

PHYSICAE AUSCULTATIONES

A Dissertation Presented

by

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CHAPTER 1

MELTING A

1.1 Background re: melting

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

1.1.1.1 3D crystallites w/ stable surfaces melt from within via Born melting

In this case, melting can be viewed as nucleation and growth of fluid phase within the solid.

1.1.1.1.1 or yet another structure.

- or even another

1.1.1.2 2D large crystallites melt by two-step process via hexatic phase

1.1.1.3 2D finite crystallites melt from perimeter

1.1.1.3.1 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 Tunable Depletion potential

1.2.3 Results

1.2.3.1 N vs. t

1.2.3.2 $\langle \psi^2 \rangle$ vs. N

1.2.3.3 C_6 vs. N , by layer

1.2.3.4 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

1.3.6.1 N vs. t

1.3.6.2 $\langle \psi^2 \rangle$ vs. N

1.3.6.3 C_6 vs. N , by layer

1.3.6.4 mean-square fluctuations in bond lengths

1.3.6.5 N vs. t for Lennard-Jones potential

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

1.3.7 Discussion

CHAPTER 2

MELTING B

2.1 Background

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

2.2 Simulation Methods

2.2.1 Gromacs system

2.2.2 Brownian Dynamics

2.2.3 Characteristics of Simulated Depletion Potential

2.2.4 Initial configurations

2.3 Results

2.3.1 N vs t

2.3.2 Order vs. N

2.3.3 Breakdown by layers

2.4 Conclusions

CHAPTER 3

DIAMETER OF RANDOM CLUSTERS

- 3.1 Background**
- 3.2 Simulations**
- 3.3 Results**

CHAPTER 4

PHASE TRANSITIONS IN COMPUTATIONAL COMPLEXITY

4.1 Background

4.1.1 Constraint Satisfaction Problems (CSP)

4.1.1.1 Examples

4.1.1.1.1 kSAT

4.1.1.1.2 Graph-coloring

4.1.1.1.3 Spin models

4.1.1.1.4 error-correcting codes

- 4.1.1.2 Observation of threshold behavior in CSP
- 4.1.1.3 Difficulties in tackling phase behavior of CSP
- 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
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- 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
 - 4.5.3.1 logarithmic or power law? (power law \rightarrow algorithm will often fail)

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