Mechanical Failure of a Small and Confined Solid

Debasish Chaudhuri and Surajit Sengupta

1Satyendra Nath Bose National Centre for Basic Sciences,
Block-JD, Sector-III, Salt Lake, Calcutta - 700098.

Abstract: Starting from a commensurate triangular thin solid strip, confined within two hard struc-
tureless walls, a stretch along its length introduces a rectangular distortion. Beyond a critical strain
the solid fails through nucleation of “smectic”-like bands. We show using computer simulations
and simple density functional based arguments, how a solid-smectic transition mediates the failure.
Further, we show that the critical strain introducing failure is inversely proportional to the channel
width i.e. thinner strips are stronger!

PACS numbers: 64.60.Cn, 61.30. v, 62.25.+g, 68.08. p
Keywords: confined solid, two dimensional smectic, fracture

I. INTRODUCTION

Studies of small systems comprising of a few thousand molecules have become increasingly important with the
advent of nano-technology. In these mesoscopic length
scales, a priori, there is no reason that mechanical behav-
ior will be governed by continuum elasticity theory. In
many situations one needs to study the effect of confine-
ment on the structural and other properties of materials.
Indeed, hard confinement, in one or more directions of-
ten induce new interesting properties; for example, the
rich phase behaviour of quasi two-dimensional colloidal
solids confined between two glass plates showing square,
triangular and “buckled” crystalline phases and
re-entrant surface melting transition of colloidal hard
spheres quite different from the bulk behaviour.

In an earlier paper we have shown that a small
confined solid in quasi one-dimension fails through nu-
cleation of “smectic” like bands. This is very unlike
a bulk solid, strained beyond it’s critical limit, fail-
ing through the nucleation and growth of cracks.

The interaction of dislocations or zones of plastic
deformation with the growing crack tip determines
the failure mechanism. Bulk solid show brittle failure
or ductile failure depending on these interactions.
On the other hand the two-dimensional confined solid shows
ductile failure along with reversible plasticity — the
plastic stress vanishes when the strain is removed and
the fractured parts join up without any discontinuity.
This is because of the high amount of orientational order
imposed by the confining walls which ensure that each smec-
tic band is confined within a dislocation - antidislocation
pair. On the removal of the strain these defects anni-
hilate in pairs leaving a perfect triangular lattice identical
to the initial solid.

In section we describe the phase structure of the two

dimensional confined strip and possible phase transitions.
We illustrate our discussion with previously published

\[ G_1, G_2, G_3 \]

\[ G_2 = G_3 \]

\[ a_x = a_0 \]

\[ a_y = \sqrt{3} a_0 \]

\[ G_1, G_2, G_3 \]

FIG. 1: The confined solid is shown along with the centered
rectangular (CR) unit cell. For an unstrained triangular lat-
tice \[ a_x = a_0 \] and \[ a_y = \sqrt{3} a_0 \]. \[ G_1, G_2, G_3 \]
denote the directions of the three reciprocal lattice vectors
(RLV). The third reciprocal lattice direction \[ G_3 \]
is equivalent to the direction \[ G_2 \], even in presence of the walls.

computer simulation data. In section we present sim-
ple density functional arguments showing the dif-
ference between a bulk solid, confined-solid and a smectic
phase as well as a Lindeman-like criterion for nuclae-
tion of the smectic. In section we give the results
and discuss their implications. We end by offering some
concluding remarks and discussions on future directions
of research in section

II. THE SYSTEM

A two dimensional bulk solid made of molecules in-
teracting via spherically symmetric potentials always
stabilizes in the triangular lattice configuration.
For specificity and simplicity we consider hard -disk
molecules, which are restricted from overlapping with
each other due to an infinitely large energy cost and remains non-interacting when they do not overlap. Apart from being easily accessible to theoretical treatment,21 experiments with nearly “hard” (macro-)molecules viz. sterically stabilized colloids21 are possible. The hard-disk free energy is entirely entropic in origin and the only thermodynamically relevant variable is the number density $\rho = N/V$ or the packing fraction $\eta = (\pi/4)\rho d^2$. The energy scale of the system is entirely set by $k_B T$ where $k_B$ is the Boltzmann constant and $T$ the (kinetic) temperature. Accurate computer simulation,2, 8 vindicated the defect unbinding theory10 of melting of the hard-disk solid below the (kinetic) temperature. Accurate computer simulation,2, 8 vindicated the defect unbinding theory10 of melting of the hard-disk solid below $\eta_m = .706$.

Imagine a narrow channel in two dimensions of width $L_y$ defined by hard walls at $y = 0$ and $L_y$ ($V_{wall}(y) = 0$ for $d/2 < y < L_y - d/2$ and $= \infty$ otherwise) and length $L_x$ with $L_x > L_y$. Therefore, $n_l$ layers of an undistorted triangular solid of lattice parameter $a_0$ and diameter $d$ may be accommodated (Fig 1) if $L_y$ is commensurate2 with the solid packing fraction, i.e.

$$L_y = \frac{\sqrt{3}}{2} (n_l - 1)a_0 + d. \quad (1)$$

For a system with a constant number of particles $N$ and $L_y$, $a_0$ is decided by the packing fraction $\eta$ alone. Note that $L_x = n_x a_0 = N a_0/n_l$, and $a_0$ is given by $\rho = N/L_x L_y$. Defining $\chi(\eta, L_y) = 1 + 2(L_y - d)/\sqrt{3}a_0$, the above condition reads $\chi = \text{integer} = n_l$. Violation of Eqn.(1) induces an internal rectangular strain measured from a reference triangular lattice of $n_l$ layers;

$$\varepsilon_d = \varepsilon_{xx} - \varepsilon_{yy} = \frac{a_x - a_0}{a_0} - \frac{a_y - a_0 \sqrt{3}/2}{a_0 \sqrt{3}/2}. \quad (2)$$

The lattice parameters of the strained, centered-rectangular (CR) unit cell $a_x$ and $a_y$ are shown in Fig 4.

The external strain, on the other hand, imposed by rescaling $L_x$ keeping $L_y$ fixed, $\epsilon = (\eta_0 - \eta)/\eta$ is measured using the initial triangular lattice as the reference state. As the solid is free to move locally, it may readjust itself to increase (or decrease) the number of layers $n_l$ in response to the external strain ensuring that the internal deviatoric strain remains small (minimization of free energy). It can be shown that2,

$$\varepsilon_d = \frac{n_l - 1}{\chi - 1} - \frac{\chi - 1}{n_l - 1}. \quad (3)$$

where the number of layers $n_l$ is the nearest integer to $\chi$ so that $\varepsilon_d$ has a discontinuity at half-integral values of $\chi$. This internal strain $\varepsilon_d$ is related non-linearly to $\epsilon$ and may remain small even if $\epsilon$ is large (Fig 2).

Walls induce density modulations, with peaks and troughs running parallel to the walls. The ensemble average of the local density $\rho(r) = \langle \sum_{i=1}^N \delta (\mathbf{r} - \mathbf{r}_i) \rangle$ shows asymmetric (ellipsoidal) density profiles at the lattice points, with the semi-major axes lying along the walls. The structure factor is defined as $\rho_{\mathbf{G}} = \left\langle \frac{1}{N} \sum_{j,k=1}^{N} \exp(-i \mathbf{G} \cdot \mathbf{r}_{jk}) \right\rangle$. For $\mathbf{G} = \pm \mathbf{G}_1(\eta)$, the reciprocal lattice vector (RLV) correspond to the set of close-packed lattice planes of the CR lattice perpendicular to the wall, and for $\pm \mathbf{G}_2(\eta)$ and $\pm \mathbf{G}_3(\eta)$ the four equivalent RLVs for close-packed planes at an angle ($= \pi/3$ and $2\pi/3$ in the triangular lattice) to the wall (see Fig. 4). It is useful to define the Lindemann parameter $l = \langle (u_i^2 - \bar{u}_i^2)^2 \rangle / a_i^2 + \langle (w_i^2 - \bar{w}_j^2)^2 \rangle / a_y^2$ where the angular brackets denote averages over configurations, $i$ and $j$ are nearest neighbors and $u_{\alpha i}$ is the $\alpha$-th component of the displacement of particle $i$ from it’s mean position. The parameter $l$ diverges at the melting transition12.

Apart from the solid phase (Fig 4 and Fig. 3(a)), the externally imposed density modulation may give rise to a modulated liquid or a smectic phase. Structurally a smectic is made up of overlapping asymmetric local density profiles along the walls generating continuous strips of density maxima running parallel to the walls. Peaks in

![FIG. 2: A plot of internal strain $\varepsilon_d$ as a function of external strain $\epsilon$. The jumps in $\varepsilon_d$ corresponds to half-integral values of $\chi$.](image-url)
the structure factor corresponding to $\pm \mathbf{G}_2(\eta)$ vanish, although for $\mathbf{G} = \pm \mathbf{G}_1(\eta)$, one continues to obtain strong peaks Fig.3b). In this phase, however, inter-layer particle exchanges are suppressed causing the Lindemann parameter to remain small. In a modulated liquid, on the other hand, this interlayer exchange is large. The structure factor of a modulated liquid (Fig.3c)) features a ring-like maximum characteristic of liquid, in addition to somewhat strong peaks corresponding to $\mathbf{G}_1$. Transitions among these phases are observed as the external strain is imposed strating from a perfect triangular solid. The sequence of phase changes is shown in Fig.4, the result of extensive Monte Carlo simulations of this system[9].

![FIG. 4: Results of Monte Carlo (MC) simulations of $N = 650$ hard -disks confined between two hard walls separated by a distance $L_y = 9d$. For each $\eta$, the system was equilibrated over $10^6$ MC steps (MCS) and data averaged over a further $10^6$ MCS. At $\eta = 0.85$ we have a strain free triangular lattice. Plots show the structure factors $\rho_{\mathbf{G}_1,i}$, $i = 1(+), 2(\circ)$ for RLVs $\mathbf{G}_1(\eta)$, averaged over symmetry related directions, as a function of $\eta$ and the Lindemann parameter $l(\square)$. The lines in the figure are a guide to the eye. At $\eta \approx .78$ $\rho_{\mathbf{G}_2}$ jumps to zero while $\rho_{\mathbf{G}_1}$ shows a small dip. The region with $.7 < \eta < .78$, therefore, contains a smectic phase which melts for $\eta < .7$, at which point the Lindemann parameter $l$ diverges.](image)

### III. THEORY

As shown earlier[9], the failure of commensurate solid under tensile strain imposed in the manner discussed in the previous section, comes about through the nucleation of smectic bands within the solid. Monte-Carlo simulations show, at half-integral $\chi$ where the local internal strain $\varepsilon_d$ becomes discontinuous, $\rho(\mathbf{r})$ at nearest neighbour sites overlap along the $x$-direction, parallel to the walls, generating smectic bands. The stress associated with $\varepsilon_d$ vanishes at these points and the solid fails under tension. In this section we shall show, using simple density functional[17, 18] arguments, that the phase transition and the consequent tensile failure (a smectic cannot support stress parallel to the smectic layers) is brought about by this overlap in the local density. Since mechanical failure in our system is a consequence of a phase transition, it is reversible — as the strain is reduced back to zero, the stress also vanishes and the perfect triangular lattice is recovered[9].

Within density functional theory[17], the excess grand potential of a non-uniform liquid containing a density modulation $\rho(\mathbf{r})$ over the uniform liquid of density $\rho_l$ is given by,

$$\frac{\Delta\Omega}{k_B T} = \int d\mathbf{r} \left( \rho(\mathbf{r}) \log(\rho(\mathbf{r})/\rho_l) - \delta\rho(\mathbf{r}) \right)$$

$$- \frac{1}{2} \int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) \delta\rho(\mathbf{r}) \delta\rho(\mathbf{r}') \quad (4)$$

Here $\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_l$ and $C(r)$ is the direct correlation function of the uniform liquid[20]. A functional minimization of the free energy yields the following self-consistency equation for the density:

$$\frac{\rho(\mathbf{r})}{\rho_l} = \exp[\int d\mathbf{r}' C(|\mathbf{r} - \mathbf{r}'|) \delta\rho(\mathbf{r}')] \quad (5)$$

In principle one should solve the above equation within the constraints imposed by the walls and obtain the equilibrium $\rho(\mathbf{r})$. Substitution of this $\rho(\mathbf{r})$ into Eqn.4 gives the equilibrium free energy and phase transitions. While we intend to carry out this procedure in the future, we must point out that for the present problem, this is complicated by surface terms and anisotropic, external, fields which are difficult to incorporate. In this paper we shall take a much simpler route in exploring the various conditions for the solid - smectic transition given the nature of the $\rho_{\mathbf{G}_1}$ (the order parameters) obtained from our simulations.

One may expand, therefore, the logarithm of the local density profile log-$\rho(\mathbf{r})$ in a Fourier series[18] around a lattice point at the origin, to get,

$$\rho(\mathbf{r}) = N \exp \left( 2C_0 \sum_{i=1}^{3} \rho_{\mathbf{G}_i} \cos(\mathbf{G}_i \cdot \mathbf{r}) \right) \quad (6)$$

where $C_0$ is a constant, of order unity, denoting the Fourier transform of the direct correlation function calculated at a q-vector corresponding to the smallest RLV set of the solid. We have kept contributions only from this set.

For a perfect triangular lattice, the RLV’s are $\mathbf{G}_1 = \hat{y} \frac{2\pi}{a}$, $\mathbf{G}_2 = \hat{x} \frac{2\pi}{a} \cos(\frac{\pi}{3}) + \hat{y} \frac{2\pi}{a} \sin(\frac{\pi}{3})$ and $\mathbf{G}_3 = \hat{x} \frac{2\pi}{a} \cos(\frac{\pi}{3}) - \hat{y} \frac{2\pi}{a} \sin(\frac{\pi}{3})$, where $a = \frac{\sqrt{3}}{2}a_0$. Using these relations and the fact that in the presence of confining walls the Fourier amplitudes denoting solid order are virtually constant up to the transition and $\rho_{\mathbf{G}_2} = \rho_{\mathbf{G}_3} \neq \rho_{\mathbf{G}_1}$, Eqn.6 gives,
\[ \rho(r) = N \exp\{C_0(2\rho G_1 + 4\rho G_2)\} \exp\left(\frac{1}{2} C_0 \left(\frac{2\pi}{d_y}\right)^2 \left\{ (2\rho G_1 + \rho G_2)\frac{y^2}{4} + 3\rho G_2 x^2 \right\} \right) \] (7)

Clearly the density profile is Gaussian, of the form, \( \rho(r) \sim \exp(-y^2/2\sigma_y^2 - x^2/2\sigma_x^2) \). Therefore, the spreads of density profile in \( x \) and \( y \) directions are given by \( \sigma_x \) and \( \sigma_y \) respectively, with

\[ \sigma_x^2 = \frac{1}{C_0} \left(\frac{d_y}{2\pi}\right)^2 \frac{1}{3\rho G_2} \] (8)
\[ \sigma_y^2 = \frac{1}{C_0} \left(\frac{d_y}{2\pi}\right)^2 \frac{1}{2\rho G_1 + \rho G_2} . \] (9)

In the absence of walls, \( \rho G_1 = \rho G_2 \) making \( \sigma_x = \sigma_y \), i.e. the density profile comes out to be symmetric in both directions, as expected for the bulk triangular solid. The presence of walls make \( \sigma_y < \sigma_x \) making the density profile elliptical with larger spread in \( x \)-direction, the direction parallel to the walls. Two neighbouring density profiles will overlap to form a smectic if \( \sigma_y > a_x \). This leads us to the definition of a measure of overlap \( O_l = (\sigma_x/\sigma_y) \).

The condition \( O_l > 1 \) is then the Lindemann criterion for nucleation of the smectic phase. Remembering \( a_x = a_0(n_l - 1)/(\chi - 1) \), we get,

\[ O_l = \frac{1}{4\pi} \frac{1}{\sqrt{C_0 \rho G_2} n_l - 1} . \] (10)

Whenever, \( \rho G_2 \to 0 \) i.e. with the loss of solid order \( O_l \) diverges although \( \sigma_y \) remains finite, since \( \rho G_1 \neq 0 \) in presence of the walls. This indicates a solid-smectic transition. However, even before \( \rho G_2 \to 0 \) the quantity \( \Delta = \frac{n_l}{\chi - 1} \) and therefore \( O_l \) shows large jumps at those internal strain \( (\varepsilon_d) \) values where \( \chi \) becomes half-integer. It is interesting to note that, at these points \( \varepsilon_d \) has discontinuities and the system fails. This shows that the mode of failure predicted by our theory is through a solid-smectic transition. The fact that \( \rho G_1 \) remains non-zero even at very small densities, due to the confinement from the walls, gives rise to the density modulations in the confined liquid.

We have shown therefore that the overlap in the density profiles may be used as an “order parameter” for the solid to smectic transition. We show below that jumps in this order parameter tantamounts to mechanical failure of the solid.

**IV. RESULTS AND DISCUSSION**

We begin with studying the overlap \( \Delta \) as a function of external strain \( \varepsilon \). For specificity, we start from a triangular solid of packing fraction \( \eta = .85 \) with \( L_y \) commensurate with a \( n_l = 10 \) layered solid. With increasing strain initially the overlap \( \Delta \) reduces due to increased separation \( (a_x) \) between neighbouring lattice points. But above a strain \( (\varepsilon) \) of about 10%, \( \chi \) reaches the half-integral mark and \( \Delta \) shows a discontinuous increase, indicating large overlap between neighbouring density profiles along the wall; indicating a solid to smectic transition (Fig.5) at the failure strain \( \varepsilon^* \). With further increase in strain the overlap reduces, again due to increased separation between neighbouring lattice points. At higher strains the smectic melts into a modulated liquid due to increased fluctuations connected with the reduced density.

We have performed this calculation for various \( L_y \) values commensurate with starting triangular solids of \( n_l = 2, 3 \ldots 20 \) layers at packing fraction \( \eta = .85 \). We found out the failure strains \( \varepsilon^* \) at each \( L_y \) and plotted them in Fig.7 as a function of \( L_y \). This clearly shows that the failure strain reduces with increase in \( L_y \). This demonstrates the fact, derived earlier from Monte-Carlo simulations, that thinner (smaller \( L_y \)) strips are stronger!

In Fig.9 we have plotted the overlap term \( \Delta \) with increasing interwall separation \( L_y \) at \( \eta = .85 \). The jumps, as usual, indicate failure strains corresponding to discontinuities in the internal strain \( \varepsilon_d \) at half-integer values of \( \chi \). The plot shows that the amount of overlap at the failure strains \( \varepsilon^* \) reduces with increasing \( L_y \) indicating that at large interwall separations the system starts to behave as a bulk solid and more conventional modes of
failure *viz.* through formation and interaction of cracks and twin boundaries starts becoming active.

V. CONCLUSION

In this paper we have described how mechanical and phase behaviour are intimately related to each other for a narrow solid strip confined between hard walls. Both may therefore be described using simple arguments based on density functional theory. The particles of the solid are assumed to interact via hard-disc interactions. Apart from constrained hard-sphere colloids [21] where our results are directly testable, a similar fracture mechanism may be observable in experiments on the deformation of mono-layer nano beams or strips of real materials provided the confining channel is made of a material which is harder and has a much smaller atomic size than that of the strip [1].

We believe that phase transition in confined systems, as described in this paper, may have future applications in nano-technology. The feature of reversible plasticity [9] may be used to produce nano scale mechanical switches. For example, thermal conductivity and electrical conductivity of such narrow strips after nucleation of smectic bands are expected to reduce drastically. These properties need to be investigated in detail. Due to reversible plasticity a small change in strain in opposite directions can vary these properties of confined nano-strips giving rise to a possible use of it as mechanical switch in nano-devices.

VI. ACKNOWLEDGEMENT

The authors thank M. Rao and V. B. Shenoy for useful discussions; D. C. thanks C.S.I.R., India, for a fellowship. Financial support from DST grant SP/S2/M-20/2001 is gratefully acknowledged.

[1] R. Giao et. al., Phys. Rev. Lett. 85, 622 (2000); A. N. Cleland and M. L. Roukes, Appl. Phys. Lett. 69, 2653 (1996).
[2] I Goldhirsh and C. Goldenberg, European Physical Journal E 9, 245 (2002).
[3] S. Nesper et al. Phys. Rev. Lett. 79, 2348, (1997).
[4] M. Schmidt and H. Loewen, Phys. Rev. Lett. 76, 4552, (1996); T. Chou and D. R. Nelson, Phys. Rev. E, 48, 4611 (1993).
[5] R. P. A. Dullens and W. K. Kegel, Phys. Rev. Lett. 92, 195702 (2004).
[6] B.J. Alder, T.E. Wainwright, Phys. Rev. B 127, 359 (1962); J.A. Zollweg, G.V. Chester, P.W. Leung, Phys. Rev. B 39 9518 (1989); H. Weber, D. Marx, Europhys. Lett. 27 593 (1994).
[7] A. Jaster, Physica A 277, 106 (2000).
[8] S. Sengupta, P. Nielaba, K. Binder, Phys. Rev. B 61, 6294 (2000).
[9] D. Chaudhuri, S. Sengupta, Phys. Rev. Lett. 93, 115702 (2004).
[10] Kosterlitz J M and Thouless D J 1973 J. Phys. C: Solid State Phys. 6 1181, Halperin B I and Nelson D R 1978 Phys. Rev. Lett. 41 121, Nelson D R and Halperin B I 1979 Phys. Rev. B 19 2457, Young A P 1979 Phys. Rev. B 19 1855.
[11] J. A. Hauch, D. Holland, M. P. Marder, and H. L. Swi-
ney, Phys. Rev. Lett. 82, 3823 (1999). D. Holland and M. Marder, Phys. Rev. Lett. 80, 746 (1998).

[12] J. S. Langer, Phys. Rev. E 62, 1351 (2000).

[13] A. A. Griffith, Philos. Trans. Roy. Soc. A 221, 163 (1920).

[14] R. Löfstedt, Phys. Rev. E 55, 6726 (1997).

[15] T. Belytschko et. al., Phys. Rev. B 65, 235430 (2002); M. F. Yu et. al., Science 287, 637 (2000).

[16] H. Ikeda et. al., Phys. Rev. Lett. 82, 2900 (1999); P. S. Branicio and J.-P. Rino, Phys. Rev. B 62, 16950 (2000).

[17] T. V. Ramakrishnan and M. Yussouff, Phys. Rev. B 19, 2775 (1979).

[18] P. M. Chaikin and T. C. Lubensky Principles of condensed matter physics, (Cambridge University Press, 1995).

[19] K. Zahn, R. Lenke and G. Maret, Phys. Rev. Lett. 82, 2721 (1999).

[20] J. P. Hansen and I. R. MacDonald Theory of simple liquids (Wiley, Chichester, 1989).

[21] I. W. Hamley Introduction to Soft Matter: polymer, colloids, amphiphiles and liquid crystals (Wiley, Chichester, 2000).