Numerical Simulation In Molecular Dynamics Numerics Algorithms Parallelization Applications

This book details the necessary numerical methods, the theoretical background and foundations and the techniques involved in creating computer particle models, including linked-cell method, SPME-method, tree codes, amd multipol technique. It illustrates modeling, discretization, algorithms and their parallel implementation with MPI on computer systems with distributed memory. The text offers step-by-step explanations of numerical simulation, providing illustrative code examples. With the description of the algorithms and the presentation of the results of various simulations from fields such as material science, nanotechnology, biochemistry and astrophysics, the reader of this book will learn how to write programs capable of running successful experiments for molecular dynamics.

The present volume is the second in a two-volume set dealing with modelling and numerical simulations in electrochemistry. Emphasis is placed on the aspect of nanoelectrochemical issues. It seems appropriate at this juncture to mention the n- growing body of opinion in some circles that George Box was right when he

stated, three decades ago, that “All models are wrong, but some are useful”. Actually, when the statement itself was made it would have been more appropriate to say that “All models are inaccurate but most are useful nonetheless”. At present, however, the statement, as it was made, is far more appropriate and closer to the facts than ever before. Currently, we are in the midst of the age of massively abundant data. Today’s philosophy seems to be that we do not need to know why one piece of information is better than another except through the statistics of incoming and outgoing links between information and this is good enough. It is why, both in principle and in practice, one can translate between two languages, without knowledge of either. While none of this can be ignored, and it may even be true that “All models are wrong and increasingly you can succeed without them” the traditional approach of scienti?c modelling is still the order of the day. That approach may be stated as hypothesize – measure – model – test. It is in this light that the present volume should be viewed.

This is an introduction to molecular and atomistic modeling techniques applied to fracture and deformation of solids, focusing on a variety of brittle, ductile, geometrically confined and biological materials. The overview includes computational methods and techniques operating at the atomic scale, and

describes how these techniques can be used to model cracks and other deformation mechanisms. The book aims to make new molecular modeling techniques available to a wider community.

Hot dense radiative (HDR) plasmas common to Inertial Confinement Fusion (ICF) and stellar interiors have high temperature (a few hundred eV to tens of keV), high density (tens to hundreds of g/cc) and high pressure (hundreds of Megabars to thousands of Gigabars). Typically, such plasmas undergo collisional, radiative, atomic and possibly thermonuclear processes. In order to describe HDR plasmas, computational physicists in ICF and astrophysics use atomic-scale microphysical models implemented in various simulation codes. Experimental validation of the models used to describe HDR plasmas are difficult to perform. Direct Numerical Simulation (DNS) of the many-body interactions of plasmas is a promising approach to model validation but, previous work either relies on the collisionless approximation or ignores radiation. We present a new numerical simulation technique to address a currently unsolved problem: the extension of molecular dynamics to collisional plasmas including emission and absorption of radiation. The new technique passes a key test: it relaxes to a blackbody spectrum for a plasma in local thermodynamic equilibrium. This new tool also provides a method for assessing the accuracy of energy and momentum

exchange models in hot dense plasmas. As an example, we simulate the evolution of non-equilibrium electron, ion, and radiation temperatures for a hydrogen plasma using the new molecular dynamics simulation capability.

In this translation of the German edition, the authors provide insight into the numerical simulation of fluid flow. Using a simple numerical method as an expository example, the individual steps of scientific computing are presented: the derivation of the mathematical model; the discretization of the model equations; the development of algorithms; parallelization; and visualization of the computed data. In addition to the treatment of the basic equations for modeling laminar, transient flow of viscous, incompressible fluids - the Navier-Stokes equations - the authors look at the simulation of free surface flows; energy and chemical transport; and turbulence. Readers are enabled to write their own flow simulation program from scratch. The variety of applications is shown in several simulation results, including 92 black-and-white and 18 color illustrations. After reading this book, readers should be able to understand more enhanced algorithms of computational fluid dynamics and apply their new knowledge to other scientific fields.

Analytical and numerical modeling of fibrous material resistance to penetration under impact by high-velocity projectiles has been of great interest not only for

personnel protection reasons but also because trial-and-error testing is costly and time-consuming. In this thesis, two PC-based models are developed for projectile impact into a multi-layer system of membrane layers with nonzero spacings between them. The projectile is a standard right circular cylinder (RCC) often used in laboratory experiments to compare material systems, and the models blend theoretical analysis and numerical simulation to characterize the interaction between the projectile and the various layers. We first consider a system of axisymmetric layers under impact by an RCC projectile. In particular, we consider such performance measures as the critical strains in layers resulting in their failure, the strains in unfailed layers, critical layer gaps, the number of layers penetrated, and the residual velocities in cases where all layers have been penetrated. The model allows variation of mechanical properties from layer to layer as well as variations in spacings between layers, in order to study their combined effects on the ballistic performance of the system. Case studies are performed on the ballistic impact response of fibrous material systems of particular interest in body armor. These are ultra-high molecular weight polyethylene (UHMWPE) fibers such as DSM's Dyneema SK76, as well as aramid fibers such as duPont's Kevlar-29. We also develop a semi-analytical model for a multi-layered biaxial, elastic membrane system impacted by an RCC

projectile. The model builds on a single-layer membrane model, which has been under development by collaborators in the overall body armor work at Cornell University. Key assumptions and parameter values in the single layer model were guided by simulation results using a code based on the finite difference method (FDM) incorporating an algorithm frequently used in molecular dynamics simulations. The code was originally developed by researchers at DSM (makers of Dyneema) and has been modified by the author and several collaborators at Cornell University to suppress local strain concentrations and dynamic artifacts resulting from the descretization of the structure, and to better handle the current geometry. Numerical simulations of impact into a flexible panel are performed where the main emphasis is on a comprehensive understanding of the strain and displacement fields, as well as on the velocity fields versus time. The panel is treated as a single biaxial membrane with negligible shear stiffness compared with the tensile stiffness, and is assigned the properties of Dyneema SK76 or Kevlar 29 biaxial fabrics and flexible composites having about 15 to 20 percent matrix content. Numerical results are obtained through incremental integration of differential equations using small time steps. Compared to simulations using the modified DSM code, there are several important improvements: (1) The calculation time has been accelerated by at least a factor of 1000; (2) Results

under different parameter combinations can be obtained for larger geometric sizes and much longer times; and (3) Modeling multi-layer systems is now possible, and we present results for several cases.

The idea of the book is to provide a comprehensive overview of computational physics methods and techniques, that are used for materials modeling on different length and time scales. Each chapter first provides an overview of the physical basic principles which are the basis for the numerical and mathematical modeling on the respective length-scale. The book includes the micro-scale, the meso-scale and the macro-scale. The chapters follow this classification. The book will explain in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution. Case studies are occasionally included to further illustrate some methods or theoretical considerations. Example applications for all techniques are provided, some of which are from the author's own contributions to some of the research areas. Methods are explained, if possible, on the basis of the original publications but also references to standard text books established in the various fields are mentioned.

This dissertation describes numerical experiments quantifying the influence of pore-scale heterogeneities and their evolution on macroscopic elastic, electrical and

transport properties of porous media. We design, implement and test a computational recipe to construct granular packs and consolidated microstructures replicating geological processes and to estimate the link between process-to-property trends. This computational recipe includes five constructors: a Granular Dynamics (GD) simulation, an Event Driven Molecular Dynamics (EDMD) simulation and three computational diagenetic schemes; and four property estimators based on GD for elastic, finite-elements (FE) for elastic and electrical conductivity, and Lattice-Boltzmann method (LBM) for flow property simulations. Our implementation of GD simulation is capable of constructing realistic, frictional, jammed sphere packs under isotropic and uniaxial stress states. The link between microstructural properties in these packs, like porosity and coordination number (average number of contacts per grain), and stress states (due to compaction) is non-unique and depends on assemblage process and inter-granular friction. Stable jammed packs having similar internal stress and coordination number (CN) can exist at a range of porosities (38-42%) based on how fast they are assembled or compressed. Similarly, lower inter-grain friction during assemblage creates packs with higher coordination number and lower porosity at the same stress. Further, the heterogeneities in coordination number, spatial arrangement of contacts, the contact forces and internal stresses evolve with compaction non-linearly. These pore-scale heterogeneities impact effective elastic moduli, calculated by using infinitesimal perturbation method. Simulated stress-strain relationships and pressure-

dependent elastic moduli for random granular packs show excellent match with laboratory experiments, unlike theoretical models based on Effective Medium Theory (EMT). We elaborately discuss the reasons why Effective Medium Theory (EMT) fails to correctly predict pressure-dependent elastic moduli, stress-strain relationships and stress-ratios (in uniaxial compaction) of granular packs or unconsolidated sediments. We specifically show that the unrealistic assumption of homogeneity in disordered packs and subsequent use of continuum elasticity-based homogeneous strain theory creates non-physical packs, which is why EMT fails. In the absence of a rigorous theory which can quantitatively account for heterogeneity in random granular packs, we propose relaxation corrections to amend EMT elastic moduli predictions. These pressure-dependent and compaction-dependent (isotropic or uniaxial) correction factors are rigorously estimated using GD simulation without non-physical approximations. Further, these correction factors heuristically represent the pressure-dependent heterogeneity and are also applicable for amending predictions of theoretical cementation models, which are conventionally used for granular packs. For predicting stress-ratios in uniaxial compaction scenario, we show the inappropriateness of linear elasticity-based equations, which use elastic constants only and do not account for dissipative losses like grain sliding. We further implement and test a computational recipe to construct consolidated microstructures based on different geological scenarios, like sorting, compaction, cementation types and cement materials. Our

diagenetic trends of elastic, electrical and transport properties show excellent match with laboratory experiments on core plugs. This shows the feasibility of implementing a full-scale computational-rock-physics-based laboratory to construct and estimate properties based on geological processes. However, the elastic property estimator (FE simulation) shows limitations of finite resolution while computing elastic properties of unconsolidated sediments and fluid-saturated microstructures.

Magnetic confinement fusion is a promising technology for electricity production due to available fuel and low waste products. However, the construction of a nuclear fusion reactor remains a scientific challenge. One of the main issues is the resistance of the plasma facing materials exposed to very harsh operating conditions. Tungsten is the leading candidate for the divertor, a crucial plasma facing component. This dissertation focuses on modeling the behavior of tungsten under irradiation conditions relevant to the divertor operations using a multi-scale modeling approach. In particular, high fluxes of helium ions at low energy impact the divertor and are responsible for changes in the tungsten microstructure such as the formation of helium blisters and "fuzz"--Like structures which can ultimately lead to erosion, degradation of materials performance and materials failure. A spatially dependent cluster dynamics model is introduced in order to model the evolution of the tungsten microstructure under irradiation. This continuum model is based on kinetic rate theory and handles each material defect type independently. Under the assumptions of a low dilute limit and no spatial correlation

between defects, this leads to a large system of non-linear reaction-diffusion equations. Hence, the results addressed in this thesis consist in the determination of the kinetic parameters for the cluster dynamics model, the construction of a solver which efficiently deals with the large non-linear system of partial differential equations, the determination of the applicability of the model to fusion relevant conditions, and the model results for a variety of irradiation conditions. The input kinetic parameters to the cluster dynamics model are the defects' diffusion coefficients, binding energies and capture radii. These can be determined using a molecular dynamics and density functional theory simulations as well as empirical data. The challenge lies in obtaining a consistent set of kinetic parameters. Therefore, a method to determine the value of the diffusion coefficients for small helium, interstitial and vacancy defects at various temperatures using only molecular dynamics simulations is presented. Binding energies are also determined using molecular dynamics, and when combined with the diffusion coefficients they form a consistent set of kinetic parameters. An efficient implementation of a parallel solver is presented to deal with the large number of stiff non linear reaction diffusion equations. The implementation of a SDIRK scheme using a modified version of the SPIKE algorithm gives excellent parallelization results and suggests that this implementation would also be efficient for an extension of the model to two or three dimensions. Convergence results for a variety of SDIRK schemes show a convergence order reduction of the numerical scheme due to the stiffness of the reaction and

diffusion terms. A comparison between simulation results using the cluster dynamics model and experimental results is essential to assess the validity of the model. Comparison with thermal helium desorption spectrometry experiments at low flux and fluence shows an excellent agreement between simulation and experiments and indicate that the model captures the key physical properties affecting the evolution of the tungsten microstructure. Further comparison with molecular dynamics simulations at extremely high fluxes provides an insight in the expected limitations of the model due to surface effects and dilute limit approximations breakdown when applied to fusion relevant conditions. Results of the model under fusion relevant conditions show the formation of large helium bubbles under the surface at a temperature dependent depth. The results are very sensitive to both irradiation flux and temperature. At large temperatures, a small concentration of large bubbles forms first deep under the tungsten surface, and forms a ``plug'' which moves towards the surface until eventually the dilute limit approximation breaks down, indicating that the sub-surfaces bubbles become interlinked. At small temperatures, a larger concentration of smaller bubbles forms close to the surface until eventually surface effects such as bubble bursting are expected to occur. These results are found to be in good agreement with a similar analytical reaction diffusion model for fusion relevant conditions. More work is needed to simulate past the dilute limit breakdown and examine the possibility of taking into account surface effects.

This book describes the mathematical underpinnings of algorithms used for molecular dynamics simulation, including both deterministic and stochastic numerical methods. Molecular dynamics is one of the most versatile and powerful methods of modern computational science and engineering and is used widely in chemistry, physics, materials science and biology. Understanding the foundations of numerical methods means knowing how to select the best one for a given problem (from the wide range of techniques on offer) and how to create new, efficient methods to address particular challenges as they arise in complex applications. Aimed at a broad audience, this book presents the basic theory of Hamiltonian mechanics and stochastic differential equations, as well as topics including symplectic numerical methods, the handling of constraints and rigid bodies, the efficient treatment of Langevin dynamics, thermostats to control the molecular ensemble, multiple time-stepping, and the dissipative particle dynamics method.

This book provides an in-depth introduction to molecular dynamics (MD) simulation, the basis for computational study of complex atomic and molecular systems. The author clarifies the role of different variables and sequences throughout, avoids excessive mathematical detail, emphasizes graphical representations, and highlights illustrative applications in materials science, biology, and biochemistry. The text also presents tips for speeding up calculations and parallelization techniques based on OpenMP. The final section offers hands-on training to open-source MD codes (NAMD) and associated

post-processing.

On May 21-24, 1997 the Second International Symposium on Algorithms for Macromolecular Modelling was held at the Konrad Zuse Zentrum in Berlin. The event brought together computational scientists in fields like biochemistry, biophysics, physical chemistry, or statistical physics and numerical analysts as well as computer scientists working on the advancement of algorithms, for a total of over 120 participants from 19 countries. In the course of the symposium, the speakers agreed to produce a representative volume that combines survey articles and original papers (all refereed) to give an impression of the present state of the art of Molecular Dynamics. The 29 articles of the book reflect the main topics of the Berlin meeting which were i) Conformational Dynamics, ii) Thermodynamic Modelling, iii) Advanced Time-Stepping Algorithms, iv) Quantum-Classical Simulations and Fast Force Field and v) Fast Force Field Evaluation.

Numerical Simulation in Molecular DynamicsNumerics, Algorithms, Parallelization, ApplicationsSpringer Science & Business Media

Multi-scale and multi-physics modeling is useful and important for all areas in engineering and sciences. Particle Methods for Multi-Scale and Multi-Physics systematically addresses some major particle methods for modeling multi-scale and multi-physical problems in engineering and sciences. It contains different particle methods from atomistic scales to continuum scales, with emphasis on molecular

dynamics (MD), dissipative particle dynamics (DPD) and smoothed particle hydrodynamics (SPH). This book covers the theoretical background, numerical techniques and many interesting applications of the particle methods discussed in this text, especially in: micro-fluidics and bio-fluidics (e.g., micro drop dynamics, movement and suspension of macro-molecules, cell deformation and migration); environmental and geophysical flows (e.g., saturated and unsaturated flows in porous media and fractures); and free surface flows with possible interacting solid objects (e.g., wave impact, liquid sloshing, water entry and exit, oil spill and boom movement). The presented methodologies, techniques and example applications will benefit students, researchers and professionals in computational engineering and sciences --

This book presents the state of the art in high-performance computing and simulation on modern supercomputer architectures. It covers trends in hardware and software development in general and specifically the future of high-performance systems and heterogeneous architectures. The application contributions cover computational fluid dynamics, material science, medical applications and climate research. Innovative fields like coupled multi-physics or multi-scale simulations are presented. All papers were chosen from presentations given at the 16th Workshop on Sustained Simulation Performance held in December 2012 at HLRS, University of Stuttgart, Germany and the 17th

Workshop on Sustained Simulation Performance at Tohoku University in March 2013.

"The investigations of three different topics of granular flows are reported in this thesis. (i) Second order solutions for granular simple shear flows are derived in the framework of granular kinetic theory. Compared to the first order solutions and the inconsistent second order solutions, the second order solutions of the present study provide better predictions of the numerical simulation results. (ii) Granular shear flows within narrow gaps and unbounded fields are studied by a molecular dynamics type discrete element simulation method. The effects of inelasticity and mean solids fraction on the distributions of granular temperatures, solids fractions and number densities of particle centers, and local mean velocities are examined. The slip velocities of bounded shear flows are calculated and the results are compared with the predictions of existing theories. (iii) Granular self-diffusion is investigated through both a kinetic theory and numerical simulation approaches by employing the time correlation function expression to determine the diffusion coefficient. The theoretical predictions agree very well with the simulation results for smooth particles at low concentrations, but at high concentrations the kinetic theory diffusion coefficients are lower than those determined in the computer simulations. The surface friction effect is examined

numerically, and it is found that rough particles are less diffusive than smooth ones." --

Evaporation and boiling is important for many processes including removal of CO2 from the anode of methanol fuel cells, electronic cooling and various microfluidic applications. Phase change over nanostructured surface is difficult to understand and control for several reasons, including the complexity of geometry, complicated formation of bubble generation between nanostructures, the multiple time and length scales involved. This thesis was concerned with evaporation and boiling over nanostructured surface on nanosecond time scales. The focus was on the effects of nanostructures shape and material. The main tool for these studies was non-equilibrium molecular dynamics simulation under NVT and NVE ensembels. The thesis consist of two main parts: a) A Molecular Dynamics (MD) simulation is carried out to investigate the normal and explosive boiling of thin film adsorbed on a metal substrate whose surface is structured by an array of nanoscale spherical particles. The molecular system was comprised of the liquid and vapor argon as well as a copper wall. The nanostructures have spherical shape with uniform diameters while the thickness of liquid film is constant; hence the effects of transvers and longitudinal distances as well as the diameter of nanoparticles are analyzed. The simulation was started from an initial

configuration for three phases (liquid argon, vapor argon and solid wall); after equilibrating the system at 90 K, the wall is heated suddenly to a higher temperature that is well beyond the critical temperature of Argon. Two different superheat degrees was selected: a moderately high temperature of 170 K for normal evaporation and much higher temperature 290 K for explosive boiling. By monitoring the space and time dependence of temperature and density as well as net evaporation rate, we obtained the detailed microscopic pictures of the normal and explosive boiling process on a flat surface with and without nanostructures. The results show that the nanostructure has significant effect on evaporation /boiling of thin film. It is found that superheat degree and size of nanoparticles have significant influences on the trajectories of particles and net evaporation rate. For the cases with nanostructure, liquid respond very quickly and evaporation rate increase with increasing the size of particles from 1 to 2 nm while it decreases for d = 3 nm. b) Nonequilibrium molecular dynamics simulations were performed to investigate the effect of size of nanocone array and wall material on explosive boiling of ultra-thin argon film on nanostructure. The numerical simulations are performed for ten systems differing in size of nanostructures and type of materials. For each case, the liquid has the constant thickness while the heights of cone-shaped nanostructure are varied from 2 to 5

nm. Two different metal materials, i.e., aluminum and silver, were used as wall material. An Embedded Atom Method (EAM) potential is used in describing the interatomic interaction between metal atoms. The results showed that the cone-like nanostructures drastically enhance heat transfer from solid to liquid and they have significant effect on temperature and pressure histories, net evaporation number, as well as the density distribution in the system. In all of the cases studied, the liquid molecules above the solid surface go into explosive boiling and a cluster of liquid is observed to move upward. It was also observed that the separation temperature associated with separation of liquid film from solid surface is strongly depending on size of nanostructure while it is not sensitive to type of material. Furthermore, in all cases in a specific time after beginning of boiling, the evaporation on the hot wall stopped and a non-evaporating layer will form on the surface.

The application of modern methods in numerical mathematics on problems in chemical engineering is essential for designing, analyzing and running chemical processes and even entire plants. Scientific Computing in Chemical Engineering II gives the state of the art from the point of view of numerical mathematicians as well as that of engineers. The present volume as part of a two-volume edition covers topics such as the simulation of reactive flows, reaction engineering,

reaction diffusion problems, and molecular properties. The volume is aimed at scientists, practitioners and graduate students in chemical engineering, industrial engineering and numerical mathematics.

This book describes the mathematical underpinnings of algorithms used for molecular dynamics simulation, including both deterministic and stochastic numerical methods. Molecular dynamics is one of the most versatile and powerful methods of modern computational science and engineering and is used widely in chemistry, physics, materials science and biology. Understanding the foundations of numerical methods means knowing how to select the best one for a given problem (from the wide range of techniques on offer) and how to create new, efficient methods to address particular challenges as they arise in complex applications. Aimed at a broad audience, this book presents the basic theory of Hamiltonian mechanics and stochastic differential equations, as well as topics including symplectic numerical methods, the handling of constraints and rigid bodies, the efficient treatment of Langevin dynamics, thermostats to control the molecular ensemble, multiple time-stepping, and the dissipative particle dynamics method. .

This book focuses on numerical simulations of manufacturing processes, discussing the use of numerical simulation techniques for design and analysis of

the components and the manufacturing systems. Experimental studies on manufacturing processes are costly, time consuming and limited to the facilities available. Numerical simulations can help study the process at a faster rate and for a wide range of process conditions. They also provide good prediction accuracy and deeper insights into the process. The simulation models do not require any pre-simulation, experimental or analytical results, making them highly suitable and widely used for the reliable prediction of process outcomes. The book is based on selected proceedings of AIMTDR 2016. The chapters discuss topics relating to various simulation techniques, such as computational fluid dynamics, heat flow, thermo-mechanical analysis, molecular dynamics, multibody dynamic analysis, and operational modal analysis. These simulation techniques are used to: 1) design the components, 2) to investigate the effect of critical process parameters on the process outcome, 3) to explore the physics of the process, 4) to analyse the feasibility of the process or design, and 5) to optimize the process. A wide range of advanced manufacturing processes are covered, including friction stir welding, electro-discharge machining, electro-chemical machining, magnetic pulse welding, milling with MQL (minimum quantity lubrication), electromagnetic cladding, abrasive flow machining, incremental sheet forming, ultrasonic assisted turning, TIG welding, and laser sintering. This

book will be useful to researchers and professional engineers alike.

In recent experiments, ultracold neutral plasmas were produced by photoionizing small clouds of laser-cooled atoms. It has been suggested that the low initial temperature of these novel plasmas leads directly to strong correlation and order. In contrast, we argue that rapid intrinsic heating raises the electron temperature to the point where strong correlation cannot develop. The argument is corroborated by a molecular dynamics simulation of the early time plasma evolution.

The primary interest of this work is in the area of flow through permeable media in the context of the subsurface. This area receives growing interest in the scientific community due to the wide range of applications that rely on an in-depth understanding of subsurface systems. The multi-scale and multi-physics nature of flow through permeable media pose significant challenges for modeling and simulation as scientific tools to understand such processes. The aim is to propose predictive mathematical models motivated by physical observations or high-fidelity simulations, and to develop reliable and robust numerical framework to predict the dynamics of flow across different scales. The first part targets discretization schemes for simulation of fractured reservoirs. A discrete fracture model is implemented using an unstructured Voronoi mesh that can capture complex fracture geometries. The mesh generation algorithm is

extended to enable modeling complex fractures in fully three-dimensional space. The proposed approach is validated against results obtained from a commercial simulator. The second part develops a high-resolution numerical framework for immiscible two-phase flow, which helps to exploit the interplay of nonlinearity and heterogeneity, as well as nonequilibrium models on the behavior of fluid mixing. A generalized analytical scaling relation is derived for two-phase flow subject to self-similar heterogeneity. Moreover, we proposed a novel, self-consistent, and physics-based mathematical formulation for multiphase flow. The proposed model generates evolving fronts that match experimental observations. The third part investigates rarefied gas flow using the lattice Boltzmann method. New optimal values for slip coefficients are proposed to capture slip velocities. Results are validated against molecular dynamics simulation reported in the literature. To capture the confined phase behavior of methane, we developed a modified extension of Peng-Robinson equation of state. The proposed equation is coupled with lattice Boltzmann method to investigate transport of methane in slit nanopores. Result indicates that pressure plays an important role in determining the transport characteristics in confined systems.

This book presents the state of the art in modeling and simulation on supercomputers. Leading German research groups present their results achieved on high-end systems of the High Performance Computing Center Stuttgart (HLRS) for the year 2003. The reports cover all fields of computational science and engineering ranging from

computational fluid dynamics via computational physics and chemistry to computer science. Special emphasis is given to industrially relevant applications. Presenting results for both vector-systems and micro-processor based systems, the book allows the reader to compare performance levels and usability of a variety of supercomputer architectures. In the light of the success of the Japanese Earth-Simulator, this book may serve as a guide book for a US response. The book covers the main methods in high performance computing. Its outstanding results in achieving highest performance for production codes are of particular interest for both the scientist and the engineer. The book comes with a wealth of color illustrations and tables of results.

The Surface Wettability Effect on Phase Change collects high level contributions from internationally recognised scientists in the field. It thoroughly explores surface wettability, with topics spanning from the physics of phase change, physics of nucleation, mesoscale modeling, analysis of phenomena such drop evaporation, boiling, local heat flux at triple line, Leidenfrost, dropwise condensation, heat transfer enhancement, freezing, icing. All the topics are treated by discussing experimental results, mathematical modeling and numerical simulations. In particular, the numerical methods look at direct numerical simulations in the framework of VOF simulations, phase-field simulations and molecular dynamics. An introduction to equilibrium and non-equilibrium thermodynamics of phase change, wetting phenomena, liquid interfaces, numerical simulation of wetting phenomena and phase change is offered for readers

who are less familiar in the field. This book will be of interest to researchers, academics, engineers, and postgraduate students working in the area of thermofluids, thermal management, and surface technology.

Attachment of particles to one another due to action of certain inter-particle forces is called as particle agglomeration. It has applications ranging from efficient capture of ultra-fine particles generated in coal-burning boilers to effective discharge of aerosol sprays. Aerosol sprays have their application in asthma relievers, coatings, cleaning agents, air fresheners, personal care products and insecticides. There are several factors that cause particle agglomeration and based on the application, agglomeration or de-agglomeration is desired. These various factors associated with agglomeration include van derWaals forces, capillary forces, electrostatic double-layer forces, effects of turbulence, gravity and brownian motion. It is therefore essential to understand the underlying agglomeration mechanisms involved. It is difficult to perform experiments to quantify certain effects of the inter-particle forces and hence we turn to numerical simulations as an alternative. Simulations can be performed using the various numerical simulation techniques such as molecular dynamics, discrete element method, dissipative particle dynamics or other probabilistic simulation techniques. The main objective of this thesis is to study the geometric characteristics of particle agglomerates using dissipative particle dynamics. In this thesis, agglomeration is simulated using the features of dissipative particle dynamics as the simulation

technique. Forces of attraction from the literature are used to modify the form of the conservative force. Agglomeration is simulated and the characteristics of the result ing agglomerates are quantified. Simulations were performed on a sizeable number of particles and we observe agglomeration behavior. A study of the agglomerates resulting from the different types of attractive forces is performed to characterize them methodically. Also as a part of this thesis, a novel, dynamic particle simulation technique was developed by interfacing MATLAB and our computational C program. Metallic glasses are amorphous materials that possess unique mechanical properties, such as high tensile strengths and good fracture toughnesses. Also, since they are amorphous, metallic glasses exhibit a glass transition, and at temperatures above this glass transition, they soften dramatically and are therefore amenable to net-shape thermoplastic forming processes. This combination of superior properties and the ability to precisely form complex geometries makes metallic glasses attractive materials for structural applications. This thesis addresses several issues related to the mechanics of these materials: " Metallic glasses are near-"ideal" isotropic materials. We have conducted numerical experiments - using molecular dynamics simulations - to develop a continuum-level isotropic elastic free energy that accounts for volumetric-deviatoric coupling effects under circumstances involving large volumetric strains." We have developed a large-deformation, elastic-plastic constitutive theory for metallic glasses that incorporates a cavitation mechanism to describe the onset of "brittle" failure. Using

this theory, we have conducted finite element simulations of fracture initiation at notch tips in a representative metallic glass under Mode-I, plane strain, small-scale-yielding conditions. We show that our theory predicts important experimentally-observed, fracture-related phenomena in metallic glasses." We have developed a large-deformation, elastic-viscoplastic constitutive theory in a temperature range, which spans the glass transition of these materials. The numerical simulation capability based on the theory is used to determine appropriate processing parameters in order to carry out a successful micron-scale hot-embossing operation for the thermoplastic forming of a Zr-based metallic glass tool for the manufacture of polymeric microfluidic devices. * The numerical simulation capability is also used to study surface tension-driven shape recovery of a Pt-based metallic glass and quantitatively determine the surface tension of this material above the glass transition.

This book presents the state-of-the-art in supercomputer simulation. It includes the latest findings from leading researchers using systems from the High Performance Computing Center Stuttgart (HLRS) in 2015. The reports cover all fields of computational science and engineering ranging from CFD to computational physics and from chemistry to computer science with a special emphasis on industrially relevant applications. Presenting findings of one of Europe’s leading systems, this volume covers a wide variety of applications that deliver a high level of sustained performance. The book covers the main methods in high-performance computing. Its outstanding

results in achieving the best performance for production codes are of particular interest for both scientists and engineers. The book comes with a wealth of color illustrations and tables of results.

This project is focus on computational solid mechanics simulation, it is the continuation and improvement of the program in development ?Alamò made by my current advisor Dr. Brandom Runnels, assistant professor of the University of Colorado Colorado Springs specialized in mechanical and aerospace engineering. ?Alamò is a numerical simulation program in continuum mechanical encompassing a range of methods from atomistic (molecular dynamics) to mesoscale (phase field) to continuum (finite element analysis). My project is about generating the numerical code into the program to simulate in 2D and 3D the comportment of the grain structure when it is brought under uniaxial traction or displacement. We study both metals and polymers, and our projects have a number of exciting applications ranging from solid rocket motors to civil infrastructure. Solid mechanics and programming (Linux server and C++).

A report on the first steps towards the numerical simulation of hypersonic flows. Intentionally, the ideal-gas assumption is used to validate the methods by comparing results with experimentally observed or theoretically obtained data in cold hypersonic flows about simple geometries. The approaches cover the continuum as well as the gas-kinetic flow regime. An implicit finite-difference method with bow-shock fitting is employed to integrate the time-dependent Navier-Stokes equations, while the gas-kinetic flow is simulated by approximations to Boltzmann's equation. The Direct-Simulation Monte-Carlo method is preferred to the

Molecular-Dynamics approach because of its larger computational efficiency. Results are compared with experimental data for the laminar flow past a blunted cone at M = 10.6 and past a hemisphere at M = 4.15. The decay of Oseen's vortex at Kn = 0.1, and the gas-kinetic flow past a cylinder at M = 5.48 with Kn = 0.1 and 0.3 have been simulated, and results are shown in comparison with theoretical data. As an application to more realistic configurations the three-dimensional laminar flow past the noise of a typical spacecraft and the gas-kinetic flow in the symmetry plane of the flow past the same configuration is being discussed. The next steps will include real-gas modelling. For hot hypersonic flows experimental data are badly needed for comparison purpose.

This book constitutes the referred proceedings of two workshops held at the 32nd ACM International Conference on Supercomputing, ACM ICS 2018, in Beijing, China, in June 2018. This volume presents the papers that have been accepted for the following workshops: Second International Workshop on High Performance Computing for Advanced Modeling and Simulation in Nuclear Energy and Environmental Science, HPCMS 2018, and First International Workshop on HPC Supported Data Analytics for Edge Computing, HiDEC 2018. The 20 full papers presented during HPCMS 2018 and HiDEC 2018 were carefully reviewed and selected from numerous submissions. The papers reflect such topics as computing methodologies; parallel algorithms; simulation types and techniques; machine learning.

This thesis deals with the liquid crystalline lamellar phase L? built by amphiphilic molecules in aqueous solutions, and its interaction with macromolecules. We perform molecular dynamics simulations to study thermal fluctuations and defects appearing in a stack of parallel amphiphilic bilayers separated by layers of solvent. The idealized, coarse-grained model

represents the solvent with soft spheres and the amphiphiles with bead-and-spring tetramers (two solvophilic beads and two solvophobic beads). The algorithm used for this thesis describes the lamellar phase in the isobaric isothermal ensemble without surface tension (N,P, T, ? = 0). First, we verify that the model exhibits a liquid-crystalline lamellar phase, which we characterize. In a second part, we study the elasticity of this smectic lamellar phase. The position fluctuation spectra of the bilayers are computed, and compared to the predictions of the “Discrete Harmonic”(DH) theory for the elasticity of smectic phases. The bilayer fluctuations observed in the simulation of a stack of fifteen bilayers are well described by the DH-theory, so that the two elastic constants - the bending rigidity Kc and the smectic compressibility modulus B - can be computed. Then, we investigate the point defects appearing in the smectic because of thermal fluctuations. It turns out that transient pores spontaneously nucleate in the bilayers of the lamellar phase. On the contrary, necks and passages between the bilayers are rarely detected. The size and shape distributions of the pores are investigated. The relationship between their area a and their contour length c is well described by the scaling law a ? c2/3 - the same scaling as two dimensional closed random walks. Additionally, the surface tension is zero. Therefore we consider that the energy of a pore depends explicitly only on the contour length of the pore. The effective free energy of individual pores and the line tension of the pore edge are then estimated from the contour-length distribution. Besides, a time-dependent analysis shows that the displacement of the pores within the bilayers during their life-time is very limited. In the last chapter of this thesis, we investigate a lamellar phase doped by a solventsoluble flexible linear polymer inserted between two bilayers. Two polymer types were simulated: adsorbing or non-adsorbing. In both

cases, the interactions between the bilayers are softened in the presence of a polymer. However, the conformations of the chain strongly depend on the interactions between the polymer and the bilayers: An adsorbing polymer remains aligned with the bilayers and confined in the thin solvent layer, whereas a non-adsorbing polymer condenses into a globule. Contrarily to standard hypothesis, a non-adsorbing polymer locally modifies the interlamellar spacing, and triggers the formation of pores in its vicinity. Diese Arbeit behandelt die flüssig-kristalline lamellare Phase (die sogenannte L? Phase), die amphiphile Moleküle in wässriger Lösung ausbilden. Diese lamellare Phase besteht aus mehrere Lagen paralleler amphiphiler Doppelschichten, die durch Lösungsmittel voneinander getrennt sind. Wir studieren mittels Molekulardynamiksimulationen die thermischen Fluktuationen der Doppelschichten und die Defekte, die in der lamellaren Phase auftreten können, und die Auswirkungen eines Makromoleküls, das zwischen die Doppelschichten gestetzt wird. In dem zugrundeliegenden, idealisierten “coarse-grained” Modell werden das Lösungsmittel als weiche Kugeln und die Amphiphile als Tetramere (zwei hydrophile Kugeln und zwei hydrophobe Kugeln) repräsentiert. Der Algorithmus, der in dieser Arbeit verwendet wird, beschreibt die lamellare Phase im isobaren isothermen Ensemble ohne Oberflächenspannung (NPT, ? = 0). Zuerst verifizieren wir, daß das Modell tatsächlich eine stabile L? Phase bildet, und charakterisieren ihre flüssig-kristalline Struktur. Um die Elastizität der lamellaren Phase zu untersuchen, berechnen wir die Fluktuationsspektren der Positionen von den Doppelschichten und vergleichen sie mit den Vorhersagen der “Discrete Harmonic Theory” (DH) f¨ur die Elastizität der smektischen Phasen. Die Ergebnisse der Simulation, die mit einem Stapel von f¨unfzehn Doppelschichten durchgeführt wurde, stimmen mit der DH Theorie überein. Daher können die elastischen

Konstanten (Steifigkeitsmodul Kc und smektischer Kompressionsmodul B) berechnet werden. Nachfolgend betrachten wir lokale Defekte, die auf Grund thermischer Fluktuationen erscheinen. Kurzlebige Poren treten spontan in den Doppelschichten der lamellaren Phase auf. Im Gegensatz dazu werden Verbindungen oder Durchgänge zwischen den Doppelschichten selten beobachtet. Die Verteilungen von Größe und Form der Poren werden bestimmt. Das Verhältnis zwischen Fläche der Poren a und ihrer Konturlänge c wird durch das Skalengesetz a ? c2/3 beschrieben (ein analoges Skalengesetz gilt für zweidimensionale geschlossene Irrfahrten). Zusätzlich ist die Oberflächenspannung null. Wir nehmen dann an, daß die Energie einer einzelnen Pore nur von ihrer Konturlänge abhängt. Diese Energie und die Linienspannung des Porenrandes werden mittels der Verteilung für die Konturlänge geschätzt. Zusätzlich zeigt eine zeitabhängige Analyse, daß die Poren innerhalb ihrer Lebensdauer nicht nennenswert diffundieren. Schließlich wird eine lamellare Phase untersucht, in der ein hydrophiles, flexibles, lineares Polymer zwischen zwei Doppelschichten eingesetzt wurde. Zwei Typen von Polymeren werden simuliert: adsorbierende und nicht-adsorbierende. In beiden Fälle werden die Wechselwirkungen zwischen den Doppelschichten in Anwesenheit des Polymer verändert. Die Konformation des Polymers hängt allerdings stark von den Wechselwirkungen zwischen dem Polymer und den Amphiphilen ab: Ein adsorbierendes Polymer verbleibt während der gesamten Simulation in der dünnen Lösungsmittelschicht zwischen den beiden Doppelschichten. Ein nicht-adsorbierendes Polymer dagegen kondensiert in einen kompakten Tropfen". Im Gegensatz zu den übliches Annahmen ändert ein nichtadsorbierendes Polymer lokal den interlamellaren Abstand und erzeugt Poren in der Doppelschicht in seiner Nähe.

The book presents the state-of-the-art in high performance computing and simulation on modern supercomputer architectures. It covers trends in high performance application software development in general and specifically for parallel vector architectures. The contributions cover among others the field of computational fluid dynamics, physics, chemistry, and meteorology. Innovative application fields like reactive flow simulations and nano technology are presented.

This dissertation, "Theoretical Modelling and Numerical Simulation of Plastic Deformation of Nanostructured Materials With High Strength and Ductility" by Jianjun, Li, ???, was obtained from The University of Hong Kong (Pokfulam, Hong Kong) and is being sold pursuant to Creative Commons: Attribution 3.0 Hong Kong License. The content of this dissertation has not been altered in any way. We have altered the formatting in order to facilitate the ease of printing and reading of the dissertation. All rights not granted by the above license are retained by the author. Abstract: ?Nanostructured materials have attracted intensive scientific interests during the past two decades due to their outstanding physical and mechanical properties. However, the brittleness of nanostructured materials posed a great challenge for their engineering applications. Recently, several strategies were successfully adopted to produce nanostructured materials with both high strength and ductility such as surface-nanocrystallized (SNC) materials, nanocrystalline materials with stress-induced nanograin growth and nanotwinned metals. A lot of molecular dynamics (MD) simulations, modelling and experiments have been conducted to investigate the deformation mechanisms and the correlated exceptional mechanical properties and considerable progress has been made. However, some problems remain unsolved. For example, the complicated structure of SNC materials due to its

grain size gradient (GSG) surface layer makes it difficult to establish a quantitative model for prediction of their strength and ductility; the main mode of nanograin growth in nanostructured materials, i.e., shear-coupled migration of grain boundaries (GBs), was experimentally observed as contributing to their enhanced ductility, but the mechanism of the enhancement remains unclear. In addition, there exist contradictory results for the grain size dependence of transitional twin thickness that corresponds to the maximum strength of nanotwinned metals. All these issues should be addressed to gain a better understanding of the mechanism-ductility correlation in order to provide some guidelines for designing lighter, stronger and ductile nanostructured materials. Therefore, an attempt was made to study the plastic deformation of nanostructured materials with high strength and ductility by theoretical modelling and numerical simulations. Firstly, the enhanced balance of strength and ductility of SNC materials was studied using a combination of theoretical analysis and finite element simulation. A criterion was established for determining the ductility of SNC materials. The results obtained showed that the ductility of a SNC sample could be comparable to that of its coarse-grained counterpart, while it simultaneously possessed a much higher strength than that of the latter if optimal GSG thickness and topmost phase grain size were adopted. Then a dislocation-density-based model was proposed to quantitatively predict the plastic deformation of SNC materials; the stress-driven nanograin growth was also incorporated in the said model. The capability of the model in predicting the strength and work hardening of SNC materials was validated by the existing experimental results. Thirdly, physical models for shear-coupled migration of GBs in nanostructured materials were developed to explain the general coupling between the shear and the normal migration of GBs observed in MD simulations and experiments. The coupled

migration process was found to be a general and effective toughening mechanism in nanostructured materials. Moreover, our study showed that the shear-coupled migration is able to enhance the intrinsic ductility considerably when it cooperates with GB sliding. Finally, an elastic-viscoplastic constitutive model based on the competition of intra-twin and twin-boundary-mediated deformation mechanisms was proposed to predict the grain size dependent transitional twin thickness o

This book presents the state-of-the-art in simulation on supercomputers. Leading researchers present results achieved on systems of the High Performance Computing Center Stuttgart (HLRS) for the year 2013. The reports cover all fields of computational science and engineering ranging from CFD via computational physics and chemistry to computer science with a special emphasis on industrially relevant applications. Presenting results of one of Europe’s leading systems this volume covers a wide variety of applications that deliver a high level of sustained performance. The book covers the main methods in high performance computing. Its outstanding results in achieving highest performance for production codes are of particular interest for both the scientist and the engineer. The book comes with a wealth of coloured illustrations and tables of results.