Contents

1 Melting A

1.1 Background re: melting

1.1.1 Theories of melting, 3D, 2D, bulk

3D crystallites w/ stable surfaces melt from within via Born melting
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In this case, melting can be viewed as nucleation and growth of fluid phase within the solid.

or yet another structure.

- or even another

2D large crystallites melt by two-step process via hexatic phase

2D finite crystallites melt from perimeter

if melt from perimeter, dN/dt goes as $N^{1/2}$

1.1.2 Expectations for 2D finite crystallites

1.2 Experiment of Savage et. al

1.2.1 Setup

1.2.2 Tuneable Depletion potential

1.2.3 Results

N vs. t

$< psi6 >^2$ vs. N

C_6 vs. N, by layer

No dependence of fast-melting feature on initial cluster size or melting rate

1.3 Simulations

1.3.1 Motivation

1.3.2 GROMACS System

1.3.3 Brownian dynamics

1.3.4 Simulated Depletion Potential

1.3.5 Simulated Lennard-Jones Potential

1.3.6 Results

N vs. t

$< psi6 >^2$ vs. N

C_6 vs. N, by layer

mean-square fluctuations in bond lengths

N vs. t for Lennard-Jones potential

Phase diagram showing lack of fluid phase with short-range potential

1.3.7 Discussion

2 Melting B

2.1 Background

2.1.1 Colloids: macroscopic system analogous to atomic system

similarites:

some phase behavior and phase transitions

can investiage atomic behavior via analogy

differences:

novel phases and phase behavior

superheated metastable states

interparticle potential readily modified

- short-range repulsion, long-range repulsion, short-range repulsion and long-range attraction

2.1.2 Experiment by Savage et. al: novel melting kinetics

system: hard spheres with short-range attraction (relative to diameter)

experiment details

two-stage melting process

first melts from perimeter until reaches critical size

then breaks up into dense amorphous phase, which is unstable and rapidly evaporates

crossover occurs at typical 'magic size'

experiments: magic size ~ 20-30 particles

simulations: magic size ~ 40-50 particles

little dependence on temperature in experiment

(?) no dependence on temp in simulation?

possible explanations ruled out:

'fast melting' behavior means rate not limited by thermal breaking of bonds

- (since this would go as $N^(1/2)$

density decreases as crystallites shrink: melting kinetics not governed by surface tension

- (?) does this contradict lacoste's argument?

- (?) can i get data re: surface tension from tony, from simulations?

melting behavior not history dependent

- no dependence on initial cluster size, melting rate in experiment
- (?) no dependence in simulation ?

not classical nucleation of liquid within solid below critical crystal size

energetically unfavorable given positive surface energy

positive difference between chemical potentials of two phases

(?) understand this argument, relevant equations

2.1.3 Our hypothesis: thermally-activated defects enhance melting rate

thermal introduction of disclinations favorable after critical size

presence of disclinations leads to concentration of stress

stress can be released through propagation of cracks

cracks propagate or not depending on range of potential

short-range, 'brittle' potential allow cracks to propagate

longer-range, 'ductile' potential doesn't

(?) is notion of a 'crack' in a liquid droplet sensible?

2.1.4 Simulations yield same result re:

2.1.5 Hypothesis: thermally-activated defects enhance melting rate in short-range, 2D system

2.1.6 Evidence:

Disclinations are implicated in breakup

GROMACS BD simulations, using depletion-like potential (from Part A)

exhibit fast-melting (from Part A)

order parameter decreases sharply (Part A)

ave disclination 'charge' reaches +1 at the magic size

Disclinations and two-stage melting affected by range of potential

Own BD simulations with screened Coulomb potential

Tune range of potential, short- and long-range (lambda values?)

Short-range: x percent fast melting; long-range: y percent fast melting; x¿¿y

2.2 Simulation Methods

2.2.1 Gromacs system

Here's a good test. [**?**]

4.1.2 Proposal: study complexity of percolation model

4.2 Percolation

4.2.1 The Model

4.2.2 Background / applications

4.3 PRAM

4.3.1 Applications in comp sci

4.3.2 PRIORITY CRCW

4.4 Parallel Algorithm for Percolation

4.5 Results

4.5.1 D_2 vs. p for several system sizes L

4.5.2 log(D_2) vs. log(L)

4.5.3 Distribution of cluster sizes

logarithmic or power law? (power law –¿ algorithm will often fail)