Hot Spots In Energetic Materials Generated By Infrared And

This book offers a comprehensive account of energetic materials, including their synthesis, computational modeling, applications, associated degradation mechanisms, environmental consequences and fate and transport. This multi-author contributed volume describes how armed forces around the world are moving their attention from legacy explosive compounds, which are heat and shock sensitive (thus posing greater challenges in terms of handling and storage), to the insensitive munitions compounds/formulations such as insensitive munitions explosive (IMX) and the Picatinny Arsenal Explosive (PAX) series of compounds. The description of energetic materials focuses on explosives, pyrotechnic compositions, and propellants. The contributors go on to explain how modern generation energetic compounds must be insensitive to shock and heat but at the same time yield more energy upon explosion. Nanoinspired and/or co-crystallized energetic materials offer another route to generate next-generation energetic materials, and this authoritative book bridges a large gap in the literature by providing a comprehensive analysis of these compounds. Additionally, it includes a valuable overview of energetic materials, a detailed discussion of recent advances on future energetic compounds, nanotechnology in energetic materials, environmental contamination and toxicity, assessment of munitions lethality, the application quantitative structure–activity relationship (QSAR) in design of energetics and the fate and transport of munition compounds in the environment.

Metal-Fluorocarbon Based Energetic Materials This exciting new book details all aspects of a major class of pyrolants and elucidates the progress that has been made in the field, covering both the chemistry and applications of these compounds. Written by a pre-eminent authority on the subject from the NATO Munitions Safety Information Analysis Center (MSIAC), it begins with a historical overview of the development of these materials, followed by a thorough discussion of their ignition, combustion and radiative properties. The next section explores the multiple facets of their military and civilian applications, as well as industrial synthetic techniques. The critical importance of the associated hazards, namely sensitivity, stability and aging, are discussed in detail, and the book is rounded off by an examination of the future of this vital and expanding field. The result is a complete guide to the chemistry, manufacture, applications and required safety precautions of pyrolants for both the military and chemical industries. From the preface: “... This book fills a void in the collection of pyrotechnic literature... it will make an excellent reference book that all researchers of pyrolants and energetics must have...” Dr. Bernard E. Douda, Dr. Sara Pliskin, NAVSEA Crane, IN, USA This book uses experimental and computational methods to rationalize and predict for the first time the relative impact sensitivities of a range of energetic materials. Using knowledge of crystal structures, vibrational properties, energy-transfer mechanisms, and experimentally measured sensitivities, it describes a model that leads to excellent correlation with experimental results in all cases. As such, the book paves the way for a new, fully ab initio approach for the design of safer energetic materials based solely on knowledge of their solid-state structures. Energetic materials (explosives, propellants, gas generators, and pyrotechnics) are defined as materials that release heat and/or gaseous products at a high rate

upon stimulus by heat, impact, shock, sparks, etc. They have widespread military and civilian uses, including munitions, mining, quarrying, demolition, emergency signaling, automotive safety, and space exploration. One of their most important properties is sensitivity to accidental initiation during manufacture, transport, storage, and operation, which has important implications for their safe use.

This book presents the latest research on the area of nano-energetic materials, their synthesis, fabrication, patterning, application and integration with various MEMS systems and platforms. Keeping in mind the applications for this field in aerospace and defense sectors, the articles in this volume contain contributions by leading researchers in the field, who discuss the current challenges and future perspectives. This volume will be of use to researchers working on various applications of high-energy research.

The papers collected together in this volume constitute a review of recent research on the response of condensed matter to dynamic high pressures and temperatures. Inlcuded are sections on equations of state, phase transitions, material properties, explosive behavior, measurement techniques, and optical and laser studies. Recent developments in this area such as studies of impact and penetration phenomenology, the development of materials, especially ceramics and molecular dynamics and Monte Carlo simulations are also covered. These latest advances, in addition to the many other results and topics covered by the authors, serve to make this volume the most authoritative source for the shock wave physics community.

Developing and testing novel energetic materials is an expanding branch of the materials sciences. Reaction, detonation or explosion of such materials invariably produce extremely

high pressures and temperatures. To study the equations-of-state (EOS) of energetic materials in extreme regimes both shock and static high pressure studies are required. The present volume is an introduction and review of theoretical, experimental and numerical aspects of static compression of such materials. Chapter 1 introduces the basic experimental tool, the diamond anvil pressure cell and the observational techniques used with it such as optical microscopy, infrared spectrometry and x-ray diffraction. Chapter 2 outlines the principles of high-nitrogen energetic materials synthesis. Chapters 3 and 4, examine and compare various EOS formalisms and data fitting for crystalline and non-crystalline materials, respectively. Chapter 5 details the reaction kinetics of detonating energetic materials. Chapter 6 investigates the interplay between static and dynamic (shock) studies. Finally, Chapters 7 and 8 introduce numerical simulations: molecular dynamics of energetic materials under either hydrostatic or uni-axial stress and ab-inito treatments of defects in crystalline materials. This timely volume meets the growing demand for a state-of-the art introduction and review of the most relevant aspects of static compression of energetic materials and will be a valuable reference to researchers and scientists working in academic, industrial and governmental research laboratories.

Incorporation of particular components with specialized properties allows one to tailor the end product's properties. For instance, the sensitivity, burning behavior, thermal or mechanical properties or stability of energetic materials can be affected and even controllably varied through incorporation of such ingredients. This book examines particle technologies as applied to energetic materials such as propellants and explosives, thus filling a void in the literature on this subject. Following an introduction covering general features of energetic materials, the first

section of this book describes methods of manufacturing particulate energetic materials, including size reduction, crystallization, atomization, particle formation using supercritical fluids and microencapsulation, agglomeration phenomena, special considerations in mixing explosive particles and the production of nanoparticles. The second section discusses the characterization of particulate materials. Techniques and methods such as particle size analysis, morphology elucidation and the determination of chemical and thermal properties are presented. The wettability of powders and rheological behavior of suspensions and solids are also considered. Furthermore, methods of determining the performance of particular energetic materials are described. Each chapter deals with fundamentals and application possibilities of the various methods presented, with particular emphasis on issues applicable to particulate energetic materials. The book is thus equally relevant for chemists, physicists, material scientists, chemical and mechanical engineers and anyone interested or engaged in particle processing and characterization technologies.

Dynamic Behavior of Materials, Volume 1 of the Proceedings of the 2018 SEM Annual Conference & Exposition on Experimental and Applied Mechanics, the first volume of eight from the Conference, brings together contributions to this important area of research and engineering. The collection presents early findings and case studies on fundamental and applied aspects of Experimental Mechanics, including papers on: Synchrotron Applications/Advanced Dynamic Imaging Quantitative Visualization of Dynamic Events Novel Experimental

Techniques Dynamic Behavior of Geomaterials Dynamic Failure & Fragmentation Dynamic Response of Low Impedance Materials Hybrid Experimental/Computational Studies Shock and Blast Loading Advances in Material Modeling Industrial Applications

Volume is indexed by Thomson Reuters CPCI-S (WoS). Explosion, shock wave, high-energy reaction and other high-rate phenomena of various materials are the main topic of this collection. The book includes papers related to explosion and shock wave phenomena driven by explosives and other impulsive phenomena including their applications. The use of such intense dynamic loading has been employed for materials processing technology and the field is currently spreading to food processing and others. The volume will bring to readers new idea for the progress in science and technology.

This book presents recently developed computational approaches for the study of reactive materials under extreme physical and thermodynamic conditions. It delves into cutting edge developments in simulation methods for reactive materials, including quantum calculations spanning nanometer length scales and picosecond timescales, to reactive force fields, coarse-grained approaches, and machine learning methods spanning microns and nanoseconds and beyond. These methods are discussed in the context of a broad range of fields, including

prebiotic chemistry in impacting comets, studies of planetary interiors, high pressure synthesis of new compounds, and detonations of energetic materials. The book presents a pedagogical approach for these state-of-the-art approaches, compiled into a single source for the first time. Ultimately, the volume aims to make valuable research tools accessible to experimentalists and theoreticians alike for any number of scientific efforts, spanning many different types of compounds and reactive conditions.

The MRS Symposium Proceeding series is an internationally recognised reference suitable for researchers and practitioners.

This volume provides an overview of current research and recent advances in the area of energetic materials, focusing on decomposition, crystal and molecular properties. The contents and format reflect the fact that theory, experiment and computation are closely linked in this field. Since chemical decomposition is of fundamental importance in energetic performance, this volume begins with a survey of the decomposition processes of a variety of energetic compounds. This is followed by detailed studies of certain compounds and specific mechanisms, such as nitro/aci-nitro tautomerism. Chapter 6 covers the transition from decomposition to crystal properties, with molecular dynamics being the primary analytical tool. The next several chapters deal with different aspects of the

crystalline state, again moving from the general to particular. There is also a discussion of methods for computing gas, liquid and solid phase heats of formation. Finally, the last portion of this volume looks at the potential of high-nitrogen molecules as energetic systems; this has been of considerable interest in recent years. Overall, this volume illustrates the progress that has been made in the field of energetic materials and some of the areas of current activity. It also indicates the challenges involved in characterizing and understanding the properties and behaviour of these compounds. The work is a unique state-of-the-art treatment of the subject, written by pre-eminent researchers in the field. - Overall emphasis is on theory and computation, presented in the context of relevant experimental work - Presents a unique state-of-the-art treatment of the subject - Contributors are preeminent researchers in the field

The development, processing, and lifecycle environmental impact analysis of energetic materials all pose various challenges and potential dangers. Because safety concerns severely limit study of these substances at most research facilities, engineers will especially appreciate a tool that strengthens understanding of the chemistry and physics involved and helps them better predict how these materials will behave when used in explosives, propellants, pyrotechnics, and other applications. Integrate Cutting-Edge Research

Sponsored by the U.S. Department of Defense Energetic Materials: Thermophysical Properties, Predictions, and Experimental Measurements covers a variety of advanced empirical modeling and simulation tools used to explore development, performance, sensitivity, and lifecycle issues of energetic materials. Focusing on a critical component of energetic materials research—prediction of thermophysical properties—this book elucidates innovative and experimental techniques being used to: Apply molecular and meso-scale modeling methodologies to measure reactivity, performance, and properties of new energetic materials Gain insight into shear initiation at the particulate level Better understand the fate, transport, and overall environmental impact of energetic materials Evaluate the performance of new materials and assess their reaction mechanisms Edited by two respected U.S. Army engineers, this book highlights cutting-edge research from leaders in the energetics community. Documenting the history, applications, and environmental behavior of energetic materials, this reference is a valuable resource for anyone working to optimize their massive potential—either now or in the future.

This unified guide brings together the underlying principles, and predictable material responses, that connect metals, polymers, brittle solids and energetic materials as they respond to extreme external stresses. Previously disparate

scientific principles, concepts and terminology are combined within a single theoretical framework, across different materials and scales, to provide all the tools necessary to understand, and calculate, the responses of materials and structures to extreme static and dynamic loading. Real-world examples illustrate how material behaviours produce a component response, enabling recognition – and avoidance – of the deformation mechanisms that contribute to mechanical failure. A final synoptic chapter presents a case study of extreme conditions brought about by the infamous Chicxulub impact event. Bringing together simple concepts from diverse fields into a single, accessible, rigorous text, this is an indispensable reference for all researchers and practitioners in materials science, mechanical engineering, physics, physical chemistry and geophysics.

The 5th revised edition expands on the basic chemistry of high-energy materials of the previous editions and examines new research developments, including plastic bonded explosives and melt-castable dinitrate esters. Applications in military and civil fields are discussed. This work is of interest to advanced students in chemistry, materials science and engineering, as well as to all those working in defense technology.

Summarizing the latest advances in experimental impact mechanics, this book provides cutting-edge techniques and methods for designing, executing, analyzing, and interpreting the results of experiments involving the dynamic responses of materials and structures. It provides tailored guidelines and solutions for specific applications and materials, covering topics such

as dynamic characterization of metallic materials, fiber-like materials, low-impedance materials, concrete and more. Damage evolution and constitutive behavior of materials under impact loading, one-dimensional strain loading, intermediate and high strain rates, and other environmental conditions are discussed, as are techniques using high temperature testing and miniature Kolsky bars. Provides cutting-edge techniques and methods for designing, executing, analyzing, and interpreting the results of experimental impact mechanics Covers experimental guidelines and solutions for an array of different materials, conditions, and applications Enables readers to quickly design and perform their own experiments and properly interpret the results Looks at application-specific post-test analysis

For a chemist who is concerned with the synthesis of new energetic compounds, it is essential to be able to assess physical and thermodynamic properties, as well as the sensitivity, of possible new energetic compounds before synthesis is attempted. Various approaches have been developed to predict important aspects of the physical and thermodynamic properties of energetic materials including (but not limited to): crystal density, heat of formation, melting point, enthalpy of fusion and enthalpy of sublimation of an organic energetic compound. Since an organic energetic material consists of metastable molecules capable of undergoing very rapid and highly exothermic reactions, many methods have been developed to estimate the sensitivity of an energetic compound with respect to detonationcausing external stimuli such as heat, friction, impact, shock and electrostatic discharge. This book introduces these methods and demonstrates those methods which can be easily applied.

Propellants are almost always ignited due to thermal processes. They can be ignited by direct application of heat or by the conversion of mechanical or electrical energy to heat. However, it

is not necessary to heat the bulk energetic for ignition. Local regions which achieve high temperatures, so called "hot spots", are sufficient to cause rapid decomposition and reaction. For "critical" hot spots, the reaction in the localized region must produce heat faster than the heat transferred to the material and losses to the surrounding environment. Otherwise, the hot spot cools and can eventually stop reacting. In their monograph work on the topic, Bowden and Yoffe (1952) estimated critical hot spots at the micron (0.1 to 10um) length scale, with duration of 10-5 to 10-3s and reaching 700K. The current research exercises a hydrocode to determine its ability to predict critical hot spot initiation of energetic materials resulting from thermo-mechanical coupling. For the simulations, the viscoSCRAM constitutive model was used to describe viscoelasticity, viscoplasticity, cracking and ignition in a double-base propellant when subjected to dynamic shear loading conditions. The effect of hot spot size and duration on the ignition threshold temperature was examined. The validity of the constitutive relations and the failure criterion are determined based on their ability to predict the observed mechanical response.

This book contains a collection of papers prepared by leading experts on selected areas of particular importance to researchers in combustion science. The editors have gathered writings on fundamental physical and chemical aspects of combustion, including combustion chemistry, soot formation, and condensed phase and turbulent combustion intended to be a source of current understanding on the topics covered. The materials were originally presented as part of a Colloquium on Combustion held in honor of Professor Irvin Glassman.

Challenges in Mechanics of Time-Dependent Materials, Volume 2 of the Proceedings of the 2016 SEM Annual Conference& Exposition on Experimental and Applied Mechanics, the

second volume of ten from the Conference, brings together contributions to this important area of research and engineering. The collection presents early findings and case studies on fundamental and applied aspects of Experimental Mechanics, including papers in the following general technical research areas: Extreme Environments & Environmental Effects Structure-Function of Performance of PE Effects of Inhomogeneities & Interfaces Characterization Across Scales Mechanics of Energy & Energetic Materials Metallic Materials Viscoelasticity & Viscoplasticity

Currently, there is a considerable gap in the level of theoretical understanding of the mechanisms triggering energy release between liquid and solid energetic/explosive materials. Although adiabatic impact-induced triggering in solid energetic /explosive materials is still treated similarly to liquid, there are qualitative differences in the impact-induced triggering of liquids and solids. In this report, we discuss our recent results related to the impact-induced triggering in solid energetic materials.

This book provides a broad and nuanced overview of the achievements and legacy of Professor William ("Bill") Goddard in the field of computational materials and molecular science. Leading researchers from around the globe discuss Goddard's work and its lasting impacts, which can be seen in today's cutting-edge chemistry, materials science, and biology techniques. Each section of the book closes with an outline of the prospects for future developments. In the course of a career spanning more than 50 years, Goddard's seminal work has led

to dramatic advances in a diverse range of science and engineering fields. Presenting scientific essays and reflections by students, postdoctoral associates, collaborators and colleagues, the book describes the contributions of one of the world's greatest materials and molecular scientists in the context of theory, experimentation, and applications, and examines his legacy in each area, from conceptualization (the first mile) to developments and extensions aimed at applications, and lastly to de novo design (the last mile). Goddard's passion for science, his insights, and his ability to actively engage with his collaborators in bold initiatives is a model for us all. As he enters his second half-century of scientific research and education, this book inspires future generations of students and researchers to employ and extend these powerful techniques and insights to tackle today's critical problems in biology, chemistry, and materials. Examples highlighted in the book include new materials for photocatalysts to convert water and CO2 into fuels, novel catalysts for the highly selective and active catalysis of alkanes to valuable organics, simulating the chemistry in film growth to develop two-dimensional functional films, and predicting ligand-protein binding and activation to enable the design of targeted drugs with minimal side effects.

Proceedings of the NATO Advanced Study Institute on Chemistry and Physics of

the Molecular Processes in Energetic Materials, Altavilla Milicia, Sicily, Italy, September 3-15, 1989

This book describes the research of Bowden, Yoffe and their collaborators on explosive initiation. What Bowden and Yoffe showed was that explosives are ignited almost invariably by thermal processes and though other processes have been identified their work still holds.

Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry, and biology. It features detailed reviews written by leading international researchers. This volume focuses on the theory of heavy ion physics in medicine. This volume presents a series of articles concerning current important topics in quantum chemistry. The invited articles are written by the best people in the field

Engineering structures may be subjected to extreme high-rate loading conditions, like those associated with natural disasters (earthquakes, tsunamis, rock falls, etc.) or those of anthropic origin (impacts, fluid–structure interactions, shock wave transmissions, etc.). Characterization and modeling of the mechanical behavior of materials under these environments is important in predicting the response of structures and improving designs. This book gathers contributions by

eminent researchers in academia and government research laboratories on the latest advances in the understanding of the dynamic process of damage, cracking and fragmentation. It allows the reader to develop an understanding of the key features of the dynamic mechanical behavior of brittle (e.g. granular and cementitious), heterogeneous (e.g. energetic) and ductile (e.g. metallic) materials.

This book summarizes science and technology of a new generation of high-energy andinsensitive explosives. The objective is to provide professionals with comprehensiveinformation on the synthesis and the physicochemical and detonation properties ofthe explosives. Potential technologies applicable for treatment of contaminated wastestreams from manufacturing facilities and environmental matrices are also be included.This book provides the reader an insight into the depth and breadth of theoreticaland empirical models and experimental techniques currently being developed in thefield of energetic materials. It presents the latest research by DoD engineers andscientists, and some of DoD's academic and industrial researcher partners. The topicsexplored and the simulations developed or modified for the purposes of energetics mayfind application in other closely related fields, such as the pharmaceutical industry.One of the key features of the book is the treatment of wastewaters

generated duringmanufacturing of these energetic materials.

The International Conference of Computational Methods in Sciences and Engineering (ICCMSE) is unique in its kind. It regroups original contributions from all fields of the traditional Sciences, Mathematics, Physics, Chemistry, Biology, Medicine and all branches of Engineering. The aim of the conference is to bring together computational scientists from several disciplines in order to share methods and ideas. More than 370 extended abstracts have been submitted for consideration for presentation in ICCMSE 2004. From these, 289 extended abstracts have been selected after international peer review by at least two independent reviewers.

The natural mission of Computational Science is to tackle all sorts of human problems and to work out intelligent automata aimed at alleviating the b- den of working out suitable tools for solving complex problems. For this reason ComputationalScience,thoughoriginatingfromtheneedtosolvethemostch- lenging problems in science and engineering (computational science is the key player in the ?ght to gain fundamental advances in astronomy, biology, che- stry, environmental science, physics and several other scienti?c and engineering disciplines) is increasingly turning its attention to all ?elds of human activity. In all activities, in fact, intensive computation, information handling, kn- ledge synthesis, the use of ad-hoc devices, etc.

increasingly need to be exploited and coordinated regardless of the location of both the users and the (various and heterogeneous) computing platforms. As a result the key to understanding the explosive growth of this discipline lies in two adjectives that more and more appropriately refer to Computational Science and its applications: interoperable and ubiquitous. Numerous examples of ubiquitous and interoperable tools and applicationsaregiveninthepresentfourLNCSvolumescontainingthecontri- tions delivered at the 2004 International Conference on Computational Science and its Applications (ICCSA 2004) held in Assisi, Italy, May 14–17, 2004.

The book gives an introduction to energetic materials and lasers, properties of such materials and the current methods for initiating energetic materials. The following chapters and sections highlight the properties of lasers, and safety aspects of their application. It covers the properties of in-service energetic materials, and also materials with prospects of being used as insensitive ammunitions in future weapon or missiles systems or as detonators in civilian (mining) applications. Because of the diversity of the topics some sections will naturally separate into different levels of expertise and knowledge.

This comprehensive book presents a detailed account of research and recent developments in the field of green energetic materials, including pyrotechnics, explosives and propellants. This area is attracting increasing interest in the community as it undergoes a transition from using traditional processes, to more environmentally-

friendly procedures. The book covers the entire line of research from the initial theoretical modelling and design of new materials, to the development of sustainable manufacturing processes. It also addresses materials that have already reached the production line, as well as considering future developments in this evolving field.
The topics discussed in this text range from quasi-static problems to dynamic problems, and are divided into 15 groups, such as: cohesion/cracking; wave propagation; and quasi-static behaviour. Each group contains theoretical, experimental and computational approaches by researchers.
' Few books cover experimental and theoretical methods to characterize decomposition, combustion and detonation of energetic materials. This volume, by internationally known and major contributors to the field, is unique because it summarizes the most important recent work, what we know with confidence, and what main areas remain to be investigated. Most chapters comprise summaries of work spanning decades and contain expert commentary available nowhere else. Although energetic materials are its focus, this book provides a guide to modern methods for investigations of condensed and gas-phase reactions. Although these energetic reactions are complex and difficult to study, the work discussed here provides readers with a substantial understanding of the behavior of materials now in use, and a predictive capability for the development of new materials based on target properties. Contents:Connecting Molecular Properties to Decomposition, Combustion and

Explosion Trends (T B Brill)Thermal Decomposition Processes of Energetic Materials in the Condensed Phase at Low and Moderate Temperatures (R Behrens)Study of Energetic Material Combustion Chemistry by Probing Mass Spectrometry and Modeling of Flames (O P Korobeinichev)Optical Spectroscopic Measurements of Energetic Material Flame Structure (T Parr & D Hanson-Parr)Transient Gas-Phase Intermediates in the Decomposition of Energetic Materials (P J Dagdigian)Role of Excited Electronic States in the Decomposition of Energetic Materials (E R Bernstein)Gas-Phase Kinetics for Propellant Combustion Modeling: Requirements and Experiments (W R Anderson & A Fontijn)Gas-Phase Decomposition of Energetic Molecules (D L Thompson)Modeling the Reactions of Energetic Materials in the Condensed Phase (L E Fried et al.)Multi-Phonon Up-Pumping in Energetic Materials (D D Dlott)Applications of Theoretical Chemistry in Assessing Energetic Materials for Performance or Sensitivity (B M Rice)Combustion and Ignition of Nitramine Propellants: Aspects of Modeling, Simulation, and Analysis (E S Kim & V Yang)Burning-Rate Models and Their Successors, A Personal Perspective (M S Miller)Ideas to Expand Thinking About New Energetic Materials (J Bottaro) Readership: Researchers studying fast chemical reactions and materials behavior under extreme conditions. Experts and beginners in energetic decomposition, combustion and detonation research. Keywords:Energetic Materials;Combustion;Thermal Decomposition;Combustion Model;Materials Design;Flames;Explosive;Propellant;Computational Chemistry;DetonationKey

Features:Summarizes the known knowns (the most important recent work) and lists the known unknowns (what remains to be investigated)Provides expert commentary on the complex behavior of materialsReviews:“This book nicely covers the application of many experimental and theoretical tools to study the difficult problem of ignition and combustion of many traditional energetic materials. It could be a valuable resource to the researchers in the field.”Journal of the American Chemical Society '