Shock-driven jamming and periodic fracture at particulate interfaces

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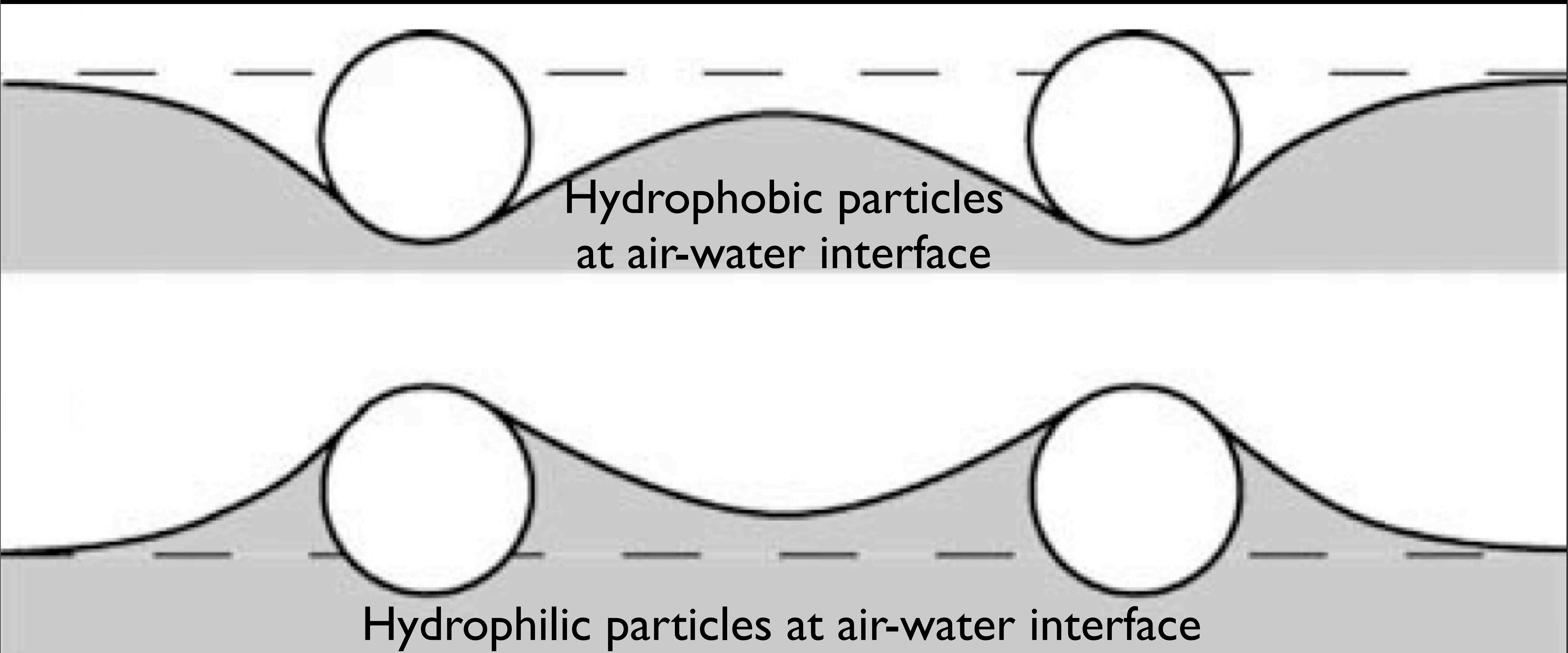
Engineering and Applied Sciences, Harvard University

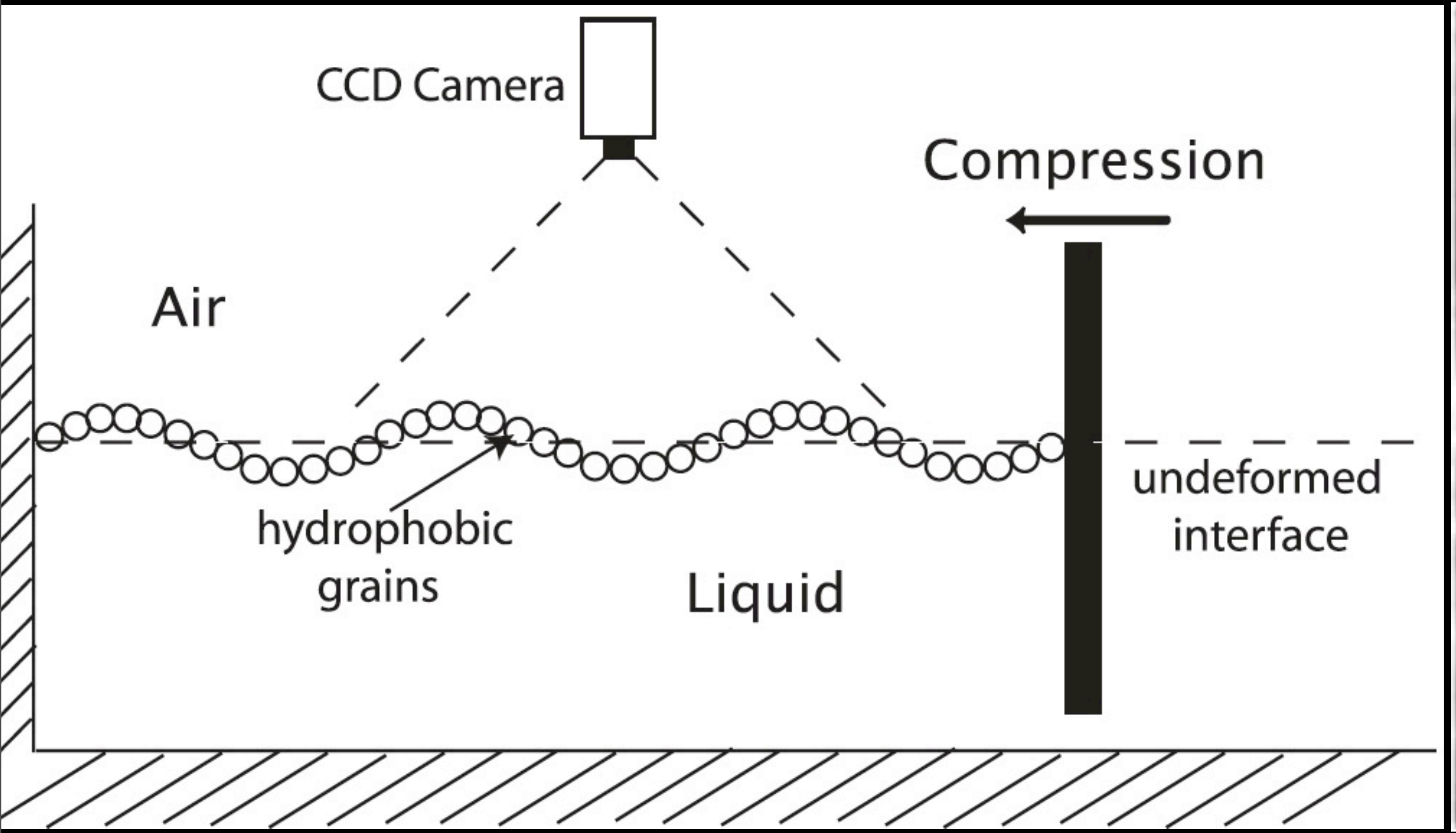
Outline

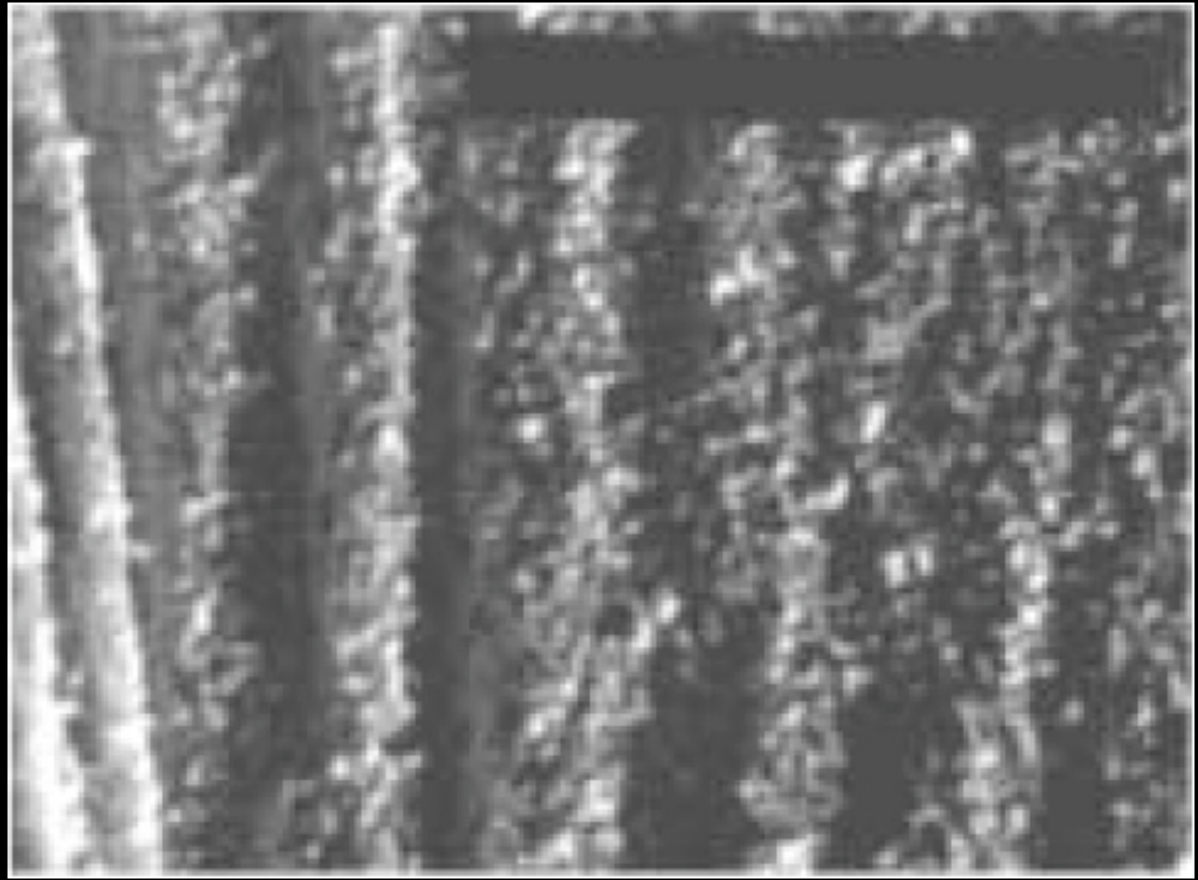
- Background
- Experiment
- Simulation
- Summary

Brief Background
&
Prior work

Particles at interfaces





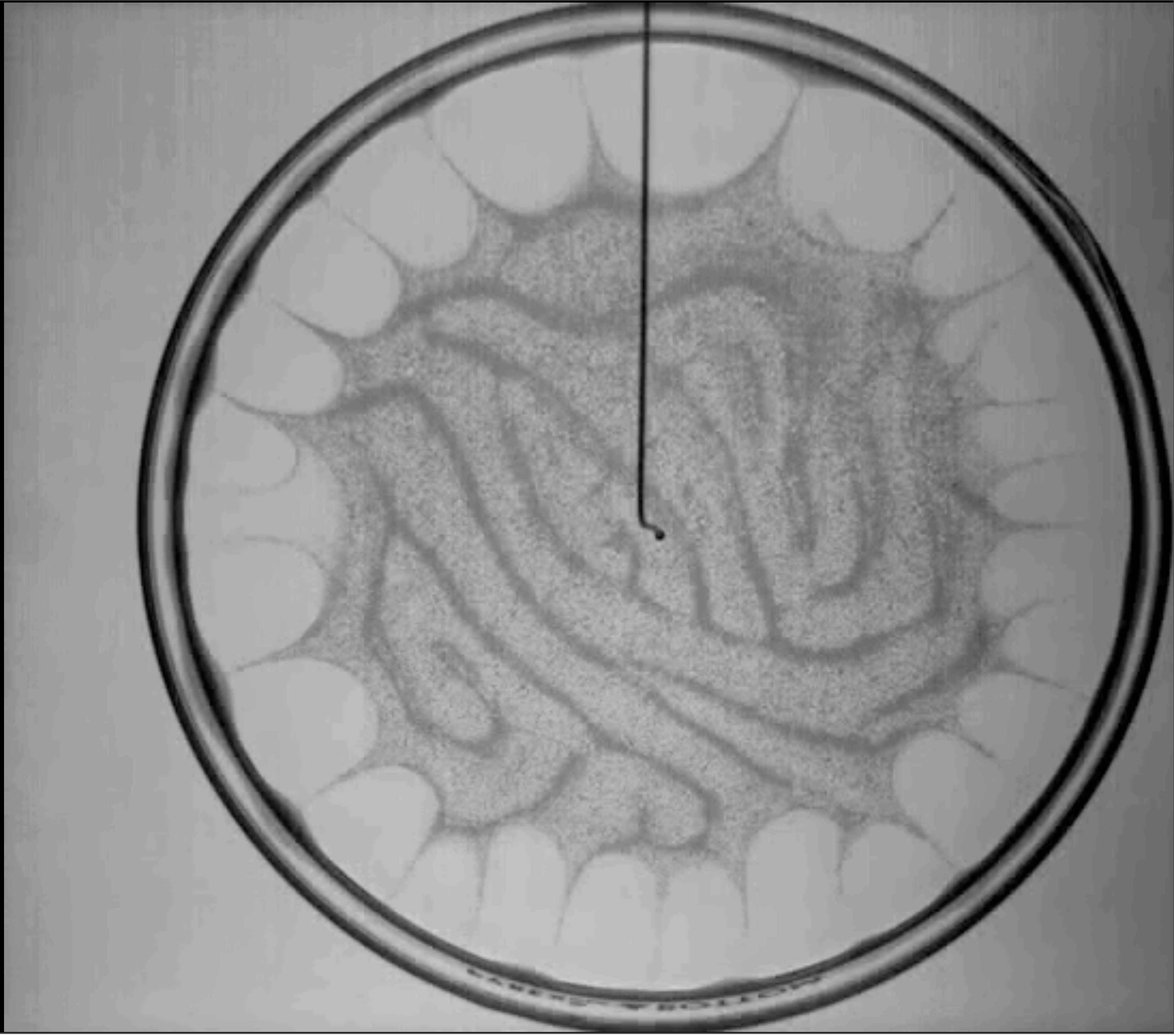


- Hydrophilic particles under compression stack up in layers.
- Wetting allows them to slide over each other.
- Hydrophobic particles under compression sustain stresses.
- They cannot slide over each other and stack up in layers.
- They collectively buckle out of plane like an elastic membrane.

D. Vella et. al., Europhys. Lett. 68, 212 (2004)

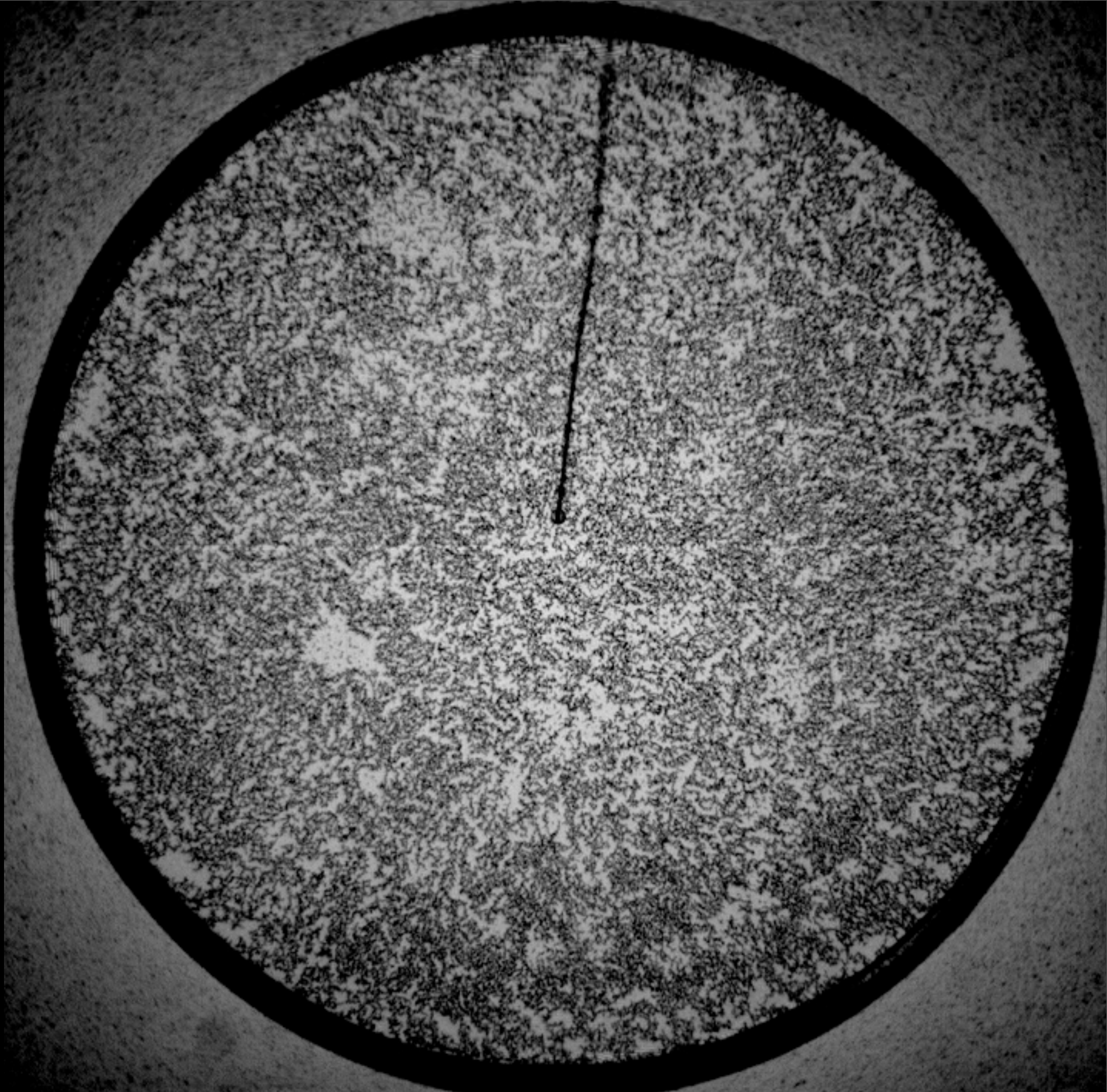
Hydrophilic particles.

Hydrophilic particles.

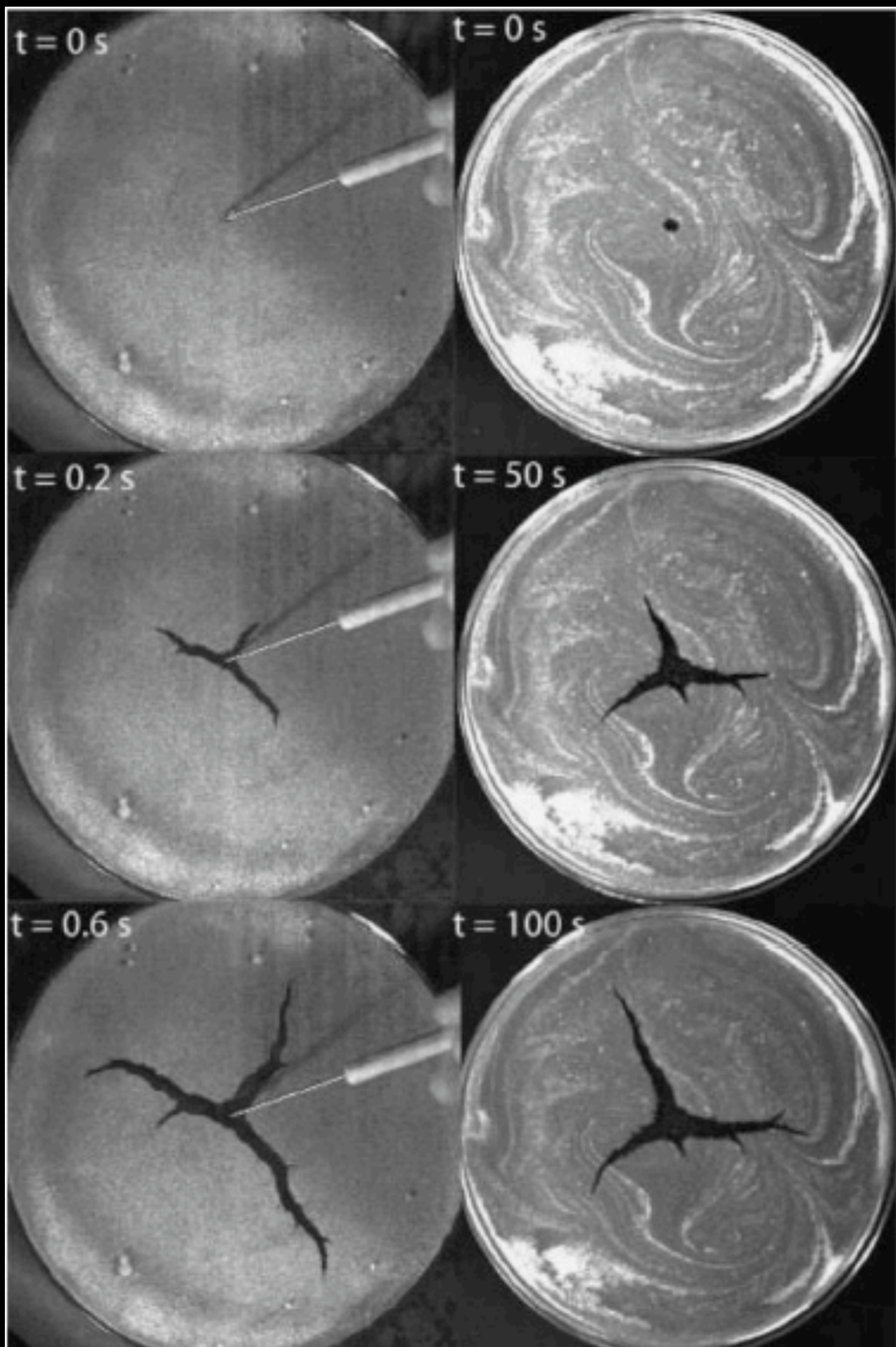


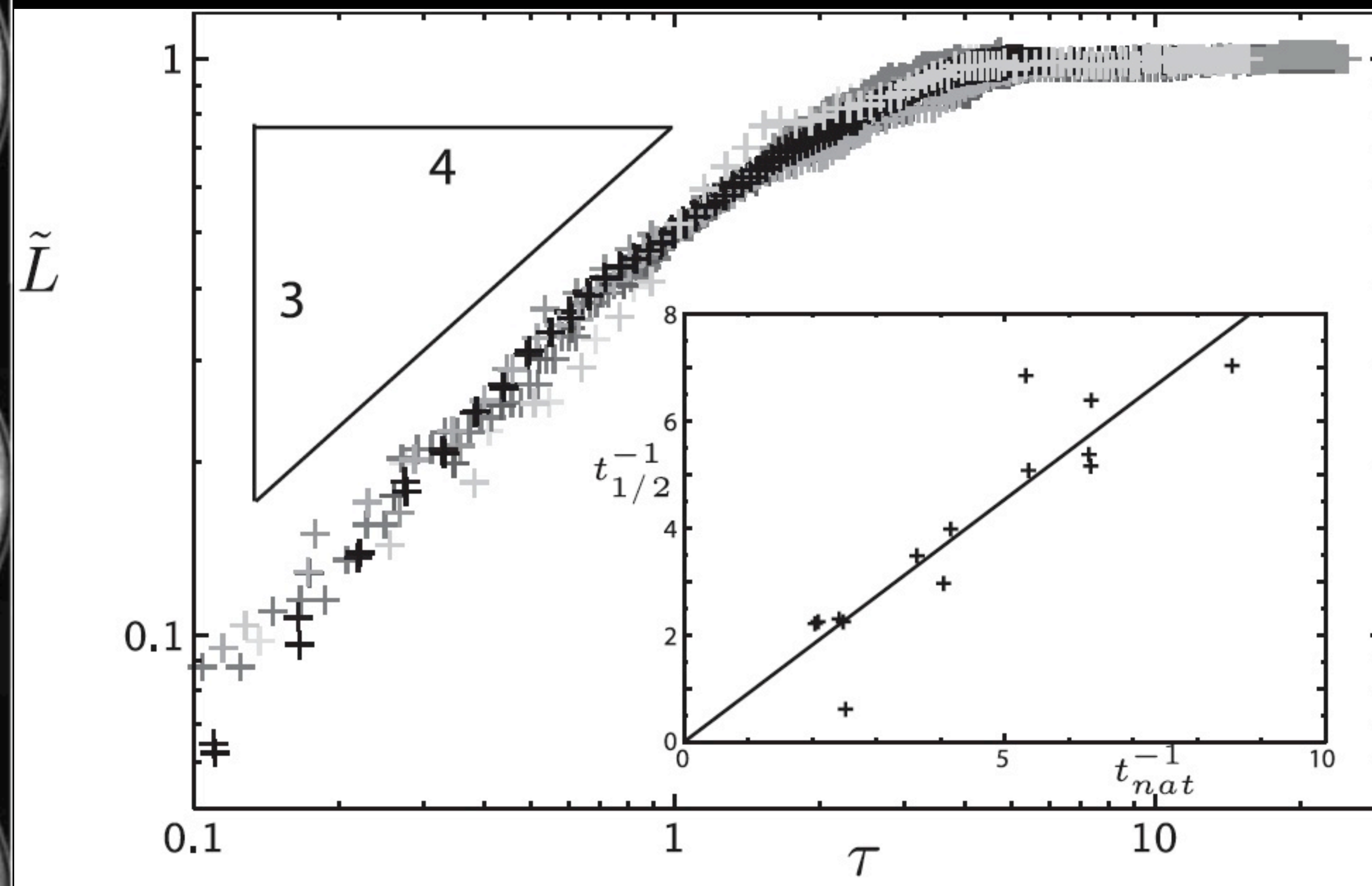
Hydrophobic particles.

Hydrophobic particles.



Localized surfactant introduction in hydrophobic particulate monolayers
Stress relieved via fracture as in solids.





Crack tip position $\widetilde{L} \sim t^{3/4}$

D. Vella et. al., Phys. Rev. Lett. 96, 178301 (2006)

Description of Experiment
&
Image Analysis

Experiment: Preparation & Protocol

- Fill distilled water in clean petri dish (diameter D = 14 cm).
  - What is clean? acid wash, water rinse, baked dry, UV treatment.

- Place dish on light tablet; we record transmitted light.

- Hydrophobic particles: Teflon coated hollow glass spheres.
  - Particles: $d = 50 \pm 10 \mu m; \rho = 0.25 g/cm^3$
  - Washed in ethanol & water, then baked dry.
  - Puffed in air and allowed to naturally sediment onto surface.
  - Cannot control packing fraction: $0.1 \leq \phi_{init} \leq 0.64$

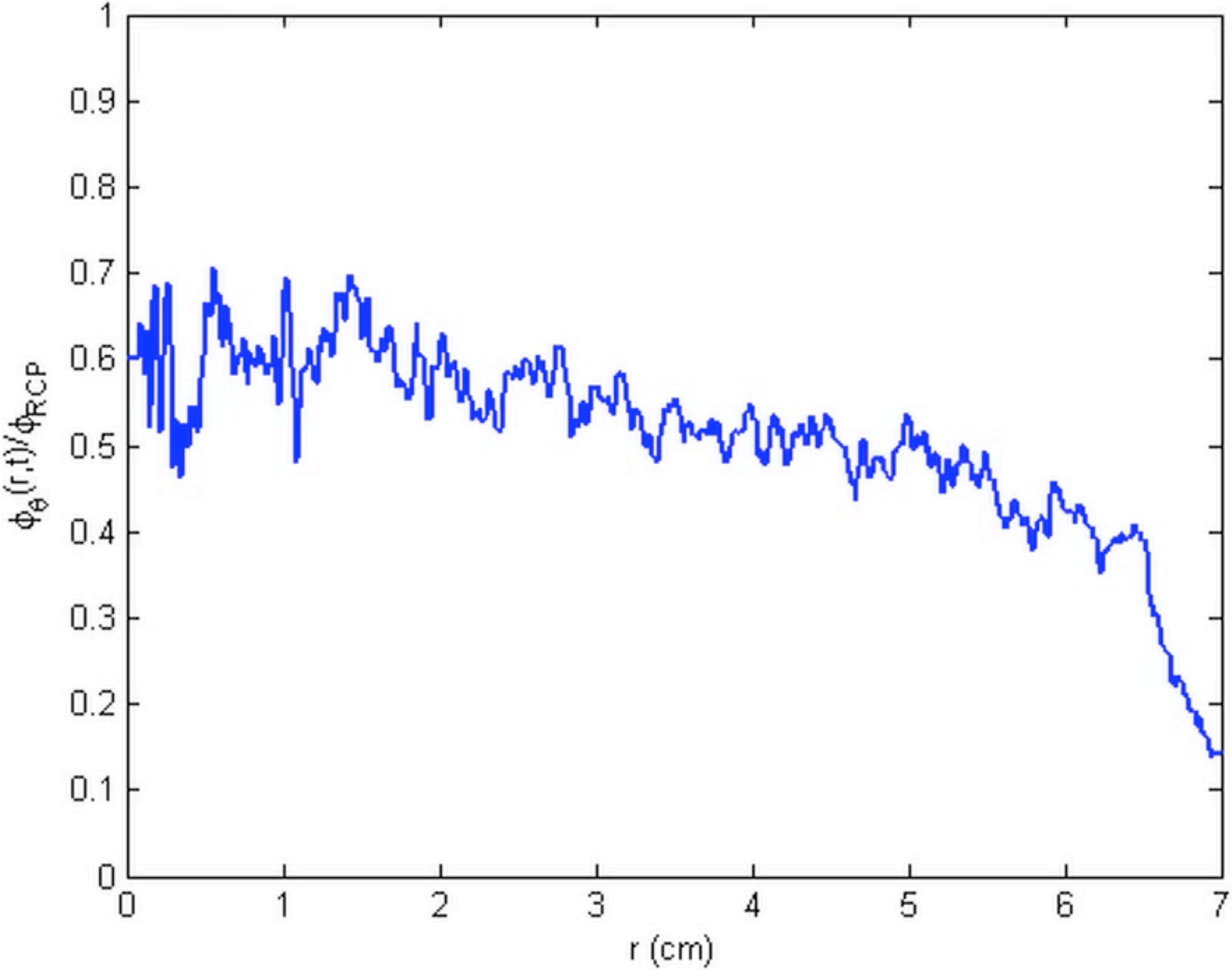
- Dip clean needle in surfactant (Oleic acid); impinge on surface.
  - Needle: Washed in ethanol & water, then flame cleaned.
  - Pure Oleic acid, no dilution in organic solvent.

- Record dynamics with high speed camera (600 frames/sec).

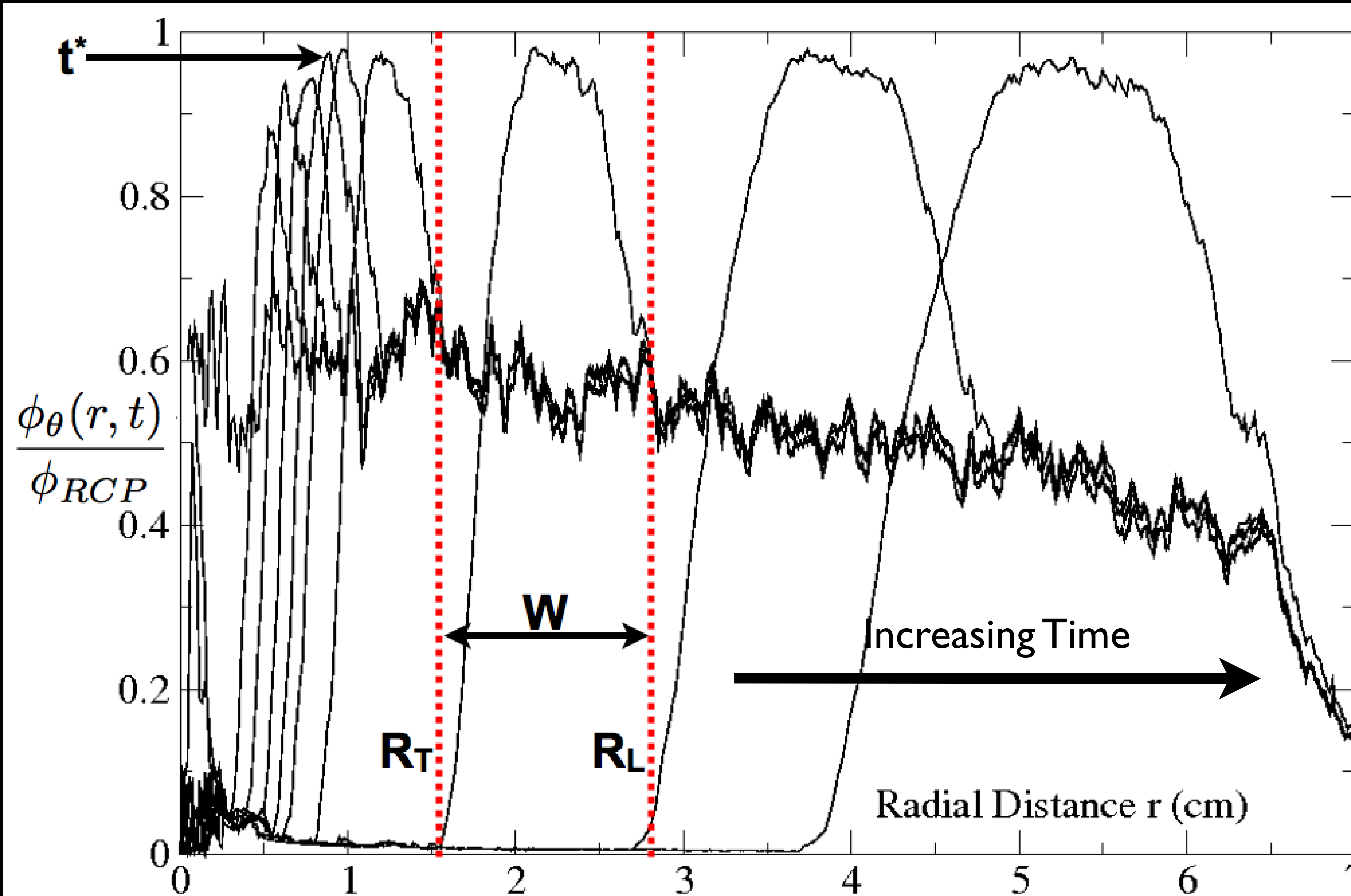
Experiment: Image Analysis

- Before Experimental run:
  - Background snapshot: water filled petri dish without particles.
- Background subtraction.
  - Removes minor spatial inhomogeneity in illumination.
  - Grayscale particle intensities on dark background.
- Apply spatial band-pass filter to remove pixel noise.
- Transform Intensity to particulate area.
- Exploit symmetry: Azimuthally avg. radial packing fraction $\phi_\theta(r,t)$

$$\phi_\theta(r,t) = \frac{1}{2\pi}\int_0^{2\pi} \phi(r,\theta,t)d\theta$$



$\phi_\theta(r,t)/\phi_{RCP}$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
r (cm)



t*
1
0.8
0.6
0.4
0.2
0
$\frac{\phi_\theta(r,t)}{\phi_{RCP}}$
W
R_T
R_L
Increasing Time
Radial Distance r (cm)
0
1
2
3
4
5
6
7

Surfactant forcing
&
response of particle raft

Position of the surfactant front

- Position of advancing surfactant on surface of a "deep" fluid layer:

$$R_s = K(\frac{\Delta\gamma^2}{\mu\rho})^{1/4} t^{3/4}$$

- Surfactant-fluid surface tension difference $\Delta\gamma$: 39.18 dyn/cm.
- Dynamic viscosity of fluid substrate (water) μ: 0.01 dyn.s/cm^2.
- Density of fluid substrate (water) ρ : 1.0 g/cm^3.
- K is a numerical prefactor in the range $(0.665 \leq K \leq 1.52)$

J. A. Fay, "Oil on the Sea", Edited by D. Hoult (Plenum, New York) (1969)

O. Jensen, J. Fluid. Mech. 293, 349 (1995)

A. D. Dussaud and S. M. Troian, Phys. Fluids 10, 23 (1998)

D. W. Camp and J. C. Berg, J. Fluid. Mech. 184, 445 (1987).

C. Huh et. al., Can. J. Chem. Engg. 53, 367 (1975).

Position of the surfactant front

- Position of advancing surfactant on surface of a "deep" fluid layer:

$$R_s = K(\frac{\Delta\gamma^2}{\mu\rho})^{1/4}t^{3/4}$$

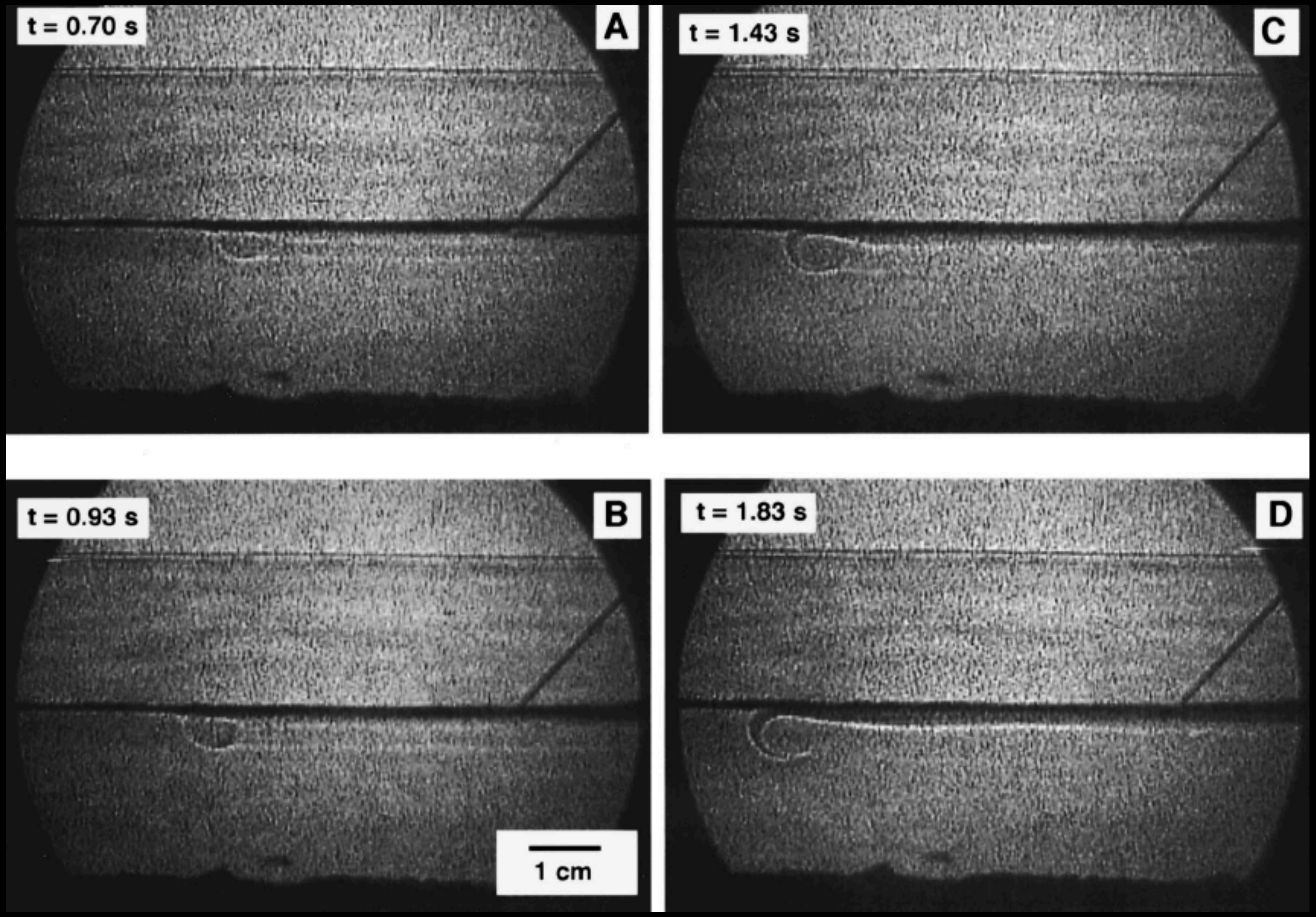
- Assumption: Surfactant introduced from constant, point source.

- Experiment:
  - Non-dilute drop of surfactant introduced.
  - Total surfactant concentration in excess of 20000 CMC.
  - Surface tension does not depend upon concentration.

Definition of “Deep” fluid layer

- Surfactant spreading generates Blasius boundary layer in the fluid.
- How long before boundary layer reaches dish bottom in experiment?

$T = H_0^2/\nu$ H_0: fluid depth (1 cm) ν: kinematic viscosity (10^{-6} m^2/s)
T ~ 100 s; Exp. duration ~ 1s.



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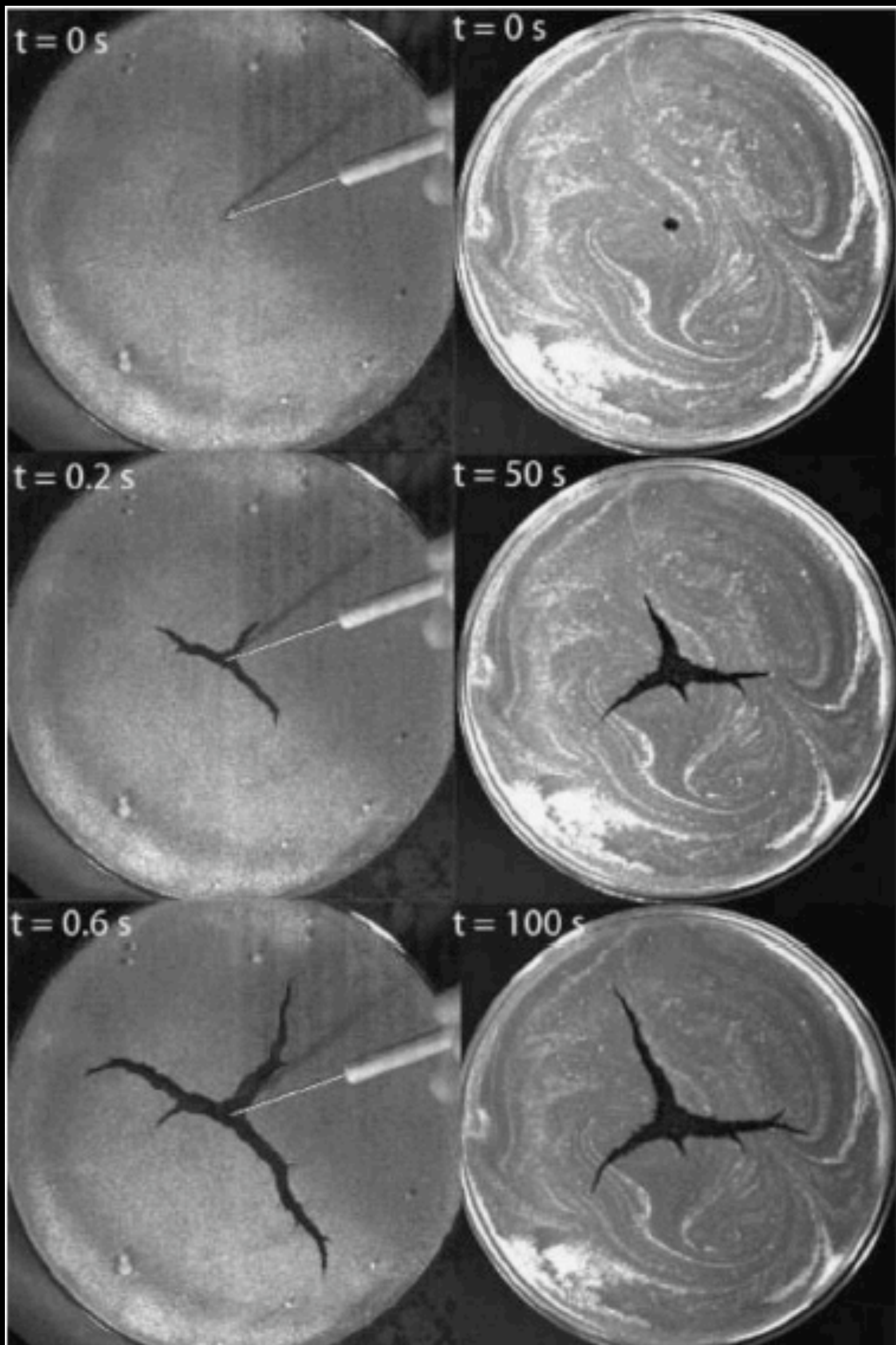

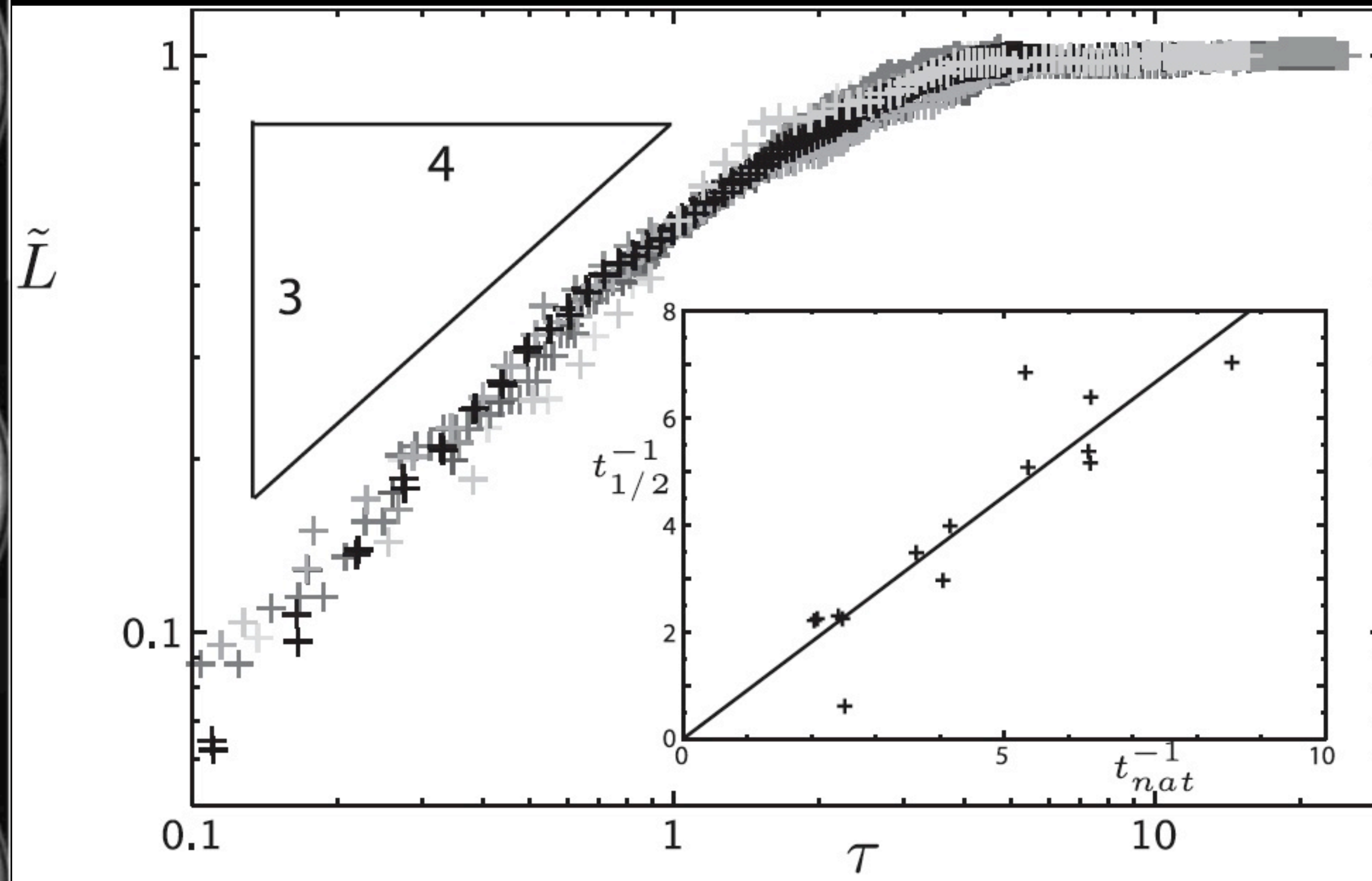

Crack tip position $\widetilde{L} \sim t^{3/4}$

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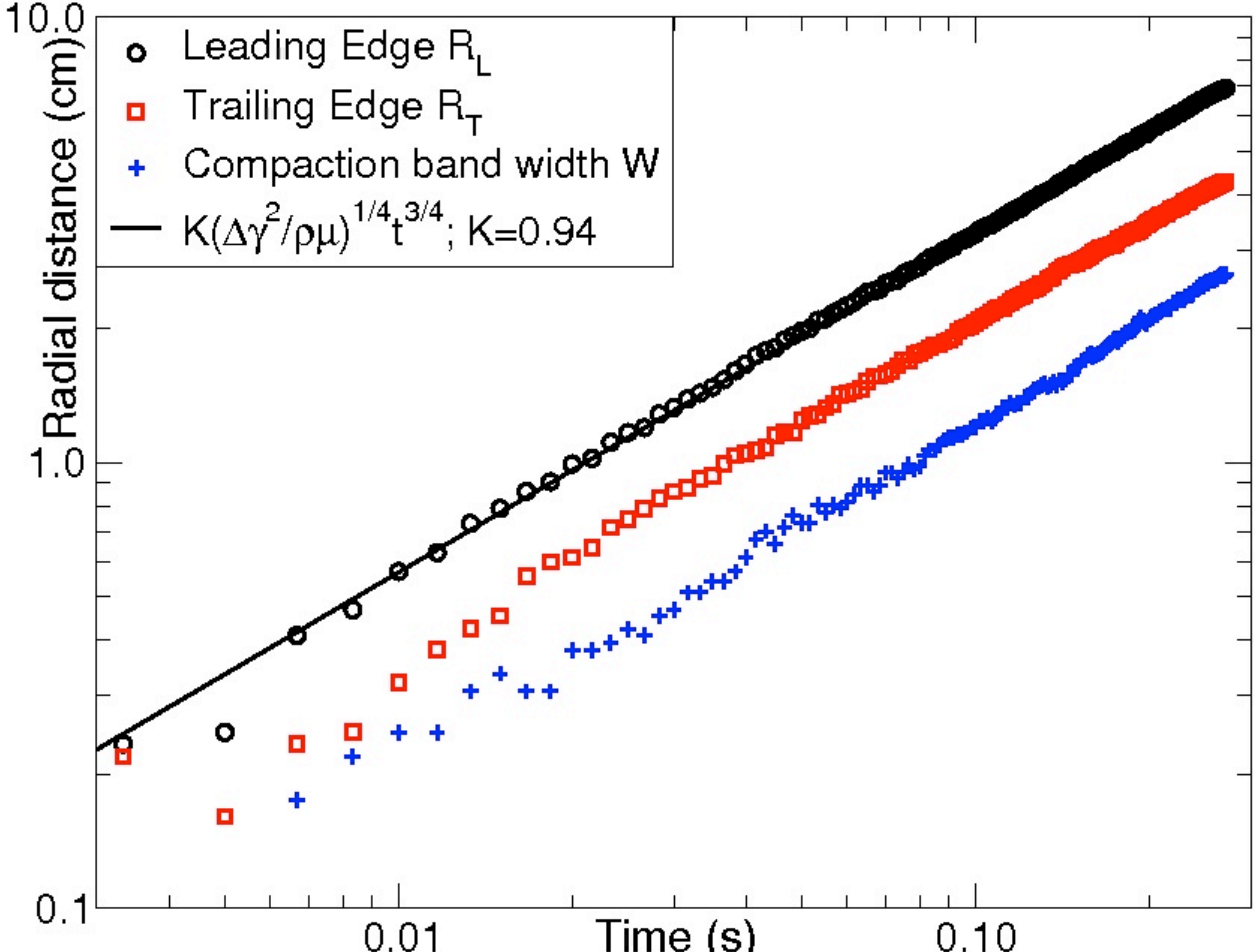
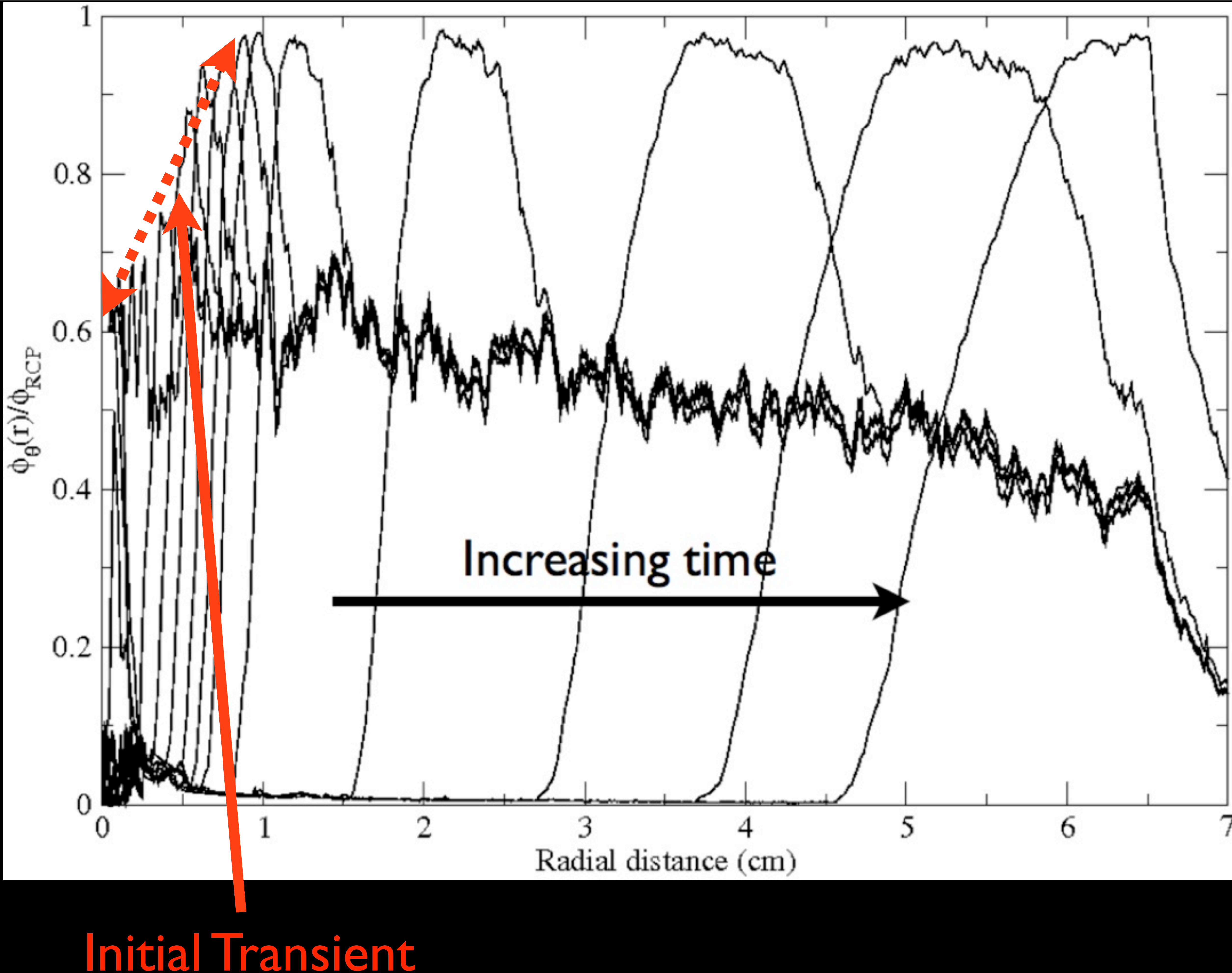


10.0
1.0
0.1
Radial distance (cm)
Leading Edge R_L
Trailing Edge R_T
Compaction band width W
$K(\Delta\gamma^2/\rho\mu)^{1/4}t^{3/4}$; K=0.94
0.01
0.10
Time (s)

Formation of a disordered, annular solid



Increasing time
Initial Transient
$\phi_\theta(r)/\phi_{RCP}$
Radial distance (cm)
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5
6
7

Transient evolution to Jamming

- $\phi_\theta(r,t)$ evolves through an initial transient.
- Saturates close to Random close packed density. $\phi_{RCP} = 0.84$ in 2D (density at which granular matter jams).
- Definition: t = t* - instant when $\phi_\theta(r,t)/\phi_{RCP} \to 1$.
- Compaction band jams to form a disordered, 2D solid.
- Develops non-zero shear modulus and yield stress.
- Definitions:
  $R_T(t = t^*) = R^*$: Compaction band's inner radius at t = t*.
  $W(t = t^*) = W^*$. Compaction band's width at t = t*.

Failure of the disordered, annular solid

Fracture onset

- Experimental observation: Fracture onset coincides with $t = t^*$.
    - Surfactant induced stress already high for crack formation.
    - But cracks cannot form until compaction band jams.
    - All stress for $t < t^*$ goes into compaction.
    - At $t = t^*$, the compacted solid has ability to sustain stress.
    - Stress relief occurs immediately via simultaneous fracture.

- *Singular aspect* of this system:
    - Same cause leads to formation and failure of the solid.
    - Almost all stress relieved on fracture onset at t^*.
    - Hardly any new cracks observed at $t > t^*$.
    - Any quantity that controls fracture matters only at t^*.

Crack selection

How many cracks relieve stress in a bar $2\pi R^*$ long and W* wide?

- Recall: All built-up stress is relieved on fracture onset at t = t*.
- No. of cracks N remains nearly constant for remaining duration.
- St. Venant: Strain applied locally does not matter far away.
- Applies if crack propagates slower than shear wave (1 m/s).
- Bar of length L and width W, with crack propagating across W: Requires N ~ L/W cracks to relieve all stress.
- We are blessed with a simple case.

$$N \sim 2\pi R^* / W^*$$

We experimentally measure, N, R*, and W*. This is testable.

Crack selection

- In fact we can do a bit better than $N \sim 2\pi R^*/W^*$
- Experimental observations:
  N monotonically decreases with initial packing fraction
  R* exhibits similar behavior.
  W* independent of ϕ_{init} because strain proportional to W/d
- Invoking Mass conservation:

$$\phi_{init}\pi(R^* + W^*)^2 = \phi_{RCP}\pi[(R^* + W^*)^2 - (R^*)^2]$$

$$\frac{\phi_{init}}{\phi_{RCP}} = \frac{1}{(1 + W^*/R^*)^2} \simeq \frac{2W^*}{R^*}$$

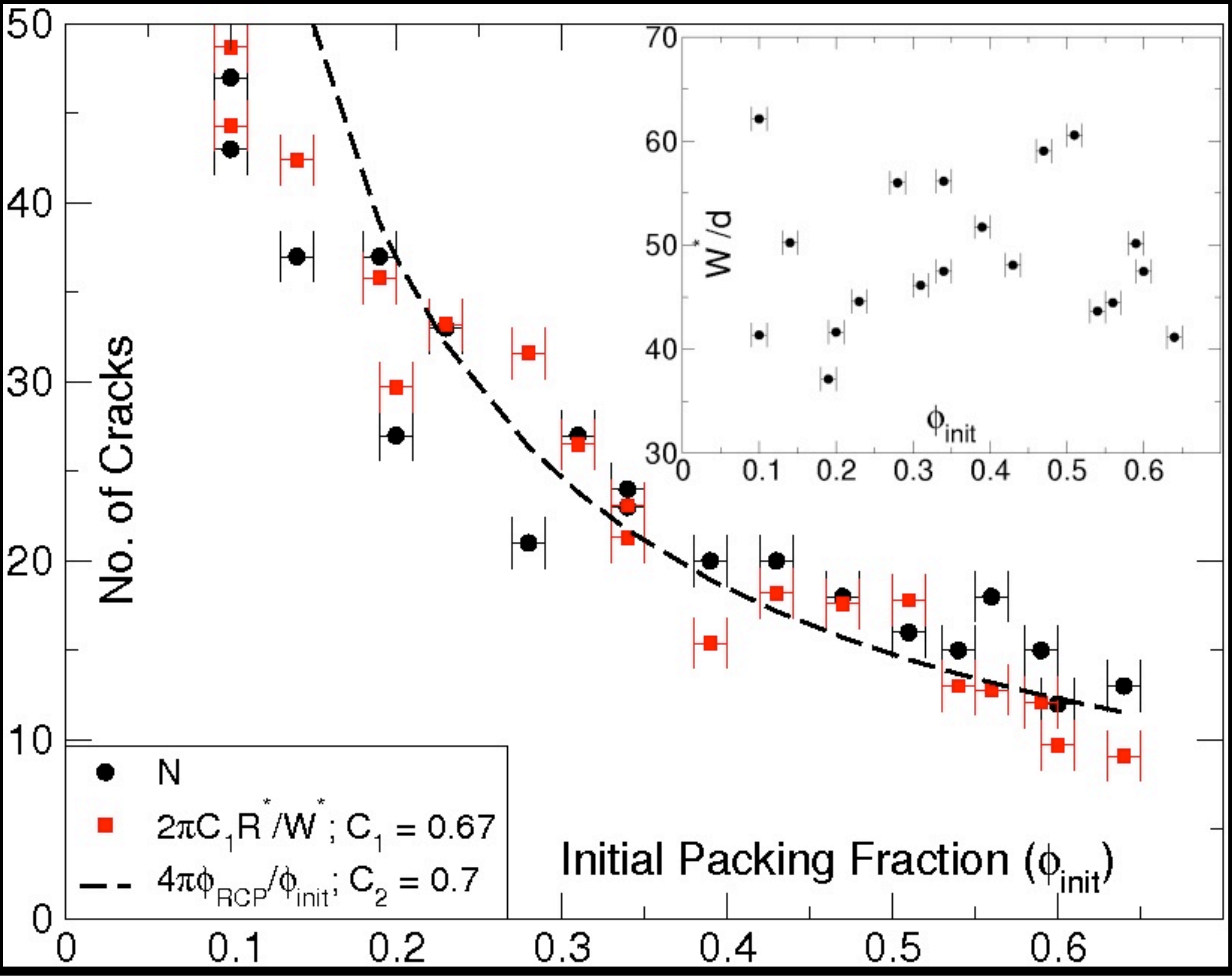
$$N \simeq \frac{2\pi R^*}{W^*} \simeq \frac{4\pi\phi_{RCP}}{\phi_{init}}$$

Caveat Emptor: works for intermediate packing fractions

$$N \simeq \frac{2\pi R^*}{W^*} \simeq \frac{4\pi \phi_{RCP}}{\phi_{init}}$$

- Relations based on several idealized assumptions.
  - $W^* << R^*$: Quadratic term is dropped.
  - Initially uniform particulate distribution (but there's drift).
  - Annulus jams exactly at $\phi_{RCP} = 0.84$ (not true).

- Both relations should fail in limiting cases:
  - Dilute limit: $\phi_{init} \to 0$
    - As $R^* \to \infty, \phi_{init} \to 0 : N \to \infty$
    - Instead, N strongly influenced by disorder.
    - There is a hard cutoff: $N \leq 2\pi R^*/d$
  - Dense limit: $\phi_{init} \to \phi_{RCP}$
    - System already jammed or close to jamming.
    - No time t^* to solid formation, R^*, W^* have no meaning.
    - Fracture type remarkably different.



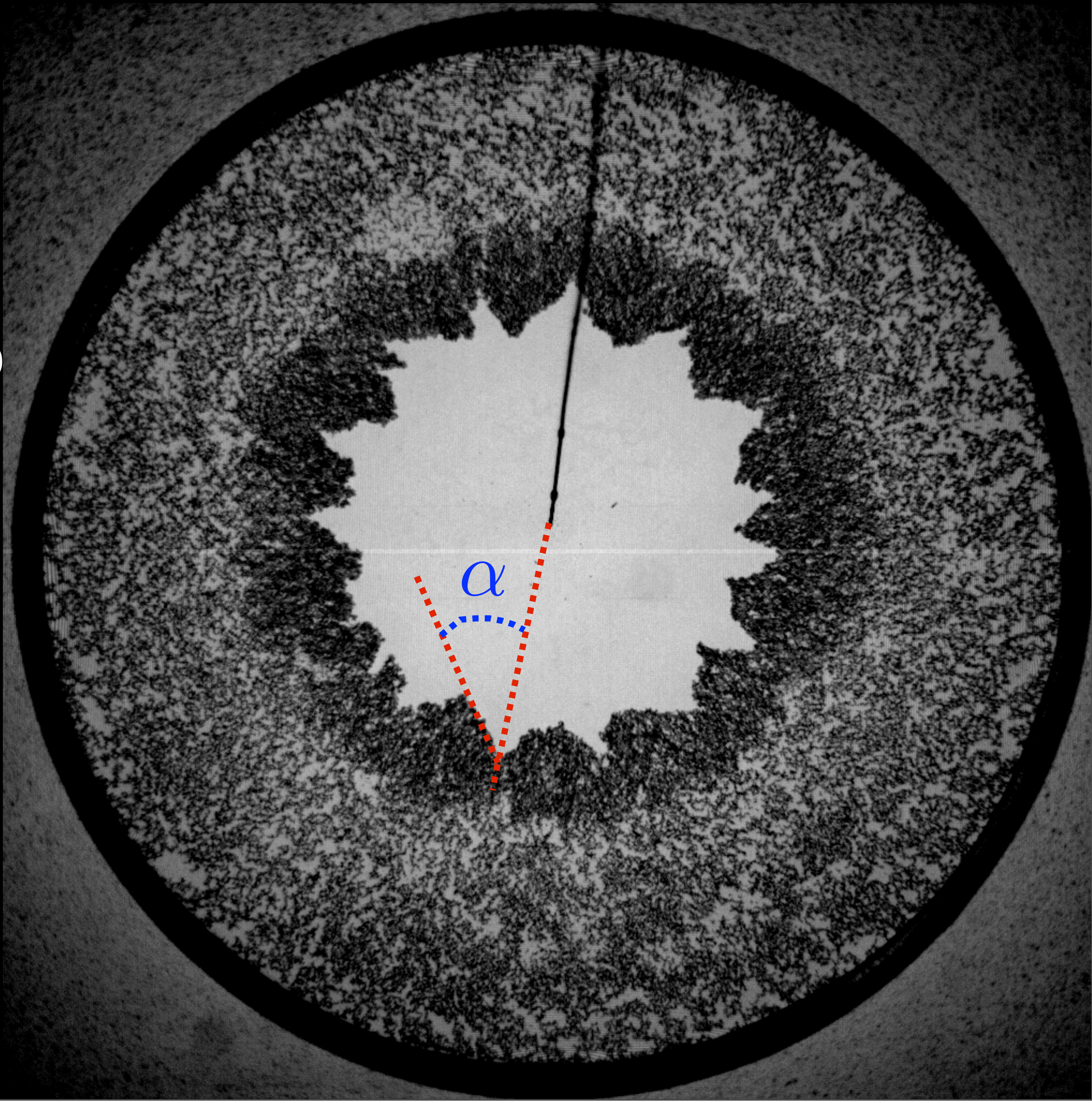
No. of Cracks
Initial Packing Fraction (ϕ_{init})
N
$2\pi C_1 R^* / W^*$; C_1 = 0.67
$4\pi\phi_{RCP}/\phi_{init}$; C_2 = 0.7
W^*/d
ϕ_{init}

Crack Geometry

Crack Geometry

$$\frac{\text{Mean}(\alpha)}{\text{Stdev}(\alpha)} = \frac{34^\circ}{6.97^\circ} = 4.9$$

Sharp distribution.



But why Triangular cracks?

- Recall, Compaction band exhibits self-similar scaling.

$$R_L, R_T, W \propto t^{3/4}$$

- Triangle area opened by a crack must scale as $Area \propto t^{3/2}$
- Any shape with curvature is not scale-free, introduces length scale.
- The set of shapes involving lines naturally fits this constraint.
- Compaction band's inner contour must have polygonoid shape.
- Hence triangular cracks.
- This does not account for the sharp angle: $\langle \alpha \rangle = 34^\circ$

Qualitative explanation for crack angle & depth.

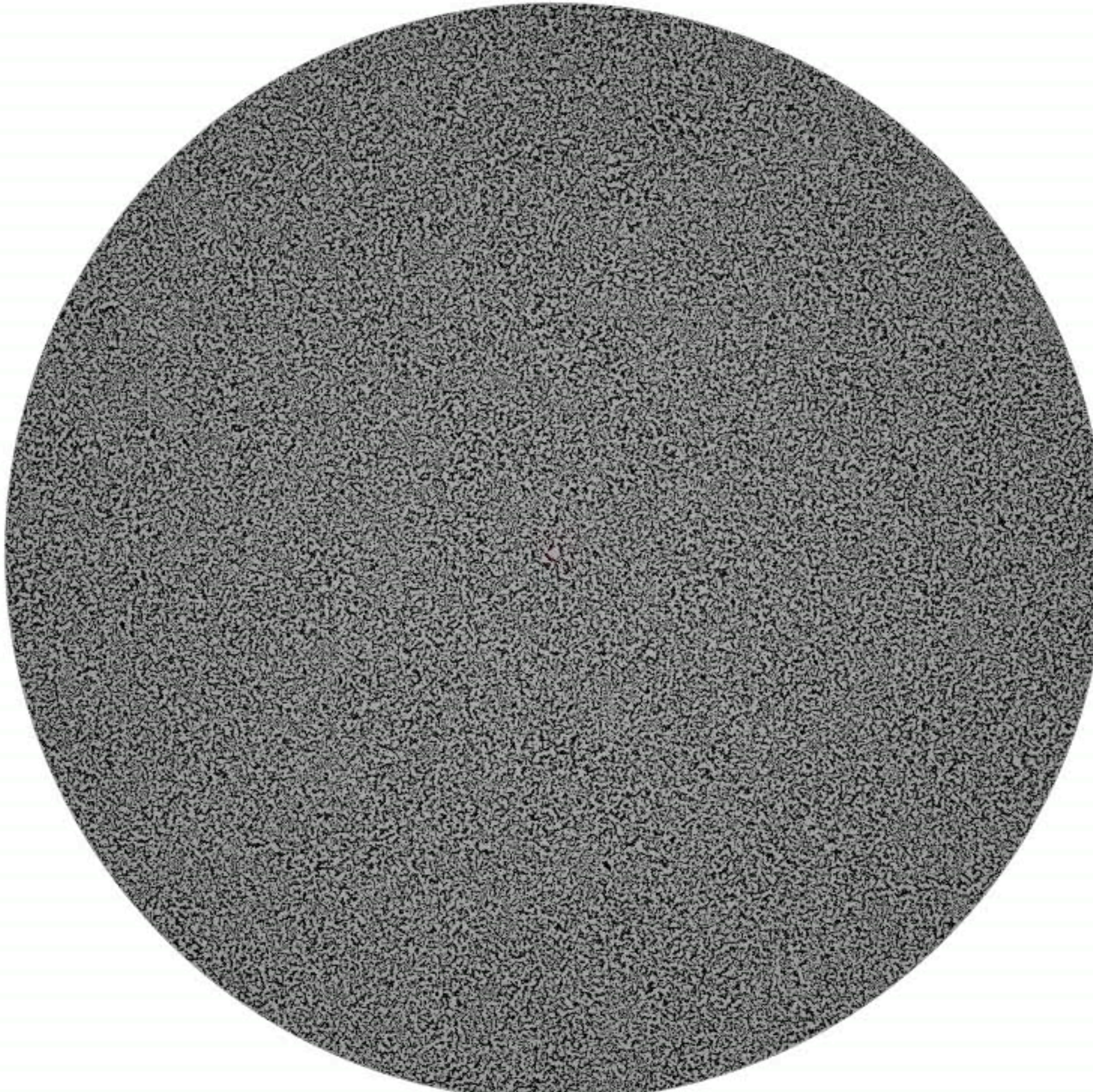
- W >> d: Compaction band may be treated as 2D continuum solid.
- No strain at shock edge, but strains exist internally.
- Blasius layer leads to compressive stress, which packs particles.
- x_c : Distance from crack tip to particulate shock edge.
- $x_c = W f(\Delta\gamma/\gamma, \nu)$.
- Crack depth and angle depend upon:
  - $\Delta\gamma/\gamma$: Ratio of surface tension contrast.
  - ν : The Poisson ratio which couples radial & azimuthal stress.

Molecular Dynamics Simulations

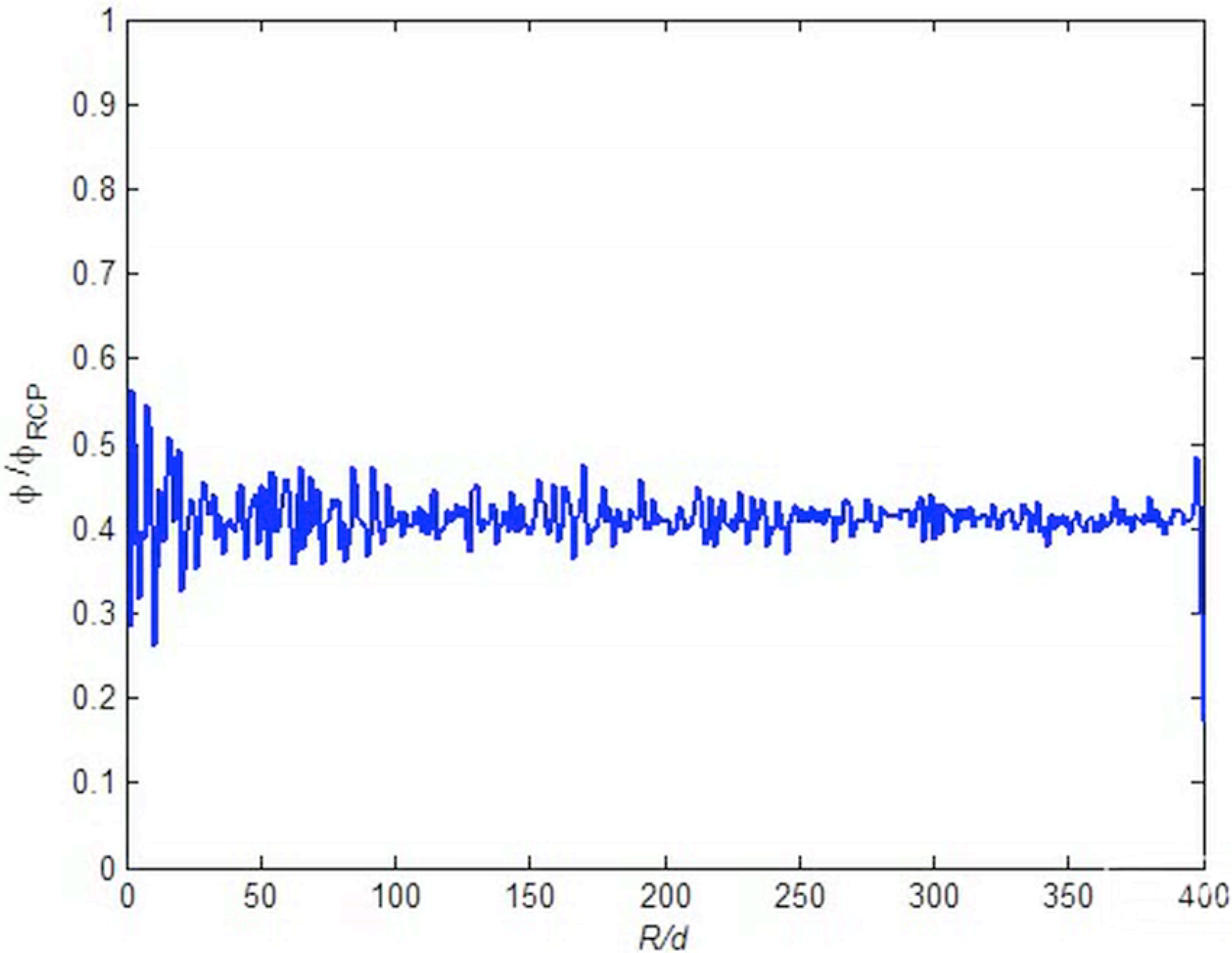
A simple Molecular Dynamics scheme

- Initial tenuous raft: randomly placed, planar system of hard spheres.
- A uniform particle diameter variation between 0.8d and 1.2d.
- Simple attractive force law: F = k (for r < 0.1d), F = 0 (r > 0.1d).
- Symplectic Euler scheme: damped Newtonian particle dynamics assuming outward radial flow with velocity $U_r = \frac{dR_s}{dt}$.
- Mimics surfactant spreading.
- Particle with velocity $\tilde{v}$ relative to fluid opposed by a drag $\tilde{\mu} d\tilde{v}$.
- $\tilde{\mu} \sim \sqrt{\mu\rho d^2/t}$: approximates mean drag/particle due to thickening of boundary layer under the raft.
- This form leads to radial integrated pressure diff. of order $\Delta\gamma$ across compaction band consistent with boundary layer arguments.
- Do these ingredients suffice to recover experimental dynamics?

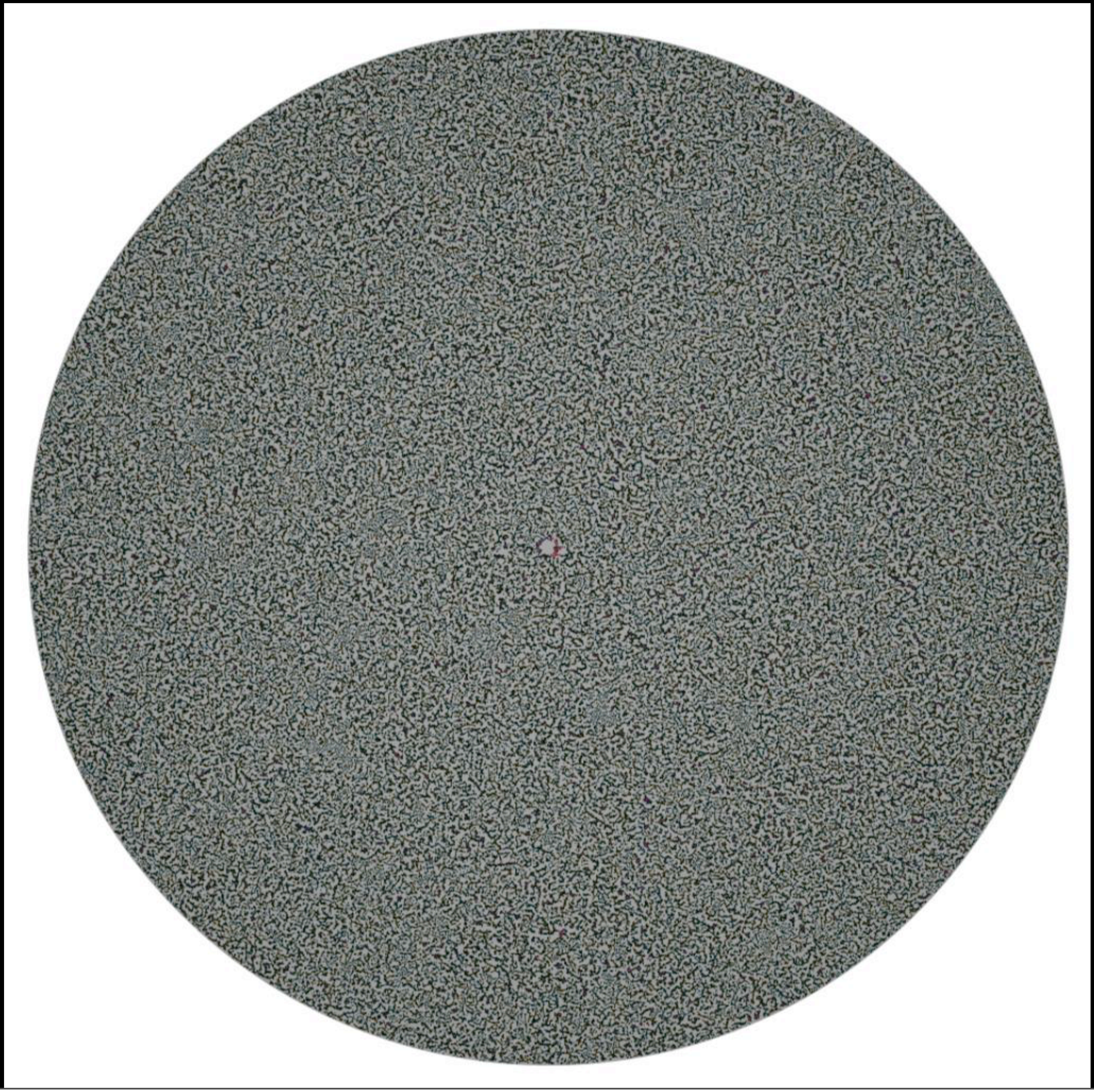
Molecular Dynamics Simulation



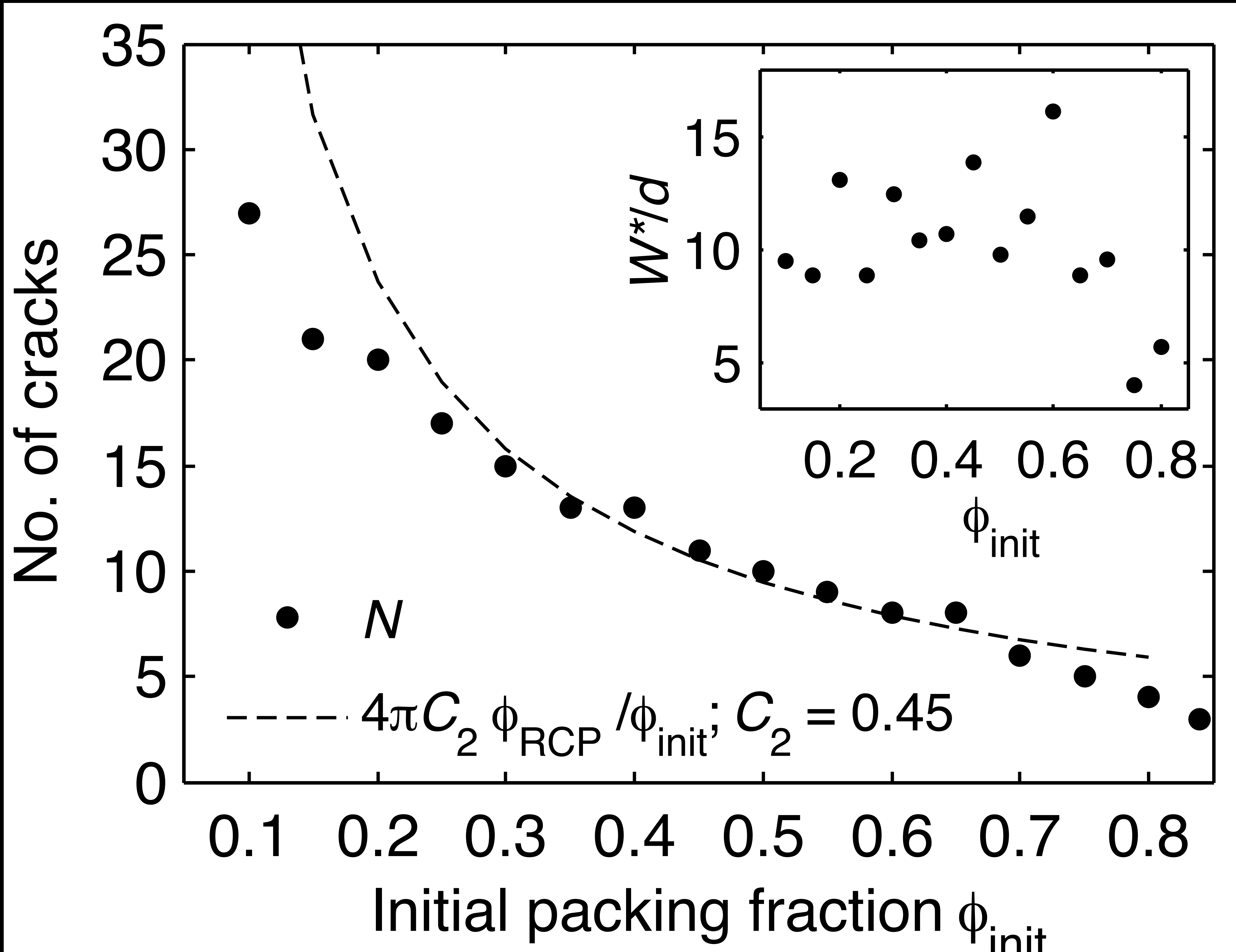
Azimuthally Avged. Packing Fraction: Simulation



Left - Azimuthal & Right - Radial Stress Component.
Blue - Tensile & Red - Compressive Stress.

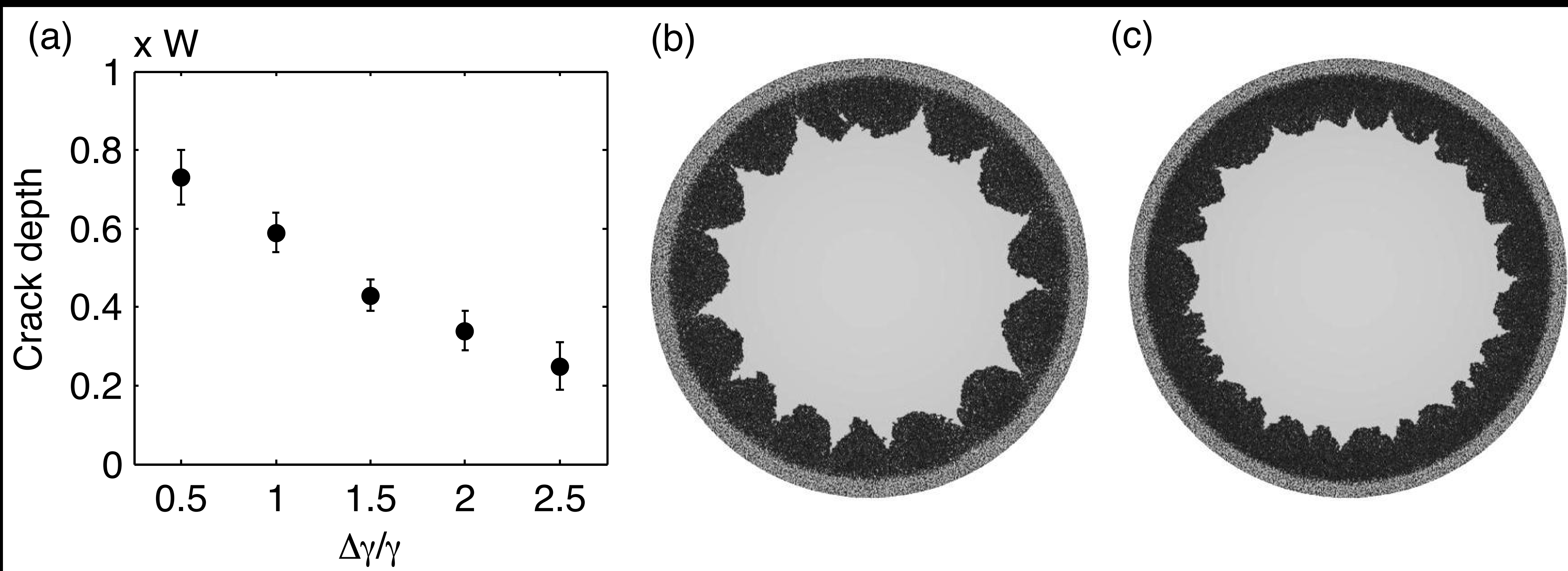


Simulation Results.



Simulation Results.

Crack depth depends upon surface tension contrast ratio.



Summary

- Phenomenon: Formation and failure of a 2D disordered solid.
  - Local surfactant introduction on hydrophobic particle monolayer.
  - Spreading surfactant sweeps up particles ahead of itself.
  - Particles are compacted into an annulus that behaves like a solid.
  - Stress relief occurs via simultaneous fracture in the annulus.
  - Nearly triangular cracks exhibit robust geometry.
  - Simple MD simulations are able to capture essential features.
- Explaining the phenomenon requires results from multiple fields:
  - Interfacial Physics (Surfactants)
  - Fluid Dynamics (Blasius Boundary Layer)
  - Granular Media (Jamming)
  - Solid Mechanics (Fracture)

MM Bandi, T Tallinen, and L. Mahadevan
Europhysics Letters 96, 36008 (2011)

Positions Available

Three experimental postdoctoral positions - July 1st or later.
Areas of interest include:

- Amorphous Solids.
- Interfacial Dynamics.
- Biophysics.
- Microfluidics.

Internship opportunities available for BS/MS/PhD students.

For details, please contact:

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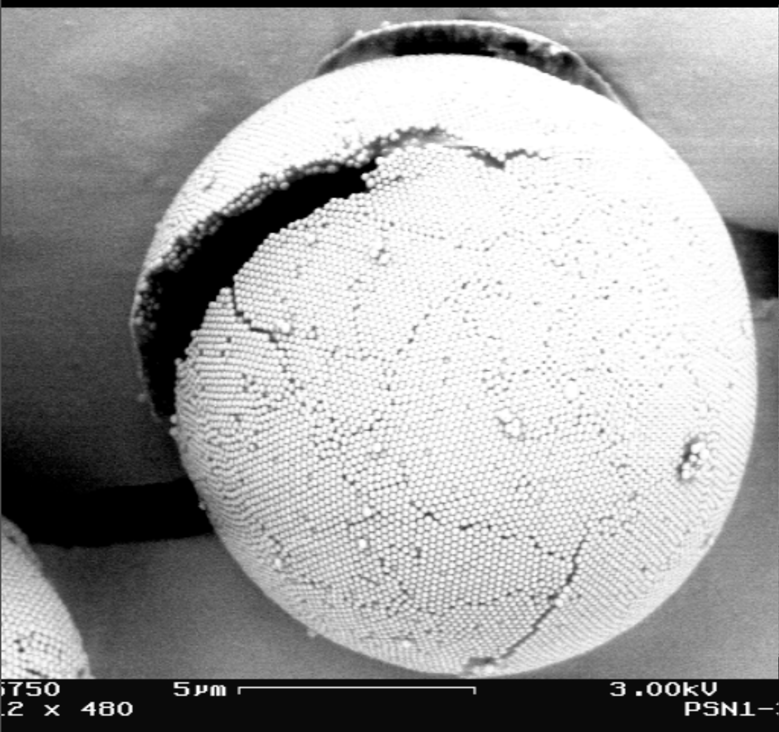
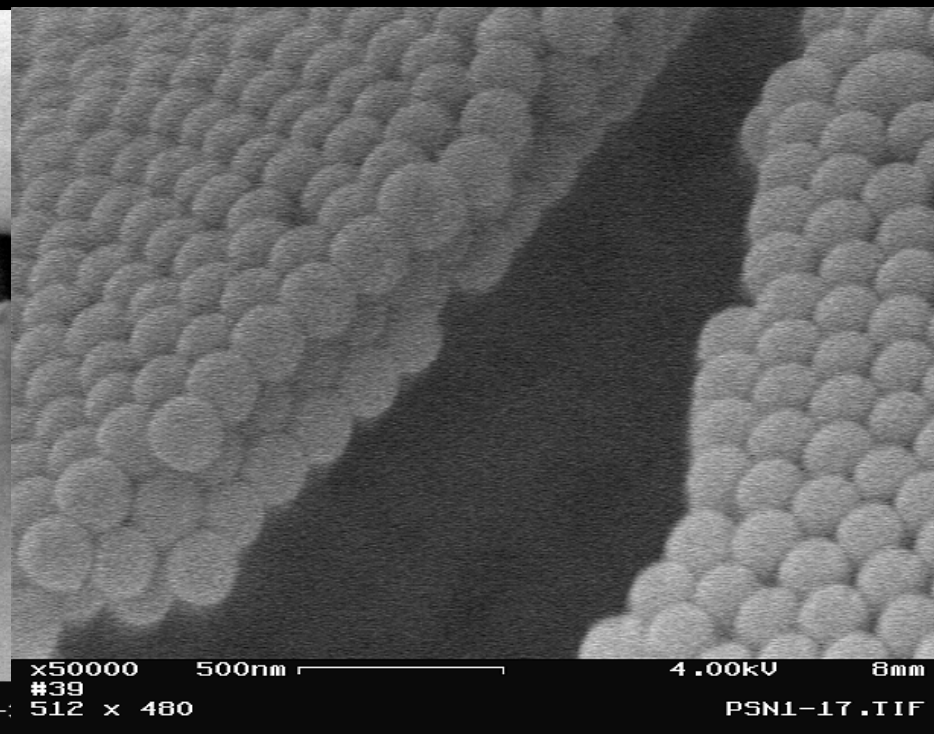
Email: bandi@oist.jp
Group Webpage: http://www.oist.jp/collective-interactions-unit

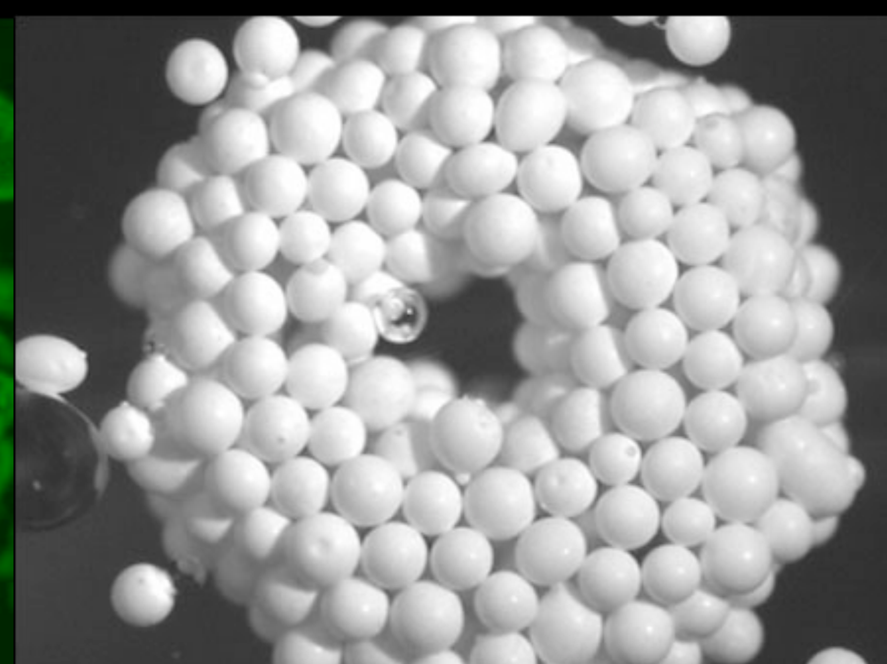
Interest in particulate interfaces





Tsapis Group
Lab de Pharmacie'
Galenique, Paris.

Colloidosomes: Drug Delivery



Stone Group, Harvard

Non-spherical bubbles