Defects in disordered solids: building blocks for avalanches?

M. Lisa Manning, Syracuse University

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Manning group and collaborators

• Manning group (SU)
  – Sven Wijtmans
  – Dapeng “Max” Bi
  – Giuseppe Passucci
  – Craig Fox
  – Contact: mmanning@syr.edu

• Liu Group (UPenn)
  – Andrea Liu
  – Sam Schoenholz
  – Carl Goodrich

• Soft Matter Theory (SU)
  – Jorge Lopez
  – Jennifer Schwartz
  – Cristina Marchetti
  – Xingbo Yang

• Schoetz-Collins lab
  – Eva-Maria Schoetz (UCSD)
  – Marcus Lanio (Princeton)
  – Jared Talbot (Princeton)
  – Ramsey Foty (Princeton)
  – Mal Steinberg (Princeton)

• Henderson Group (SU)
  – Jay Henderson
  – Megan Brasch
  – Richard Baker

• SUNY Upstate Medical
  – Chris Turner
  – Nick Deakin
  – Jeff Amack
  – Guangliang Wang
  – Agnik Dasgupta
Motivation: what leads to catastrophic failure in disordered solids?

Bulk metallic glasses

Granular fault gouge

W. Johnson Group, Caltech

Is there a basic unit of deformation in disordered solids? What is it? How do they interact to form avalanches?

- Liquids: rearrangements can occur anywhere

- Crystalline solids: rearrangements occur at dislocations
Theoretical framework for solids

- The dynamical matrix describes linear response
  - harmonic approximation for a spring network

\[ m\ddot{u} = Mu \]

\[ M_{ij} = \frac{\partial^2 V(|r_i - r_j|)}{\partial r_i \partial r_j} \]

- For an ordered solid, phonons are eigenmodes of the Dynamical Matrix
  - eigenvalues give phonon frequencies
  - matrix is small for crystals (lots of symmetry)
Yes, but we’re interested in plasticity – that’s a nonlinear response.

e.g. ordered solids flow via dislocations, locations where geometric order parameter is small.
Linear modes identify defects!

Barker and Sievers, Rev. Mod. Phys. 47 (1975)
Particle packing

Sum of lowest vibrational modes

experiment

Chen et al, 
PRE 88, 022315 (2013)

simulations

MLM
Plan: do the same thing in disordered solids

problem: disordered solids are horrible and messy
Dynamical Matrix for disordered solids

- Simulated frictionless 2D soft repulsive discs

\[ V(r) = \begin{cases} -1 & r < r_s \\ 0 & r > r_s \end{cases} \]

- Dynamical matrix (DM):
  - Much larger: \( Nd \) by \( Nd \)
  - Ignores changes to nearest neighbor contacts

\[ m \ddot{u} = Mu \]

\[ M_{ij} = \begin{cases} 2V(|r_i - r_j|) & i \neq j \\ -r & r_i = r_j \end{cases} \]
All solids have a Debye regime in their density of states.

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL 95, 098301 ('05)

Decreasing pressure

Debye ($\propto \omega^{d-1}$)
Debye regime

But these aren’t just plane waves!
Correlation between short-time vibrations and rearrangements

Widmer-Cooper and Harowell, PRL 96 185701 (2006)

• Black spots: long time propensity (particle rearrangements)
• colormap: local Debye Waller factor (soft vibrational modes)
Correlation between lowest energy mode and particle rearrangement

- Local failure under shear (L. M. Manning)
- Two-level systems
- Quasi-localized mode
- Rearrangement at higher strain

Before

Normal modes analyzed at $10^{-6}$ units of strain from plastic rearrangement
Does the lowest energy mode determine the rearrangement?

No!

Initial particle rearrangement is only the same as lowest mode close to rearrangement
Original soft spot algorithm:

- Identify clusters of **localized excitations** inside **Debye regime**
  - characteristic length scale and energy scale
  - matches rearrangement locations
  - also works in 2D experimental colloidal systems

- **Cons:**
  - does not identify directions of displacements
  - does not allow energy barrier calculations
  - systematic errors at low packing fractions

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MLM and A. J. Liu PRL **107** 108302 (2011)

Problem:

extended modes are messy, so it is difficult to filter them

long range elastic tails “pollute” our basic units of deformation
Idea: Add an artificial term to the energy that acts as a high pass filter:

\[ \tilde{V} = u^T \tilde{M} u \]

Particles no longer at a minimum of this new energy functional, but can still calculate eigenvectors of this new (symmetric, real) matrix.
New method: Change the dynamical matrix by adding a mechanical high pass filter.

\[ \tilde{V} = u_i M_{ij} u_j + K_{lk} (\tilde{u}_l - \tilde{u}_k)^2 \]
\[ \tilde{u}_k = \sum_{i} u(x_i) e^{-(x_i-ka)^2/\sigma^2} \]
\[ \tilde{V} = u_i \tilde{M}_{ij} u_j \]
\[ \tilde{M}_{ij} = M_{ij} + \tilde{K}_{ij} \]

“Augmented Matrix (AM)”

Data shown for 2500-particle systems at packing fraction of 0.90 generated by infinite temperature quenches.
Is it acting as a high-pass filter?  
Test on “pure” plane waves

Yes, though not perfect. We choose \( g=5 \) for the rest of the simulations shown here.
Is it acting as a high-pass filter?

In real jammed packings

Yes, low frequency plane waves are shifted to higher frequencies
It works!

Eigenvalues (DM) vs. defects (AM)
Unweighted sum of lowest 30 modes

Normal

Augmented
“Great, now all we have to do is show that the AM modes have lower energy barriers than the DM modes, and we’re done!”
Energy Barriers

New state = new contact network

Definitions for a “new state”

- Different contact network (Xu et al)
- Different contact network (rattlers excluded)
- More than two particles with new contacts
- Cutoff on largest (average) particle displacement between old state and new state
- Cutoff on difference in energy between old state and new state
- Mark Robbins (with inertia – kinetic energy increases rapidly)
Definitions for a “new state”
Finally, AM vs. DM energy barrier

\[ \text{Log10(most similar AM barrier/DM barrier)} \]
Localized modes generically cost more energy

- DM: Weighted cutoff
- DM: Sharp cutoff
- AM: most similar (dot product)
- AM: (dot product or distance)
One slide (sort of) about avalanches

![Graph showing correlation between soft spot distributions and average strain between rearrangements. The X-axis represents the amount of strain between soft spot distributions, ranging from $10^{-4}$ to $10^{-2}$. The Y-axis shows the correlation and average strain values.](image-url)
Conclusions:

• Our mechanical high-pass filter:
  – generates truly localized modes (in same places as soft spots)
  – first method to isolate mode frequencies, directions, energy barriers for structural defects

• Strongly supports hypothesis that localized structural defects hybridize with phonon-like modes in disordered solids

• Energy barriers are higher for localized excitations compared to quasi-localized excitations
  – long-range quadrupolar tails lower energy barriers
  – somewhat artificial reaction coordinate (different from nudged rubber band, etc.)

• Still open: what is the best way to think about this?
  – elastically interacting localized defects OR
  – extended defects
five minutes about the boson peak
What sets the “edge” of the Debye regime? The Boson Peak

Sometimes defined as “an excess of modes above the Debye prediction” in the density of states:

Polymers (Jain & Pablo JCP 2004)

Sodium silicate glass (Chumakov et al PRL 2011)
Boson peak modes are extended and disordered.
Surprise!

• Boson peak modes look almost identical

MLM and A. J. Liu PRL 107 108302 (2011)
Introduce Boson Peak Wigner Matrix: (BPW)

- Symmetric
- Off-diagonal elements: mean $\mu$ and variance $\sigma^2$
- On-diagonal elements: mean $-N\mu$ and variance $N\sigma^2$

THIS matches the boson peak!!
What happens for sparse matrices with coordination number $z$?

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL 95, 098301 ('05)

http://arxiv.org/abs/1307.5904

sparse positive definite random matrices
Conclusions

• We propose a new random matrix definition of the Boson Peak, defined by eigenvector statistics
  – new Boson Peak Wigner Matrix (BPW) universality class
  – this also explains the dependence of boson peak location on pressure/packing fraction

http://arxiv.org/abs/1307.5904
One slide about biological tissues

CHEAT SHEET:
- Average energy barrier height $\sim$ yield stress
- Inverse perimeter modulus $r \sim$ strain rate
- Preferred perimeter $p_0 \sim$ density

Bi, Lopez, Schwarz, MLM submitted (2014)
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http://www.phy.syr.edu/~mmanning/