ENERGETIC MATERIALS

Advanced Processing Technologies for Next-Generation Materials

Edited by
Mark J. Mezger
Kay J. Tindle
Michelle Pantoya
Lori J. Groven
Dilhan M. Kalyon

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MATERIALS ENGINEERING

ENERGETIC MATERIALS

Advanced Processing Technologies for Next-Generation Materials

"This book is unique in so far as it does not only describe the synthesis of (new) energetic materials, but also discusses thermodynamic aspects, physical properties, and diagnostics of such materials. Another equally important feature that makes this book highly valuable is its inclusion of the discussion of the transition from laboratory scale to industrial production. I am sure this book is going to become a "must" for all researchers in the field of energetic materials – whether they are academic- or industrially-based people."

—**Thomas M. Klapötke**, Ludwig-Maximilians-Universität München, Germany

"By expertly discussing long-standing grand challenges to EM research, development, and production, this book serves as a Rosetta Stone; it enables our researchers, managers, and government officials to clearly understand each other's language, constraints, and priorities. The broad-reaching scope of this book will help make possible the necessary retooling of administrative and EM manufacturing infrastructures including the introduction of science-based principles into the energetic materials enterprise. In short, it is an essential business and PLM guidebook for modernizing the energetic materials industry."

—**Joseph M. Zaug**, Lawrence Livermore National Laboratory, Livermore, California, USA

"This book is set apart from all others in the related field. It meshes a good bit of technical aspects with the program management of how business is done as it relates to the energetic materials enterprise."

—**Scott Iacono**, US Air Force Academy, Chemistry Research Center, USA

This book reviews some of the promising energetic compounds and addresses the major issues and technical aspects of using novel processing methods for their manufacture, including their synthesis, characterization, mixing, rheology, and shaping. The science necessary to implement the next generation processes and to understand the resulting process/property relationships is elucidated in conjunction with various mathematical modeling and simulation approaches. The adaptation and utilization of promising new materials and novel means for their manufacture will be disruptive, and will change the business environment for the energetic materials industry. ***Energetic Materials: Advanced Processing Technologies for Next-Generation Materials*** presents a new business model based on academic/industry/government partnership to focus on the changes necessary to develop and transition these technologies into the industrial base.

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Energetic Materials

Preface

Explosives, propellants, and pyrotechnics are energetic materials (EMs) that have been utilized for the munitions, mining, oil well perforation, construction, and demolition industries for hundreds of years. In each of these industries, the trend has been to develop and/or acquire EMs that display greater performance and improved sensitivity characteristics, that are less expensive and of better quality, and that are easy and safe to manufacture. Historically, scientists have explored the development of new materials through organic chemical synthesis that resulted in the identification of many EMs with varying properties. Several of these compounds were originally intended for commercial applications before their energetic properties were discovered. One such example is trinitrotoluene (TNT) invented in Germany during the early 1800s as a yellow dye. TNT was found to be an insensitive explosive that was later used for main charges in munitions by the end of the 1800s.

There was much progress in the development of EMs during World War I and II. Before and during World War I, EMs for munitions were produced at small arsenals and ordnance stations, and at a few contractor facilities across the United States. After World War II, the nation consolidated EM production into large army ammunition plants. The entire complex, termed the National Technology and Industrial Base (NTIB) for Conventional Munitions, is still utilized for EM manufacturing today. Constructed in the 1940s and 1950s with the most modern manufacturing methods of the day, production lines in the NTIB were dedicated single product lines required to produce materials in extremely high volumes and at the lowest possible costs. The NTIB had a manufacturing capacity that was designed to supply the munitions for the United States and its allies through a conflict based on the magnitude of World War II. For example, this complex was capable of producing a million pounds of TNT per day with similar capacities for other legacy EMs.

One of the major conundrums associated with the NTIB is how to *right size* a base so that it can efficiently and cost effectively produce ammunition in peacetime and yet maintain the ability to ramp up the capacity for readiness in the event of a major war. Since the 1950s, the military has undergone several changes that have had a significant impact on the NTIB. Several facilities have been closed as a result of multiple rounds of Base Realignment and Closure actions and in 2010 changes in the scope of military strategy. No longer is the nation concerned about being ready at any moment to fight a major conflict on two separate fronts. Military strategy is now based on short-duration, small-unit operations primarily focused in various regions of the world. Under this type of strategy, the material requirements between peacetime and readiness are diminished. The net result of all of these changes is an NTIB that is operating between 3% and 5% of its total capacity now and for the foreseeable future.

The military is looking to develop systems that will create leap-ahead advances in warfighting capabilities. The vision is to transition new technologies to the warfighter at the speed of development. For EMs, this translates into compounds with increased power that are more effective and more survivable in a combat environment. Developing new products within the process constraints of the existing NTIB is a long and arduous endeavor. The immense capacity and inflexibility of these lines form a significant barrier to the transition of many new energetic products into the field. Retooling and revising line layouts require capital expenditures that make a cost–benefit analysis work against adopting any new technology.

University, commercial, and government laboratories are developing new EMs that go beyond standard C–H–N–O-type EMs and use processes that are not necessarily traditional organic chemistry methods. These materials include metastable interstitial compounds, organic–metallic compounds, nanophase and amorphous phase metallic and organic compounds that are referred to as *next-generation EMs*. The nation has a significant capacity within its laboratories to create these materials using novel processes; however, there is little or no capacity to develop or produce these innovations. Therefore, potential solutions that could be utilized to create leap-ahead advances in warfighter capability may never be produced.

Other industries have moved from dedicated production lines and batch processes to flexible agile manufacturing techniques. The nation is at a point in history where perhaps the NTIB needs to be rethought to more efficiently meet the challenges and requirements of the changing military strategy. The scope of this book will be to look at the development of *next-generation EMs* that will be developed using new and novel ingredients and modern manufacturing processes.

Section I focuses on the studies that have been conducted to assess EM physical and chemical characteristics and the capability to synthesize innovative solutions. This section will summarize the findings for the purpose of pointing the direction for the future.

This section will also consider the sciences associated with recent material and process advances of next-generation EMs. Advances in energetics technology are making use of new chemical techniques, such as vapor deposition of fine particle metals as high-density fuels. They look to nanomorphologies of organic crystals, nontraditional energy release mechanisms, amorphous phases of C–H–N–O compounds, spray coating and drying, acoustic mixing, twin-screw extrusion, and two-dimensional/three-dimensional printing. This portion of the book will focus on how basic sciences are being developed and employed to model and design the fabrication methods to produce inexpensive high-quality EMs. This will include the development of these processes for both legacy and next-generation EMs.

Section II examines how to conduct business in a new manner. Forming as a subgroup in the National Armaments Consortium (NAC), the National Energetic Materials Initiative (NEMI) is being created to focus and coordinate the development efforts for next-generation EMs. Through the NAC, the NEMI will facilitate the interactions between academia, private organizations, and government agencies to generate solutions for both the warfighter and commercial industry.

Editors

Mark J. Mezger is a senior technology advisor for Energetics Development Initiatives at the U.S. Army Armament Research, Development and Engineering Center at Picatinny Arsenal, Wharton, New Jersey, where he earlier held positions in the Office of the Director of Technology and the Business Interface Office.

Through the establishment of public–private partnerships, Mezger created a national nanotechnology network with regional areas of expertise. He also served as the RDECOM (Research, Development, and Engineering Command) Nanotechnology Integrated Product Team Chairman. Through his associations with the National Nanotechnology Manufacturing Center in Swainsboro, Georgia, NanoMaterials Commercialization Center technical advisory board, Pittsburgh, Pennsylvania, the Lehigh Valley Nanotechnology Network in Bethlehem, Pennsylvania, the State University of Missouri at Columbia (MIZZU) in Columbia, Missouri, and the Greater Garden State Nanotechnology Alliance, he has established for the Army one of the largest nanoparticle reactor facilities in North America and is currently involved in applying this technology to explosive and reactive materials.

He earned his ExMT in technology management from the Wharton School at the University of Pennsylvania–Philadelphia, Pennsylvania, and Bachelor's of Science degrees in math–physics and in engineering science are from the State University of New York at Buffalo, Buffalo, New York.

Kay J. Tindle currently serves as the senior director for the Research Development Team in the Office of the Vice President for Research at Texas Tech University, Lubbock, Texas. She earned her BA in teaching English as a foreign language from Oklahoma Christian University, Edmond, Oklahoma, her MEd in adult and higher education from the University of Central Oklahoma, Edmond, Oklahoma and her Ph.D. in higher education research from Texas Tech University, Lubbock, Texas. Her research focuses on multidisciplinary teams as mechanisms of accountability, communication practices and innovations among multidisciplinary teams, and women leaders in higher education.

Michelle Pantoya is the J.W. Wright Regents Chair in mechanical engineering and a professor at Texas Tech University, Lubbock, Texas. Her research focuses on developing new nanoscale energetic materials used for both industrial and military applications. Her vision is to promote cleaner, safer, and more effective energetic composites through an understanding of their basic combustion behavior. Her advances have been recently aired on a segment of the Discovery Channel's *Daily Planet* entitled *Green Ammunition*. The news story explains her scientific contributions to remove lead-based materials engrained in most ordnance systems with environmentally safe and more reactive nanoparticle formulations. She is making tremendous strides through creating new diagnostic techniques for probing combustion reactions on the nanoscale; and then bridging these findings to describe a reactive material's macroscopic behavior. Her ability to establish the link between how phenomena occurring on the nanoscale affect the energetic performance of a pyrotechnic on the macroscale is one example of a scientific contribution that has made her a leader at the frontiers of knowledge in energetic materials combustion. Another more fundamental impact that broadly advances science is her research to introduce an entirely new mechanism by which a reaction can occur based on a dispersion rather than a classical diffusion process. She received U.S. Presidential recognition for her work as a recipient of the prestigious National Science Foundation Presidential Early Career Awards for Scientists and Engineers award in 2004.

Lori J. Groven is an assistant professor of chemical and biological engineering at South Dakota School of Mines and Technology, Rapid City, South Dakota. Prior to this appointment, she served as an assistant research faculty in the School of Mechanical Engineering at Purdue University, West Lafayette, Indiana. She is an experimentalist focused on the combustion, characterization, processing, and improvement of materials ranging from traditional materials to the nanoscale for propulsion and energy storage. Her research has included the study of combustion of nanosized powders to synthesize intermetallic and ceramic materials, small-scale propagation of gasless reactions, and direct write of biocidal materials, and most recently has focused on additive manufacturing routes for energetic materials, to name a few. She has been the author or coauthor of more than 30 peer-reviewed publications since 2010.

Dilhan M. Kalyon holds the Institute Professor Chair at Stevens Institute of Technology, Hoboken, New Jersey, and is affiliated jointly with the Department of Chemical Engineering and Materials Science and the Departments of Chemistry, Chemical Biology, and Biomedical Engineering. He has also been the founding director of the Highly Filled Materials Center at Stevens since 1989. Professor Kalyon has received the International Research award of the Society of Plastics Engineers (2008), the Thomas Baron award in Fluid-Particle Systems of the American Institute of Chemical Engineers (2008), the Harvey N. Davis Distinguished Teaching Assistant Professor award (1987), Exemplary Research Award (1992), Henry Morton Distinguished Teaching Full Professor award (2000), honorary MEng degree (*honoris causa*) (1994) and the Davis Memorial award for Research Excellence (2009) from Stevens Institute of Technology, the Founder's award of JOCG Continuous Extrusion and Mixing Group (2004), and various fellowships, including DuPont Central Research and Development Fellowship (1997), Exxon Education Foundation Fellowship (1990), and Unilever Education Fellowship (1991). He was elected Fellow of the Society of Plastics Engineers (2004) and Fellow of American Institute of Chemical Engineering (2006).

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Introduction

DEPARTMENT OF DEFENSE ENERGETIC MATERIALS DOMAIN

Scope

The Department of Defense (DoD) Energetic Materials (EM) mission encompasses the entire life cycle of the products. As depicted in Figure I.1, the life cycle of products within the DoD is broken out in discrete sections, taking technology from concepts investigated in the laboratory through development to production, operational sustainment, and removal from service.

Depending on the service and system under consideration, the life cycle elements of a product are managed by different organizations. In the specific case for EMs, there is no overarching plan for the complete life cycle between the managing organizations.

Products

The EM products associated with DoD weapon systems are explosives, gun propellants, rocket propellants, and pyrotechnics. Explosives are generally used for terminal effects in firing trains and warhead main charges, whereas gun and rocket propellants are used for the propulsion systems of munitions and missiles. Pyrotechnics are utilized for several purposes: to generate visible light, smoke as obscurants, and heat as anti-aircraft decoys. Each of these products has its own type of reaction, which occurs in microseconds in the case of explosives, or in several minutes as in the case of pyrotechnics.

For each material, the output and its corresponding sensitivity to reaction from various stimuli are critical to handling safety and weapon system survivability. For explosives, the goal is to maximize energy output in terms of Gurney energy (an explosive's ability to accelerate metal) or its brisance (an explosive's ability to move earth), while minimizing its sensitivity to impact, friction, heat, and electrostatic shocks. Gun propellants are different from explosives in that the material development seeks to create compounds that maximize a specific impulse (I_{sp}) during burning with minimal flame temperatures. Gun propellant formulators also have to be concerned with material sensitivity to external stimuli in order to maximize safety in service during the product's usable life. Rocket propellants also try to maximize

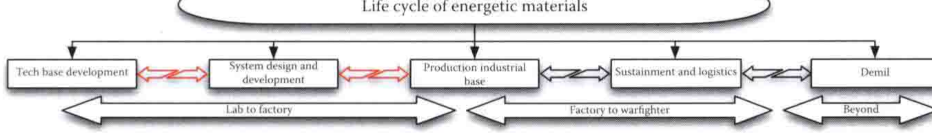

FIGURE I.1 The life cycle of EMs as used by the DoD.

burning characteristics while minimizing their smoke signature along with material sensitivity concerns.

The processing, storage, and handling of these materials are also uniquely different. Certain materials cannot be stored and/or processed in close proximity due to safety compatibility concerns. This is true not only in case of primary and secondary explosives, but also with explosives and some pyrotechnic or propellant ingredients. As a result of these material incompatibilities, safety protocols and material allowances for processing have to be strictly regulated.

Mission

The DoD is always looking to identify and employ the best technology that will provide warfighters with the most effective weaponry possible. To accomplish this mission, the energetics community within the DoD must monitor advanced technology developments nationally and internationally to identify the best technologies to address issues with military systems. Once unique and innovative technologies are identified, it is up to the people in the service laboratories to coordinate and facilitate the linkage between technology providers and people who understand military systems to realize creative solutions for the warfighter.

NATIONAL CAPABILITIES FOR ENERGETIC MATERIALS DEVELOPMENT AND PRODUCTION

Introduction

EM research and development (R&D) for the DoD stands at a crossroad. In order to meet the requirements for asymmetrical warfare, more powerful and less-sensitive energetics are required. To achieve these results, scientists and engineers have had to break with the traditional means for creating these materials and employ more innovative approaches for new types of materials. However, the nation's infrastructure is primarily built around the carbon, hydrogen, nitrogen, oxygen (CHNO) chemistry that has been the principal basis for EMs for more than a century. This is a major limiting factor in the transition and fielding of new materials. This challenge is how to achieve a disruptive warfighting capability that employs next-generation EMs (NGEMs) utilizing an industrial complex built upon 1940s' equipment and manufacturing processes. There exists little capability to scale technologies being developed in today's laboratories, that is, to raise Manufacturing Readiness Levels (MRLs) so that they are comparable with Technology Readiness Levels (TRLs), and virtually no capability to produce them in large quantities. The DoD has undertaken many studies in the previous decade for the purpose of understanding the nation's capacity for developing and producing EMs.

Congress

The House Armed Services Committee in the 2009 Defense Authorization Act directed the Secretary of Defense to assess the current state of—and future advances