. 5.17). We build them by first centering the individual profiles in this direction and subsequent averaging over all samples of one particular lattice size. Indeed, a central peak in damage starts to be visible around the maximum-stress point in both considered cases. The shapes of the damage profiles suggest that our fracture simulation in its final stage might be compared more successfully with the percolation in a gradient [31] rather than with the random percolation of damage. If one looks only at the damage snapshots and the damage-density profiles, it might be tempting to conclude that for high, moderate and uniform disorder the picture before the maximum-stress point remains qualitatively the same: visually damage appears to develop in a percolation-like way up to the maximum-stress point. However, as made clear above, our analysis of the scaling laws and anisotropy factor show a clear difference in the damage evolution for lattices with low ($\alpha \leq 0.6$) and high ($\alpha > 0.6$) disorder strength.

Thus, macroscopic localization limits the percolation-like regime from above in the case of strong disorder. For low disorder it takes over from the
initial regime without any percolation-like intermediate phase. A question re-
mains to which extent the distinction in disorder is size dependent, but here
computing resources remain the dominant limiting factor.

5.4 Summary and conclusions

In the present chapter we show the results of the systematic numerical study of
the fracturing of 2D central-force networks with power-law disorder, with the
latter changing from uniform ($\alpha = 0$) to strong ($\alpha = 0.75$). In particular, we
have analyzed the macroscopic stress-strain behavior and microscopic dam-
age development, and compared the microscopic statistics of the damage clus-
ters with that for random damage percolation. The major conclusion from this
work is that the pattern of damage development is qualitatively different for
high and low disorder. This sheds new light on conclusions from similar studies
in the literature which use a variety of disorder strengths [33, 65, 31, 53, 54, 45]
and come to varying results as regards percolation. We have also analyzed the
dependence of our results on system size, but rigorous conclusions in this re-
spect will require significantly more computer power that currently available to
us; more attention could first be paid to improving the algorithmic aspects of
the simulations.

For high disorder, i.e. a high power-law exponent $\alpha = 0.75$, we confirm our
earlier findings (for $\alpha = 0.7$, Chapter 4) that damage in fracture develops in
three stages: short-range localization at low damage concentration $p$, random-
percolation behavior in a middle range, and macroscopic localization towards
a final anisotropic crack. The percolation-like regime rapidly shrinks with de-
creasing disorder exponent and vanishes around $\alpha = 0.6$.

For still lower values of $\alpha$ the damage development is anisotropic from the
beginning, with a 90 degree change in anisotropy with increase of the damage;
the short-range localization at low $p$ is no longer observed. These results can
be rationalized from the disorder statistics.

Both for low and high disorder macroscopic localization of damage sets in
around the maximum stress, and leads to a final crack oriented perpendicular
to the direction of load.
5. The effect of disorder strength...
Chapter 6

Fracture-surface morphology

Damage clusters that form in the simulation of random percolation of damage are on average isotropic, and the largest one is not much larger than others. Therefore it is impossible to recognize a cluster that looks like a crack. To apply RP to fracture and identify a final crack, the concept of gradient percolation or stress-weighted percolation has been introduced. This approach leads to a prediction for the roughness exponent [31], but has also met with serious criticism. Contrary to this, in our brittle-fracture simulation it is always possible to identify the dominant final damage cluster that contains a path connecting opposite sides of the lattice, i.e. the crack. The obvious question then is whether the roughness of this crack scales like it does in experimental observations and what is the influence of the disorder strength.

In this chapter we analyze the scaling properties of crack profiles obtained in our brittle-fracture simulations. First we summarize the gradient-percolation arguments. Next we analyze the simulated crack as a self-affine profile. The analysis itself consists of two non-trivial steps: identification of the crack profile and estimation of the self-affinity scaling exponent. Each of the steps can be performed in a few possible ways. For the former we employ three different methods, each of which having its own arguments to be appropriate. For the latter we use only one method, which has been reported in the literature as the most precise and least size-sensitive for the present purpose.

6.1 Prediction of crack roughness from gradient percolation

A way of estimating the roughness scaling exponent directly from percolation theory was suggested by Hansen and Schmittbuhl, who used the concept of percolation in a gradient [31]. They argue that at breakdown the damage den-
Fracture-surface morphology

Figure 6.1: Clusters of broken bonds for a single lattice with linear size $L = 100$; (a) for RP simulation at the threshold, (b) for fracture simulation with strong disorder ($\alpha = 0.7$) at the stress-drop point.

The use of this method for fuse networks is based on the applicability of the arguments of percolation in a gradient and on the RP-like scaling of $\xi$ in this case. With the RP value $\nu = 4/3$ in 2D it leads to the value $\zeta = 8/11 = 0.73$ for the roughness exponent.

We need to note here that even for the case of the highest disorder with $\alpha = 0.75$ the damage profiles look like a gaussian (Fig. 5.17-b) rather than a parabola. The shape of the profile would most likely become more parabola-like for larger values of $\alpha$.

6.2 Identification of crack profiles

As already mentioned, the final damage patterns are completely different for RP and for fracture. For the former case one sees several big isotropic damage clusters, one of which spans through the lattice (Fig. 6.1-a). In the case of fracture, anisotropy of a final damage pattern can be easily noticed by the naked eye (Fig. 6.1-b). It is also seen that the biggest fracture cluster is far larger than any other, suggesting that the damage pattern is localized; the damage pattern...
6.2. Identification of crack profiles

![Figure 6.2](image)

**Figure 6.2:** Example of the final crack profile (red line) obtained by means of horizontal averaging (a), by the burning algorithm (b), and by solid-on-solid approximation (c), for a single simulation with $L = 100$; inserts represent the scaling of crack roughness for the corresponding profiles.

at the point of maximum stress still remains rather isotropic and does not reveal pronounced localization, although the major cluster has been nucleated by this moment (Fig. 6.1-b).

The crack path can be defined in at least three ways: averaging, in the direction of load, within the biggest cluster; identifying the so-called backbone of the biggest cluster by means of the "burning" algorithm [34]; and defining the
border of intact material touching the biggest cluster from each side. The latter is sometimes called "solid-on-solid approximation". In the case of averaging, we first average in the direction of applied strain the coordinates of bonds of the heaviest damage cluster of an individual lattice (Fig. 6.2-a) in order to obtain the crack profile as a function of the transversal coordinate. The "burning" method defines the shortest path from one side of the lattice to another (Fig. 6.2-b), deleting dangling ends and parallel loops of longer path length. In the solid-on-solid approximation, one defines two boundaries (left and right if the load is applied horizontally) between the biggest damage cluster and surrounding intact bonds, by finding the minimum and maximum horizontal coordinate of the cluster at constant vertical position (see Fig. 6.2-c, where only one side of the cluster is shown). In all cases the averaging over different samples is only done in the roughness exponent.

The three methods give different profiles and, consequently, different results of roughness analysis. The above procedure of averaging in the horizontal direction of loading to get the position of the crack implies that the correspondence with real experimental cracks cannot be made down to the level of individual lattice elements; it is in line with the way in which the horizontal fluctuation of the crack position is described in the original paper [31] which derives the roughness exponent from damage correlations in gradient percolation. This is indeed a rather vague way of defining the real-crack roughness, and as an alternative we can choose the backbone of the infinite cluster, however, with at least one important caveat. The infinite cluster may have loops, leading to non-unique crack paths in the backbone, and possibly also vertical overhangs, for which the backbone makes one choice. Comparison with real cracks is then probably only meaningful on a length scale larger than the typical local width of the infinite cluster, i.e. the depth of the subsurface damage. The solid-on-solid method also contains an embedded drawback: it treats a dangling part of the biggest cluster by producing a sharp step connecting the dangling part with the main profile of the crack. It should be noted that in each case the crack is related here to damage profiles, not to profiles of rigidity clusters.

6.3 Estimation of crack-roughness exponents

We analyze the crack-roughness scaling defined by the following equation (already introduced in Chapter 2)

$$\Delta h = \langle \max(h(y_1) - h(y_2) ; y_1, y_2 \in [y_0, y_0 + d]) \rangle_{y_0}, \quad (6.2)$$

where $y$ is the coordinate along the average crack-propagation direction and $h(y)$ is the height of the crack profile. We employ only the simulations with
6.4 Numerical results

We recognize from Table 6.2 that the difference between the three methods of crack identification is systematic, so the definition of crack path is important. But, more relevant to the subject of the present research, we notice that in each definition the roughness is independent of the disorder strength, and hence independent of the damage-development scenario up to the maximum stress. This reinforces the idea that around the maximum-stress point the random-damage scenario is replaced by a different, more catastrophic mechanism as will be considered in Chapter 8. The latter mechanism should then possibly be invoked to explain the experimentally observed (near-) universality in crack roughness, but sound theoretical arguments for this are still lacking.

Nevertheless, the average value of $\zeta$ that we found for the backbone roughness almost coincides with that following from random percolation in a gradient ($\zeta = 8/11 = 0.73$) [31]. Our results for $\zeta$ corresponding to this “burning” method also agree very well with the results of another recent simulation of central-force lattices ($\zeta = 0.75 \pm 0.03$), with even stronger disorder ($\alpha = 0.95$) [8], although there a different assumption has been made about the scaling of the correlation length. The values for $\zeta$ from the other methods are somewhat lower, and close to one another. All values of $\zeta$ are sufficiently near those observed experimentally for quasi-two-dimensional cracks in wood ($0.68 \pm 0.04$) [24].
6. Fracture-surface morphology

Table 6.2: Roughness exponents obtained from the fracture simulations

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>Roughness exponent (averaging method)</th>
<th>Roughness exponent (&quot;burning&quot; method)</th>
<th>Roughness exponent (&quot;solid-on-solid&quot; method)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.68 ± 0.10</td>
<td>0.77 ± 0.10</td>
<td>0.63 ± 0.09</td>
</tr>
<tr>
<td>0.3</td>
<td>0.66 ± 0.11</td>
<td>0.74 ± 0.11</td>
<td>0.63 ± 0.09</td>
</tr>
<tr>
<td>0.5</td>
<td>0.66 ± 0.11</td>
<td>0.74 ± 0.11</td>
<td>0.62 ± 0.11</td>
</tr>
<tr>
<td>0.7</td>
<td>0.65 ± 0.11</td>
<td>0.75 ± 0.11</td>
<td>0.63 ± 0.10</td>
</tr>
<tr>
<td>0.75</td>
<td>0.64 ± 0.10</td>
<td>0.76 ± 0.12</td>
<td>0.62 ± 0.11</td>
</tr>
</tbody>
</table>

6.5 Summary and conclusions

Surprisingly enough, scaling is still present in the last regime of damage development, although the damage pattern is then strongly localized and anisotropic. A power-law dependence is obeyed very nicely by the crack roughness. In fact, the scaling of crack roughness is observed over more than three decades in lengthscale, only limited by the maximum size of the lattice. In the damage growth towards the final fracture clear differences are visible between high and low disorder, but both for low and high disorder macroscopic localization sets in around the maximum stress. The roughness of the final crack "surface" is surprisingly independent of $\alpha$, and can be characterized by an accurate size-scaling law. The precise value of the roughness-scaling exponent depends on details of the definition of the crack surface, but is anyway in good agreement with other numerical and experimental results.
Chapter 7

Simulation of brittle fracture in 3D

Real failure obviously happens in three dimensions, unless quasi-two-dimensional conditions are fabricated in special experiments. Therefore, 3D simulation is a natural extension of our two-dimensional study. We do not expect dramatic qualitative differences from the 2D case in the macroscopic response, i.e. in stress vs strain. Nevertheless, changes in aspects related to random percolation should be present since RP in all its results is dependent on the dimensionality of a problem.

Obviously, 3D simulations are much more demanding. They also require more complex post-simulation analysis: the analysis of crack roughness, for example, becomes the analysis of a surface instead of a curve. But it is worth the effort because 3D simulations allow to get closer to the real phenomena and also, with sufficient simulation data, to understand more deeply our earlier findings from the two-dimensional modelling.

This chapter is organized in the following way. We first discuss some methodological changes that are necessary for simulation in 3D. Then we show some results related to the macroscopic behavior of our model. Next we briefly address the comparison between fracture and damage percolation, which is more complex now than in the 2D case of Chapters 4 and 5. After that we perform a roughness analysis of crack surfaces, both for uniform and strong disorder. We finish the chapter with summary and conclusions.

7.1 Simulation of fracture in 3D lattices

Three-dimensional simulation of fracture by means of lattice models is not frequently met in literature. The main reason is of course in the fact that it is com-
Figure 7.1: Average 3D stress-strain (upper graphs) and damage-strain (lower graphs) dependencies for (a) uniform ($\alpha = 0$) and (b) strong disorder ($\alpha = 0.7$); data are calculated over all samples of size $L = 16$.
usually smaller, is believed to be universal. Batrouni and Hansen [10] observed only one scaling exponent that was independent of disorder strength and equal to $0.62 \pm 0.05$ within the range of lattice sizes from $L = 8$ to $L = 48$. Nukala et al. [55] reported the local and global roughness exponents to be equal respectively to 0.4 and 0.52 for the case of uniform disorder. They based their findings on the simulation of fuse networks with good statistics for maximum lattice size $L = 64$. Authors of [58] used a three-dimensional Born model with regular geometry which, for one particular set of parameters, corresponds to a central-force model. They obtained for lattice sizes up to $50 \times 50 \times 25$ a universal value of the roughness scaling exponent equal to 0.5.

Our three-dimensional lattice model is a natural extension of the 2D one. Topologically the lattice is a Delaunay tessellation of a cubic region with randomly distributed nodes. The bonds of the lattice form tetrahedrons instead of triangles in 2D. In terms of simulation the difference of the 3D case is in the presence of an additional degree of freedom per node which needs to be taken into account. We used only the "busbars" boundary conditions: load is applied in one direction to two opposite sides of the lattice; the other four sides remain free. This allows us to simulate larger lattices than we would be able to do with periodic boundaries (due to presence in the latter case of Lagrange multipliers, which constitute additional degrees of freedom).

Our 3D simulations are done for a limited range of lattice sizes; the statistics per sample size is presented in Table 7.1.

As one can expect, the macroscopic stress-strain dependencies of our three-dimensional simulations are qualitatively very similar to those of the 2D case (Fig. 7.1). Stress builds up during the initial quasi-elastic regime, then reaches

Figure 7.2: Damage $p$ as a function of the reduced stress $\sigma/\sigma_Y$ for uniform and strong disorder, showing a diverging damage rate $dp/d\sigma$ on approach of the yield stress $\sigma_Y$; data are calculated over all samples of size $L = 16$
Table 7.1: Statistics of the simulation runs, both for uniform ($\alpha = 0$) and strong ($\alpha = 0.7$) disorder

<table>
<thead>
<tr>
<th>Linear lattice size $L$ (3D)</th>
<th>Number of samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>100</td>
</tr>
<tr>
<td>12</td>
<td>50</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>5</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
</tr>
</tbody>
</table>

its maximum and drops, leading to a macroscopic breakdown. The shapes of damage-strain curves are also similar to those for the two-dimensional case and so are the differences between different disorders. The initial part of the curve is steeper for higher disorder and the damage density at the maximum-stress point is larger for higher disorder. The critical strain (strain at the maximum-stress point) decreases with increasing disorder strength, because higher disorder means a larger fraction of weak bonds (those with low thresholds). In the end the damage saturates close to failure. As seen from Fig. 7.2 the damage growth rate $dp/d\sigma$ diverges on the approach of the yield (maximum) stress $\sigma_Y$ both for uniform and for strong disorder.

7.2 Damage percolation vs fracture in 3D

While in terms of methodology the main difference between 2D and 3D is simply in the presence of the third degree of freedom, there is an important distinction between two- and three-dimensional cases in the interpretation of the results, namely in the correspondence between percolation of damage and loss of integrity. In 2D, the formation of a spanning damage cluster was not coinciding with, but nevertheless happened very close to, the failure point, i.e. to the state when a lattice fails to transmit load. This situation is very different in three dimensions. Failure of a three-dimensional lattice happens when damage spans through the lattice forming a failure surface, not a path; this means that the lattice must be broken into pieces that do not have remaining connections. The formation of a percolating damage cluster is geometrically different. Such a cluster should just connect at least two points lying on opposite sides of the lattice, while the lattice can remain rigid and connected. As a result, percolation of damage occurs earlier (in terms of connectivity) than failure.

If nevertheless the analysis of damage clusters is made up to the former damage-percolation point, one can observe (not shown) that the second moment of the cluster-size distribution as well as the correlation length of damage clusters develops in a very similar way in fracture and in random percolation, both for uniform ($\alpha = 0$) and strong ($\alpha = 0.7$) disorder. One can conclude from it that in the range of damage density $p$ from zero to this critical point the dam-
7.3. Analysis of crack-surface roughness

7.3.1 Definition of the crack surface

Contrary to our 2D roughness analysis of Chapter 6 here we literally need to deal with fracture surfaces instead of one-dimensional fracture profiles. The first step of the roughness analysis should be therefore the identification of a fracture surface from the simulation results. To that end we choose the so-called solid-on-solid approximation. We used this method, together with two others, in the 2D roughness analysis of Chapter 6. The solid-on-solid approximation is chosen for 3D as it is relatively easy to realize technically with our three-dimensional results; also it allows a clear physical interpretation. In this
method one finds a surface of most distant points of intact material measured parallel to the load direction and from one of the two sides of the lattice to which load is applied. First one needs to define the set of connected intact bonds that are also connected to one side of the lattice (the side with \( x = 0 \) if the load is applied in the \( x \) direction). Then the fracture surface \( x(y, z) \) is defined as the \( x \) coordinate of the most distant (from the side with \( x = 0 \)) point of intact material at \( y, z \). In order to obtain the opposite fracture surface the procedure needs to be repeated for the opposite side of the lattice (with \( x = 1 \)). In the end the method gives two fracture surfaces, exactly like in a real experiment.

Technically we realize this method as follows. First, we identify two parts of a broken lattice by means of a connectivity analysis (Fig. 7.3). Then we separately analyze each of them. From the set of tetrahedrons that were obtained during three-dimensional Delaunay tessellation, we define the set of all tetrahedron facets. Among the facets we leave only those that are associated with the considered fragment. Then we remove the facets lying on the sides of the lattice and in the bulk of the material. In the end only the fracture surface is left. Then we eliminate the average tilt of each surface by rotating it appropriately, with typical results as shown in Fig. 7.4.

Ideally the described method would lead to two fracture surfaces for each lattice sample. However, some of the samples cannot be used for further roughness analysis because one or both fracture surfaces touch one of the boundaries to which load is applied.
7.3. Analysis of crack-surface roughness

Figure 7.5: Roughness power-law scaling for single samples with disorder exponent $\alpha = 0$ (a) and $\alpha = 0.7$ (b), and lattice size $L = 20$; the window size $d$ varies only in the limited range $0.1L - 0.2L$.

7.3.2 Scaling of the surface roughness

The next step is measuring the roughness exponent itself. Here we use the same minimum-maximum method as in Chapter 6 (see equation (6.2)) for fracture profiles, with the only difference that the observation window is now a square of size $d$. For each sample surface we change the size of the observation window stepwise from $1/10$ to $1/5$ and, for each window size, average the roughness over windows with different origin. In other words, the window of a certain size ($1/10, 1/9, ... 1/5$) scans with a certain step throughout the entire fracture surface and then the roughness is averaged over windows with different locations. Window sizes larger than $1/5$ are not considered to exclude edge effects of the finite sample. Finally we calculate the roughness scaling exponent for each sample by means of least-square fitting of the relation between the roughness and window size. We perform the procedure described above only for relatively large samples ($L = 16$ and $20$). The maximum lattice size $L = 24$ is not considered in view of the lack of statistics, only one sample being available. We observe that even within the limited range of length scales accessible in 3D the power-law scaling of fracture roughness is followed rather nicely for each sample (Fig. 7.5).

The values thus obtained for the roughness scaling exponents are presented in Table 7.2. These values seem to be somewhat lower for high disorder ($\alpha = 0.7$) though the scatter of the data is big and does not allow to draw definite conclusions. The possibility that the roughness exponent is independent of $\alpha$ (as in 2D) and of lattice size can not be excluded, in view of the overlap of the accuracy intervals. If this is indeed the case, the resulting exponent will be
Table 7.2: Roughness exponent for different disorders and samples sizes

<table>
<thead>
<tr>
<th>Disorder strength $\alpha$</th>
<th>Linear lattice size $L$ (3D)</th>
<th>Roughness exponent $\zeta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>16</td>
<td>$0.71 \pm 0.06$</td>
</tr>
<tr>
<td>0</td>
<td>20</td>
<td>$0.67 \pm 0.05$</td>
</tr>
<tr>
<td>0.7</td>
<td>16</td>
<td>$0.54 \pm 0.16$</td>
</tr>
<tr>
<td>0.7</td>
<td>20</td>
<td>$0.66 \pm 0.05$</td>
</tr>
</tbody>
</table>

0.66 ± 0.10. Calculating the exponent separately for different disorder leads to $\zeta = 0.67 \pm 0.06$ for $\alpha = 0$ and $\zeta = 0.59 \pm 0.13$ for $\alpha = 0.7$. Obviously, better statistics is needed to define the exponent with more acceptable accuracy. The values we obtain for roughness are close to those obtained from the simulations with fuse networks [55, 10] and with the Born model [58] that we have mentioned in the beginning of this chapter. The experimental value of the local roughness scaling-exponent is found to approximately equal 0.8 [15, 13, 14] for an extremely broad range of materials. So this universal value is somewhat higher than our results and the results of other simulations.

7.4 Summary and conclusions

In this chapter we present the first results obtained from the simulation with our three-dimensional lattice model. These results, still limited by sample size, show a direction for future research and define the methods rather than allow to make some rigorous statements. However, a few conclusions may be drawn already now.

The comparison between fracture and random percolation of damage as was done in 2D simulation is much less sensible in 3D. Contrary to the two-dimensional case the correspondence between the percolation of damage and the loss of integrity is not valid in 3D. Looking for similarities is still possible, and indeed we find that up to the damage-connectivity-percolation point the damage clusters develop in a very similar way for fracture and random-percolation simulations. However, this point is lower in damage density than the maximum-stress point; what should be compared in fracture and random percolation is the vanishing of the spanning cluster of intact bonds. This comparison is however beyond the present scope and numerical capabilities, and has to our knowledge not been made in the literature either.

We identify the 2D fracture surfaces of our 3D samples by means of a solid-on-solid approximation and estimate their roughness scaling exponents. Our results show that for each sample the power-law scaling is followed quite nicely, even within the limited range of length scales. The obtained values are somewhat lower than the experimentally observed exponents [15], but lie reasonably close to those found in simulations of 3D fuse networks [10, 55] and of the
7.4. Summary and conclusions

Born model [58]. However, much better statistics than available to us is needed to estimate the roughness exponent with acceptable accuracy and to find out whether the exponent depends on the disorder strength or not.

Further work on 3D simulations is in progress, the first objective being acceleration of the simulation code.
7. Simulation of brittle fracture in 3D
Chapter 8

Local fracture avalanches and self-organized criticality in brittle and polymer-like failure

In the present chapter we focus our research on the statistics of the avalanches of fracture events. We study brittle fracture first, exploiting the model for brittle failure that we used in Chapters 4 and 5. Next we concentrate on polymer-like failure, that is, on the large-deformation behavior up till plastic flow; final fracture after strain hardening is beyond our scope. In molecular terms, we concentrate on the rupture of cohesive bonds between polymer segments. We show that such failure can be mimicked by extending our model via the introduction of a fraction of unbreakable bonds. In both cases the analysis is performed in the spirit of self-organized criticality, but the results also shed further light on our earlier findings regarding random percolation at high disorder.

The extended model is described by two parameters: the disorder strength $\alpha$ of the breakable (weak) bonds, and the fraction $\beta$ of such bonds. For the extended model we also investigate the effect of disorder strength on macroscopic features of deformation and breakdown. We suggest the idea that disorder alone can be responsible for dramatic qualitative differences in macroscopic response of polymer-like systems. A parallel can be drawn between this idea and the continuum-mechanics research on the influence of thermomechanical history and aging on the post-yield response of glassy polymers [41]. Aging and rejuvenation influence the yield peak and the extent of softening and can indeed be interpreted as reducing, respectively increasing, the disorder in the weak Van der Waals bonds.
Figure 8.1: Stress (upper graph) and damage (lower graph) vs strain for brittle lattices with uniform disorder (the case with $\alpha = 0, \beta = 1$, which is treated as the reference case) and for lattice linear size $L = 50$; the data are averaged at constant strain over all samples.

### 8.1 Brittle failure

We have chosen the case of a fully breakable lattice ($\beta = 1$) with uniform threshold disorder ($\alpha = 0$) as the reference one, in view of the fact that a similar system (a fuse model with uniform disorder) was already extensively analyzed in terms of SOC [79]. Therefore we first validate the findings of this publication for our more complex spring model, next investigate the effect of disorder strength and only then introduce a fraction of unbreakable bonds.
8.1. Brittle failure

8.1.1 Self-organized criticality in the brittle fracture of lattices with uniform disorder

Macroscopically the behavior of the lattices with $\alpha = 0, \beta = 1$ looks as follows (Fig. 8.1). Stress builds up from zero level to the maximum almost linearly with an insignificant decrease of the slope. After the maximum the stress drops down rather rapidly. On the stress-strain curve averaged over many samples the decay of the stress looks quite smooth, while for each individual sample the drop is much more rapid and saw-tooth-like. The process can be also described in terms of damage development. The damage $p$ grows with a nearly constant rate within the initial phase but the growth accelerates on approach of the maximum-stress point (Fig. 8.1). Damage quickly saturates near the point of final failure.

When we consider $p$ as the order parameter of a system developing towards failure, and plot it against the driving parameter $\sigma$ (see Chapter 2, Section 2.4) we can recognize the approach of a critical point, with a diverging damage rate $dp/d\sigma$ at the yield stress $\sigma_Y$ (Fig. 8.2). Following [79] we will analyze this in terms of self-organized criticality (SOC). To that end we divide the range between zero and the maximum-stress point into bins and calculate the distribution of avalanches (collective fracture events between two subsequent stable points of applied load, see Sections 2.4 and 3.3) for every bin; for practical purposes we take these bins evenly spread in strain rather than stress, which may be easily corrected for via a proper normalization. As can be seen in Fig. 8.3,

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure8_2.png}
\caption{Damage vs reduced stress up to the yield point for the case with $\alpha = 0, \beta = 1$ and for lattice linear size $L = 50$; the data are averaged over all samples}
\end{figure}
Failure avalanches and self-organized criticality...

Figure 8.3: Unnormalized avalanche-size distributions (a), normalized avalanche-size distributions with curves shifted for clarity (b), and the corresponding scaling function (c) for 10 bins (yield point at $\varepsilon = 0.005$), for the case of $\alpha = 0, \beta = 1$ and for lattice size $L = 50$; black solid lines demonstrate the slope with $\gamma = 1.9$, i.e. the power-law SOC scaling

\[ n_a(\varepsilon) = \left( \frac{a}{a_0} \right)^{-\gamma} f\left(\frac{a}{a^*(\varepsilon)}\right); \quad (8.1) \]

the scaling function $f$ is constant for $x \lesssim 1$ and has a strain-dependent cut-off $a^*(\varepsilon)$. We observe the same power-law exponent $\gamma = 1.9$ as found by the authors of [79] for a random-fuse model (Fig. 8.3). The cut-off of the distribution as well as the maximum avalanche size noticeably increase with increasing strain, which is best seen in Fig. 8.3-b. The appropriateness of the chosen
8.1. Brittle failure

Figure 8.4: Divergence of the cut-off $a^*$ of the avalanche-size distribution (a), and scaling divergence of the second moment $\langle a^2 \rangle$ of the avalanche-size distribution with the exponent $\delta = \tau - \gamma$ (b); both singularities correspond with $\sigma_c$ equal to $\sigma_Y$; data are for the case of $\alpha = 0, \beta = 1$ and for lattice size $L = 50$.

Figure 8.5: Cumulative avalanche-size distributions up to strains $\varepsilon = 0.003, \varepsilon = 0.004, \varepsilon = 0.005$ for the case of $\alpha = 0, \beta = 1$ and for lattice size $L = 50$; the solid lines correspond to least-square fitting of the scaling parts of the curves, with fitted slopes approximately equal $-3.0$.

scaling exponent $\gamma = 1.9$ is supported by Fig. 8.3-c where we plot the scaling function of the distribution. In spite of the high noise it can be observed that the function has a plateau at low arguments followed by a fast decay. It
8. Failure avalanches and self-organized criticality...

Figure 8.6: Density of breaking events in the early stage of deformation at $\varepsilon = 0.00075$ (a), and right before the maximum-stress point at $\varepsilon = 0.00425$ (b); breaking events of all avalanches are artificially displaced in such a way that each avalanche has its center of mass in the origin; plots contain avalanches of all samples of size $L = 50$; the intensity of gray indicates the density of events (white means no events, black - maximum density of events at $\varepsilon = 0.00425$)

is rather complicated to estimate the value of the cut-off of the avalanche-size distribution directly from the shape of distribution but this cut-off can be easily related (as shown in Chapter 2) to the second moment of the distribution as $a^* \propto <a^2>^{1/(3-\gamma)}$, provided that the distribution itself has the form of equation (8.1); this relation has been used to construct Fig. 8.3.

As may be derived from Fig. 8.3-a, the average level of the unnormalized distribution decreases with increasing strain, showing that for higher strain less avalanches happen within one bin. Indeed, the number of avalanches per strain bin, which is the normalization constant of the distribution, is found to have a mild, nearly linear decrease with strain (not shown).

The cut-off $a^*$ rapidly diverges on the approach of the point of maximum stress (Fig. 8.4-a). There is not much qualitative difference for the shape of the curves in Fig. 8.4 whether the bins are equally spread in strain or in stress. However, if we want to apply the formalism of SOC, it is important to use stress as a driving variable to describe the behavior of the cut-off and, consequently, of the damage rate in the range till the maximum-stress point. If stress is employed as a driving parameter, yield naturally becomes a critical point, while in the description with strain the determination of the critical point is not that clear. As seen from Figs 8.1 and 8.2, $dp/d\sigma$ truly diverges on the approach of $\sigma_Y$, contrary to $dp/d\varepsilon$, which always remains limited. We assume therefore that the
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Figure 8.7: Average squared gyration radius $< R_g^2 >$ of single avalanches (a), and squared avalanche correlation length $\psi^2$ (b), as functions of the applied strain for the case of $\alpha = 0, \beta = 1$ and for lattice size $L = 50$

distribution cut-off scales as

$$a^* \propto a^2 >^{1/(3-\gamma)} (\sigma - \sigma_c)^{-1/\delta}.$$  

(8.2)

This scaling law, together with equation (8.1), results in a scaling law for the cumulative distribution in the following form:

$$C_a(\sigma) = \left( \frac{a}{a_0} \right)^{-\tau} G(a/a^*(\sigma)),$$  

(8.3)

where $\tau = \gamma + \delta$. This result follows (as shown in Chapter 2, Section 2.4) directly from the integration of the appropriately normalized avalanche size distribution (8.1).

Indeed we find that the cumulative distribution of avalanche sizes over an interval from 0 to strain values within the regime where the scaling of the local avalanche-size distribution $n_a$ is noticeable, scales with the exponent $\tau = 3.0$ (Fig. 8.5). This value is in a good agreement with the value $\tau = 3.05$ obtained by the authors of [79] for the random-fuse model. It implies that $\delta = \tau - \gamma = 1.1$. If we plot $< a^2 >^{\delta/(\gamma-3)}$ against $\sigma$ taking the thus estimated values of the exponents ($\gamma = 1.9, \tau = 3.0$), the result looks like a straight line only in the range corresponding to the last six bins (Fig. 8.4-b), i.e. exactly those bins for which a noticeable scaling part of the avalanche size distribution is observed (Fig. 8.3). The resulting value for $\sigma_c$ nicely corresponds with $\sigma_y$.

The picture above is not complete without information about the spatial extent of the avalanches. Spatial characteristics of avalanches can be visually depicted by plotting them in such a way that the centers of mass of all avalanches coincide (Fig. 8.6). It is seen that avalanches are quite broad from the
very beginning, i.e. the maximum spread of avalanches does not increase significantly. Nevertheless, the average extent of avalanches turns out to increase; this observation indicates that the typical range of influence of a breaking event increases. A slight anisotropy of the central part of the avalanche cloud can be noticed near the point of maximum stress (Fig. 8.6-b). Quantitatively the spatial behavior of avalanches can be described similar to damage clusters in percolation theory: by their gyration radius and correlation length. The former is defined for each avalanche as

$$\rho^2 = \sum_{i=1}^{a} \frac{|r_i - r_{cm}|^2}{a},$$

(8.4)

where $a$ is the size of an avalanche, $r_i$ stands for the location of a breaking event and $r_{cm}$ is the center of mass of all breaking events of one avalanche. The correlation length is defined as the weighted average distance between two events of the same avalanche and is calculated as

$$\psi^2 = \frac{2}{a} \sum_{i} \frac{a_i^2 \rho_i^2}{\sum_i a_i^2},$$

(8.5)

where index $i$ is the number of an avalanche and summation covers all avalanches.

The average avalanche gyration radius and avalanche correlation length have a similar behavior until the maximum-stress point: they are both monotonically increasing concave functions of $\varepsilon$ (Fig. 8.7). After the maximum-stress point the gyration radius slightly increases till its own maximum which is located at somewhat higher strain than the maximum-stress point. Then the gyration radius decreases rapidly near final breakdown. Contrary to this behavior the correlation length stays at a high level and insignificantly decreases just before the final failure. The drop of the gyration radius can be explained by the presence of small (in terms of spatial extent and number of events) avalanches that are required for the coalescence of already existing ruptures. The high level of the correlation length shows the presence of large (in spatial extent and in number of events) avalanches, which are however not so many in number compared with the smaller avalanches.

8.1.2 Influence of disorder strength on avalanche statistics and damage build-up in brittle fracture

A change in disorder strength does not lead to a serious qualitative difference of the stress-strain dependence. As seen from Fig. 8.8 increase in disorder mostly influences the length of the post-yield regime by increasing it. The shapes of the pre-yield parts of the curves change as well though not significantly. At the same time the behavior of the damage and damage growth rate does change
8.1. Brittle failure

Figure 8.8: Stress-strain dependencies for brittle fracture ($\beta = 1$) and varying disorder strength $\alpha$. Stresses have been scaled to have the same maximum while strains have been scaled to have either a common failure point (a) or a common maximum-stress points (b); data are averaged over all samples of size $L = 50$.

Dramatically. In the reference case with $\alpha = 0, \beta = 1$ the damage growth rate $\frac{dp}{d\varepsilon}$ maintains nearly a constant level during the initial phase of deformation, dramatically rises on the approach of the maximum-stress point and rapidly drops to zero after that (Fig. 8.9-a). Already for $\alpha = 0.3$ the picture is different: the damage growth rate has a much higher value in the beginning, steeply drops and then rises up again while passing the maximum-stress point (Fig. 8.9-b); in the end it rapidly drops to zero as in the case of $\alpha = 0$. The initial peak of $\frac{dp}{d\varepsilon}$ becomes higher with increasing disorder while the second peak gets smaller (relative to the first one) and practically vanishes for $\alpha$ above 0.6 (Fig. 8.9-c,d). Note that this peak near $\varepsilon_Y$ in the damage growth rate vanishes around the same disorder strength ($\alpha = 0.6$) beyond which in Chapter 5 a percolation-type regime of damage development could be identified.

The scaling law (8.1) of the avalanche-size distribution is followed nicely for all considered values of $\alpha$. Moreover, the value of the scaling exponent $\gamma = 1.9$ found for $\alpha = 0$ remains the same for all cases. We show only the results for $\alpha = 0.7$ (Fig. 8.10) in view of the similarity for all values of disorder strength. Contrary to this similarity, the behavior of the number of avalanches per bin (Fig. 8.11-a) and the cut-off $a^*$ of the distribution (as calculated from the second moment $< a^2 >$, Fig. 8.11-b) are different from the reference case. The number of avalanches decreases much more steeply for stronger disorder. The behavior of the cut-off remains qualitatively the same though it seems to diverge faster for weaker disorder.

The cumulative avalanche-size distribution for the case with $\alpha = 0.7$ and at the point of maximum stress shows two scaling regimes, with distinct expo-
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Figure 8.9: Damage growth rate $\frac{dp}{d\varepsilon}$ vs strain for brittle fracture ($\beta = 1$) and with different values of $\alpha$, for lattice linear size $L = 50$; the data are averaged over all samples; the increase at moderate strain and the post-yield peak disappear for disorder strengths above $\alpha = 0.6$.

components: $\tau_1 = 1.9$ and $\tau_2 = 3.3$ (Fig. 8.12). The latter is close to the exponent $\tau = 3.0$ obtained for $\alpha = 0$, while $\tau_1 = 1.9$ equals the scaling exponent $\gamma$ for $\alpha = 0$. This behavior of the cumulative distribution deviates from the pure SOC statistics seen in the reference case $\alpha = 0$, and indicates the presence of small avalanches with different cut-off statistics and hence a different type of distribution. It fits into the picture presented in Chapter 4, of initial short-range localization of fracture before, at larger scales, the strong disorder induces random percolation of damage. In terms of SOC it could mean growing avalanches of small, fixed-size avalanches rather than of single fracture events. The scaling of the second moment of the avalanche-size distribution with the exponent $\delta = 1.4$ following from the values of $\gamma = 1.9$ and $\tau_2 = 3.3$ is confirmed by Fig.
8.1. Brittle failure

Figure 8.10: Development with strain (yield point at $\varepsilon_Y = 0.247 \times 10^{-3}$) of the unnormalized avalanche-size distribution for brittle fracture with high disorder ($\beta = 1$, $\alpha = 0.7$) and for lattice size $L = 50$; black solid lines demonstrate the power-law exponent $\gamma = 1.9$.

Figure 8.11: Number of avalanches (a) and the cut-off of the avalanche distribution (b) as functions of reduced stress for brittle fracture ($\beta = 1$) and for different values of the disorder strength $\alpha$; lattice size $L = 50$.

8.13. In other words, $\delta = 1.4$, $\gamma = 1.9$ and $\tau_2 = \delta + \gamma = 3.3$ form a consistent picture for $\alpha = 0.7$, similar to that for the case with $\alpha = 0$. These values of exponents are also numerically close to those for $\alpha = 0$. In this respect of avalanche size (mass) scaling, disorder has little influence, the most striking effect being
the deviation in the cumulative distribution at small sizes (Fig. 8.12).

However, the spatial behavior significantly changes for higher disorder. The dependence of the avalanche correlation length $\psi$ as a function of the reduced
stress becomes less steep with increasing disorder (Fig. 8.14-a) and its level is higher. This observation tells that for high disorders the average range of influence of a breaking event is large from the beginning and does not increase very much up to the yield point. It supports, in turn, the idea of similarity between fracture with high disorder and percolation: damage spreads more evenly throughout the sample from a very early stage of deformation onwards. We have now noticed similar trends in the dependence on disorder strength of the behavior of the correlation length $\psi$ and of the second moment $<a^2>$: for high disorder they are both quite large already in a early stage of deformation, and grow with stress less steeply. The dependence of $\psi^2$ on the second moment of the avalanche-size distribution is surprisingly universal for the considered values of $\alpha$ (Fig. 8.14-b). Hence, irrespective of disorder strength, for a given correlation length one finds roughly the same value of $<a^2>$, i.e. the relation between the average spatial extent of avalanches and their number size is universal, independent also of marked differences in the anisotropy of the fracture patterns (see Chapter 5).

8.2 Polymer-like failure

The new simulation feature which we introduce in our model in order to reproduce polymer-like behavior is that only a certain fraction of bonds, denoted $\beta$, remains breakable, whilst the rest of bonds (with the same modulus) are unbreakable, i.e. they have infinitely high thresholds. The thresholds of breakable
bonds remain distributed according to a power law (3.11), as they did in the initial model.

We consider two cases, with different disorder: $\alpha = 0$, which corresponds to the uniform threshold distribution, and $\alpha = 0.7$, which gives a distribution with an algebraically diverging tail of very weak bonds. From the point of view of mathematical description, the existence of unbreakable bonds can be interpreted as an additional peak of threshold distribution at infinity. The analogy between our model and real polymers is based on the idea that breakable (weak) bonds represent Van der Waals interactions while unbreakable (strong) ones stand for chemical bonds in polymer chains and topological entanglement constraints between chains. It is obviously a very idealized toy-model analogy, which nevertheless qualitatively captures, as our results show, some important features of polymer behavior under large deformation, i.e. when equilibrium Van der Waals bonds are ruptured.

Our simulation is done for sets of samples, each for a particular lattice size $L$, in order to obtain statistically reliable data. As before, by size we mean the number of bonds per lattice side, while the actual width and height of the lattices remain equal to 1. Simulations are performed for a range of sizes ($L = 25, 50, 100, 200$) and for various fractions $\beta$ below 1; the fraction $\beta = 0.33$ thereby represents the threshold value below which for the present type of (infinite) lattice the percolation of permanent bonds is guaranteed. In the present chapter we, as earlier in Chapters 4 and 5, base our detailed analysis on one particular lattice size $L = 50$ which has sufficient statistics of samples and still is not too small.
As seen from the stress-strain curves of our model (Fig. 8.15), the behavior of lattices drastically change for $\beta$ around 0.33. For small values of $\beta$, the small amount of breakable bonds in the system are only able to slightly bend the curve downwards. Around $\beta = 0.3$ a yield peak first appears. This peak is followed by a hardening regime when $\beta$ remains below 0.33. The cases with $\beta = 0.33$ and higher have a long flow regime. In particular the case with the fraction of breakable bonds equal to 0.3 resembles a typical response of polymers.

To reveal the effect of disorder in the breakable bonds we compare the stress-strain curves corresponding to two different disorder cases (uniform disorder and power-law disorder with $\alpha = 0.7$) for $\beta = 0.3$ (Fig. 8.16). The graphs clearly show that increasing disorder suppresses the yield peak on the softening-
hardening curve, leaving the value of strain at which the inflexion occurs unchanged. We may more generally define this inflexion point as the yield point, also in absence of a peak. In real polymers a yield peak is similarly superimposed upon a monotonous stress-strain curve when the material ages, i.e. when the Van der Waals interactions induce local ordering with time [41].

The damage-stress relationship on approach of the yield point strongly depends on the disorder strength (Fig. 8.17). In the initial phase damage accumulates much faster for $\alpha = 0.7$. Then, in the intermediate regime, damage grows with comparable rates for both cases. Close to yield, damage growth accelerates, with a diverging rate both for $\alpha = 0$ and $\alpha = 0.7$, though the growth is steeper for the uniform-disorder case.

### 8.2.1 Damage development before the yield point

Before studying for the polymer-like lattices the avalanche statistics, as in Section 8.1 for the brittle lattices, we will first analyze the damage development before yield in terms of percolation patterns, as in Chapters 4 and 5. To that end we consider the statistics of the damage clusters, in particular the second moment $M_2$ of the cluster-size distribution and the spatial cluster correlation length $\xi$. Our results make clear that for uniform disorder ($\alpha = 0, \beta = 0.3$) the second moment of the cluster-size distribution as well as the correlation length are deviating very significantly from the random-percolation data (not shown); this is in line with the results of Chapters 4 and 5. Based on those chapters, some similarity in the behavior of $M_2$ and $\xi$ between random percolation and our deformation simulation with high disorder ($\alpha = 0.7, \beta = 0.3$) might be ex-
Figure 8.18: Second moment $M_2$ of the damage cluster-size distribution and correlation length $\xi$ of the clusters, as functions of $|p - p_c|$ in the pre-yield regime for the polymer-like case with strong disorder ($\alpha = 0.7, \beta = 0.3$), and for lattice linear size $L = 50$; the data are averaged over all samples; the straight lines are consistent with RP scaling.

8.2. Polymer-like failure

Expected. Surprisingly enough, the data corresponding to this polymer-like case (Fig. 8.18) not only lie very close to the random-percolation results but also suggest an improvement of the similarity to the latter when compared with the brittle case $\alpha = 0.7, \beta = 1$. In particular, the scaling regimes of $M_2$ and $\xi$ become slightly larger (Fig. 8.18). It is interesting to note that the initial short-range localization that we observed for fracture of fully breakable lattices (see Chapter 4) and that caused deviation of the correlation length from the percolation-like scaling behavior at low values of $p$, is less pronounced in the presence of unbreakable bonds. Apparently, unbreakable bonds bear some stress redistributed due to breaking and, consequently, screen breakable ones from each other.

In order to verify the presence of the percolation-like scaling regime more
8. Failure avalanches and self-organized criticality...

![Figure 8.19: Scaling function of the cluster-size distribution within the pre-yield scaling regime for the polymer-like case with strong disorder (α = 0.7, β = 0.3), and for lattice linear size L = 50; the data represent averages over all samples; scattered data for large s are excluded; curves are levelled vertically to match one another]

profoundly we test the possibility to construct a scaling cluster-size distribution according to (4.8). From Fig. 8.18 we thereby define the scaling regime to run from \( p = 0.09 \) to \( p = 0.2 \). The result (Fig. 8.19) indeed allows to say that the percolation-like cluster statistics is nicely followed. Hence we can conclude that the approach of the yield peak in polymer-like lattices is qualitatively the same as in the brittle case: a percolation-like regime is clearly present, but only for high disorder. The agreement between the failure data and the data for random percolation is even better than in the brittle case.

8.2.2 Fracture-avalanche statistics before and after yield

After studying the percolation statistics and confirming for polymer-like lattices our earlier findings as regards similarity to random percolation for high disorder, we will analyze the statistics of avalanches in terms of self-organized criticality. We consider first the case with \( \alpha = 0 \) (for which we have confirmed the validity of SOC statistics in the brittle case) but now with only a finite fraction of breakable bonds (\( \beta = 0.3 \)) and for the two ensuing deformation regimes: the one before and the one after yield.

The detailed avalanche statistics for \( \alpha = 0, \beta = 0.3 \) (not shown) in the range up to the yield point is very similar to our results for \( \alpha = 0, \beta = 1 \), though the scaling exponent of the distribution slightly changes, from \( \gamma = 1.9 \) to \( \gamma = 1.7 \). The cumulative distribution of avalanche sizes in the range up to yield also behaves similar to the brittle case (Fig. 8.20-a). Again, only the governing exponent becomes lower: \( \tau = 2.3 \) instead
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Figure 8.20: The case of $\alpha = 0, \beta = 0.3$

(a) The cumulative avalanche-size distribution for the polymer-like case with strong disorder ($\alpha = 0, \beta = 0.3$) with interval end points before and after the yield peak $\varepsilon_Y = 0.027$; the latter intervals show an upcoming shoulder with a different slope within the distribution; curves are shifted for clarity;

(b) The cumulative distribution for the separate pre-yield and post-yield intervals, with distinct slopes $-2.3$ and $-1.6$ respectively

of previously observed $\tau = 3$. Soon after the yield point $\varepsilon_Y$ a shoulder with a new slope emerges within the distribution, and gets wider when $\varepsilon$ increases. The difference in the avalanche statistics before and after yield becomes more clear if we split the full strain range into two parts (Fig. 8.20-b): $[0, \varepsilon_Y]$ and $[\varepsilon_Y, \varepsilon_D]$, where $\varepsilon_D = 0.08$ is the strain at which stress starts to build up again after drop. Apparently, the avalanche-size distribution is described by different scaling laws (or, at least, by the same law with different exponents) before and after yield. The scaling exponent of the post-yield regime is found to be $1.6$, which is very close to $\gamma$ in this case. One can recall (see Section 2.4) that the scaling exponent $\tau$ of the cumulative distribution is a sum of $\gamma$, which comes from the form of the distribution per strain bin, and $\delta$, which is the scaling exponent of the cut-off $a^*$. If the distribution changes in such a way that it does not have a cut-off anymore or that its cut-off is constant, equation (2.60) will have only $a^{-\gamma}$ in the pre-factor of the integral. Consequently, $\tau$ will become equal to $\gamma$. This explains the exponent of the post-yield cumulative distribution. To confirm this explanation we study in the next section more closely the case which corresponds to a long post-yield flow regime: the one with $\alpha = 0, \beta = 0.33$. 


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8.3 Self-organized criticality around the yield point

8.3.1 Avalanche scaling during stress build-up, stress drop and flow

In this section we will focus on the influence of a polymer-like yield peak on
SOC, in particular on commonalities and differences with SOC as observed in
the brittle reference case ($\alpha = 0, \beta = 1$). To eliminate the effects of the
permanent strain-hardening network we choose the critical case $\alpha = 0, \beta = 0.33,$
which has a long flow regime after the stress drop.

![Figure 8.21](image)

Figure 8.21: Normalized avalanche-size distributions for 10 bins within the pre-yield
(a) and post-yield (b) regimes, for the polymer-like case with uniform disorder and no
strain hardening ($\alpha = 0, \beta = 0.33, L = 50$); curves are shifted for clarity; black solid lines
demonstrate the power law with exponent $\gamma = 1.7$

Fig. 8.21-a gives the avalanche statistics for subsequent strain bins up to the
yield point. Comparison with Fig. 8.3-b shows that the presence of unbreakable
bonds does not change the statistical size properties of avalanches significantly
within the pre-yield regime. The avalanche-size distribution obeys the same
scaling law, although with a somewhat lower exponent (1.7 instead of 1.9). Also
other aspects of SOC scaling (not shown) are in this regime similar to those for
brittle lattices, with minor deviations in the exponents: $\delta = 0.9$ (instead of 1.1)
for the power-law divergence of the cut-off $a^*$ (equation (8.2)) and $\tau = 2.4$ (in-
stead of 3.0) for the cumulative distribution of avalanche sizes (equation (8.3)).
Qualitatively the behavior of the spatial characteristics (avalanche gyration ra-
dius $\rho$ and correlation length $\psi$) remains the same as well. Deviations may still
be due to statistical errors. A clear contrast is seen when the avalanche statistics
is analyzed for bins after the yield peak (Fig. 8.21-b). The power-law scaling,
with a constant exponent, extends over almost the full range of avalanche sizes.
8.3. Self-organized criticality around the yield point

Clearly, the cut-off size $a^*$ has been replaced by another, constant cut-off, likely determined by sample size. Detailed analysis shows that in this region of very large avalanches and strong noise the average distribution actually slightly tilts upwards. In any case the full distribution can no longer be represented by a law like (8.1), with the dependence on $\varepsilon$ (or $\sigma$) only via a cut-off $a^*$.

The damage growth rate $dp/d\varepsilon$ in the present polymer-like case behaves similar to that for the brittle case with $\alpha = 0$ up to $\varepsilon_Y$ which, in the former case, almost coincides in strain with the maximum of $dp/d\varepsilon$ (see Fig. 8.22-a). The damage growth rate in respect to stress, $dp/d\sigma$, strongly diverges on the approach of the yield point which is again similar to the corresponding brittle case (see Fig. 8.22-b).

We consider again the spatial characteristics of avalanches as described by the correlation length, to study any possible effect of finite size. As seen from Fig. 8.23-a, $\psi^2$ on average keeps the level it has reached by the yield point. This saturation is likely related to the finite size of the samples. The relation of the correlation length with $a^*$ can no longer be determined, but with $< a^2 >$ it can (see Fig. 8.14-b). As seen from Fig. 8.23-b the dependence of $\psi^2$ on $< a^2 >$ is qualitatively the same, up to the yield point, as for the reference brittle case. In the post-yield regime the curve fluctuates around its state at the yield point, which is completely logical since both $\psi^2$ and the avalanche-size distribution do not exhibit noticeable changes after yield.

Figure 8.22: Damage growth rate $dp/d\varepsilon$ for a wide range of strain (a) and $dp/d\sigma$ in the range up to the yield point (b) for the polymer-like case with uniform disorder and no strain hardening ($\alpha = 0$, $\beta = 0.33$, $L = 50$); $\sigma = \sigma_Y$ is again a critical point.
8. Failure avalanches and self-organized criticality...

Figure 8.23: Squared avalanche correlation length $\psi^2$ as a function of strain (a) and vs the second moment of the avalanche-size distribution $<a^2>$ for the polymer-like case with uniform disorder and no strain hardening ($\alpha = 0, \beta = 0.33, L = 50$); both graphs cover the same range of strain.

8.3.2 Influence of disorder

The main effect of the disorder on the macroscopic response of the lattices is in the behavior of the yield peak. As we have seen, increasing the disorder strength suppresses the yield peak, i.e. makes it wider and ultimately vanishing. For the critical fraction of permanent bonds $\beta = 0.33$ a yield peak is still visible even at the highest disorder considered ($\alpha = 0.7$). However, if the fraction of breakable bonds is slightly lowered, high disorder is capable of suppressing the yield peak completely, like it happens for $\alpha = 0.7, \beta = 0.3$ (Fig. 8.16). To study avalanche behavior in absence of a yield peak we therefore choose the latter case.

Similar to the case of fully breakable lattices, we find that in the presence of permanent bonds the scaling exponent of the avalanche-size distribution is independent of disorder strength and equals $\gamma = 1.7$ both for uniform disorder with a pronounced yield peak ($\alpha = 0, \beta = 0.3$ and 0.33) and for strong disorder with a suppressed yield peak ($\alpha = 0.7, \beta = 0.3$, not shown). In fact, increasing the disorder strength does not change the general picture, and all the differences are in details. The presence of a lower initial slope in the cumulative avalanche-size distribution for the case $\alpha = 0.7, \beta = 0.3$ is noticeable already at the yield point (see Fig. 8.24-a), i.e. earlier than for the cases with uniform disorder. We note again that in absence of a yield peak, the yield point is defined as the inflexion point of the stress-strain curve. The cumulative distribution over the interval from the yield point to the end of simulation shows a good scaling with the exponent $-1.6$ close to $\gamma$ (Fig. 8.24-b), exactly like in the case with low disorder (Fig. 8.20-b).
Figure 8.24: Cumulative avalanche-size distribution for the polymer-like case without a yield peak, but with the yield point $\varepsilon_Y = 0.015$ defined as an inflexion point ($\alpha = 0.7, \beta = 0.3, L = 50$) in the range from $\varepsilon = 0$ to $\varepsilon_Y$ (a) and for the post-yield range from $\varepsilon_Y$ to $\varepsilon = 0.3$; solid lines in (a) correspond to the slopes $-2.3$ and $-2.8$; the solid line in (b) follows the slope $-1.6$.

Figure 8.25: Squared correlation length $\psi^2$ vs second moment $< a^2 >$ of the avalanche-size distribution for the pre-yield (a) and post-yield (b) regimes; data are for the case of $\beta = 0.3$, two different values of $\alpha$ and for lattice size $L = 50$, and show a marked universal trend.

Having now studied both brittle and polymer-like behavior, with both uniform and strong disorder, it is interesting to look again at the avalanche correlation length $\psi$ and the average squared avalanche (number) size $< a^2 >$. Already in Fig. 8.14-b (brittle fracture) we observed a surprising universality of
the relation between $\psi^2$ and $<a^2>$ for different values of disorder strength. Combining all data for $\beta = 1$ and $\beta = 0.3$ and for two extreme values of $\alpha$ (0 and 0.7) we continue to see the same universality of the dependence, both in the pre-yield (Fig. 8.25-a) and post-yield (Fig. 8.25-b, only for $\beta = 0.3$) regimes. For the post-yield phase the curves turn backwards due to the decrease of $<a^2>$ after yield, with a strong scatter. So both for the brittle and polymer-like cases, disorder strength does not change the relation between $\psi^2$ and $<a^2>$, but only defines the part of the curve that is traversed by a system. Systems around yield correspond to a saturation of the avalanche correlation length, likely due to a finite-size effect. The systems with high disorder also occupy the upper part of the universal curve, which supports the idea of random damage development and similarity to random percolation.

8.4 Summary and conclusions

In the present chapter we demonstrate the possibility to control the yield peak and post-yield behavior of a two-component lattice model by means of changing the fraction of breakable bonds and the disorder strength in these bonds. This relatively simple model turns out to be capable of reproducing qualitatively a polymer-like stress-strain behavior. Clearly, the disorder strength governs the behavior of the yield peak, while together with the fraction of breakable bonds it changes the post-yield response from brittle to flow or hardening.

The value of $\beta$ at which a yield peak and stress drop start to be observed is close to percolation threshold ($0.3333$) for infinite random lattices. The range of $\beta$ for which sufficient hardening is observed after softening, is extremely small. For $\beta$ slightly above the percolation threshold the softening part of the response is not followed by hardening but by flow.

Localization of damage is dependent on both $\alpha$ and $\beta$. Weakening the disorder strength or increasing the fraction of breakable bonds leads to escalated aggregation of damage. Diluting the lattice with unbreakable bonds acts against localization rather strongly although it is not an effective means if the disorder is weak. The effect of the disorder strength on the yield peak in our model is in line with experimentally observed influence of thermomechanical history (aging vs rejuvenation) of polymer samples on the strength of the yield peak. In this analogy aging is interpreted as ordering in the breakable cohesive bonds, while rejuvenation represents a return to the initial disordered state.

The percolation-like statistics is nicely followed in the case of strong power-law disorder ($\alpha = 0.7$) not only for high fractions of breakable bonds, which is obvious, but also for a relatively small one ($\beta = 0.3$). The latter is understandable since the similarity regime lies way before the formation of a sample-spanning percolating cluster and also due to the fact that the universal behavior of percolating lattices is not disturbed by dilution. In fact, in approach of the yield peak the correspondence is even better than in the brittle case.
The progress of damage with increasing strain is via avalanche-like, spatially distributed fracture events. We show that the avalanche statistics in our model can be described using the viewpoint of self-organized criticality. In the reference case of fully breakable lattices with uniform disorder ($\beta = 1, \alpha = 0$) the distribution of avalanche sizes follows a power law with a cut-off that diverges on approach of the maximum stress. The governing exponent is found to be $\gamma = 1.9$, which coincides with the value obtained for fuse networks [79]. Increasing the disorder strength from $\alpha = 0$ to $\alpha = 0.7$ does not destroy the power-law scaling of the avalanche-size distribution. Moreover, the exponent $\gamma = 1.9$ remains unchanged. Contrary to that, the behavior of the number of avalanches per strain interval and of the cut-off in the distribution do change considerably.

For the lattices with polymer-like behavior ($\alpha = 0, \beta = 0.3$ and $0.33$) the power-law scaling of the avalanche-size distribution is still followed, though with a somewhat lower governing exponent $\gamma = 1.7$. The statistics in polymer-like lattices within the post-yield regime is clearly different from the one before yield. The difference manifests itself via a distinct, constant behavior of the cut-off and, consequently, via a different scaling exponent of the post-yield cumulative distribution of avalanche sizes. All sizes of avalanches appear, seemingly only restricted by sample dimensions.

A major increase of the disorder strength ($\alpha = 0.7$) within polymer-like lattices does not change the scaling exponents of the avalanche-size distribution. Exactly like in the brittle case, disorder mostly influences the behavior of the spatial correlation length and the average squared size of avalanches. For the cases with uniform disorder, the squared correlation length increases about ten times within the interval from zero strain till yield. Contrary to that, for high-disorder cases the correlation length is high already at low strain and does not change much when approaching and going beyond the yield point. The long range of spatial correlation within an avalanche for strong disorder supports our earlier conclusions about the similarity between random percolation and fracture of highly disordered lattices.

The dependence of the correlation length of avalanches on the second moment of the avalanche-size distribution is found to be surprisingly universal (independent of the disorder strength) both for the brittle case and the polymer-like pre-yield and post-yield cases. Within statistical error, disorder does not change the shape of the curve, but defines what range of the curve is traversed. This numerical universality is in marked contrast with the large differences in many detailed aspects of the failure process of the different systems.
Chapter 9
Conclusions and outlook

9.1 General aim of the work

The general goal of the present thesis can be formulated as "understanding the role of disorder in brittle and polymer-like material failure". The main focus was therein on generic and universal aspects of pattern formation. Following other authors we chose to use the method of simulations, as such a problem is hardly possible to handle analytically, unless formulated in an extremely simplified form. Lattice models were chosen as they had already proved to be a convenient tool to handle the simulation of breakdown in disordered materials. We did not want to sacrifice the vectorial nature of material deformation for the sake of reducing the numerical complexity. Therefore central-force lattices were preferred to more frequently used fuse networks, which represent a scalar analogy of vectorial elasticity. Key questions to be addressed were: the validity of claimed similarity between fracture and random percolation of damage, the emergence of the universal scaling in the crack-surface roughness, the possibility to describe fracture as a self-organized critical phenomenon, and the extension of such models, concepts and findings to polymer-like behavior. In our work we mostly dealt with two-dimensional lattices, though some simulations could also be done in 3D for a limited range of lattice sizes.

9.2 Summary of main results and conclusions

The first results of our two-dimensional simulations that are described in Chapter 4 address the question of similarity between fracture with a strong power-law disorder of local thresholds and random percolation of damage. Comparing the two is important since it allows to reveal those aspects of fracture that are driven by disorder. We find that for the case of strong disorder (with the
exponent of the threshold distribution $\alpha = 0.7$) damage develops in three different stages. Initially a localized growth of small fractures occurs everywhere in a sample. In the second stage the effect of disorder takes over and damage progresses in a percolation-like way, with random coalescence of different damage clusters. Already before the point of maximum stress easily noticeable macroscopic localization sets in, with a rough final crack preferentially growing in the direction perpendicular to the loading.

Next to the analysis of the similarity between random percolation and fracture with one particular disorder strength, we analyzed in Chapter 5 systematically the influence of disorder on the fracture process. The main conclusion of this analysis is that the pattern of damage development is qualitatively different for high and low disorder. The highest degree of disorder that computationally could be handled was $\alpha = 0.75$, while theoretically the limit of infinite disorder is $\alpha = 1$. For the former case we confirmed our earlier findings of Chapter 4 that damage in fracture develops in the three aforementioned stages. The percolation-like regime rapidly shrinks with decreasing disorder exponent and vanishes around $\alpha = 0.6$ (at least for the considered sample sizes). For even weaker disorder the damage development is anisotropic from the beginning, which rules out any similarity with random percolation. For all disorder strengths macroscopic localization of damage sets in around the maximum stress, and leads to a final crack. Our analysis for different disorders creates a more clear picture on the conclusions from similar studies in the literature, which use a variety of disorder strengths and come to varying results as regards percolation. The theoretical claim of similarity between random percolation and breakdown (at least in the fuse picture) in the limit $\alpha \to 1$ of infinite disorder, is not inconsistent with our results.

In Chapter 6 we analyze the roughness scaling exponents that result from our 2D fracture simulations. We find that power-law dependence is obeyed very nicely over more than three decades in lengthscale, only limited by the maximum size of the lattice. The roughness of the crack profile is surprisingly independent of disorder strength. However, the precise value of the roughness-scaling exponent turns out to depend on details of the definition of the crack surface, but is anyway in good agreement with other numerical and experimental results.

In the analysis of our 3D simulations in Chapter 7 we mainly focus on the roughness of fracture surfaces. Although the available range of lattice sizes is small, the roughness within this size range is found to follow a power-law dependence, with exponents reasonably close to values found by other studies. It is plausible that the exponent is independent of disorder like in 2D simulations, though the statistical quality of our 3D results is not enough to make rigorous conclusions. The question of similarity between fracture and random damage percolation is left out of the scope, in view of the fact that an analogy - if any - is more complex in three dimensions, being related to the vanishing of the infinite massive cluster, rather than to the percolation of the damage cluster.
Chapter 7 serves more as a demonstration of the method we were able to develop for 3D than as a report of solid numerical results we obtained, due to the still strong limitation in system size.

In order to mimic the more complex behavior of materials with post-yield mechanical response we modified our 2D model in such a way that only a certain fraction of bonds, denoted $\beta$, remain breakable, while the other bonds have an infinitely high threshold. As described in Chapter 8, it turns out that this simple modification is enough for reproducing qualitatively polymer-like stress-strain curves for values of $\beta$ around 0.3. The effect of the disorder strength on the yield peak in our model is in line with the experimentally observed effect of ordering of weak cohesive bonds by aging: order strengthens the yield peak. In the pre-yield regime percolation-like statistics is followed in the case of strong power-law disorder ($\alpha = 0.7$), even better for $\beta = 0.3$ than for the brittle case ($\beta = 1$).

The progress of damage with increasing strain is via avalanche-like fracture events. We show that the avalanche statistics in our model can be described using the viewpoint of self-organized criticality, with the yield point as a critical point. In the case of fully breakable lattices with uniform disorder ($\beta = 1, \alpha = 0$) the distribution of avalanche sizes follows a power law with a cut-off that diverges on approach of the maximum stress. The influence of high disorder is seen in details. In particular, avalanches spread more widely sooner, confirming the random-percolation picture; this spreading is recognized by an avalanche correlation length. Also for lattices with polymer-like behavior the power-law scaling of the avalanche-size distribution is followed in the pre-yield regime, though with a somewhat lower power-law exponent. The post-yield regime shows a power-law distribution of avalanche sizes at all scales, only limited by system size. In both the brittle and polymer-like cases, disorder mostly influences the behavior of the spatial correlation length and the average squared mass of the avalanches. The relation between the two is found to be surprisingly universal, independent of the disorder strength, for all considered cases. Within statistical error, disorder does not change the form of the relation, but defines what range of the curve is traversed by the various systems. For diverging avalanche sizes there is obviously a finite-size effect, with an important physical interpretation. However, our limited system sizes here still prevent qualitative conclusions.

### 9.3 Recommendations

Finally we want to mention a few directions for future research. First of all, both 2D and 3D simulations need to be extended to larger system sizes and to more massive sample statistics, in order to study finite-size effects with a sufficient accuracy of the results. Secondly, establishing a possible relation of avalanche statistics and the universal roughness scaling may be attempted. The analysis
of fracture in terms of self-organized criticality can be extended both theoretically and by means of simulations. The effect of threshold distributions other than the considered power laws might be promising to look at. The comparison of three-dimensional fracture with the percolation of intact material is still uncovered. Introduction of additional competing length scales and their effects on fracture patterns, e.g. related to reinforcing fillers, can lead to more insight in composite behavior. In order to bridge the present subject with more practical fracture studies, a first promising approach is to search for patterns as observed here also in more realistic particle and polymer models, e.g. via molecular dynamics.
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May 15, 2007
Summary

Pattern Formation and Fracture in Brittle and Polymer-like Failure of Disordered Materials

The aim of the present work is understanding cooperative phenomena that lead to failure in disordered materials. Our research is an attempt to understand fundamental microscopic aspects of materials behavior related to disorder via sufficiently simple but at the same time sufficiently representative models. The main topics of our research are:

- Finding out to what extent the failure of disordered materials is similar to random percolation (RP) of damage or, in other words, whether the failure process of disordered materials is random and delocalized.
- Searching for size-scaling of stress-strain dependencies, and for universality in the size-scaling of crack profiles.
- Analyzing the role of disorder strength systematically.
- Modelling the transition from brittle to polymer-like (ductile) failure by means of changing the statistics of microscopic material properties.
- Analyzing and comparing mechanisms of damage development in the pre-yield and post-yield phases, i.e. within the quasi-elastic regime of the stress-strain dependence and beyond, in particular in terms of self-organized criticality (SOC).

In order to achieve the goal of our research we resort to a computer simulation and analysis of brittle and polymer-like failure by means of two- and three-dimensional lattice models undergoing uniaxial tension. The choice in favor of lattice models has been done because it allows a natural way of introducing disorder and heterogeneity. Another argument for choosing this approach is in the possibility of benchmarking our results with random percolation of damage on the same lattices. Direct comparison with random percolation, for which a lot of theoretical results are known, helps to identify those regimes of failure that are driven by disorder rather than localization.

Our model is not a replacement or a competitor of comprehensive rheological models but a way to understand the underlying physics. Unlike many other works which also exploit lattice (or network) models, we use central-force spring lattices instead of fuse network models (a scalar analogy of mechanical breakdown). Obviously, the use of spring lattices is more realistic due to vectorial displacement field they allow to model. In our simulation disorder is introduced in two ways: via random lattice geometry and via random thresholds of individual springs which are generated according to a certain distribution.

In the 2D simulation of the brittle failure we clearly observe three different regimes in the full strain range, of which only one can be identified as similar to the random
percolation of damage while the other two have a sufficient extent of damage localization. The similarity with random percolation manifests itself via the fact that the proper scaling exponents of random percolation theory are followed. The presence and the width of the percolation-like regime are dependent on disorder strength. This regime is only present in strongly disordered lattices anyway, while for a weak disorder it is totally suppressed by crack localization and anisotropy in the failure pattern.

We analyze the morphology of cracks obtained from the results of our simulation. The roughness of crack profiles shows universal scaling. The connection of the roughness scaling behavior with the scaling laws of random percolation is nevertheless doubtful since the final rupture happens outside the RP regime. The crack-roughness exponent is found to be consistent with the simulation results of other authors as well as with some quasi-two-dimensional fracture experiments.

We find that critical stress and strain scale as a power law with lattice size. However, we present arguments that this scaling may well be accidental or at least unrelated to scaling properties associated with RP.

The behavior of our model in the brittle case beyond the point of maximum stress is characterized by avalanche-like breaking events, with power-law scaling of the distribution of avalanche sizes in agreement with SOC.

Although our 2D lattice model is simple, an extension proves possible for modeling polymer-like stress-strain dependence, i.e. for modeling the sequence of (quasi-)elastic regime, yield peak, softening and hardening. This is achieved by introducing additional unbreakable elastic bonds into the lattice. We show that the disorder strength is responsible for the existence and size of the yield peak, which has a very natural interpretation. It is in line with ideas on the roles of aging and rejuvenation in macroscopic response of polymers. For the pre-yield regime of polymer-like response corresponding to strongly disordered lattices we find that random-percolation features are followed at least to the same extent as for lattices with the brittle behavior. The scaling of avalanches within the post-yield regime of damage in polymers is different from the one in the pre-yield regime of both types (brittle and polymer-like) lattices, consistent with the picture of polymer flow after yield.

As a natural extension of the analysis described above we repeat some parts of it in three dimensions.
Curriculum Vitae

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Bibliography


