Hot Spots In Energetic Materials Generated By Infrared And

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 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.

Introduction of discontinuities increases the sensitivity of energetic material to initiation by shock waves. We have experimental evidence that

the particular nature of these discontinuities significantly changes this sensitivity. The observations are preliminary, but they are

significant in our understanding of heterogeneous initiation. Data from these studies, combined with literature data on the shock sensitivity of

pressed explosives, show quantitatively different responses for materials with the three types of voids. In materials with the same porosity,

damage creates the most sensitive material, but pressed explosives are affected less, and the addition of microballoons creates the smallest

change in sensitivity. The analysis of these data employs an interesting, and as yet unexplored, representation of shock sensitivity as a function of

density. 7 refs., 5 figs. The strict safety requirements associated with experimental studies of energetic materials warrant a com

puter-aided approach for the investigation and design of safe and powerful explosives or propellants. Models must therefore be developed to

allow evaluation of significant properties from the structure of constitutive molecules. Much recent effort has been put into modeling sensitivities, with most work focusing on impact sensitivity, leading to a lot of experimental data in this area. Modern machine learning

techniques, new physics-based models, and new reactive molecular dynamics and multiscale simulation methods have subsequently led to

quantitative procedures applicable to large datasets and yielded valuable insight into the underlying initiation mechanisms. Molecular Modeling of the Sensitivities of Energetic Materials highlights these latest developments. Beginning with an introduction to experimental

aspects in Part I, Parts II and III then explore relationships between sensitivity, molecular structure, and crystal structure, before going

on to discuss insights from numerical simulations in Part IV. Part V then highlights applications of these approaches to the design of new materials.

Providing practical guidelines for implementing predictive models and their application to the search for new compounds, Molecular

Modeling of the Sensitivities of Energetic Materials is an authoritative guide to this exciting field of research. Highlights a range of approaches for

computational simulation and the importance of combining these to accurately understand or estimate different parameters Provides an

overview of experimental findings and knowledge in a quick, accessible format Presents guidelines to implement sensitivity models using

open-source python-related software, supporting easy implemen tation of flexible models, and allowing fast assessment of hypotheses Towards

Coherent Control of Energetic Material Initiation Chemistry of High-Energy Materials Predictive Capability for Hot Spot Ignition of

Double Base Propellants Part 1. Decom position, Crystal and Molecular Properties Micromechani cal Modeling of Heterogeneou s Energetic

Materials
This book represents a collection of lectures presented at the NATO Advanced study Institute(ASI) on "Chemistry & Physics of the Molecular Processes in

Energetic Materials", held at Hotel Torre Normanna, Altavilla Milicia, Sicily, Italy, September 3 to 15, 1989. The institute was attended by seventy participants including

twenty lecturers, drawn from thirteen countries. The purpose of the institute was to review the major ad vances made in recent years in the theoretical and experi

mental aspects of explosives and propellants. In accordance with the format of the NATO ASI, it was arranged to have a relatively small number of speakers to *present in depth, re view type lectures emphasizing the basic research aspects of the subject, over a two week period. Most of the speakers gave two lectures, each*

in excess of one hour with addition al time for discussions. The scope of the meeting was limit ed to molecular and spectroscopic studies since the hydro dynamic aspects of

detonation and various performance crite ria of energetic materials are often covered adequately in other international meetings. An attempt was made to have a

coherent presentation of various theoretical, computational and spectroscopic approaches to help a better understanding of energetic materials from a molecular

point of view. The progress already made in these areas is such that structure property (e. g. ' 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. Con* *tents: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 Kor

obeinichev)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 B ernstein)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;Computati *onal Chemistry; DetonationKey Features:Summarizes the known knowns (the most important recent work) and lists the known unknowns (what remains to be investigat* *ed)Provides expert commentary on the complex behavior of mat erialsReviews:" 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 ' *Currently, there is a considerable gap in the level of theoretical understanding of the mechanisms triggering*

energy release between liquid and solid energ etic/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. 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 micro encapsulation, 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.*

Role of "hot Spots" in the Initiation of Energetic Materials Chemistry and Physics of Energetic Materials Proceedings of the 2018 Annual Conference on

Experimental and Applied Mechanics

Shock Compression of Condensed Matter--1997

Particle Processing and Characterization

In this work, the mesoscale

processes of consolidation, deformation and reaction of shocked porous energetic materials are studied using shock physics analysis of impact on a collection of discrete HMX crystals. High resolution three-dimensional CTH

simulations indicate that rapid deformation occurs at material contact points causing large amplitude fluctuations of stress states having wavelengths of the order of several particle diameters. Localization of energy produces hot-spots due to shock

focusing and plastic work near grain boundaries as material flows to interstitial regions. These numerical experiments demonstrate that hot-spots are strongly influenced by multiple crystal interactions. Chemical reaction processes also *produce multiple wave structures associated with particle distribution effects. This study provides new insights into the micromechanical behavior of heterogeneous energetic materials strongly suggesting that initiation and reaction of shocked* *heterogeneous materials involves states distinctly different than single jump state descriptions.*

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. 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. 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.
"Hot Spots"
Military Explosives
Initiation and Growth of Explosion in Liquids and Solids
Static Compression of Energetic Materials
Deformation and Thermal Properties of Energetic

Materials
In the brief instant of a high-explosive detonation, the shock wave produces a pressure 500,000 times that of the Earth's atmosphere, the detonation wave travels as fast as 10 kilometers per second, and

internal temperatures soar up to 5,500 Kelvin. As the shock propagates through the energetic material, the rapid heating coupled with compression that results in almost 30% volume reduction, initiate complex chemical reactions. A dense, highly reactive supercritical fluid is established behind the propagating detonation front. Energy release from the exothermic chemical reactions serve in turn to drive and sustain the detonation process until complete reactivity is reached. Several experimental results suggest the existence of strong correlations between the applied mechanical stress and shocks, the local heterogeneity and defects (dislocations, vacancies, cracks, impurities, etc.), and the onset of chemical reactions. The reaction chemistry of energetic materials at high pressure and temperature is, therefore, of considerable importance in understanding processes that these materials experience under impact and detonation conditions. Chemical decomposition models are critical ingredients in order to predict, among other things, the measured times to explosion and the conditions for ignition of hot spots, localized regions of highly concentrated energy associated with defects. To date, chemical kinetic rates of condense-phase energetic materials at detonation conditions are virtually non-existent, and basic questions such as: (a) which bond in a given energetic molecule breaks first, and (b) what type of chemical reactions (unimolecular versus bimolecular, etc.) that dominate early in the decomposition process, are still largely unknown. In solid explosive materials, the holes filled with gas can portray explosion-triggering hot spots. We explore the form factor on the generation of the hot spots. As a

result, we consider the Eshelby approach in the two-dimensional problem of determining the thermoelastic field of an elastic plane weakened by an elliptic hole and the field with liquid or gaseous media.
This book

summarizes science and technology of a new generation of high-energy andinsensitive explosives. The objective is to provide professionals with c omprehensiveinfor mation 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 duringm anufacturing of

these energetic materials.
In a condensed energetic material an understanding of the dynamics and microscopic mechanisms underlying energy transfer between a shock front and various defects is of prime importance

for a realistic description of ''hot spot'' formation and explosives initiation. A wide variety of simulations using the well-established technique of computer molecular dynamics has enabled us to obtain a general and very useful microscopic description of the processes beneath the macroscopic behavior of shocked systems. The calculation of the influence of heterogeneities such as point and line defects, voids, and grain boundaries is made possible by computer codes that can handle totally heterogeneous dynamical systems and track the dynamics of energy concentration and partitioning among the molecular bonds in the defect and the nearby region. One and two-dimensional calculations will be discussed in which the spatial and temporal dependence of the energy flux in a general lattice-defect system is calculated quantitatively as a

function of shock strength, initial temperature, and initial parameters defining the lattice and defect.
CCC7-119 Reactive Molecular Dynamics Simulations of Hot Spot Growth in Shocked Energetic Materials
The Properties of

Energetic Materials
A Thermo-mechanical Analysis of Hot Spot Formation in Condensed-phase, Energetic Materials
From Cradle to Grave
A Thermochemical Transport Model for the Analysis of Hot Spot Formation in

Energetic Materials
The 6th revised edition expands with new research developments, including new melt casts, reactive structure materials, a computational study on the detonation velocity of mixtures of solid explosives with non-explosive liquids, calculation of craters

after explosions. This work is of interest to advanced students in chemistry, materials science and engineering, as well as to all those working in military and defense technology.

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. 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/f ormulations 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. Annotation Presents 236 papers from the July/August, 1997 conference. Included are sections on* *equations of state; phase transitions; mechanical properties of reactive and nonreactive materials; material properties and synthesis; optical, electrical, and laser studies; hypervelocity phenomenology; and impact and penetration mechanics. Attention is focused on the strain* *and failure behavior, the weak impulse initiation, and the safety aspects of explosives. Developments in measurement techniques, particularly those employing fast optical methods, are also discussed. The CD-ROM contains the contents of the text.*

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Molecular Modeling of the Sensitivities of Energetic Materials

Fundamentals and Applications

Dynamic Behavior of Materials, Volume 1

Materials in Mechanical Extremes

Emerging Energetic

Materials: Synthesis, Physicochemical, and Detonation Properties
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 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
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. 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
Mechanochemical Processes in Energetic Materials
Shock Compression of Condensed Matter - 1991

All Hot Spots" are Not Equal
A Computational and Experimental Investigation
Energetic Materials
A UNIFYING FRAMEWORK OF HOT SPOTS FOR ENERGETIC MATERIALS.Role of "hot Spots" in

the Initiation of Energetic MaterialsThe Impact-Induced Triggering of Hot Spots in Energetic/ Explosive Materials Part 2: Adiabatic Temperature Distribution Near a Spherical Hole

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
The purpose of this work is to understand how defects control initiation in energetic materials used in stockpile components; Sequoia gives us

the core-count to run very large-scale simulations of up to 10 million atoms and; Using an OpenMP threaded implementation of the ReaxFF package in LAMMPS, we have been able to get good parallel efficiency running on 16k nodes of Sequoia, with 1 hardware thread per core.

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.

A Numerical Study of Shock-induced Hot Spot

Generation in Energetic Material Reactive Molecular Dynamics Simulations of Hot Spot Growth in Shocked Energetic Materials CCC8-133 Proceedings of the Conference of the American Physical

Society Topical Group on Shock Compression of Condensed Matter Held at Amherst, Massachusetts, July 27-August 1, 1997
Proceedings of the American Physical Society Topical Conference Held

in Williamsburg, Virginia, June 17-20, 1991

Laser Ignition of Energetic Materials

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.
Direct optical initiation (DOI) of energetic materials using coherent control of localized energy

deposition requires depositing energy into the material to produce a critical size hot spot, which allows propagation of the reaction and thereby initiation, The hot spot characteristics needed for growth to initiation can be studied using quantum controlled initiation (QCI).

Achieving direct quantum controlled initiation (QCI) in condensed phase systems requires optimally shaped ultrafast laser pulses to coherently guide the energy flow along the desired paths. As a test of our quantum control capabilities we have successfully demonstrated our ability to control the reaction pathway of the chemical system stilbene. An acousto-optical modulator based pulse shaper was used at 266 nm, in a shaped pump/supercontinuum probe technique, to enhance and suppress th relative yields of the

cis- to trans-stilbene isomerization. The quantum control techniques tested in the stilbene experiments are currently being used to investigate QCI of the explosive hexanitroazobenzene (HNAB).
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 report covers four areas of work. In the first it is shown that some polymers can sensitise explosives in impact situations. The effect is primarily a mechanical one with the production of free radicals by the polymer only of secondary importance. Chemical effects were assessed using TG. High speed photography, with the sample between transparent anvils, was used to photography impacts on polymers, explosives and layers of explosive with polymers added.

Polymers which sensitise are those which fail catastrophically, either by fracture or localised adiabatic shear, and which have a low specific heat, latent heat and thermal conductivity. Hot spots in these polymers during rapid deformation can greatly exceed the polymers softening point. This was confirmed by separate experiments with a friction apparatus with hot spot temperatures recorded using I.R. techniques. The second study describes a graphical computer method for analysing TG and DSC traces which gives all three reaction parameters (E, A, n) characterising an nth order reaction from a single trace. The final areas of research described are concerned with the analysis of (i) isothermal kinetic data and (ii) dynamic kinetic data from solid-state reactions. (Author).

Dynamic Damage and Fragmentation

Overviews of Recent Research on Energetic Materials

June 16-19, 1981, Annapolis, Maryland

Simulating the Chemistry of Energetic Materials at

Extreme Conditions