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Theoretical studies of breakdown in random media

Progress Report

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by

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Abstract

Failure initiates in local regions of a material microstructure which are either especially weak, or which carry an especially large field. The size and location of these weak or “hotspots” depends on the microstructure, and is especially sensitive to microstructural disorder. Using model random microstructures, we have developed analytic and numerical tools to predict where failure initiates, its initiation field, and how it propagates from the initiation sites. We have found it useful to divide the failure process into a nucleation stage, in which damage occurs quite randomly throughout the material, a localisation stage, where a critical crack nucleates, and a catastrophic failure stage during which an unstable crack propagates through the material. The results are being compared with experiments on: highly porous materials (porous glass, and porous gold); dielectric breakdown of metal loaded insulators (e.g. aluminum in poly-ethylene) and; the critical current of superconductors containing cracks (Nb and Nb_3Ge). This report summarises our efforts in these areas, while full details are contained in the published papers and preprints attached to the report.

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Appended to this progress report are copies of all papers published or prepared using support from this grant.

I. Introduction

This project develops scaling theories and numerical algorithms for predicting how a disordered microstructure affects material failure. We apply concepts developed in statistical mechanics and disordered systems in combination with conventional fracture mechanics, damage mechanics and dielectric breakdown theory to develop a new, more unified perspective of breakdown phenomena. This unified perspective helps us to better understand the similarities and the differences between the effect of a random microstructure on the various types of material failure. Our approach is to develop the simplest theoretical models which illustrate the effects of disorder on material failure, and then to generalise and specialise these models to applications in mechanical, dielectric and superconducting failure.

This progress report begins (section II) with some general results in the failure of random networks. Section III describes work on random spring networks, with bond bending terms. Section IV outlines work on the effect of a crack on the critical current of superconductors, while section V summarises results on the effect of random metal inclusions on the dielectric breakdown field of insulators. The final section (section VI) describes some work on the growth morphology of thin films. This work started with efforts to understand void coalescence processes in fracture, and it turned out that during film growth there can be an extended island coalescence regime. From a theoretical standpoint there are some interesting similarities between these two types of coalescence process.

II. General theory/ generic models and methods [3,4,8,9,11]

We have developed a simple equation to predict the damage and external field at which catastrophic failure occurs, in models where the bond failure thresholds are randomly distributed [3,4]. This theory is applicable to any distribution of bond strengths, but does not consider variations in the bond elastic or transport moduli.

To include variations in the bond resistance and critical current, we randomly assign the bond of a random resistor network the conductances, G_2 and G_1 , and the bond failure thresholds, I_2 and I_1 . When an external current is applied to the network, there is first a nucleation stage, during which bond failure occurs almost randomly. At a critical applied current, damage localises onto a single path, and soon after catastrophic failure occurs. This is illustrated for a random resistor network in figure 1a.

Figure 1. *Failure of random electrical composites a) nucleation and localisation in a 200x200 network, with volume fraction 0.25 of G_2 bonds in a G_1 background. $G_2/G_1 = \infty$ and $I_2/I_1 = \infty$. b) N_b is the number of bonds which fail before localisation, for various lattice sizes L and various values of the conductance ratio $g = G_2/G_1$. The calculations are at $p = 0.25$ and at strength ratio $I_2/I_1 = 2$.*

In this figure, the crosses that lie off the final failure path failed first, and once localisation had occurred, essentially all further bond failure occurred on the final failure path. By defining the number of bonds that fail prior to localisation, N_b , as an order parameter, we have calculated a “failure map” for the model. If $N_b \rightarrow \infty$ as $L \rightarrow \infty$, we consider the material to be quasi-brittle, while if $N_b \rightarrow \text{constant}$ as $L \rightarrow \infty$, we consider the system to be brittle. A study of N_b for various $g = G_2/G_1$

with $I = I_2/I_1 = 2$ and $f = 0.25$, for various L is shown in figure 1b. At $g \sim 3.0$, a brittle to quasi-brittle transition occurs. We have developed a scaling theory which predicts the behavior of N_b [11]. To develop this scaling theory, we needed to refine previous understanding of the scaling behavior of the largest current in random resistor networks, and these results are contained in ref. [9].

Motivated by questions concerning the size and location of field “hotspots” in fractal or hierarchical geometries, we have carried out an analysis of the way in which an applied field is distributed in disordered hierarchical topologies [8]. We found that disorder in tree structures (e.g. the human lung and the circulatory systems) leads to very large fluctuations in the current flow at outer levels of the tree. Calculations on models for continuous fiber composites suggest that a hierarchical layup may enhance longitudinal and transverse toughness [8].

III. Fracture of disordered systems [10]

We have been studying the elasticity and brittle fracture of random honeycombs, which have both bond bending and central force terms in the energy. The honeycombe lattice model is interesting as a primitive model for the fracture of graphite sheets containing random vacancies, and for cellular materials, which are dominated by bond bending and beam bending terms in the elastic energy. We presented a paper [10] discussing these issues at CASMEII in Yokohama Japan, and plan to continue this analysis during this contract period. Our analysis of these honeycombs was initiated by a desire to understand the effect of disorder on the elasticity and failure of cellular materials, and calculations on this problem, with beam bending terms added into the strain energy, are now in progress.

IV. Cracks and critical current [5]

In type II superconductors, defects can either: act as pinning sites for vortex motion and enhance critical current (such as point defects), or; act as barriers to

supercurrent and hence decrease critical current. Extended defects are especially effective at degrading critical current when the superconducting coherence length, ξ , is small. Because most low temperature superconductors have $\xi > 5nm$, the primary effect of defects in these materials is as pinning sites. In high temperature superconductors, $\xi < 5nm$ and can be as small as atomic dimensions, so that grain boundaries, cracks and other extended defects can seriously reduce the critical current of these materials. Driven by the need to develop a better understanding of the effect of extended defects on critical current, we have initiated a study of the effect of cracks of width $\geq \xi$ on critical current. We have developed a simple theory for the effect of such a crack on the critical current of thin superconducting films [5], which has two important limiting cases. In the strong pinning limit, the critical current, j_c , is determined by the cross-section available for flow of supercurrent, so for a crack perpendicular to the direction of current flow, $j_c(a)/j_c(0) \sim (1 - a/W)$, where a is the crack length and W is the width of the film. In the weak pinning limit, we find that $j_c(a)/j_c(0) \sim (\rho/a)^{1/2}$ for $a > \rho$. This predicts that critical current reduces very rapidly at small crack sizes in weak pinning systems, in a similar manner to the reduction in tensile fracture strength produced by small cracks in brittle materials such as glass. The physical intuition leading to this effect is as follows. In superconductors, vortices are produced at the end of a crack in much the same way that eddies are produced near the end of a pier protruding into a flowing river. In the case of a flowing river the eddies are governed by hydrodynamic equations, while in superconductors, they are described by superconducting electrodynamics, but the effects of a protrusion (surface crack in the case of a superconductor) are intuitively similar.

Funded by a grant from the state of Michigan, Professor Pratt's group at MSU has tested the strong pinning result using polycrystalline films of Nb , which have crit-

ical currents of around $10^6 \text{ amp}/(\text{cm}^2)$, and finds (see figure 2c) remarkable agreement with the theoretical predictions.

Figure 2 a) The geometry of the four probe experiment used to measure the critical current. The crack is lithographically drawn in the central region. b) A closer view of a crack which was lithographically drawn in a Nb film. The crack is about $50\mu\text{m}$ wide and 0.3mm long. The transport current is injected in the y-direction. c) The measured critical current $j_c(a)/j_c(0)$, as a function of crack length a . The solid line is the strong pinning prediction $j_c(a)/j_c(0) = 1 - a/W$, where $W = 1.0\text{mm}$ in this experiment.

Experiments to test the weak pinning theory using thin films of amorphous Nb_3Ge are currently under way. The experimentalists have recently made an apparatus which has field and temperature control, so that the experiments can be performed near T_c and H_{c2} , where the pinning is known to be weak, even in polycrystalline Nb. In

order to better understand the way in which the vortices depin and flow we have developed a new model which incorporates vortex-vortex interactions, pinning and inhomogeneous supercurrent flow. During the next grant period, this model will be used to analyse several new issues in the depinning and flow of vortices in disordered superconductors.

V. Dielectric breakdown of metal-loaded dielectrics [1]

Dilute metal inclusions markedly reduce the dielectric breakdown field of insulators. For this reason, there are strict limits placed on the volume fraction of such inclusions that are allowed in commercial insulating materials. We have applied our theory to the dependence of the dielectric breakdown field and its statistics on the volume fraction of metal inclusions in insulators, and have compared our results with experiment [1] (see below).

Figure 3 The capacitance ratio $C(0)/C(f)$ ($\square$) and the dielectric breakdown field ratio $E_b(f)/E_b(0)$ ($\circ$) as a function of the volume fraction of metal inclusions, f . a) Theoretical calculations on random networks. b) Experimental results on samples of paraffin wax containing steel balls.

One set of experiments was performed at Michigan State University by Professor Schroeder's group, on a rather idealised system. A second set of experiments was done by an independent group in England, on materials of more direct practical relevance. In both cases, the dependence of the average dielectric breakdown field on volume fraction of metal inclusions, agreed with the theory remarkably (perhaps fortuitously) well. The experimental and theoretical data are presented in figures 3a and 3b.

The dielectric breakdown of these materials was measured using a relatively short voltage ramp time (of order minutes). In applications, the interest is often in dielectric failure at lower electric fields, but on longer times. In this case, dielectric trees nucleate and grow, until catastrophic failure occurs. This problem is a focus of our analysis during the next grant period.

VI. Growth morphology of thin metal films [6]

This work was not part of the original proposal, and began when I asked a student to look into void coalescence models of ductile fracture. It turns out that during evaporation of thin film metal coatings onto non-wetting substrates, an early stage growth and coalescence process plays an important role in determining the eventual structure of the continuous thin film. One feature of these films is the high percolation coverage that is observed, and we have developed a theoretical model which explains this effect.

VII. Papers published or prepared during last grant period

1. P.M. Duxbury, P.D. Beale, H. Bak and P.A. Schroeder *Capacitance and Dielectric Breakdown of Metal Loaded Dielectrics*. J. Phys. **D23**, 1546-1553 (1990)
2. P.M. Duxbury and Y.S. Li, *Scaling Theory and Fluctuations of the Strength of Percolation Networks*. in *Disorder and Fracture*, J.C. Charmet, S Roux and E. Guyon eds., pp141-147, NATO, ASI series 1990.
3. P.M. Duxbury and S.G. Kim, *Scaling Theory and Simulations of Fracture in Disordered Media*. P.M. Duxbury and S.G. Kim Proceedings of the ASME symposium on *Damage Mechanics* Dallas, Texas Nov, 1990
4. P.M. Duxbury and S.G. Kim, *Scaling Theory of Elasticity and Fracture in Disordered Networks* P.M. Duxbury and S.G. Kim, MRS Symp. Proc. **207**, 179-195 (1991).
5. S.G. Kim and P.M. Duxbury, *Cracks and Critical Current*, J. Appl. Phys. **70**, 3164-3170 (1991).
6. X. Yu, P.M. Duxbury, G. Jeffers and M.A. Dubson, *Coalescence and Percolation in Thin Metal Films*, Phys. Rev. **B44**, 13163-13166 (1991).
7. P.M. Duxbury, *Disorder brings order to fracture theory*, Physics World, June issue, 27-28 (1992)
8. P.M. Duxbury, *Disorder and scaling in regular and hierarchical composites*, Proc. **MRS** in symposium on "hierarchically structured materials" in press
9. P.M. Duxbury, *Comment on "Large currents in random resistor networks"*, submitted to Phys. Rev. B.
10. S.K. Chan, S.G. Kim and P.M. Duxbury, *Elasticity and Fracture of Tubular Honeycombs containing random vacancies*, Proceedings of CASME 1992 in press.
11. P.D. Beale and P.M. Duxbury, *Electrical Breakdown of random composites*,

in preparation.

12 Y.S. Li and P.M. Duxbury, *The 3-d random fuse network*, in preparation.

13 P.M. Duxbury and X. Yu, *Contact line depinning and the growth morphology of thin metal films*, in preparation.

VIII. Significant invited conference lectures during last grant period

1. MRS Fall 1990 Meeting in Boston, Nov 1990 In symposium on "Scaling in Disordered Systems" Lecture entitled "Scaling theory for elasticity and strength of disordered materials".
2. ASME winter meeting in Dallas, Nov. 1990 In Symposium on "Damage Mechanics". Lecture entitled "Scaling Theory and Simulations of Fracture in Disordered Media."
3. DARPA Workshop on "Mechanical Properties of Thin Films", San Diego, July 1991. Lecture entitled "Role of Defects in Super- conducting Thin Films".
4. MRS Fall 1991 Meeting in Boston, Dec. 1991. In symposium entitled "Heirarchically structured materials". Lecture entitled "Disorder and Scaling Relationships in Composites".
5. Midwest Thermo. conf., Waldan Woods MI, April 1992. Lecture entitled "Coalescence and percolation during non-equilibrium growth".
6. AFOSR workshop "Problems involving mechanics and physics", Chicago, July 1992. Lecture entitled "Fracture of disordered systems"
7. CASME 2nd international conference, Sept. 1992, Yokohama, Japan. Lecture entitled "Elasticity and fracture of tubular honeycombes containing random vacancies".

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