Modelling Phase Change In A 3d Thermal Transient Analysis

The main goal of this work is to numerically simulate convection phenomena in solid-liquid phase change processes and its application in the analysis of a thermal energy storage system with phase change materials. First two chapters consist in the resolution of two well-known numerical problems used as an introduction to the governing equations of uid ows and heat transfer. Here, the necessary tools for discretizing and solving these equations are brie y described. Third chapter speci cally deals with the problem of modelling solid-liquid phase change and its application into the simulation of a special thermal storage system.

The primary objective of this work is to propose a state-of-the-art physics based multiscale modeling framework for simulating material phase change problems. Both ice melting and copper crystallization problems are selected to demonstrate this multiscale modeling and simulation. The computational methods employed in this thesis include: classical molecular dynamics, finite element method, phase-field method, and multiscale (nano/micro coupling) methods. Classical molecular dynamics (MD) is a well-known method to study material behaviors at atomic level. Due to the limit of MD, it is not realistic to provide a complete molecular model for simulations at large length and time scales. Continuum methods, including finite element methods, should be employed in this case. In this thesis, MD is employed to study phase change problems at the nanoscale. In order to study material phase change problems at the microscale, a thermal wave method one-way coupling with the MD and a phase-field method one-way coupling with MD are proposed. The thermal wave method is more accurate than classical thermal diffusion for the study of heat transfer problems especially in crystal based structures. The second model is based on the well-known phase-field method. It is modified to respond to the thermal propagation in the crystal matrix by the thermal wave method, as well as modified to respond to temperature gradients and heat fluxes by employing the Dual-Phase-Lag method. Both methods are coupled with MD to obtain realistic results. It should be noted that MD simulations can be conducted to obtain material/thermal properties for microscopic and/or macroscopic simulations for the purpose of hierarchical/sequential multiscale modeling. These material parameters include thermal conductivity, specific heat, latent heat, and relaxation time.

Provides a comprehensive coverage of the basic phenomena. It contains twenty-five chapters which cover different aspects of boiling and condensation. First the specific topic or phenomenon is described, followed by a brief survey of previous work, a phenomenological model based on current understanding, and finally a set of recommended design equations or correlations. Detailed references are listed at the end of each chapter for further reading.

This monograph collects research and expository articles reflect ing the interaction and the cooperation of different groups in several European institut ions concerning current research on mathematical models for the behaviour of materials with phase change. These papers were presented and discussed in a Workshop held at Obidos, Portugal, du ring the first three days of October, 1988, and grew out of a two year period of intensive exploitation of differ ent abilities and mathematical experiences of the six participating groups, namely, in the University of Augsburg, wh ich was the co ordination center of this project, the Laboratoire Central des Ponts et Chaussees of Paris, the Aristoteles University of Thessaloniki, the University of Florence, the University of Lisbon and the University of Oxford. This project was carried out under the title "Mathemat ical Models of Phase Transitions and Numerical Simulation" , in the framework of twinning program for stimulation of cooperation and scientific interchange, sponsored by the European Community. The underlying idea of the project was to create and study the mathematical models arising in applied engineering problems with free boundaries in a broad sense, namely in melting and freezing problems, diffusion-reaction processes, solid-solid phase transition, hysteresis phenomena, "mushy region" descriptions, contact prob lems with friction andjor adhesion, elastoplastic deformations, etc. vi This large spectrum of applied problems have in common the main feature of brusque transitions of their qualitative behaviour that correspond, in general, to non-classical discontinuous monotone or non monotone strong nonlinearities in the mathematical equations.

Foreword by Walter J. Freeman. The induction of unconsciousness using anesthetic agents demonstrates that the cerebral cortex can operate in two very different behavioral modes: alert and responsive vs. unaware and quiescent. But the states of wakefulness and sleep are not single-neuron properties---they emerge as bulk properties of cooperating populations of neurons, with the switchover between states being similar to the physical change of phase observed when water freezes or ice melts. Some brain-state transitions, such as sleep cycling, anesthetic induction, epileptic seizure, are obvious and detected readily with a few EEG electrodes; others, such as the emergence of gamma rhythms during cognition, or the ultra-slow BOLD rhythms of relaxed free-association, are much more subtle. The unifying theme of this book is the notion that all of these bulk changes in brain behavior can be treated as phase transitions between distinct brain states. Modeling Phase Transitions in the Brain contains chapter contributions from leading researchers who apply state-space methods, network models, and biophysically-motivated continuum approaches to investigate a range of neuroscientifically relevant problems that include analysis of nonstationary EEG time-series; network topologies that limit epileptic spreading; saddle--node bifurcations for anesthesia, sleep-cycling, and the wake--sleep switch; prediction of dynamical and noise-induced spatiotemporal instabilities underlying BOLD, alpha-, and gamma-band Hopf oscillations, gap-junction-moderated Turing structures, and Hopf-Turing interactions leading to cortical waves.

This monograph collects research and expository articles reflect ing the interaction and the cooperation of different groups in several European institut ions concerning current research on mathematical models for the behaviour of materials with phase change. These papers were presented and discussed in a Workshop held at Obidos, Portugal, du ring the first three days of October, 1988, and grew out of a two year period of intensive exploitation of differ ent abilities and mathematical experiences of the six participating groups, namely, in the University of Augsburg, wh ich was the co ordination center of this project, the Laboratoire Central des Ponts et Chaussees of Paris, the Aristoteles University of Thessaloniki, the University of Florence, the University of Lisbon and the University of Oxford. This project was carried out under the title "Mathemat ical Models of Phase Transitions and Numerical Simulation", in the framework of twinning program for stimulation of cooperation and scientific interchange, sponsored by the European Community. The underlying idea of the project was to create and study the mathematical models arising in applied engineering problems with free boundaries in a broad sense, namely in melting and freezing problems, diffusion-reaction processes, solid-solid phase transition, hysteresis phenomena, "mushy region" descriptions, contact prob lems with friction andjor adhesion, elastoplastic deformations, etc. vi This large spectrum of applied problems have in common the main feature of brusque transitions of their qualitative behaviour that correspond, in general, to non-classical discontinuous monotone or non monotone strong nonlinearities in the mathematical equations.

Various memory devices are being widely used for a wide range of applications. There has not been any universal memory device so far because each memory device has a unique set of features. Large performance gaps in various dimensions of features between memory devices and a new set of features required by new electronic systems such as portable electronics open up new opportunities for new memory devices to emerge as mainstream memory devices. Besides, the imminent scaling limit for existing mainstream memory devices also motivates development and research of new memory devices which can meet the increasing demand for large memory capacity. Phase change memory (PCM) is one of the most promising emerging memory devices. It has the potential to combine DRAM-like features such as bit alteration, fast read and write, and good endurance and Flash-like features such as non-volatility and a simple structure. PCM is expected to be a highly scalable technology extending beyond scaling limit of existing memory devices. Prototypical PCM chips have been developed and are being tested for targeted memory applications. However, understanding of fundament physics behind PCM operation is still lacking because the key material in PCM devices, the chalcogenide, is relatively new for use in solid state devices. Evaluation and development of PCM technology as successful mainstream memory devices require more study on PCM devices. This thesis focuses on issues relevant to scalability and reliability of PCM which are two of the most important qualities that new emerging memory devices should demonstrate. We first study basic scaling rule based on thermoelectric analysis on the maximum temperature in a PCM cell and show that both isotropic and non-isotropic scaling result in constant programming voltage. The minimum programming voltage is determined by material properties such as electrical resistivity and thermal conductivity regardless of the device size. These results highlight first-order principles governing scaling rules. In the first-order scaling rule analysis, we assume that material properties are constant regardless of its physical size. However, when materials are scaled down to the nanometer regime, material properties can change because the relative contribution from the surface property to the overall system property increases compared to that from the bulk property. We study scaling effect on material property and device characteristics using a novel device structure -- a PCM cell with a pseudo electrode. With the pseudo electrode PCM cell, we can accurately relate the observed properties to the amorphous region size. We show that threshold switching voltage scales linearly with thickness of the amorphous region and threshold switching field drifts in time after programming. We also show that the drift coefficient for resistance drift stays the same for scaled devices. These property scaling results provide not only estimates for scaled device characteristics but also clues for modeling and understanding mechanisms for threshold switching and drift. To make scaled memory cells in an array form, not only memory device elements but also selection devices need to be scaled. PCM requires relatively large programming current, which makes it challenging to scale down selection devices. We integrate Ge nanowire diodes as selection devices in search for new candidates for high density PCM. Ge nanowire diode provides on/off ratio of ~100 and small contact area of 40 nm in diameter which results in programming current below 200 [mu]A. The processing temperature for Ge nanowire diode is below 400°C, which makes Ge nanowire diode a potential enabler for 3D integration. As memory devices are scaled down, more serious reliability issues arise. We study the reliability of PCM using a novel structure -- micro-thermal stage (MTS). The high-resistance-state (RESET) resistance and threshold switching voltage are important device characteristics for

A thermal model which simulates combined conduction and phase change characteristics of thermal energy storage (TES) materials is presented. Both the model and results are presented for the purpose of benchmarking the conduction and phase change capabilities of recently developed and unvalidated microgravity TES computer programs. Specifically, operation of TES-1 is simulated. A two-dimensional SINDA85 model of the TES experiment in cylindrical coordinates was constructed. The phase change model accounts for latent heat stored in, or released from, a node undergoing melting and freezing. Skarda, J. Raymond Lee Glenn Research Center RTOP 506-41-31

The transverse field Ising and XY models (the simplest quantum spin models) provide the organising principle for the rich variety of interconnected subjects which are covered in this book. From a generic introduction to in-depth discussions of the subtleties of the transverse field Ising and related models, it includes the essentials of quantum dynamics and quantum information. A wide range of relevant topics has also been provided: quantum phase transitions, various measures of quantum information, the effects of disorder and frustration, quenching dynamics and the Kibble-Zurek scaling relation, the Kitaev model, topological phases of quantum systems, and bosonisation. In addition, it also discusses the experimental studies of transverse field models (including the first experimental realisation of quantum annealing) and the recent realisation of the transverse field Ising model using tunable Josephson junctions. Further, it points to the obstacles still remaining to develop a successful quantum computer.

The heat transfer and analysis on laser beam, evaporator coils, shell-and-tube condenser, two phase flow, nanofluids, complex fluids, and on phase change are significant issues in a design of wide range of industrial processes and devices. This book includes 25 advanced and revised contributions, and it covers mainly (1) numerical modeling of heat transfer, (2) two phase flow, (3) nanofluids, and (4) phase change. The first section introduces numerical modeling of heat transfer on particles in binary gas-solid fluidization bed, solidification phenomena, thermal approaches to laser damage, and temperature and velocity distribution. The second section covers density wave instability phenomena, gas and spray-water quenching, spray cooling, wettability effect, liquid film thickness, and thermosyphon loop. The third section includes nanofluids for heat transfer, nanofluids in minichannels, potential and engineering strategies on nanofluids, and heat transfer at nanoscale. The forth section presents time-dependent melting and deformation processes of phase change material (PCM), thermal energy storage tanks using PCM, phase change in deep CO2 injector, and thermal storage device of solar hot water system. The advanced idea and information described here will be fruitful for the readers to find a sustainable solution in an industrialized society.

Efforts have been devoted over the last decades towards modelling phase change kinetics of fats in chocolate. The fats in chocolate have a number of crystal forms and manufacturers must deliver a product with the right polymorph to the consumer. In this work a simplifed mathematical model was developed that clusters six polymorphs into two, namely stable and unstable, depending on their Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD) characteristics. This simplification allowed the phase change kinetics to be estimated from a set of DSC experiments conducted at different cooling and heating rates. The phase change reactions were coupled with the heat transfer equation and used to model temperature profiles and concentration of polymorphs in a model geometry. The model was able to predict both the temperature profiles measured by thermocouples (\(\pm\)2\(^\circ\)C) and the fat crystals concentration as measured using XRD (\(\pm\)10%) at various locations in a chocolate slab. The model was applied to the recently developed processes using very high cooling rates such as the FrozenCone process, to explain their capabilities to produce "good" chocolate in spite of the high cooling rates used. Such modelling was not possible with existing models, which usually deal with either heat transfer or isothermal crystallisation kinetics.

The main outcomes of this work are (i) the coupling of the reactions kinetics with heat transfer which can be expanded to other processes, (ii) the novel XRD method and (iii) the application to fast cooling processes and their explanation.
Describing the physical properties of quantum materials near critical points with long-range many-body quantum entanglement, this book introduces readers to the basic theory of quantum phases, their phase transitions and their observable properties. This second edition begins with a new section suitable for an introductory course on quantum phase transitions, assuming no prior knowledge of quantum field theory. It also contains several new chapters to cover important recent advances, such as the Fermi gas near unitarity, Dirac fermions, Fermi liquids and their phase transitions, quantum magnetism, and solvable models obtained from string theory. After introducing the basic theory, it moves on to a detailed description of the canonical quantum-critical phase diagram at non-zero temperatures. Finally, a variety of more complex models are explored. This book is ideal for graduate students and researchers in condensed matter physics and particle and string theory.
Predictive theories of phenomena involving phase change with applications in engineering are investigated in this volume, e.g. solid-liquid phase change, volume and surface damage, and phase change involving temperature discontinuities. Many other phase change phenomena such as solid-solid phase change in shape memory alloys and vapor-liquid phase change are also explored. Modeling is based on continuum thermo-mechanics. This involves a renewed principle of virtual power introducing the power of the microscopic motions responsible for phase change. This improvement yields a new equation of motion related to microscopic motions, beyond the classical equation of motion for macroscopic motions. The new theory sensibly improves the phase change modeling. For example, when warm rain falls on frozen soil, the dangerous black ice phenomenon can be comprehensively predicted. In addition, novel equations predict the evolution of clouds, which are themselves a mixture of air, liquid water and vapor.
Most storage materials exhibit phase changes, which cause stresses and, thus, lead to damage of the electrode particles. In this work, a phase-field model for the cathode material NaxFePO4 of Na-ion batteries is studied to understand phase changes and stress evolution. Furthermore, we study the particle size and SOC dependent miscibility gap of the nanoscale insertion materials. Finally, we introduce the nonlocal species concentration theory, and show how the nonlocality influences the results.
Presents mathematical models of melting and solidification processes that are the key to the effective performance of latent heat thermal energy storage systems, utilized in a wide range of heat transfer and industrial applications.
... "What do you call work?" "Why ain't that work?" Tom resumed his whitewashing, and answered carelessly: "Well. Il1a), he it is, and maybe it aill't. All I know, is, it suits Tom Sawvc/:" "Oil CO/lll!, IIOW, Will do not mean to let 011 that you like it?" The brush continued to move. "Likc it? Well, I do not see wlzy I oughtn't to like it. Does a hoy get a chance to whitewash a fence every day?" That put the thing ill a Ilew light. Ben stopped nibhling the apple ... (From Mark Twain's Adventures of Tom Sawyer, Chapter II.) Mathematics can put quantitative phenomena in a new light; in turn applications may provide a vivid support for mathematical concepts. This volume illustrates some aspects of the mathematical treatment of phase transitions, namely, the classical Stefan problem and its generalizations. The in tended reader is a researcher in application-oriented mathematics. An effort has been made to make a part of the book accessible to beginners, as well as physicists and engineers with a mathematical background. Some room has also been devoted to illustrate analytical tools. This volume deals with research I initiated when I was affiliated with the Istituto di Analisi Numerica del C.N.R. in Pavia, and then continued at the Dipartimento di Matematica dell'Universita di Trento. It was typeset by the author in plain TEX.
Thermal enhancement of the phase change material (PCM) using nanoparticle and porous medium is studied analytically, numerically and experimentally for melting and freezing processes of the PCM. Copper nanoparticle of 30nm is dispersed into the base PCM of Paraffin Wax to prepare the PCM with nanoparticle (NanoPCM). NanoPCM is poured into the Aluminum solid matrix of 95% porosity to have NanoPCM and porous medium matrix. Copper nanoparticle and Aluminum solid matrix are used as enhancer for thermal conductivity improvement of Paraffin Wax without affecting the effective volume of PCM and other thermophysical properties such as viscosity, latent heat of fusion and melting temperature. Initially, a conduction model is developed for constant temperature boundary condition. The effect of the volume fraction of nanoparticle and porosity of the porous medium are studied for temperature distribution, heat transfer and melt fraction inside the cavity analytically and numerically. A scale analysis is executed to establish simplified relationships between different non-dimensional parameters such as Fourier number, Stefan number, porosity and volume fraction. The model is compared with the exact solution of existing literature for equivalent thermophysical properties of NanoPCM with porous medium and found good agreement between the exact solution and numerical result of this research. The conduction model is modified by incorporating both convection and conduction heat transfer with constant temperature boundary condition from side. Because of the boundary condition from side, convection and conduction both heat transfer are responsible for phase change initially. After the top melts completely, the melting of remaining part occurs mostly due to conduction heat transfer. The model executes scale analysis to estimate the extent of the complete phase change process. The scale analysis results in simplified relationships among different non-dimensional parameters such as Fourier number, Stefan number, Raleigh number, Nusselt number, porosity of the porous medium and volume fraction of nanoparticles. The natural convection melting process of NanoPCM inside the porous medium is solved numerically. The numerical simulation verifies the correctness of the relationships proposed by scale analysis and identifies the effects of nanoparticle volume fraction, time, Rayleigh number, flow field, thermal field and heat transfer process during the melting of NanoPCM inside the thermal energy storage system. A nearly closed form analytical model with conduction heat transfer is developed to satisfy the application of phase change material under constant heat flux input conditions. From the exact solutions of the models, the temperature distribution and movement of the melting interface inside the phase change region are predicted. The model data is compared with experimental data for interface movement rate and temperature profile at one location of the melting interface. An extensive experimental research is carried out to observe the thermal performance of PCM, NanoPCM, PCM with porous

medium and NanoPCM with porous medium for conduction and convection heat transfer with constant heat boundary condition from bottom, side and top. The better thermal performance is observed for heating from bottom because of higher influence of convection heat transfer. The heating from side performs better than the heating from top. The heating from top is mostly conduction heat transfer because of insignificant presence of convection heat transfer. The results are compared with the thermal performance of base PCM, NanoPCM and PCM with foam for similar experimental conditions. From the result, the desired thermal enhancement of NanoPCM with porous medium is observed for conduction heat transfer by improving the charging/discharge time along with low temperature rise. This pioneering research with NanoPCM with porous medium may lead to many future researches for replacing the sensible energy storage system with latent heat energy storage system for various transient thermal applications.

Air conditioning electricity consumption in summer represents a challenge in many areas with hot and humid climates. When incorporated into lightweight residential building walls, phase change materials (PCMs) can increase the effective thermal mass of the wall, which in turn will shift part of the cooling load to off-peak times and lower the peak space cooling load of the building. From analyses of experimental data, it was found that it was very likely that the PCMs, once integrated into the walls, would "start" the phase change process from partially melted states. Currently used simulation models, including the most widely accepted models, such as the effective heat capacity method and the enthalpy method, come short when handling phase change processes that start from partially melted states. The characteristics of how the heat is absorbed or released during the phase change process were studied through experimental and theoretical analyses. A differential scanning calorimeter (DSC) method and its detailed steps, used to obtain latent heat of fusion distribution along the phase change temperature range, are presented. Based on the DSC test data, a modified PCM model for a paraffin-based PCM was developed.

Solid-liquid phase change phenomena are present in a large number of industrial applications and natural processes like material processing, crystal growth, heat storage, icebergs or magma eruption. Numerical modelling of strongly non-linear, moving boundary, thermal and fluid flow problems is a challenging task. The book gives a review of modelling methods of phase change problems, numerical and experimental methods used in the field. It combines experience of theoreticians with those using numerical tools for modelling problems of solidification. It offers researchers and engineers knowledge and critical assessment of numerical approaches, physical models and validation methods used in the field of modelling industrial problems. The book collects in an unique way most recent knowledge on modelling of phase change problems, from micro scale problems and the interface (growth of dendrites) to macro scale models.

Proceedings of the NATO Advanced Research Workshop, held in Volga River, Russia, 24-28 May 2001

To increase the efficiency of energy-intensive industrial processes, thermal energy storages can offer new possibilities. A novel approach is investigated in the project HyStEPs. In this concept, containers filled with PCM are placed at the shell surface of a Ruths steam storage, to increase storage efficiency. In this work, a two-dimensional model using the finite element method is developed to simulate the PCM of the hybrid storage as designed in the HyStEPs project. The apparent heat capacity method is applied in a MATLAB implementation, considering heat transfer by both conduction and natural convection. This successfully validated code can handle any desired layout of materials arranged on a rectangular domain. Furthermore, a parameter study of different dimensions and orientations of the PCM cavity was conducted. The impact of natural convection was found to lead to significantly varying behaviour of the studied cavities with different orientation during the charging process, while it was found to be negligible during the discharging process.

I simulate phase change including stochastic nucleation and growth of discrete grains with a finite element framework which captures the latent heat of phase change and heterogeneous melting. I model the electrical conductivity, thermal conductivity, Seebeck coefficient, and specific heat in TiN, SiO2, and the face centered cubic and amorphous phases of Ge2Sb2Te5 as well as the thermal boundary conductance at interfaces of these materials over the temperatures and fields encountered during phase change memory device operation. Simulations show reset, set, and read of phase change memory devices including mushroom cells, encapsulated pillar cells, double mushroom cells, and threshold switch controlled mushroom cells. My results show that the latent heat of phase change increases the temperature at crystalline-amorphous interfaces during crystallization, heterogeneous melting can help account for the experimentally observed improvement in reset and set speeds as grain size decreases, and that threshold switching can be captured using a closed form model of independent thermal and electric field contributions to electrical conductivity.

Efforts have been devoted over the last decades towards modelling phase change kinetics of fats in chocolate. The fats in chocolate have a number of crystal forms and manufacturers must deliver a product with the right polymorph to the consumer. In this work a simplifed mathematical model was developed that clusters six polymorphs into two, namely stable and unstable, depending on their Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD) characteristics. This simplification allowed the phase change kinetics to be estimated from a set of DSC experiments conducted at different cooling and heating rates. The phase change reactions were coupled with the heat transfer equation and used to model temperature profiles and concentration of polymorphs in a model geometry. The model was able to predict both the temperature profiles measured by thermocouples (\(\pm\)2\(\circ\)C) and the fat crystals concentration as measured using XRD (\(\pm\)10%) at various locations in a chocolate slab. The model was applied to the recently developed processes using very high cooling rates such as the FrozenCone process, to explain their capabilities to produce "good" chocolate in spite of the high cooling rates used. Such modelling was not possible with existing models, which usually deal with either heat transfer or isothermal crystallisation kinetics. The main outcomes of this work are (i) the coupling of the reactions kinetics with heat transfer which can be expanded to other processes, (ii) the novel XRD method and (iii) the application to fast cooling processes and their explanation.

During the operation of phase-change ink-jet printers a bubble formation phenomenon often occurs. These bubbles are detrimental to the operation of the printer and substantial efforts are made to remove them. The objective of this research was 1: to develop a fundamental understanding of how bubble or void formation occurs during the phase-change process, and, 2: to develop a simple computer model to simulate this behavior which can then be used as a tool for better design of print-head geometries. Preliminary experimental work indicated the void formation to be a result of the density change accompanying the phase-change process. The commercial numerical code, Flow 3-D, was used to model the phase-change process in print-head geometries and substantiate certain simplifying assumptions. These assumptions included the effect of convection on the process and the effect of the varying material properties. For channel sizes less than 0.5 cm the phase-change process was found to be a pure conduction process. Convection effects are thus negligible and can be eliminated from the

model. The variability of density, specific heat and thermal conductivity must be included in the model, as they affect the phase-change process dramatically. Specific heat is the most influential of the properties and determines, along with the conductivity, the rate at which the phase change takes place. The density must be included since it is directly linked to the void formation.

This unique volume offers a review of state-of-the-art modelling methods of phase change problems, numerical and experimental methods used in the field. It combines the experience of theoreticians with those using numerical tools for modelling problems of solidification.

As an introductory account of the theory of phase transitions and critical phenomena, this book reflects lectures given by the authors to graduate students at their departments and is thus classroom-tested to help beginners enter the field. Most parts are written as self-contained units and every new concept or calculation is explained in detail without assuming prior knowledge of the subject. The book significantly enhances and revises a Japanese version which is a bestseller in the Japanese market and is considered a standard textbook in the field. It contains new pedagogical presentations of field theory methods, including a chapter on conformal field theory, and various modern developments hard to find in a single textbook on phase transitions. Exercises are presented as the topics develop, with solutions found at the end of the book, making the text useful for self-teaching, as well as for classroom learning.

Continuum Models for Phase Transitions and Twinning in Crystals presents the fundamentals of a remarkably successful approach to crystal thermomechanics. Developed over the last two decades, it is based on the mathematical theory of nonlinear thermoelasticity, in which a new viewpoint on material symmetry, motivated by molecular theories, plays a central role. This is the first organized presentation of a nonlinear elastic approach to twinning and displacive phase transition in crystalline solids. The authors develop geometry, kinematics, and energy invariance in crystals in strong connection and with the purpose of investigating the actual mechanical aspects of the phenomena, particularly in an elastostatics framework based on the minimization of a thermodynamic potential. Interesting for both mechanics and mathematical analysis, the new theory offers the possibility of investigating the formation of microstructures in materials undergoing martensitic phase transitions, such as shape-memory alloys. Although phenomena such as twinning and phase transitions were once thought to fall outside the range of elastic models, research efforts in these areas have proved quite fruitful. Relevant to a variety of disciplines, including mathematical physics, continuum mechanics, and materials science, Continuum Models for Phase Transitions and Twinning in Crystals is your opportunity to explore these current research methods and topics.

This monograph develops a unified microscopic basis for phases and phase changes of bulk matter and small systems, based on classical physics. It describes the thermodynamics of ensembles of particles and explains phase transition in gaseous and liquid systems. The origins are derived from simple but physically relevant models of how transitions occur between rigid and fluid states, of how phase equilibria arise, and how they differ for small and large systems.

Phase transitions--changes between different states of organization in a complex system--have long helped to explain physics concepts, such as why water freezes into a solid or boils to become a gas. How might phase transitions shed light on important problems in biological and ecological complex systems? Exploring the origins and implications of sudden changes in nature and society, Phase Transitions examines different dynamical behaviors in a broad range of complex systems. Using a compelling set of examples, from gene networks and ant colonies to human language and the degradation of diverse ecosystems, the book illustrates the power of simple models to reveal how phase transitions occur. Introductory chapters provide the critical concepts and the simplest mathematical techniques required to study phase transitions. In a series of example-driven chapters, Ricard Solé shows how such concepts and techniques can be applied to the analysis and prediction of complex system behavior, including the origins of life, viral replication, epidemics, language evolution, and the emergence and breakdown of societies. Written at an undergraduate mathematical level, this book provides the essential theoretical tools and foundations required to develop basic models to explain collective phase transitions for a wide variety of ecosystems.

This book describes the physics of phase change memory devices, starting from basic operation to reliability issues. The book gives a comprehensive overlook of PCM with particular attention to the electrical transport and the phase transition physics between the two states. The book also contains design engineering details on PCM cell architecture, PCM cell arrays (including electrical circuit management), as well as the full spectrum of possible future applications.

In recent years the phase-change paint technique has evolved into an accepted diagnostic tool in high-speed wind-tunnel testing. This report documents use of the method at the Naval Surface Weapons Center, White Oak Laboratory, to study aerodynamic interference heating on fin-body configurations. Various aspects of both the underlying theory and the experimental method are enumerated based on experience and on information from other researchers. Analytic relationships are presented which indicate how uncertainties in the various input parameters affect the uncertainty in the heat-transfer coefficient. Advantages and disadvantages of the phase-change paint method are discussed.

In recent decades, latent heat storage in phase change materials (PCMs) received considerable attention. This is due to their high latent heat capacity, which is essentially required for managing and overcoming the temporal mismatch between energy supply and demand. Thus, at the time of energy availability at supply side, it is stored in PCMs so as to be extracted later on when it is needed. In order to provide continuous operation, there are some periods when a thermal storage has to be simultaneously charged and discharged. Most studies focused either on charging, discharging, or consecutive charging and discharging process, while limited work has been conducted for the case of simultaneous charging and discharging (SCD). The first objective of this dissertation is to develop a numerical model to analyze the heat transfer mechanism within a horizontal PCM storage under SCD. Since the possible heat transfer mechanisms within PCMs are conduction, convection or a combination of both, two models are used to identify the mechanism under SCD; i.e. the pure conduction (PC) model and combined conduction and natural convection (CCNC) model. The PC model is a hypothetical model, which neglects the natural convection during phase change process; however, the CCNC model is the real case one. Validation of the model results by comparison with experimental data shows an acceptable agreement both under melting and solidification. Therefore, the developed model can be used to numerically study the phase change process in PCMs.Natural convection is the result of density changes, which create buoyancy forces within melted PCM and plays a significant role during melting. Currently, the most widely used method to account for natural convection is the effective thermal conductivity method. The method considers an artificial increase in thermal conductivity values to take into consideration the effect of natural convection by comparing the results with experimental data. Two major shortcomings of this method are that first, it is tedious to obtain the proper value and second, the method does not provide information about the melting front location. In this dissertation, a novel simplified front tracking method is presented to replace the thermal conductivity method. The novel method is based on considering two separate melting fronts for the upper and lower halves of a horizontal thermal storage system. Therefore, two dimensionless correlations are developed to map the results of the simple PC model to that of the complicated CCNC model based on the presented logic. The method essentially creates a link between CCNC and PC models, which is also missing in the literature. Based on verification, the correlations can provide results within ±15% discrepancy.

The aim of this research was to evaluate the thermal performance of an organic phase change material that absorbs latent heat at nearly isothermal conditions while changing phase.This BioPCM exhibits similar thermophysical properties to paraffin while eliminating flammability issues as installed in buildings. The investigation was performed using the finite element method through a computer simulation of the ambient temperature for a typical Phoenix summer day for different wall arragenments. It was found that a typical wall with a 1 inch PCM layered after the interior gypsum board does improve the ability of lowering the interior wall temperature by 0.5 C and to shift the peak temperature for 2 h. This small temperature difference may play a more important role if we were evaluating the entire building. The

importance of these results is on setting an analytical model for this BioPCM and further analyze its properties, as performed herein, to determine a set of characteristics that impact its performance in a building.

Phase Change with Convection: Modelling and ValidationSpringer

This work deals with modeling and numerical simulation of fluid flow and heat transfer associated with phase change process inside both isotropic and anisotropic porous media, based on the Two-Phase Mixture Model (TPMM) along with the assumption of Local Thermal Equilibrium (LTE) and Non-Equilibrium (LTNE) conditions. In particular, it demonstrates the necessity and usefulness of a newly proposed smoothing algorithm for handling the sharp discontinuities in the effective diffusion coefficient in order to avoid the occurrence of non-physical “jump” in the predicted temperature distribution during the numerical simulation of the complete phase change process inside porous media. For the purpose of demonstration, one- and two-dimensional phase change problems operated in the Darcy flow regime have been considered.The Finite Volume Method (FVM) has been used on both staggered and non-staggered grid layouts in order to solve the governing conservation equations. In this work, after critically analyzing the drawbacks of the existing enthalpy formulation based on TPMM, a modified formulation has been also developed that can easily accommodate substantial density variations in the single phase regions. The results obtained from the modified enthalpy formulation have been compared with that predicted by the existing modified volumetric enthalpy formulation and excellent agreements have been observed for all tested cases. A thorough parametric study, using both LTE and LTNE models, indicates that the adoption of the proposed smoothing algorithm successfully eliminates “jump” in the predicted temperature distribution and does not alter the overall energy and momentum balance. All tested cases, covering applicable ranges of parametric variations, could be physically interpreted. The methodology is, therefore, recommended for future simulations of complete phase change process inside porous media. The results also show that the modified enthalpy formulation requires significantly less computation time thanmodified volumetric enthalpy formulation.