Thesis Outline, Don Blair (July 6, 2010)

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CHAPTER

CHAPTER 1

MELTING A

1.1 Background re: melting

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

a. 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

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

c. 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

a. N vs. t

b. $< psi6 >^2$ vs. N

c. C_6 vs. N, by layer

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

1.3 Simulations

1.3.1 Motivation

a. Rule out any hydrodynamic effects causing fast-melting

b. Determine whether range of potential plays role in fast melting

c. Justification for using Brownian dynamics

1.3.2 GROMACS Simulations

a. Brownian dynamics option

b. Interparticle 'depletion' potential

- **Mimics that in experiment**

- $U(r) = 0$ **for** $r > r_0$

- $U(r) = 4/(10r - 9)^{12} - 400a_0(r - r_0)^2$ **for** $r \leq r_0$ with the first term resembling hard sphere repulsion and the second term representing a two-body depletion potential. The parameters $a_0 = 1.0$ and $r_0 = 1.1$ were chosen to allow for a potential with a narrow width compared to the particle diameter. This potential has an effective particle diameter $\sigma = 1.0$, a width equal to 0.1 and an equilibrium inter-particle spacing $a \approx 1.01637$

c. Temperature

d. Effective well depth: $3.5k_BT$

e. Time step: 2.5×10^{-5} **(in GROMACS time units)**

f. $N = 100$ **particles**

g. periodic box of size $L = 18.0\sigma$

h. particle area fraction of 24%