Fracture phenomena of disordered media

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1

INTRODUCTION

The year was 1635: Galileo, seventy-two years old completed his 'Dialogues concerning two *new* sciences' [1]. The first science was his study of what holds solids together and why do they fall apart. The second science was on the dynamics of objects, specifically related to the trajectory of projectiles, the topic for which he is renown. It is fair to say that since Galileo's 'Dialogues' this question 'what holds solids together' has developed to the core of interests in condensed matter physics, whereas the topic 'why do they fall apart' became an important branch of engineering. Both fields have developed independently and almost never united again[2]. Condensed matter physics explained that the cohesive properties of solids are based on electron/phonons and collective excitations. These concepts were very successful in explaining electrical and optical properties and led to advances in devices that form the basis of the semiconductor industry. In contrast, a similar success was not achieved in explaining the mechanical properties, and the question 'why do they fall apart' is still not properly answered. Mechanical properties are determined by the collective behaviour of defects rather than by the individual bonding between atoms and electrons. Even the behaviour of one singular defect is often irrelevant. Despite the enormous effort that has been put in both theoretical and experimental work, a clear physical picture that could even predict a stress-strain curve and failure by crack propagation is still lacking. The reason is quite

obvious: in plastic deformation and in fracture we are faced with very non-linear effects. In addition the phenomena are irreversible and far from equilibrium and consequently cannot be treated by common solid state physics approaches. As a result this area of research has largely been ignored by condensed matter physics. The problem was too tough to be 'cracked', so to speak. However, like in all sciences he who would eat the kernel must crack the nut.

Luckily enough the tide has been turning for two reasons. The first reason is new instrumental developments in the field of microscopy [3,4] that make it possible to do controlled *in-situ* deformation and fracture experiments under controlled conditions to obtain structural and chemical information on various length scales. The second reason is the availability of novel theoretical methods[5,6,7,8,9] to describe the collective behavior of defect structures incorporating the properties of individual defects as known from both linear elasticity theory and experiments. In particular the fields of statistical physics[10] and solid mechanics[11,12] have given impetus to these novel developments. Together with the advent of advanced electron microscopy they provided new concepts for the description of the co-operative behavior of defects that determine failure of materials.

The first question to ask when dealing with rupture is when fracture will develop and when it will not. It was the first problem to be attempted by fracture mechanics and may well prove the last to be solved. An important criterion has been formulated by Griffith [13] based on the idea that a crack will progress, if and only if the energy needed to create a new free surface area is smaller than the elastic energy released when the crack moves. A somewhat different approach to obtain a fracture criterion is to consider the stress fields near a crack. Within the framework of linear elasticity the stress distribution can be easily obtained for a semi-infinite crack in an infinite medium with a simple stress state imposed at infinity. The elastic energy release rate in the case of a single crack can be calculated from an arbitrary contour, the so-called J-integral, that contains the stress field and encircles the crack; the method is due to Jim Rice[14]. The stress function is singular at the tip of the crack[15] and reads:

$$\sigma_{ij}(r,\theta) \propto \frac{K}{\sqrt{r}} f_{ij}(\theta) \tag{1.1}$$

θ is measured from the crack plane at $\theta = 0$ and K is called the stress intensity factor. The divergence of $\sigma_{ij}(r,\theta)$ if $r \to 0$ is very general, i.e. independent of a specific geometry. Of course this divergence is very unphysical and depending whether the material is ductile[15] like a metal or brittle like a ceramic material [16]; effective cut-offs of the elastic solutions are known. Even if the material is neither plastic nor susceptible to damage, a cohesive zone can be introduced producing a cut-off of the elastic solution[17]. So far, Eq. (1.1) refers to a single crack in an infinite medium and the real situation of many cracks in a finite system becomes complex because the singular stress fields may interact.

It is fair to say that fracture enhances locally the amount of 'disorder'; either by the nucleation and propagation of cracks or by the complex heterogeneity of stress fields of existing cracks. The precise evolution of the amount of disorder makes fracture becoming a collective phenomenon, which is responsible for statistical fluctuations in the fracture stress and for size effects. Sample to sample variations are seen in most materials at all scales. In general the fracture load increases with decreasing sample size or increases with decreasing microstructural sizes keeping the sample size constant. These aspects underline the idea that mechanical response of a material cannot be reduced to its average and that both in strain hardening and strain softening of materials either delocalization or localization of 'disorder', respectively, play an essential role.

According to its definition, size effects are determined by the so-called representative volume[18], meaning that they vanish when the representative volume has been reached. Besides size and scale effects also shape effects can be distinguished but the latter is not fully examined in this thesis. Basically there are various approaches to tackle the size and scale effects on fracture phenomena. One class is focused on providing a description of the mechanical behavior without concentrating on a physical explanation. The model descriptions by Bažant's[19] size effect law and multi fractal scaling law by Carpinteri[20] are known best. Other suggestions include models by taking into

account higher order derivatives of the displacement field[21], non-local damage[22] following non-local models of elasticity first proposed by Kröner[23] and further developed by other researchers[24,25]. These models are very useful to reproduce the mechanical behavior and can be used as efficient tools for applications but they *cannot* provide physical information about the relevant length scale ξ because ξ is a free parameter. In contrast, if one likes to understand size and scaling effects 'disorder' has to be taken into account explicitly and this has been the main objective in this thesis.

Although molecular dynamics is still the purest discrete approach to study the evolution of 'disorder' during fracturing, the method is actually only numerically tractable in a study of the behavior of a single crack[26, 27] in a nanometer-sized sample of material. The presence of several cracks requires too large system sizes and too long equilibration times to make this method very attractive and doable in practice. Instead, lattice models have been developed in which the material is reduced to a set of points, termed 'nodes', which are connected by coupled springs. As a matter of course these models do not describe fracture phenomena on an atomic scale but they intend to give a physical description on a much larger scale. In contrast to molecular dynamics, rupture is not a natural outcome of the computation but has to be implemented explicitly by assuming a preset threshold value for fracture of the springs that may lean on experimental information. The big advantage of the lattice spring models is that 'disorder' can be introduced and studied easily, but fracture of the springs is well defined, i.e. the method is more 'rigid' than molecular dynamics to recognize the actual development of fracture.

In particular, elastic networks of springs are frequently used to model the relation between the mechanical properties and the microstructure of (highly) porous media. In this thesis disordered three-dimensional spring networks [28, 29] are used to study the size effect in brittle failure. In the past, simulations were carried out both in two [30, 31, 32, 33] and three[34,35,36,37,38,39] dimensions, mainly exploring regular spring networks. In general, the research so far on size effects [40,41] and crack growth [42], seems to underline the importance of heterogeneities in random resistor network models[43]. Further, experimental and numerical

investigations of size-effects have been pursued in the field of concrete fracture mechanics using deterministic models [44,45,46,47].

In order to incorporate a specific microstructure of highly porous ceramic media, we explore a new method of generating dynamically a node distribution. This rather mesoscopic approach provides a possibility to incorporate microstructural properties. It is important to realize that any strength distribution during the fracturing process is due to the node distribution itself. So, even a homophase sample may not be homogeneous in strength neither on a local or global scale.

The major part of this thesis can be connected to a description of the mechanical stability of a single extrudate particle of a highly porous ceramics that is used in the chemical industry as catalyst carrier[48,49]. These extrudates are very interesting also from a scientific point of view because their porosity is so high that it reaches the percolation limit of the network models. Generally speaking a catalyst carrier should have a high porosity and small pores. But the pore size should not be too small because otherwise transport of the raw material is severely hampered. Besides these microstructural considerations, these materials must be able to operate in typical petrochemical conditions and must therefore have suitable mechanical properties in order to withstand the applied load under operation. Problems will arise when catalyst carriers at the bottom of the reactor crumble under the load of other carriers. This affects the flow through the reactor and the efficiency of the process will diminish. Thus the mechanical properties of a collection of extrudates are of great importance to the practical performance of the carrier.

The thesis is organized as follows:

In chapter 2 details of a new computational methodology are presented that can generate correlated node distribution. A 'correlated node distribution' means that the position of the nodes is not independent of the positions of the other nodes. Those node distributions are converted into spring networks by connecting the nodes with springs that are within a preset value of a connectivity threshold. These resulting spring networks are used to model the highly porous extrudates on the mesoscopic scale. This chapter has been

published in the Physical Review-B [29]. Chapter 3 concentrates on an examination of the effect of the various parameters in the model on the failure characteristics. This part was already published in the Physical Review-B[50]. In particular we investigate the effects of several fracture criteria and of the connectivity at the nodes in the network. From this investigation it is concluded that it is not sufficient to examine only the fracture strain. In particular, the connectivity threshold C_0, which controls the spring entanglement between nodes, has a substantial effect on the crack morphology.

In chapter 4 the size effect is studied using the networks as generated by the method described in chapter 2. It concentrates on the scaling of the failure stress of a three-dimensional spring network as a function of its volume and its aspect ratio. In particular the influences of the geometry and the local structure are examined. Both homophase disordered 3D structures and composite systems are studied containing a more or less ordered slab. It is found that the failure stress at constant base area could be described by:

$$\sigma_{\text{fail}} \propto \left(\log \frac{h}{\xi} \right)^{-1/\mu} \tag{1.2}$$

where ξ represents the correlation length within the sample (logarithm is to the base *e*) and h is the height The values of μ are effective values. Only within the same kind of failure mechanism and microstructure the exponent μ becomes more or less universal. Actually, the modulus μ appears to depend on the system size but in all cases thin samples are stronger than thick samples under uniaxial compression and the failure stress increases with increasing coordination number. The failure stress of heterophase materials differs considerably in our calculations from that of homophase materials. Also chapter 4 has been accepted for publication in the Physical Review-B [51]. In chapter 5 different types of morphologies are generated to illustrate the importance of the details of the network structure in relation with its mechanical strength while keeping the density fixed. By varying the disorder parameter in a dynamical system of weakly interacting void volume spheres, it is possible to generate various correlated node distributions. A network of springs is constructed from the correlated node distribution, which can be used to examine the failure

characteristics of materials that are not governed by systems commonly derived from regular spring networks. Within a single phase the correlation length is the predominant parameter that determines the failure stress of the network. The chapter shows that node distributions can be produced with a remarkable increase in strength while maintaining the same density. The work has been submitted for publication [52]. An outlook to further research on various length scales is presented in chapter 6, together with some preliminary results. In particular, calculated Atomic Force Microscopy (AFM) images can be compared with experimental AFM height mode images[53,54]. These analyses of AFM images can be used to scrutinize the scaling behavior of the surface roughness of brittle fracture making a connection to the mechanical behavior [55,56]. This approach is related to studies using a random fuse network of fracture [57], which predicted universal scaling behavior of fracture surfaces, not depending on details in the microstructure. Further, in chapter 6 a possible computational method is delineated to study of mechanical properties of a collection of extrudates.

Chapter 7 contains a representative selection of visualizations of the fracture process.

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