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Fracture phenomena of disordered media

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SUMMARY

The introductory chapter 1 formulates the objectives of this thesis, namely to understand fracture of disordered brittle media on a mesoscopic scale, in particular the corresponding size and scaling effects.

In chapter 2 details of a new computational methodology are presented that can generate correlated node distributions so as to describe brittle fracture of highly porous random media. Geometrical heterogeneity in the ‘open cell foam’ structure of the porous medium on a mesoscopic length scale (100 nm) is mapped directly onto a three-dimensional, 3D, elastic network by using molecular dynamics techniques to generate starting configurations. The aspects in our description are that the elastic properties of an *irregular 3D-network* are described using not only a potential with a two-body term (change in bond length) but also a three-body term (change in bond angle, or bending) and a four-body term (torsion). The equations for minimum energy are written and solved in matrix form. If the changes in bond lengths, bond- or torsion angles exceed pre-set threshold values, then the corresponding bonds are irreversibly removed from the network. Brittleness is mimicked by choosing small (1%) threshold values. The applied stress is increased until the network falls apart into two or more pieces.

Chapter 3 concentrates on the failure stress of a disordered three-dimensional spring network. In particular we investigate the effects of several fracture criteria and of the connectivity at the nodes in the network. A node cannot be connected with another node if its relative distance is larger than the so-called connectivity threshold. In our modeling approach the spring networks were loaded in compression and the network configuration with the lowest energy was calculated after each force increment. Subsequently, the mechanical properties of the relaxed network structures were investigated using various fracture criteria. The largest threshold value of displacement was set to the commonly used criterion for brittle fracture, i.e. a fraction criterion of 1%, but also lower values (0.75%, 0.50% and 0.25%) were examined. In addition, for each of these fracture criteria the stress calculations were repeated with different connectivity thresholds. From this investigation it is concluded that it is not sufficient to evaluate only the fracture strain. In particular, the connectivity, i.e. the connectivity threshold C_0 , which controls the spring entanglement between the nodes, has a substantial effect on the crack morphology. Larger C_0 s result in smaller fragments caused by a crack branching morphology.

Chapter 4 focuses on the scaling of the failure stress of a three-dimensional spring network as a function of its volume. In particular the influences of the geometry and the local structure are examined. Both homophase disordered 3D structures and heterophase systems are studied containing a more or less crystalline slab. The structures are generated by starting with a node distribution. A molecular dynamics based algorithm uses void volume spheres, which all have a Lennard-Jones interacting outer surface. The generated distributions of nodes form the basis of a procedure to interconnect the nodes with springs. In the calculation of the failure stress the total elastic energy is described by a two-body central force, a three-body bond bending and a four-body torsion contribution. The areas under uniaxial compression are varied in the range of $0.64 \mu\text{m}^2$ to $5.76 \mu\text{m}^2$ and the height h ranges between $0.80 \mu\text{m}$ and $6.4 \mu\text{m}$. It is found that the failure stress at constant base area could be described by:

$$\sigma_{\text{fail}} \sim \left(\log \frac{h}{\xi} \right)^{-1/\mu} \quad (8.1)$$

where ξ represents the correlation length within the sample. The modulus μ appears to depend on the system size but in all cases thin samples are stronger than thick samples and the failure stress increases with increasing coordination number. The failure stress of heterophase materials differs considerably from that of homophase materials. The composite materials exhibit an increase in strength by a factor of 4, in comparison to the disordered structures of the same size where the enhancement in strength due to the slab depends also on the size of the slab. In fact, the size of a heterophase sample could have been chosen 15 to 25 times larger than a homophase disordered structure while maintaining the same strength.

In chapter 5 the focus is on the four kinds of network morphologies, generated to illustrate the importance of the microstructure in relation with its strength while keeping the density fixed. By varying the disorder parameter in a dynamical system of weak interaction void volume spheres, it is possible to generate correlated node distribution. The spring networks constructed from the correlated node distribution can be used to model strength properties of materials ungoverned by random annihilated regular spring networks. Within a phase, the correlation length effect is the dominant property in network failure stress. The spring network property, namely the coordination number, shows to be proportional to the correlation length. The radial distribution function, RDF, of the nodes can characterize the materials microstructure and also their phase state. The failure stress is in agreement with experimental findings.

The outlook of this thesis is presented in chapter 6. In this chapter, an overall view on this subject in terms of length scale is being made. Some preliminary studies with qualitative results are included on other length scales than the mesoscopic length-scale that is the core of this thesis.

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

CHAPTER 8