

Hanna Vehkamäki

Classical Nucleation Theory in Multicomponent Systems



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Classical Nucleation Theory In Multicomponent Systems:

Classical Nucleation Theory in Multicomponent Systems Hanna Vehkamäki, 2006-03-22 Nucleation is the initial step of every first order phase transition and most phase transitions encountered both in everyday life and industrial processes are of the first order Using an elegant classical theory based on thermodynamics and kinetics this book provides a fully detailed picture of multi component nucleation As many of the issues concerning multi component nucleation theory have been solved during the last 10 15 years it also thoroughly integrates both fundamental theory with recent advances presented in the literature Classical Nucleation Theory in Multicomponent Systems serves as a textbook for advanced thermodynamics courses as well as an important reference for researchers in the field The main topics covered are the basic relevant thermodynamics and statistical physics modelling a molecular cluster as a spherical liquid droplet predicting the size and composition of the nucleating critical clusters kinetic models for cluster growth and decay calculating nucleation rates and a full derivation and application of nucleation theorems that can be used to extract microscopic cluster properties from nucleation rate measurements The assumptions and approximations needed to build the classical theory are described in detail and the reasons why the theory fails in certain cases are explained Relevant problems are presented at the end of each chapter

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The Validity of Classical Nucleation Theory and Its Application to Dislocation Nucleation Seunghwa Ryu, 2011 Nucleation has been the subject of intense research because it plays an important role in the dynamics of most first order phase transitions The standard theory to describe the nucleation phenomena is the classical nucleation theory CNT because it correctly captures the qualitative features of the nucleation process However potential problems with CNT have been suggested by previous studies We systematically test the individual components of CNT by computer simulations of the

Ising model and find that it accurately predicts the nucleation rate if the correct droplet free energy computed by umbrella sampling is provided as input This validates the fundamental assumption of CNT that the system can be coarse grained into a one dimensional Markov chain with the largest droplet size as the reaction coordinate Employing similar simulation techniques we study the dislocation nucleation which is essential to our understanding of plastic deformation ductility and mechanical strength of crystalline materials We show that dislocation nucleation rates can be accurately predicted over a wide range of conditions using CNT with the activation free energy determined by umbrella sampling Our data reveal very large activation entropies which contribute a multiplicative factor of many orders of magnitude to the nucleation rate The activation entropy at constant strain is caused by thermal expansion with negligible contribution from the vibrational entropy The activation entropy at constant stress is significantly larger than that at constant strain as a result of thermal softening The large activation entropies are caused by anharmonic effects showing the limitations of the harmonic approximation widely used for rate estimation in solids Similar behaviors are expected to occur in other nucleation processes in solids

Nucleation Theory and Applications Jörn W. P. Schmelzer, 2006-03-06 An overview of recent developments in the field of first order phase transitions which may be considered a continuation of the previous work Aggregation Phenomena in Complex Systems covering work done and discussed since then Each chapter features a different aspect of the field written by international specialists and covers such topics as nucleation and crystallization kinetic of silicate glasses nucleation in concentration gradients the determination of coefficients of emission of nucleation theory diamonds from vitreous carbon

Nucleation Theory V.I. Kalikmanov, 2012-11-28 One of the most striking phenomena in condensed matter physics is the occurrence of abrupt transitions in the structure of a substance at certain temperatures or pressures These are first order phase transitions and examples such as the freezing of water are familiar in everyday life The conditions at which the transformation takes place can sometimes vary For example the freezing point of water is not always 0 C but the liquid can be supercooled considerably if it is pure enough and treated carefully The reason for this phenomenon is nucleation This monograph covers all major available routes of theoretical research of nucleation phenomena phenomenological models semi phenomenological theories density functional theories microscopic and semi microscopic approaches with emphasis on the formation of liquid droplets from a metastable vapor Also it illustrates the application of these various approaches to experimentally relevant problems In spite of the familiarity of the involved phenomena it is still impossible to calculate nucleation accurately as the properties and the kinetics of the daughter phase are insufficiently well known Existing theories based upon classical nucleation theory have on the whole explained the trends in behavior correctly However they often fail spectacularly to account for new data in particular in the case of binary or more generally multi component nucleation The current challenge of this book is to go beyond such classical models and provide a more satisfactory theory by using density functional theory and microscopic computer simulations in order to describe the properties of small clusters Also semi

phenomenological models are proposed which attempt to relate the properties of small clusters to known properties of the bulk phases This monograph is an introduction as well as a compendium to researchers in soft condensed matter physics and chemical physics graduate and post graduate students in physics and chemistry starting on research in the area of nucleation and to experimentalists wishing to gain a better understanding of the efforts being made to account for their data

Crystallization Technology Handbook A. Mersmann, 2001-05-08 This handbook facilitates the selection design and operation of large scale industrial crystallizers that process crystals with the proper size distribution shape and purity sought including cooling evaporation drowning out reaction melt and related crystallization techniques This new edition offers new results on direct contact cooling crystallization It lists the properties of over 170 organic and inorganic crystallization systems

Thermal Analysis and Thermodynamic Properties of Solids Jaroslav Sestak, 2021-08-09 Thermal Analysis and Thermodynamic Properties of Solids Second Edition covers foundational principles and recent updates in the field presenting an authoritative overview of theoretical knowledge and practical applications across several fields Since the first edition of this book was published large developments have occurred in the theoretical understanding of and subsequent ability to assess and apply principles of thermal analysis Drawing on the knowledge of its expert author this second edition provides fascinating insight for both new and experienced students researchers and industry professionals whose work is influenced or impacted by thermo analysis principles and tools Part 1 provides a detailed introduction and guide to theoretical aspects of thermal analysis and the related impact of thermodynamics Key terminology and concepts the fundamentals of thermophysical examinations thermostatics equilibrium background thermotics reaction kinetics and models thermokinetics and the exploitation of fractals are all discussed Part 2 then goes on to discuss practical applications of this theoretical information to topics such as crystallization kinetics and glass states thermodynamics in superconductor models and climate change Includes fully updated as well as new chapters on kinetic phase diagrams thermokinetics in DTA experiments and crystallization kinetics Discusses the influence of key derivatives such as thermostatics thermodynamics thermotics and thermokinetics Helps readers understand and describe reaction kinetics in solids both in terms of simplified descriptions of the reaction mechanism models and averaged descriptions using fractals

Nucleation in Condensed Matter Ken Kelton, Alan Lindsay Greer, 2010-03-19 In Nucleation in Condensed Matter key theoretical models for nucleation are developed and experimental data are used to discuss their range of validity A central aim of this book is to enable the reader when faced with a phenomenon in which nucleation appears to play a role to determine whether nucleation is indeed important and to develop a quantitative and predictive description of the nucleation behavior The third section of the book examines nucleation processes in practical situations ranging from solid state precipitation to nucleation in biological systems to nucleation in food and drink Nucleation in Condensed Matter is a key reference for an advanced materials course in phase transformations It is also an essential reference for researchers in the field Unified treatment of key theories

experimental evaluations and case studies Complete derivation of key models Detailed discussion of experimental measurements Examples of nucleation in diverse systems Kinetic Theory of Nucleation Eli Ruckenstein, Gersh Berim, 2016-07-06 Explore a Kinetic Approach to the Description of Nucleation An Alternative to the Classical Nucleation Theory Kinetic Theory of Nucleation presents an alternative to the classical theory of nucleation in gases and liquids the kinetic nucleation theory of Ruckenstein Narsimhan Nowakowski RNNT RNNT uses the kinetic theory of fluids to calculate t

Advances in Ion Mobility-Mass Spectrometry: Fundamentals, Instrumentation and Applications, 2019-01-10 Ion Mobility Spectrometry Volume 83 will focus on new trends methods and instrumentation in the field starting from the innovations of each technique to the most progressive challenges of IM MS Chapters include section on Recent advances in IM MS IM MS Principles and Theory IM MS Applications and Instrumentation and the Future of IM MS Presents the latest advancements in IM MS that are essential for new applications Helps readers understand the state of the art in the currently available IM MS interfaces and their principle uses Provides information on different IM MS instrumentation Delves into key applications of IM MS

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