

Table of Contents

Introduction	1
1.1 Vapor Phase Synthesis of Materials.....	1
1.2 Applications Motivating Vapor Phase Process Development.....	3
1.3 Goals of the Dissertation.....	6
Background	10
2.1 Vapor Creation Using an Electron Beam Gun.....	12
2.1.1. Pure metal / metal alloy processing.....	12
2.1.2. Compound processing.....	16
2.1.3. Vacuum regime.....	17
2.2 Vapor Transport.....	20
2.2.1. High vacuum vapor transport.....	21
2.2.1.1 Spatial distribution	
2.2.1.2 Angular distribution	
2.2.1.3 Kinetic energy	
2.2.1.4 Deposition efficiency	
2.2.2. Modification of vapor transport characteristics.....	26
2.2.2.1 Spatial distribution	
2.2.2.2 Angular distribution	
2.2.2.3 Kinetic energy	
2.2.2.4 Deposition efficiency	
2.2.2.5 Evaporated material form	
2.2.3. Jet Vapor Deposition TM	34
2.2.4. Supersonic gas jet structure.....	37
2.2.5. Vapor transport modeling.....	39
2.3 Vapor Adsorption and Diffusion on a Substrate.....	46
2.4 Summary.....	49
Invention of Directed Vapor Deposition	50
DVD System Design	56
4.1 Electron Beam Gun.....	57
4.1.1. Maximum e-beam gun power requirements.....	57
4.1.2. Accelerating voltage selection.....	60
4.1.3. Selection of an e-beam generation source.....	63
4.1.4. A modified e-beam deflection system was required.....	65
4.1.5. Final e-beam gun configuration.....	68
4.2 Processing Chamber.....	69

4.2.1. X-ray shielding for system user protection	70
4.2.2. The chamber could accommodate various sources and substrates	72
4.3 Crucible.....	74
4.4 Gas System	76
4.5 Vacuum Pumps.....	81
4.6 Vacuum Gauges	82
4.7 Substrate Temperature Control System	83
4.8 Computer Control Methodology.....	84
4.9 Concluding Remark	88
 Experimental Investigation of Vapor Transport 90	
5.1 Overview	90
5.2 Accessible Processing Regime	91
5.3 Visual Observations of Gas Stream	97
5.4 Gas Flow / Vapor Stream / Substrate Interactions	102
5.4.1. Carrier gas flux	103
5.4.2. Mach number	106
5.4.3. Carrier gas type / e-beam power	109
5.4.4. Carrier gas flux / vapor stream interaction with substrate / crucible . .	112
5.5 Concluding Remarks.....	115
 Materials Synthesis Via Directed Vapor Deposition 116	
6.1 Overview	116
6.2 Contamination Study of Nonreactive Deposition	117
6.3 Study of Silicon Deposition.....	119
6.4 Study of Reactive Deposition	126
6.5 Concluding Remarks.....	128
 Experimental Investigations of Deposition Efficiency 129	
7.1 Overview	129
7.2 Deposition Efficiency Experimental Procedures	131
7.3 Flat Substrate Results.....	132
7.3.1. Carrier gas flux / Mach number	133
7.3.1.1 Vapor transport visualizations help explain efficiency results	
7.3.1.2 A discussion of evaporation rate variations	
7.3.1.3 Deposited film appearance, adhesion depend on process conditions	
7.3.1.4 A summary of initial deposition efficiency results	
7.3.2. E-beam power (evaporation rate effects)	142
7.3.2.1 Low beam power experiments generate inconsistent results	
7.3.2.2 Visual inspection of films revealed chamber pressure and beam power effects	

7.3.2.3	A summary of evaporation rate results	
7.3.3.	Crucible to nozzle separation effects	147
7.3.3.1	Initial vapor distribution effects upon deposition efficiency	
7.3.3.2	Summary of nozzle position experiments	
7.4	Fiber Substrates.....	151
7.4.1.	Fiber coating deposition efficiency trends mirror flat substrate results	152
7.4.2.	Non line-of-sight deposition enhances deposition efficiency	155
7.4.3.	Inspection of coated fiber characteristics.	155
7.4.4.	Summary of fiber coating study.	157
7.5	Clustering.....	158
7.5.1.	Clustering probabilities for various process conditions.	160
7.5.2.	Ionization effects upon cluster formation probability	163
7.6	Summary	164
Vapor Transport Model Development		166
8.1	Direct Simulation Monte Carlo (DSMC) Modeling of the Flowfield	168
8.1.1.	Selection of discrete atom modeling method.	168
8.1.2.	Adaptation of DSMC code to DVD.	170
8.2	Biatomic Collision Theory (BCT) Modeling of Vapor Transport	177
8.2.1.	Initial conditions	178
8.2.2.	Distance between collisions.	181
8.2.3.	Calculation of the directed momentum transfer cross-section (σ_d) . . .	183
8.2.4.	Determination of the range of atomic interaction (b_{max}).	186
8.2.5.	Collision event	191
8.3	Summary	196
Vapor Transport Model Verification		198
9.1	Verification of DSMC Results	198
9.2	BCT Model Verification.....	200
9.2.1.	Random walk	201
9.2.2.	Atomic energy loss	205
9.3	Summary	211
Vapor Transport Modeling of DVD		212
10.1	Vapor Transport Predictions.....	213
10.1.1.	Model predicts redirection at lower pressures than experiments.	216
10.1.2.	Dissipation of jet's fast flow limits vapor direction to substrate	217
10.1.3.	Adatom kinetic energies are below initial evaporation energies	218
10.1.4.	Adatom angle of incidence determined by gas near the substrate	220
10.1.5.	Flowfield temperature and pressure.	221
10.2	Vapor Deposition Predictions	223

10.2.1. Model predicted deposition efficiency trends	223
10.2.2. Vapor concentration effects	226
10.2.3. Predicted efficiencies	226
10.2.4. Deposition energy distributions change little with process conditions	227
10.2.5. Deposition angle distributions	228
10.2.6. Deposition distribution.	229
10.3 Summary	231
DVD System Development	234
11.1 Reconfiguration of the Gun, Vapor Source, and Carrier Gas Flow	235
11.1.1. Justification for system reconfiguration.	235
11.1.2. Model-based analysis of system reconfiguration.	237
11.2 Substrate Bias	242
11.3 Experimental Work	243
11.4 Model Development.	245
11.5 Concluding Remarks.	248
Discussion	249
12.1 Focus, Efficiency, and Angular Distribution	250
12.2 Non-line-of-sight Coating.	251
12.3 Vapor Stream Mixing	253
12.4 Enhanced Energy Deposition.	253
12.5 Rapid, Continuous Processing of Pure Materials and Compounds	255
12.6 Other Applications	256
12.7 Other System Configurations	257
12.8 Summary	257
Conclusions	258
13.1 Specific Conclusions	259
13.2 Final Thought	262
References	263
Appendix A - DVD Specifications	276
A.1 E-beam Gun Design Drawings	276
A.2 Processing Chamber Design Drawings	281
A.3 Water-Cooled Crucible Design Drawings	282
A.4 Processing Chamber Pumping Capacity Design Calculations	283
Appendix B - Clustering Calculations	286
Appendix C - Flowfield Modeling Code	287

Appendix D - Atom Tracking Code 329

Appendix E - E-beam Vapor Distribution 348