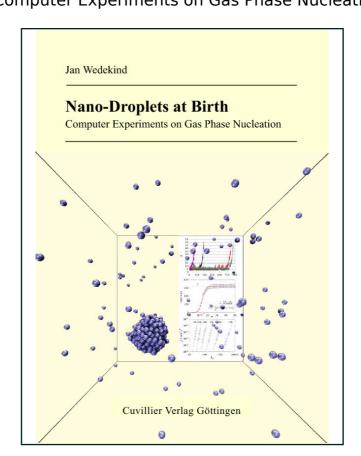


Jan Wedekind (Autor) Nano-Droplets at Birth Computer Experiments on Gas Phase Nucleation



https://cuvillier.de/de/shop/publications/1972

Copyright:

Cuvillier Verlag, Inhaberin Annette Jentzsch-Cuvillier, Nonnenstieg 8, 37075 Göttingen, Germany

Telefon: +49 (0)551 54724-0, E-Mail: info@cuvillier.de, Website: https://cuvillier.de

Table of Contents

Lis	List of Important Symbols and Abbreviations			
1	Introduction			
	1.1	Phase Transitions and Nucleation	11	
	1.2	Research on Vapor-Liquid Nucleation	15	
	1.3	Task Description	21	
2	Theory of Vapor-Liquid Nucleation			
		The Nucleation-and-Growth Picture	23	
	2.2	The Thermodynamics of a Vapor-Drop System	27	
		2.2.1 General Thermodynamic Relations	27	
		2.2.2 A Hypothetical Vapor-Drop System	28	
		2.2.3 Equilibrium Conditions: The Generalized Laplace Equation	31	
	2.3	Classical Nucleation Theory (CNT)	34	
		2.3.1 The Nucleation Barrier	34	
		2.3.2 Steady-State Nucleation Rate	39	
	2.4	The Nucleation Theorem	44	
	2.5	Corrections and Extensions of CNT	46	
		2.5.1 The "Self-Consistent" Correction	46	
		2.5.2 Density Functional Theory (DFT)	47	
		2.5.3 Dynamical Nucleation Theory (DNT)	47	
		2.5.4 The Scaled Model	48	
		2.5.5 Other Recent Models	48	
	2.6	The Modified Liquid Drop Model (MLD)	49	
	2.7	The Extended Modified Liquid Drop Model (EMLD)	53	
	2.8	The Reguera-Reiss Theory (EMLD-DNT)	56	
		2.8.1 Basic Concept	56	
		2.8.2 The Nucleation Barrier in the RR Theory	58	
3	Mo	lecular Dynamics Simulations	61	
	3.1	Basic Concepts and Techniques	62	
		3.1.1 Classical Mechanics	63	
		3.1.2 Integration of the Equations of Motion	65	
		3.1.3 Periodic Boundary Conditions	67	
		3.1.4 Cluster Identification	68	
	3.2	The Lennard-Jones Potential	71	
	3.3	Details of the Simulations in this Work	73	
	3.4	Rate Evaluation, Thermostat, and Finite-Size Effects	73	
4	A New Method to Analyze Rates in Simulations of Nucleation			
	4.1	The Problem of Determining Rates in a Simulation	75 75	
	4.2	Rates and Mean First-Passage Times	80	
	4.3	Practical Implementation and Application in this Work	85	
	4.4	Different Cluster Definitions and the Critical Cluster Size	89	
	4.5	Early Times and Steady-State	90	
		•	_	

5	The Influence of Different Thermostats on Simulations of Vapor-Liquid			
	Nuc	leation	93	
	5.1	The Different Thermostating Methods	95	
		5.1.1 Velocity Scaling	95	
		5.1.2 The Andersen Thermostat	95	
		5.1.3 The Nosé-Hoover Thermostat	96	
	5.2	MD Simulations with Different Thermostats	97	
		5.2.1 Details of the simulations	97	
		5.2.2 Results	99	
		5.2.3 Mean Cluster Temperatures	101	
		5.2.4 Discussion of the Simulation Results	106	
6	Finite-Size Effects in Phase Transitions in Small Systems			
	6.1	Theoretical Framework: MLD	113	
	6.2	Evaporation	115	
	6.3	The "Strey-Approach" to Evaporation	118	
	6.4	Nucleation	119	
		6.4.1 General Case Study	119	
		6.4.2 Optimizing the System Size in Simulations of Nucleation	122	
		6.4.3 Optimum System Sizes in this Work	125	
	6.5	MD Simulations of Smaller System Sizes	126	
7	Homogeneous Nucleation Rates of Argon from MD Simulations			
	7.1	Nucleation Rates and Critical Cluster Sizes	133	
	7.2	Comparison with Nucleation Theory and Experiment	138	
		7.2.1 Nucleation Rates	138	
		7.2.2 Critical Cluster Sizes	144	
		7.2.3 Nucleation Rates in the Scaled Model	147	
		7.2.4 Concluding Remarks	149	
8	Summary and Outlook			
	8.1	Summary and Conclusions	153	
	8.2	Outlook	155	
App	endix		157	
	A.1	Argon Parameters	157	
	A.2	Simulation Results	158	
	A.3	Computer Resources	160	
	A.4	New Subroutines and Analysis Tools	161	
		Details of 2D Simulations	164	
	Refe	erences	165	
	Erkl	ärung (Statement)	175	
	Lebe	enslauf (Curriculum vitae)	177	