

STRUCTURE FORMING PROCESSES IN MESOSCOPIC POLYMER SYSTEMS

by

TOMAS KOCI

(Under the direction of Michael Bachmann)

ABSTRACT

This is going to be the best abstract ever :)

INDEX WORDS: Index word or phrase, Index word or phrase, Index word or phrase,
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MESOSCOPIC POLYMER SYSTEMS

by

TOMAS KOCI

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Tomas Koci

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TOMAS KOCI

Approved:

Major Professor: Michael Bachmann

Committee: Steven P. Lewis
Heinz-Bernd Schuttler

Electronic Version Approved:

Alan Dorsey
Dean of the Graduate School
The University of Georgia
July 2016

Structure Forming Processes in Mesoscopic Polymer Systems

Tomas Koci

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Chapter 1

Introduction

Kickass Intro...

Chapter 2

Elements of Statistical Mechanics

Statistical mechanics explains microscopic origins of the macroscopic properties of systems with large numbers of degrees of freedom. The exact solution for a phase space trajectory of a complex system requires enormous computational efforts and contains little useful information. On the other hand, the collective properties such as the entropy, pressure, or temperature often display relatively simple behavior. The formalism of statistical mechanics allows us to study these properties by considering the average behavior of a large number of identically prepared systems; the statistical ensemble. It is well established that in the thermodynamic limit all ensembles are equivalent. However this is emphatically not true for intrinsically finite systems for which the choice of an ensemble is non-trivial. Therefore, I shall first discuss several prominent statistical ensembles starting with the most fundamental one; the *microcanonical ensemble*.

2.1 The microcanonical ensemble

2.2 The canonical ensemble

2.3 Generalized ensembles

Chapter 3

Computational Methods

3.1 Markov chain Monte Carlo

3.1.1 Master equation and detailed balance

3.1.2 Metropolis sampling

3.2 Generalized ensemble Monte Carlo

3.2.1 Parallel tempering

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Coarse-grained Homopolymer Model

4.1 Flexible elastic homopolymer

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Chapter 5

Confinement Effects on Structural Transitions in Flexible Homopolymers

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Chapter 6

Impact of Bonded Interactions on the Ground-State Geometries of Flexible Homopolymers

6.1 Structural order parameters

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Chapter 7

Aggregation of Flexible Elastic Homopolymers

7.1 Introduction

7.2 Microcanonical analysis

7.2.1 Subphases and subphase transitions

7.2.2 Missing subphases and translational entropy

7.2.3 Density effects on the latent heat

Chapter 8

Summary and Outlook

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Figure 8.1: Example of a figure.

Table 8.1: Example of a table.
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