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Deformed Materials: Towards a Theory of Materials Morphology Dynamics

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Executive summary

This grant supported work on the response of crystals to external stress. Our primary work described how disordered structural materials break in two (statistical models of fracture in disordered materials), studied models of deformation bursts (avalanches) that mediate deformation on the microscale, and developed continuum dislocation dynamics models for plastic deformation (as when scooping ice cream bends a spoon, Fig. 9).

Glass is brittle -- it breaks with almost atomically smooth fracture surfaces. Many metals are ductile -- when they break, the fracture surface is locally sheared and stretched, and it is this damage that makes them hard to break. Bone and seashells are made of brittle material, but they are strong because they are disordered -- lots of little cracks form as they are sheared and near the fracture surface, diluting the external force. We have studied materials like bone and seashells using simulations, mathematical tools, and statistical mechanics models from physics. In particular, we studied the extreme values of fracture strengths (how likely will a beam in a bridge break far below its design strength), and found that the traditional engineering tools could be improved greatly. We also studied fascinating crackling-noise precursors -- systems which formed microcracks of a broad range of sizes before they broke.

Ductile metals under stress undergo irreversible plastic deformation -- the planes of atoms must slide across one another (through the motion of dislocations) to change the overall shape in response to the external force. Microscopically, the dislocations in crystals move in bursts of a broad range of sizes (termed 'avalanches' in the statistical mechanics community, whose motion is deemed 'crackling noise'). In this grant period, we resolved a longstanding mystery about the average shape of avalanches of fixed duration (using tools related to an emergent scale invariance), we developed the fundamental theory describing the shapes of avalanches and how they are affected by the edges of the microscope viewing window, we found that slow creep of dislocations can trigger an oscillating response explaining recent experiments, we explained avalanches under external voltage, and we have studied how avalanches in experiments on the microscale relate to deformation of large samples.

Inside the crystals forming the metal, the dislocations arrange into mysterious cellular structures, usually ignored in theories of plasticity. Writing a natural continuum theory for dislocation dynamics, we found that it spontaneously formed walls -- much like models of traffic jams and sonic booms. These walls formed rather realistic cellular structures, which we examined in great detail -- our walls formed fractal structures with fascinating scaling properties, related to those found in turbulent fluids. We found, however, that the numerical and mathematical tools available to solve our equations were not flexible enough to incorporate materials-specific information, and our models did not show the dislocation avalanches seen experimentally. In the last year of this grant, we wrote an invited review article, explaining how plastic flow in metals shares features with other stressed materials, and how tools of statistical physics used in these other systems might be crucial for understanding plasticity.

Project activities

Below find a list of publications supported by this grant. A selection of these publications is described in detail. Publications since the last reporting period (end of this section) are in green.

"Bending crystals: Emergence of fractal dislocation structures", Yong S. Chen, Woosong Choi, Stefanos Papanikolaou, and James P. Sethna, ***Phys. Rev. Lett.*** 105, 105501, 2010, see [Computer models explain patterns in bent crystals]() (Anne Ju).
This article presents a definitive 2D analysis of the predictions of dislocation dynamics theory that motivated our original proposal (Fig. 1). We present the grain-boundary and cell-structure patterns formed by our theory in two dimensions with and without glide, with comparisons to experiments, correlation function analysis of the self-similar cell structures we observed, and fractal and scaling analysis of the strained crystals, replicating previous analytical approach to these experimental systems.

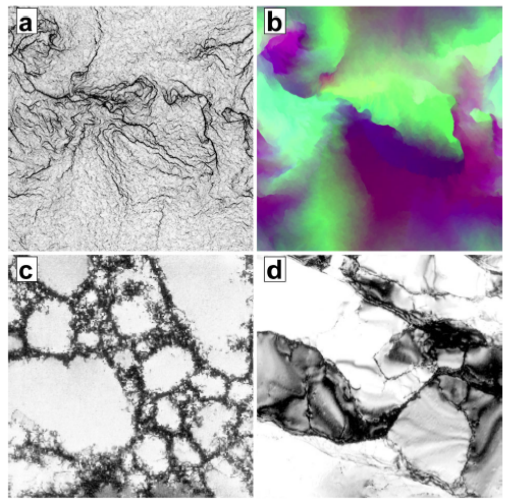

Fig. 1: Our dislocation dynamics model (a,b), compared to experiment (c,d), showing the formation of cellular dislocation structures.

A. Mesaros, S. Papanikolaou, C. F. J. Flipse, D. Sadri and J. Zaanen *Electronic states of Graphene grain boundaries* Phys. Rev. B 82, 205119 (2010), (Phys. Rev. B Editors' Suggestion), arxiv:1007.1137.

D. G. Galanakis and S. Papanikolaou *Nodal-Antinodal dichotomy from pairing disorder in d-wave superconductors, Phys. Rev. B* **82**, 060507(R) (2010).

S. Papanikolaou and J. J. Betouras *First- order versus unconventional phase transitions in three-dimensional dimer models Phys. Rev. Lett.* **104**, 045701 (2010).

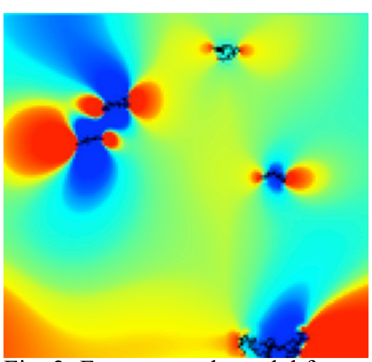
Fig. 2: Fuse network model for fracture

Fracture strength of disordered media: Universality, interactions and tail asymptotics, Claudio Manzato, Ashivni Shekhawat, Phani K. V. V. Nukala, Mikko J. Alava, James P. Sethna, and Stefano Zapperi, *Phys. Rev. Lett.* **108**, 065504, 2012. See ["Physicists predict when brittle materials fail"]() (Anne Ju).
Our fuse-network model for fracture (Fig. 2) addressed several key questions for rare event failure estimation. (1) The failure distribution (crucial for practical engineering applications) is not well described by the commonly used universal extreme-value distributions (Weibull, Gumbel, or Fréchet), even for relatively large systems. (2) The distribution does obey the weakest link

hypothesis for rather small sizes; the long-range interactions between cracks do not qualitatively change the failure mechanisms. This hypothesis underlies the coarse-graining renormalization-group transformation that underlies extreme value statistics: why doesn't it work? (3) The failure distribution is nicely described by a disorder-based nucleation theory (originally due to Duxbury). (4) The nucleation theory, for large enough sizes, will eventually converge to the Gumbel distribution – but very slowly. Two sigma into the tails, the convergence reaches 1% accuracy only for samples larger than the observable universe.

Avalanche Spatial Structure and Multivariable Scaling Functions; Sizes, Heights, Widths, and Views through Windows, Yan-Jiun Chen, Stefanos Papanikolaou, James P. Sethna, Stefano Zapperi, and Gianfranco Durin, *Phys. Rev. E* ***84***, 061103 (2011). *(Selected for PRE Kaleidoscope)*

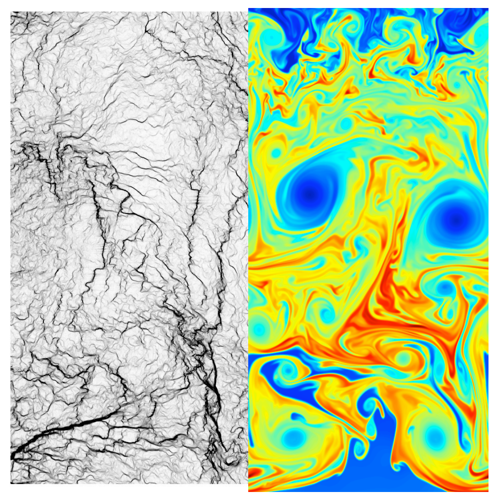

Figure 3: Dislocation dynamics (left) has strong analogies to turbulence (right).

"Is dislocation flow turbulent in deformed crystals?", Woosong Choi, Yong S. Chen, Stefanos Papanikolaou, and James P. Sethna, *Computing in Science and Engineering* **14**, 33 (2012).
Our invited paper on the analogies between dislocation evolution and fully-developed turbulence, *Is dislocation flow turbulent in deformed crystals?,* was published in a special issue of CiSE (Fig. 3). It addresses in detail the subtle issues of defining good convergence in the continuum limit of theories that form delta shocks and fractals that inevitably extend to the lattice scale.

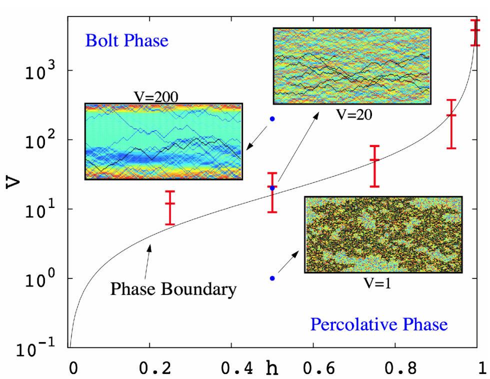

Fig. 4: Nonequilibrium phase diagram for metal-insulator avalanche behavior.

"Theory of dielectric breakdown and avalanches at the non-equilibrium Mott transition", Ashivni Shekhawat, Stefanos Papanikolaou, Stefano Zapperi, and James P. Sethna, *Phys. Rev. Lett.* **107**, 276401 (2011).
Our manuscript explained the avalanche behavior seen during metal-insulator transitions in strongly correlated electron materials. Ashivni's analysis used classical dielectric breakdown models – strongly related to the fuse network models we use to study fracture – demonstrating that the electronic physics that underlies the transition isn't relevant for understanding the macroscopic non-equilibrium behavior. We also predict a new phase transition at lower resistive contrast (Fig. 4).

"Universality beyond power laws and the average avalanche shape", Stefanos Papanikolaou, Felipe Bohn, Rubem L. Sommer, Gianfranco Durin, Stefano Zapperi, and James P. Sethna *Nature Physics* **7** 316-320 (2011).

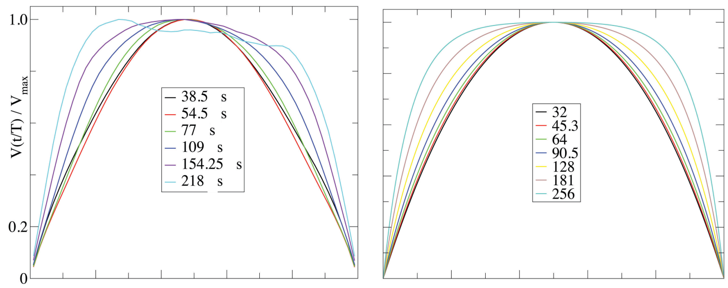

Fig. 5: Average temporal avalanche shape: thin film magnets (left) and mean-field theory (right).

This paper extracted universal, multiparameter scaling predictions from the mean-field theory, applicable both to the thin-film magnet experiments presented by our collaborators in the paper and also to most models of dislocation avalanches in crystals (where long-range elastic interactions make mean field theory valid). Stefanos Papanikolaou's triumph in the paper was an analytic calculation of the average temporal shape of avalanches of fixed duration (Fig. 5) showing a crossover from parabolic behavior to a flattened shape as the duration becomes suppressed by the demagnetization factor – precisely matching experiments.

A Striped Holographic Superconductor, R. Flauger, E. Pajer and S. Papanikolaou, *Phys. Rev. D* **83**, 064009 (2011).

"Minimal model of plasma membrane heterogeneity requires coupling cortical actin to Ising criticality", Benjamin B. Machta, Stefanos Papanikolaou, James P. Sethna, and Sarah L. Veatch, *Biophysical Journal* **100**, 1668-1677 (2011).

Straining the identity of Majorana fermions, A. Mesaros, S. Papanikolaou and J. Zaanen, *Phys. Rev. B* **84**, 041409(R) (2011).

From damage percolation to crack nucleation through finite size criticality, Ashivni Shekhawat, Stefano Zapperi, and James P. Sethna, Physical Review Letters **110**, 185505 (2013). (Editor's choice for a viewpoint, The Breaking of Brittle Materials by Elisabeth Bouchaud.)

Quasi-periodic events in crystal plasticity and the self-organized avalanche oscillator, Stefanos Papanikolaou, Dennis M. Dimiduk, Woosong Choi, James P. Sethna, Michael D. Uchic, Christopher F. Woodward, and Stefano Zapperi, Nature **490**, 517-521 (2012). See Slow avalanches 'oscillate' toward new power law (Anne Ju).
We figured out why Dimiduk's group was finding rate-dependent critical exponents in the dislocation avalanches seen in micropillar experiments. We hypothesized that there was a slow relaxation process competing with the avalanches, and developed several models to incorporate and explore this competition. We discovered that these models exhibited a new mechanism for avalanches – not self-organized criticality, not plain old depinning, but an oscillatory approach to the critical point. Large, rare avalanches throw one far from the critical point, leading to a quasi-periodic series of large avalanches with a build-up in between. This behavior is captured in a simple model, in more realistic simulations, is exhibited in Dimiduk's experiments, and appears also to be observed in earthquakes deep under the earth's crust.

Scaling theory of continuum dislocation dynamics: Self-organized critical pattern formation, Yong S. Chen, Woosong Choi, Stefanos Papanikolaou, and James P. Sethna, International Journal of Plasticity **46**, 94-129 (2013). It gives full descriptions of the motivation and derivations of our

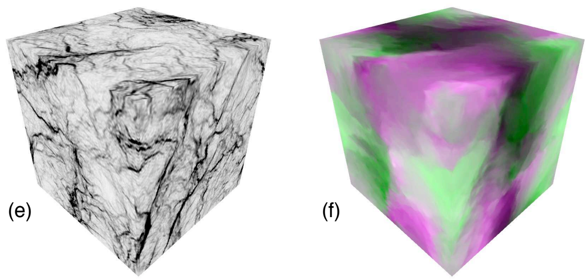

Fig. 6: 3D simulations of dislocation evolution with climb forbidden by vacancy-diffusion backpressure: dislocation density (left) and orientation field (right).

equations of motion. It introduces a new model for forbidding climb, by coupling climb to a vacancy field (below) and then making the vacancies expensive; this reproduces a model originally proposed by Acharya (Fig. 6). It introduces true three-dimensional simulations of our model, which continue to show realistic cellular structures and evolution (Fig. 6). The clear distinction between cell walls (allowing climb) and grain boundaries (forbidding climb) that we reported in our PRL disappeared in three dimensions, where all three models have similar morphologies and correlation functions.

Visualization, coarsening and flow dynamics of focal conic domains in simulated Smectic-A liquid crystals, Liarte, Danilo B., Bierbaum Matthew, Zhang Muxin, Leahy Brian D., Cohen Itai, and Sethna James P., *Phys. Rev. E* **92**, 062511 (2015).
Metals and insulators form polycrystalline domains when cooled from the melt – almost perfect crystalline regions separated by sharp walls. Smectic A liquid crystals organize into focal conic domains, each of which contains almost perfect cyclides of Dupin, with singularities forming a confocal ellipse and hyperbola. (See also Fig. 8 below.) Our work appears to be the first to simulate these structures with a continuum theory; we also explored the coarsening behavior, compared to experiments in Itai Cohen's group on the behavior under periodic shear, and confirmed a theoretical prediction and experimental realization for a continuous instability under dilation. We are refining our numerical approaches, and exploring alternative theoretical formulations. In an unexpected development, we find large regions in our simulations (and presumably in the experiments) that appear to decompose into fine, ramified wedges of focal domains. These appear to be a generalization of the lameller structures seen in martensites (see Weirdest Martensite below).

Fracture strength: Stress concentration, extreme value statistics and the fate of the Weibull distribution, Zsolt Bertalan, Ashivni Shekhawat, James P. Sethna, and Stefano Zapperi, Phys. Rev. Applied, 09/2014, Volume 2, p.034008, (2014).

"Irregularization" of Systems of Conservation Laws, Hunter Swan, Woosong Choi, Stefanos Papanikolaou, Matthew Bierbaum, Yong S. Chen, James P. Sethna (https://arxiv.org/abs/1506.05743, unpublished).
Mathematically and numerically our continuum dislocation equations are pushing new ground – they form δ-shocks, which are far less studied or understood than the standard step-like Riemann shocks that arise in hydrodynamics and traffic. Here these δ-shocks are physically representing grain boundaries and cell walls – clearly of physical interest even if dangerous mathematically. We explored why previous theories (Park and Arsenlis, Koslowski and LeSar) did not generate these δ-shocks, and what is missing from current numerical and mathematical methods that is needed to incorporate materials-specific information about the dynamics of the cellular walls.

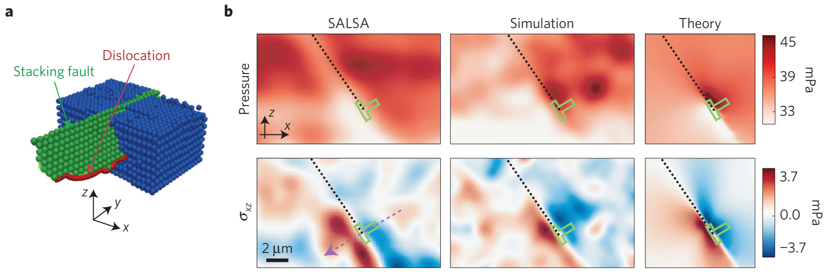

Fig. 7: Here we use experimental colloidal particle positions at a dislocation line (a) to extract the xy component of the stress tensor (SALSA), showing good agreement both with stress measured by a simulation of the same particle configuration and with traditional elastic theory.

Measuring nonlinear stresses generated by defects in 3D colloidal crystals, Neil Y. C. Lin, Matthew Bierbaum, Peter Schall, James P. Sethna, and Itai Cohen, *Nature Materials* **15**, 1172 (2016). Themechanical, structural and functional properties of crystals are determined by their defects, and the distribution of stresses surrounding these defects has broad implications for the understanding of transport phenomena. When the defect density rises to levels routinely found in real-world materials, transport is governed by local stresses that are predominantly. Such stress fields however, cannot be measured using conventional bulk and local measurement techniques. Here, we develop SALSA, a method for theoretically calculating local stresses in an experimental colloidal system We report direct and spatially resolved experimental measurements of the nonlinear stresses surrounding colloidal dislocation defect cores (Fig. 7), and show that the nonlinear stresses at vacancy cores generate attractive interactions between them.

Weirdest martensite: Smectic liquid crystal microstructure and Weyl-Poincaré invariance, Danilo B. Liarte, Matthew Bierbaum, Ricardo A. Mosna, Randall D. Kamien, and James P. Sethna, *Phys. Rev. Lett.* **116**, 147802 (2016), pdf. (Cover story and Editor's Choice for PRL, Cornell chronicle story, and "Two different crystals can be described by the same mathematical rules", by Lisa Zyga at Phys.org.) Smectic A liquid crystals are crystalline in one direction and liquid in two (some are made, e.g., from stacks of soap films). They exhibit what must be the oddest of all materials morphologies: they show defects forming geometrically perfect ellipses and hyperbolas. Using our GPU simulations developed as an offshoot of our dislocation dynamics code, we have simulated these defect structures (Fig. 8). In this manuscript, we show that these defects are a kind of martensite, where the variants have circular and linear defects and the external symmetry group (usually crystalline rotations) is promoted to include Lorentz boosts and dilations.

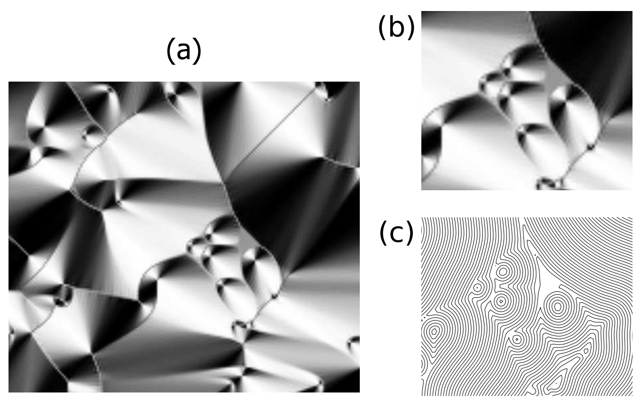

Fig. 8: Simulated focal conic structures in smectic liquid crystals.

Deformation of crystals: Connections with statistical physics, James P. Sethna, Matthew K. Bierbaum, Karin A. Dahmen, Carl P. Goodrich, Julia R. Greer, Lorien X. Hayden, Jaron P. Kent-Dobias, Edward D. Lee, Danilo B. Liarte, Xiaoyue Ni, Katherine N. Quinn, Archishman Raju, D. Zeb Rocklin, Ashivni Shekhawat, Stefano Zapperi, *Annual Review of Materials Research,* **47** (2017).

In this invited review article, we give a bird's-eye view of the plastic deformation of crystals aimed at the statistical physics community, and a broad introduction into the statistical theories of forced rigid systems aimed at the plasticity community. Memory effects in magnets, spin glasses, charge density waves, and dilute colloidal suspensions are discussed in relation to the onset of plastic yielding in crystals. Dislocation avalanches and complex dislocation tangles are discussed via a brief introduction to the renormalization group and scaling. Analogies to emergent scale invariance in fracture, jamming, coarsening, and a variety of depinning transitions are explored. Dislocation dynamics in crystals challenges nonequilibrium statistical physics. Statistical physics provides both cautionary tales of subtle memory effects in nonequilibrium systems, and systematic tools designed to address complex scale-invariant behavior on multiple length and time scales.

Fig. 9: Bending a spoon: review of stat mech related to plasticity

Training yield-precursor avalanches over cyclic loading in small-scale crystals, Xiaoyue Ni, Julia Greer, Danilo Liarte, Karin Dahmen, Will McFaul, and James P. Sethna (manuscript in preparation).

We have been working with Julia Greer's group, exploring the irreversible microscale response ofcrystals to external stress -- dislocation avalanches and plastic deformation of metallic micropillars. We examine the connection between microscale and macroscale plasticity. We discover that the textbook description of yield stress and work hardening is clearly violated in the micropillars. Their experiments, averaged over many load and unloading cycles, clearly show substantial precursor avalanches upon reloading (avalanches below the previous stress maximum), at a level which for a macroscopic system would be a significant departure from the textbook scenario (Fig. 10) (No avalanches, however, are observed upon unloading, which appears to follow Hooke's law just as for macroscopic systems.) We study the pillar size dependence of the precursor avalanches, and do see a reduction with increasing pillar size. We then examine the behavior of these micropillar precursor avalanches upon repeated cycling of stress. We are inspired by studies of 'reversible-irreversible' transitions (RIT) in dilute colloids and other systems including simulated plastic deformation of metallic glasses. In these systems, 'reversible' denotes the ability of a system to stabilize to a steady periodic state under cyclic deformation. They find that their micropillars stay in the reversible state in this sense -- upon repeated cycling to the same maximum stress, they find that the precursor avalanches die away after some number of cycles. Just as in these other systems, the number of precursor avalanches and

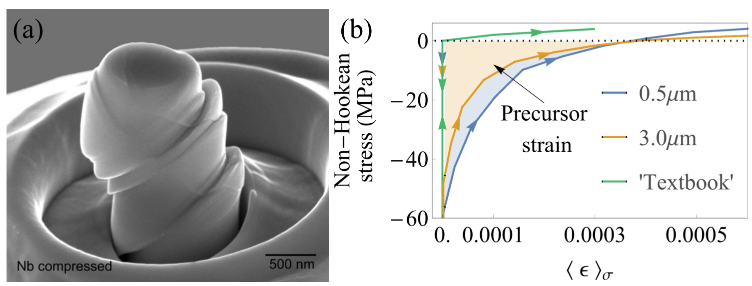

Fig. 10: Precursor avalanches in micropillar compression. Usually in macroscopic samples there is little plastic deformation below a yield stress, which grows to match the previous stress maximum. We find substantial plastic deformation below the previous maximum in micropillar experiments. This deformation disappears under repeated cycling, with intriguing relation to other nonequilibrium systems. (Figure from *Deformation of crystals: Connections with statistical physics* above.)

the number of cycles needed for them to disappear grows as we increase the maximum stress -- suggesting the approach to an irreversible state where precursor avalanches would continue indefinitely under cycling. We find that this transition point is either associated with, or lies above, the stress at which the pillar undergoes catastrophic failure.

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