Nucleation And Growth Kinetics Modeling Using Matlab

Magnetic Nanomaterials
Handbook of Industrial Crystallization
Cement Based Materials
Handbook of Thermal Analysis and Calorimetry
Classical Nucleation Theory in Multicomponent Systems
Flash Ironmaking
Pseudoelasticity of Shape Memory Alloys
Kinetics of Water-Rock Interaction
Modeling and Simulation of Heat/mass Transport, Nucleation and Growth Kinetics in Phase Transformations
Kinetics of Geochemical Processes
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Integral Materials Modeling
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FAA/NASA International Symposium on Advanced Structural Integrity Methods for Airframe Durability and Damage Tolerance
Computational Fluid Dynamics and Population Balance Modeling of Particulate Systems
10th International Symposium on Process Systems Engineering - PSE2009
Extract von denen Fürstlichen Sachsen-Hildburghäusischen getreuen Land-Ständen an Ritterschafft und Städten auf die Ihnen vorgelegte Landes-Herrschaftliche gnädigste Propositions-Puncta vom 6. Juni erstatteten Berichts vom 8. eiusdem mensis
10th International Symposium on Process Systems Engineering
Advances in III-V Semiconductor Nanowires and Nanodevices
The Atomistic Nature of Crystal Growth
Nanomaterials Chemistry
Magnesium Technology 2013
Understanding of the Nucleation Induced Cooperative Behavior in Complex Macromolecular Systems
Chemical Engineering in the Pharmaceutical Industry, Active Pharmaceutical Ingredients
Deterministic Kinetics in Chemistry and Systems Biology
Heterogeneous Nucleation of Active Pharmaceutical Ingredients on Polymers
Crystallization Processes
Theory of Particulate Processes
Nucleation, Growth, and Solid Phase Transformations During Precipitation Processes
Crystal Growth for Beginners
Comprehensive Materials Processing
Handbook of Crystal Growth
Thermal Spray
Kinetics and Heat Transfer During Crystallization of Gas Hydrates and Ice
Science and Engineering of Casting Solidification
Computer Modelling of Heat and Fluid Flow in Materials Processing
The Handbook of Continuous Crystallization
Numerical Studies of Domain-growth Kinetics and Nucleation Processes in Models of Adsorption

EILEEN SHANNON

Magnetic Nanomaterials Springer
The understanding and control of transport phenomena in materials processing play an important role in the improvement of conventional processes and in the development of new techniques. Computer modeling of these phenomena can be used effectively for this purpose. Although there are several books in the literature covering the analysis of heat tra
Handbook of Industrial Crystallization John Wiley & Sons
In this thesis work, we aimed to explore crystallization processes for small molecule API compounds based on engineered polymer surfaces that could be used in continuous manufacturing. First, we identified a library of polymers that can be used and selected PVA as the model polymer based on its solution and film properties. We also illustrated a rational approach for designing and fabricating PVA film surfaces for increasing heterogeneous nucleation rate of different compounds and enable polymorph selection. The design philosophy was to select prevalent angles between major faces of crystals according to a selection of compounds, and to create substrate surfaces with indentations that include these angles. Nucleation induction time trends showed that heterogeneous nucleation rates were accelerated by at least an order of magnitude in the presence of PVA due to the favorable interactions between the model compounds and the polymer. Nucleation rates were further increased for patterned substrates with matching geometries. Surface indentations with non-matching angles resulted in faster nucleation rates than flat films but slower than matching geometries because they only increased the effective area of the films and their roughness. X-ray diffraction was used to reveal faces that preferentially interacted with the PVA side chains and to deduce possible arrangement of solute molecules at the corners of the indentations. Combining X-ray data and morphology of the crystal product, we suggest that matching geometries on the substrate enhanced nucleation of compounds. In addition to enhancing nucleation rate, polymorph selection was possible in the

presence of the polymer substrate to yield a higher percentage of thermodynamically stable gamma indomethacin. Offline Raman experiments and in-line morphology determination confirmed that polymorph control of the final crystal product via kinetic control of the nucleation process was viable. For the aspirin system, the 85 degree angle lead to the highest rate of nucleation; for the polymorphic indomethacin system, XRPD results showed that gamma form preferentially formed on the PVA films with 65 and 80 degree angles leading to the largest reduction in nucleation induction time. Kinetic Monte Carlo simulation showed that a crystallizer incorporating both nucleation and crystal growth in the absence of active mass transfer would have too small a throughput and too large a footprint to be useful. The main reasons were long average nucleation induction times and slow crystal growth in the absence of convection. A set of batch desupersaturation experiments showed that mass transfer limited growth dominate the crystal growth kinetics at low supersaturations when nucleation events were suppressed. An increase in the bulk fluid velocity increased the effective growth kinetics in the system when mass transfer kinetics dominated. Steady state modeling based on the first principle approach was performed using a combination of Navier Stokes Equations and diffusion-convection mass transport equations. The modeling result demonstrated that for mass transfer from a moving fluid to a stationary surface, a thin momentum and concentration boundary layer existed at the leading edge, which resulted in much higher local mass transfer rates. In the absence of momentum boundary layers, mass transfer could only occur via diffusion, which resulted in slow growth kinetics. The first principle model was used to derive dimensionless number correlations for the continuous crystallizer.

Cement Based Materials Butterworth-Heinemann

The 10th International Symposium on Process Systems Engineering, PSE'09, will be held in Salvador-Bahia, Brazil on August 16-20, 2009. The special focus of PSE 2009 is Sustainability, Energy and Engineering. PSE 2009 is the tenth in the triennial series of international symposia on process systems engineering initiated in 1982. The meeting is brings together the worldwide PSE community of researchers and practitioners who are involved in the creation and application of computing-based methodologies for planning, design, operation, control and maintenance of chemical and petrochemical process industries. PSE'09 will look at how the PSE methods and tools can support sustainable resource systems and emerging technologies in the areas of green engineering: environmentally conscious design of industrial processes. PSE methods and tools support: - sustainable resource systems - emerging technologies in the areas of green engineering - environmentally conscious design of industrial processes

Handbook of Thermal Analysis and Calorimetry Bentham Science Publishers

Cement-based materials have been used by humans nearly since the dawn of civilization. The Egyptians used lime and gypsum cement to bind their aggregate materials, mud and straw, resulting in bricks that are used for building their famous Egyptian pyramids (between 3000 and 2500 BC). Hydrated cement is a cement material bonded together with water and used for building construction; it is characterized by acceptable chemical, physical, thermal, mechanical, and structural stability. It plays a main role in the creation of vessels for storage, roads to travel on, weather-resistant structure for protection, inert hard stabilizer for hazardous wastes, and so on. Due to the composition of these materials and their advantages, it has been practiced in different applications. Cement is an essential component of making concrete, the single most prevalent building material used worldwide for construction, skyscrapers, highways, tunnels, bridges, hydraulic dams, and railway ties. Besides their numerous desired properties, there are some undesirable features. To overcome these disadvantages, several studies were established to prepare, improve, and evaluate innovative cement-based materials. Despite its oldness and deep research, every year several methods and materials evolve and so do cement technology. This book intends to provide a comprehensive overview on recent advances in the evaluation of these materials.

Classical Nucleation Theory in Multicomponent Systems CRC Press

Handbook of Thermal Analysis and Calorimetry: Recent Advances, Techniques and Applications, Volume Six, Second Edition, presents the latest in a series that has been well received by the thermal analysis and calorimetry community. This volume covers recent advances in techniques and applications that complement the earlier volumes. There has been tremendous progress in the field in recent years, and this book puts together the most high-impact topics selected for their popularity by new editors Sergey Vyazovkin, Nobuyoshi Koga and Christoph Schick—all editors of Thermochimica Acta. Among the important new techniques covered are biomass conversion; sustainable polymers; polymer nanocompsoties; nonmetallic glasses; phase change materials; propellants and explosives; applications to pharmaceuticals; processes in ceramics, metals, and alloys; ionic liquids; fast-scanning calorimetry, and more. Features 19 all-new chapters to bring readers up to date on the current status of the field Provides a broad overview of recent progress in the most popular techniques and applications Includes chapters authored by a recognized leader in each field and compiled by a new team of editors, each with at least 20 years of experience in the field of thermal analysis and calorimetry Enables applications across a wide range of modern materials, including polymers, metals, alloys, ceramics, energetics and pharmaceutics Overviews the current status of the field and summarizes recent progress in the most popular techniques and applications

Flash Ironmaking Springer Science & Business Media

This book gives a concise overview of the mathematical foundations of kinetics used in chemistry and systems biology. The analytical and numerical methods used to solve complex rate equations with the widely used deterministic approach will be described, with primary focus on practical aspects important in designing experimental studies and the evaluation of data. The introduction of personal computers transformed scientific attitudes in the last two decades considerably as computational power ceased to be a limiting factor. Despite this improvement, certain time-honored approximations in solving rate equations such as the pre-equilibrium or the steady-state approach are still valid and necessary as they concern the information content of measured kinetic traces. The book shows the role of these approximations in modern kinetics and will also describe some common misconceptions in this field.

Pseudoelasticity of Shape Memory Alloys Elsevier

This textbook is for graduate students and young scientists, who are looking for an introduction to the physics and physical chemistry of crystal growth and nucleation phenomena.

Kinetics of Water-Rock Interaction Elsevier

An overview of crystallization processes of organic and inorganic substances from various homogeneous liquids. Crystal

structures, phase transitions and crystallization rates are described in the book in connection with the structure of ions, complexes and molecules of the solution phase.

Modeling and Simulation of Heat/mass Transport, Nucleation and Growth Kinetics in Phase Transformations John Wiley & Sons

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.

Kinetics of Geochemical Processes CRC Press

Volume 8 of Reviews in Mineralogy treats a Short Course in Kinetics, which brings together the fundamentals needed to explain field observations using kinetic data. It is hoped that this book may serve, not only as a reference for researchers dealing with the rates of geochemical processes, but also as a text in courses on geochemical kinetics. The book is organized with a rough temperature gradient in mind, i.e. low temperature kinetics at the beginning and igneous kinetics at the end. However, the topics in each chapter are general enough that they can be applied often to any geochemical domain: sedimentary, metamorphic or igneous. The theory of kinetics operates at two complementary levels: the phenomenological and the atomistic. The former relies on macroscopic variables (e.g. temperature or concentrations) to describe the rates of reactions or the rates of transport; the latter relates the rates to the basic forces operating between the particular atomic or molecular species of any system. This book deals with both descriptions of the kinetics of geochemical processes.

Kinetic Processes Springer

Computational models are developed in an effort to aid in the design of process equipment for the crystallization of pharmaceutical compounds. The models focus on the combination of population balance equations and computational fluid dynamics software. For the simulation of antisolvent crystallization, knowledge of kinetics at high supersaturation are necessary. Chapter 2 describes the concentration profile within a high-throughput, evaporation platform that can be used to create conditions of high supersaturation for the study of crystal polymorphs as well as nucleation and growth kinetics. An equation is derived which provides the maximum concentration difference within an evaporating droplet. Chapter 3 discusses the secondary nucleation phenomena of breakage due to ultrasonic irradiation of crystals dispersed in a fluid. The simulation provides optimal kinetic parameters for the breakage kernel found by comparison to experimental data. Chapter 4 implements fouling along the walls in the simulation of cooling crystallization of seeds in an agitated tank. Future goals include adding breakage and aggregation/agglomeration to the model described in Chapter 4 and using the increasing computational power of modern supercomputers to simulate the multiphase system.

Handbook of Heterogenous Kinetics John Wiley & Sons

Crystallization refers to a liquid-to-solid phase transition and has been extensively studied due to its relevance in wide-ranging engineering systems. Although the thermodynamics of crystallization is well understood, the kinetics of liquid-solid phase transitions remains an area of active research. Unlike the reverse process of melting, crystallization consists of two different stages: nucleation of a seed crystal, followed by growth into the liquid medium. The kinetics of nucleation primarily depends on interfacial energies and temperature, whereas growth is influenced by heat and mass transfer characteristics of the system. Understanding the overall kinetics of liquid-solid phase transitions is therefore quite complex, and is the focus of this dissertation. This dissertation focuses on the crystallization of gas hydrates and ice. Hydrates are ice-like crystalline solids which form under high pressure and low temperature conditions from water (cage of host molecules) and another liquid or gas (guest molecule). Hydrates can enable novel applications in areas such as carbon capture and sequestration (CCS), flow assurance, natural gas transportation/storage and desalination. Understanding ice formation/melting is critical in the fields of atmospheric sciences, global warming, cryopreservation, infrastructure protection and desalination. Specific topics of this dissertation center around the nucleation and growth kinetics of hydrates and ice. The first task aims at improving the significantly sluggish nucleation kinetics of carbon dioxide (CO2) hydrates. CO2 hydrates offer promising new options for carbon dioxide capture and sequestration. However, nucleation times of CO2 hydrates can range from hours to days, which is too slow and stochastic for any practical application. Building up on previous research, it is discovered that magnesium and magnesium alloy surfaces can nucleate CO2 hydrates in a few minutes. This represents a 20X improvement in nucleation time over previous research and makes possible on-demand nucleation, which is critical for industrial applications. XPS and FTIR characterization of these surfaces reveal interesting mechanistic insights into the phenomena underlying this ultrafast nucleation. The second task studies the influence of three-phase contact lines and interfacial chemistry on the nucleation kinetics of ice. From classical understanding of nucleation, it is well-known that homogenous nucleation is much slower than heterogeneous nucleation, with the latter occurring on a metal surface with high surface energy. Heterogeneous nucleation is therefore analytically modeled at the conjunction of two phases. It is shown that the conjunction of three-phases at contact lines can further accelerate nucleation. Experimentally, this is often observed in bulk water where ice nucleation originates at the three-phase contact lines present in the system, and not inside the bulk water. Controlled experimentation investigating ice nucleation at fluid-fluid-solid interfaces and modeling using classical nucleation theory show the importance of considering three-phase line contacts during ice nucleation. The third task models the film growth kinetics of hydrates on a stagnant gas-water interface. Film growth of hydrates is the stage of hydrate growth

after nucleation where a layer of hydrate grows at the interface of gas and water. It has been conventionally understood that the kinetics of film growth is controlled by the rate of heat transfer in the system. Using scaling arguments, this dissertation shows that heat transfer is not a significant factor, as previously believed. It is shown that hydrate film growth can be effectively modelled using gas diffusion-limited kinetics. The new model shows excellent agreement with multiple experimental datasets (from literature) on hydrate formation from a single as well as mixture of gases. This work enables a novel understanding of the kinetics underlying film growth and provides a fundamentals-based equation for describing the reaction model of hydrate formation. The fourth task explores the coupling between heat and mass transfer during hydrate growth. Hydrate growth kinetics has been modeled in studies spanning several decades; however, most models tend to focus on heat and mass transfer separately; there is inadequate understanding on how these effects are coupled. The focus of this task is to develop a mathematical formulation to capture such effects. The developed mathematical formulation is incorporated in a framework to simulate hydrate growth in bubble column reactors. Bubble column reactors exhibit one of the highest growth rates and the process can be significantly heat transfer-limited if not designed appropriately. The simulation captures the evolution of bubble velocities, bubble radius, temperature, conversion rate etc. for various flow rates of gas and operating conditions. This work also identifies methods to enhance heat dissipation and captures the influence of various operating parameters on hydrate growth. In summary, this dissertation significantly advances the current understanding of crystallization of hydrates and ice. Via experimentation and modeling (analytical, numerical), this dissertation reports novel approaches to speed up hydrate formation, while also providing a deeper understanding of the mechanisms underlying the nucleation of hydrates and ice

Integral Materials Modeling Newnes
The formation of solids is governed by kinetic processes, which are closely related to the macroscopic behaviour of the resulting materials. With the main focus on ease of understanding, the author begins with the basic processes at the atomic level to illustrate their connections to material properties. Diffusion processes during crystal growth and phase transformations are examined in detail. Since the underlying mathematics are very complex, approximation methods typically used in practice are the prime choice of approach. Apart from metals and alloys, the book places special emphasis on the growth of thin films and bulk crystals, which are the two main pillars of modern device and semiconductor technology. All the presented phenomena are tied back to the basic thermodynamic properties of the materials and to the underlying physical processes for clarity.

Protein Crystal Nucleation and Growth John Wiley & Sons
The Magnesium Technology Symposium, the event on which this volume is based, is one of the largest yearly gatherings of magnesium experts in the world. Papers reflect all aspects of the field including primary production to applications, recycling, basic research findings, and industrialization. Readers will find broad coverage of current topics, including alloys and their properties, cast products and processing, wrought products and processing, corrosion and surface finishing, ecology, and more. New and emerging applications in such areas as hydrogen storage are also examined.

Modeling for Casting and Solidification Processing World Scientific
Theory of Particulate Processes: Analysis and Techniques of Continuous Crystallization, Second Edition covers the numerous population balance-based particulate studies. This edition emerged from the notes for an industrial short course on crystallization. This book is divided into 10 chapters and begins with an outline of the methods for representation of particle distributions and a systematic approach to the predictive modeling of processes where there is a need to characterize distributions in time and space and by some identifying property. The succeeding chapters provide a specific and more elementary approach to modeling crystal size distributions, as well as the modeling the kinetics of crystal nucleation and growth rates. Other chapters discuss a wide range of system analysis and design considerations specific to crystallization for both the steady state and unsteady state. The final chapters illustrate the use of a population balance analysis to interpret data from both laboratory and process equipment. These chapters also explore a wide variety of particulate processes and systems for which the population balance analysis is useful. This book is of great value to graduate students with particulate systems course.

FAA/NASA International Symposium on Advanced Structural Integrity Methods for Airframe Durability and Damage Tolerance BoD – Books on Demand
Geochemical kinetics as a topic is now of importance to a wide range of geochemists in academia, industry, and government, and all geochemists need a rudimentary knowledge of the field. This book summarizes the fundamentals of geochemical kinetics with examples drawn especially from mineral dissolution and precipitation. It also encompasses discussion of high temperature processes and global geochemical cycle modeling. Analysis of textures of rocks, sediments, and mineral surfaces are incorporated throughout and provide a sub-theme of the book.

Computational Fluid Dynamics and Population Balance Modeling of Particulate Systems Elsevier
This is the first-ever textbook on the fundamentals of nucleation, crystal growth and epitaxy. It has been written from a unified point of view and is thus a non-eclectic presentation of this interdisciplinary topic in materials science. The reader is required to possess some basic knowledge of mathematics and physics. All formulae and equations are accompanied by examples that are of technological importance. The book presents not only the fundamentals but also the state of the art in the subject. The second revised edition includes two separate chapters dealing with the effect of the Enrich-Schwoebel barrier for down-step diffusion, as well as the effect of surface active species, on the morphology of the growing surfaces. In addition, many other chapters are updated accordingly. Thus, it serves as a valuable reference book for both graduate students and researchers in materials science.

10th International Symposium on Process Systems Engineering - PSE2009 Butterworth-Heinemann
A guide to the development and manufacturing of pharmaceutical products written for professionals in the industry, revised second edition The revised and updated second edition of Chemical Engineering in the Pharmaceutical Industry is a practical book that highlights chemistry and chemical engineering. The book’s regulatory quality strategies target the development and manufacturing of pharmaceutically active ingredients of pharmaceutical products. The expanded second edition contains revised content with many new case studies and additional example calculations that are of interest to chemical engineers. The 2nd Edition is divided into two separate books: 1) Active

Pharmaceutical Ingredients (API's) and 2) Drug Product Design, Development and Modeling. The active pharmaceutical ingredients book puts the focus on the chemistry, chemical engineering, and unit operations specific to development and manufacturing of the active ingredients of the pharmaceutical product. The drug substance operations section includes information on chemical reactions, mixing, distillations, extractions, crystallizations, filtration, drying, and wet and dry milling. In addition, the book includes many applications of process modeling and modern software tools that are geared toward batch-scale and continuous drug substance pharmaceutical operations. This updated second edition: • Contains 30new chapters or revised chapters specific to API, covering topics including: manufacturing quality by design, computational approaches, continuous manufacturing, crystallization and final form, process safety • Expanded topics of scale-up, continuous processing, applications of thermodynamics and thermodynamic modeling, filtration and drying • Presents updated and expanded example calculations • Includes contributions from noted experts in the field Written for pharmaceutical engineers, chemical engineers, undergraduate and graduate students, and professionals in the field of pharmaceutical sciences and manufacturing, the second edition of Chemical Engineering in the Pharmaceutical Industry focuses on the development and chemical engineering as well as operations specific to the design, formulation, and manufacture of drug substance and products.

Extract von denen Fürstlichen Sachsen-Hildburghäusischen getreuen Land-Ständen an Ritterschafft und Städten auf die Ihnen vorgelegte Landes-Herrschaftliche gnädigste Propositions-Puncta vom 6. Juni erstatteten Berichts vom 8. eiusdem mensis CRC Press

"Semiconductor nanowires exhibit novel electronic and optical properties due to their unique one-dimensional structure and quantum confinement effects. In particular, III-V semiconductor nanowires have been of great scientific and technological interest fo"

10th International Symposium on Process Systems Engineering Springer Science & Business Media

Details the frontier of magnetic nanotechnology from the persepctive of scientists, engineers and physicians that have shaped this unique and highly collaborative field of research.