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## 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

CLOSED: 2010-07-04 Sun 15:28

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.  $\langle \psi^2 \rangle$  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:  $3.5k_B T$
- e. Time step:  $2.5 \times 10^{-5}$  (in GROMACS time units)
- f.  $N = 100$  particles
- g. periodic box of size  $L = 18.0\sigma$
- h. particle area fraction of 24%