

MONTE CARLO SIMULATIONS OF NANOTUBES IN SUSPENSION

by

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ABSTRACT

Nanotube suspensions have been modeled via Monte Carlo simulation. A computer model was used to realize networks of nanotubes with random placement and orientation. The nanotubes were modeled as capped interpenetrating cylinders placed in a unit volume. The problem was formulated as a percolation process, where the critical fractional volume (CFV) of cylinders (associated with the onset of percolation) was realized multiple times and analyzed. The aim of the study was to consider nanotubes of high aspect ratio, a (a =length/diameter; as high as 2000), and to determine the effects that aspect ratio may have on the CFV. It was determined that the CFV is inversely proportional to the aspect ratio in the limit of high aspect ratios. This results in the need for very low percent volume loadings ($\%volume \leq 0.01\%$) of nanotubes to create a conductive network (percolation infinite cluster). These findings are in good agreement with recent experimental data involving the thermal conductivity of carbon nanotube suspensions.

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Table of Contents

Abstract	ii
Acknowledgements.....	iii
Table of Contents.....	iv
1.0 Introduction.....	1
2.0 Background on Percolation Theory.....	4
2.1 History and Nature of Percolation Problems.....	4
2.2 Random Site Problems.....	4
2.3 The Thermodynamic Limit.....	5
2.4 Percolation in Summary.....	6
3.0 Defining the Percolation Problem for Nanotube Suspensions.....	7
3.1 Nanotubes as Capped Cylinders.....	7
3.2 The Percolation Algorithm.....	8
3.2.1 Input.....	8
3.2.2 The Initial Seed Number, N	8
3.2.3 Seeding of the Space and Checking for Connections.....	9
3.3 The Connectivity Criterion and Resulting Conditions.....	9
3.4 The Distance Between Two Line Segments in Space.....	11
3.5 Derivations of Conditions of Connectivity.....	11
3.5.1 <i>Case I</i> : Side to Side Touching.....	13
3.5.2 <i>Case II</i> : Cap to Cap Touching.....	14
3.5.3 <i>Case III</i> : Side to Cap Touching.....	16
3.6 Checking for Percolation.....	18

4.0 Calculations.....	19
5.0 Discussion of Main Results of Simulations.....	23
5.1 Resulting Curves.....	23
5.2 Excluded volume considerations.....	23
5.3 Comparison with the excluded volume model.....	25
5.4 Conclusions based on B_c	26
5.5 Comparison with experiment.....	26
6.0 Conclusions.....	28
Appendices.....	29
Appendix A: Thermodynamic Limits of Average Critical Volume.....	30
Appendix B: C Computer Code for the Percolation Simulations.....	55
References.....	87
Vita.....	88