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Research progress in sensitivity test and simulation of energetic materials

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Abstract: *Energetic materials are widely used in military, civil and aerospace fields. With the rapid development of energetic materials technology, the inherent contradiction between high energy and high stability of energetic materials becomes more intense. How to obtain high energy, reduce its sensitivity and improve its safety is an important challenge for scientists. At present, the research on measuring the sensitivity of energetic materials has received great attention in the field of energetic materials. This paper aims to summarize the main sensitivity testing devices and equipment, testing methods and contents, and the research progress of simulation, so as to provide reference for sensitivity testing of energetic materials.*

Keywords: *Energetic Materials; Sensitivity Test; Simulation*

1. Introduction

Energetic Materials (EMs) are a kind of metastable materials that can release a large amount of energy through rapid chemical reactions and do external work, covering explosives, propellants, pyrotechnics and other aspects, and are the core energy of national defense weapons and equipment, aerospace power systems and civil blasting engineering. Because of its high energy density, its explosion energy can reach hundreds of times that of ordinary fuel, and it plays an irreplaceable role in the fields of military precision strike, spacecraft propulsion and resource exploitation [1-6]. However, the inherent contradiction between the high-energy characteristics of energetic materials and their safety exists for a long time: the higher the energy density, the higher the sensitivity (i.e. sensitivity) to external stimuli (such as impact, friction, heat, static electricity, etc.), which leads to the burning or explosion easily caused by accidental stimuli in the production, storage, transportation and use [7]. Painful lessons caused by out-of-control sensitivity are not uncommon in history, such as the self-explosion of US aircraft carrier ammunition during the Vietnam War and the torpedo detonation of Russian nuclear submarine Kursk, which caused heavy casualties and equipment damage [8]. Such incidents have prompted countries to improve the status of sensitivity testing of energetic materials to test various thresholds of energetic materials and evaluate their safety.

Sensitivity, as the core index to measure the safety of energetic materials, represents the difficulty of chemical reaction under external stimulation, including mechanical sensitivity (impact, friction), thermal sensitivity, electrostatic sensitivity and shock wave sensitivity. Many researchers at home and abroad accurately measure the sensitivity of different energetic materials in different ways, characterize the explosion (or combustion) limit of energetic materials, and further standardize their use and operation methods to ensure their safety.

2. Sensitivity Test Experiment

Sensitivity test of energetic materials is a key link to evaluate its safety performance and reliability, and its importance stems from the potential risk of unexpected combustion or explosion of materials under external stimuli (impact stress, electrostatic spark power, etc.). Based on the core mechanism of hot spot theory, energetic materials will form local high-temperature regions (usually＞500 ℃) through stress concentration at crystal defect sites, frictional heat generation at particle interfaces or adiabatic compression of bubbles under mechanical load. When the hot spot temperature exceeds the critical threshold of materials, it will trigger a self-sustaining chemical chain reaction and trigger the phenomenon of combustion to detonation [9]. Through standardized multi-dimensional tests such as impact sensitivity (H50 value), friction sensitivity (critical pressure), thermal stability (peak value of DTA or DSC) and electrostatic sensitivity (E50 value), the safety boundary of energetic materials under different working conditions can be quantitatively evaluated, which provides for material formula optimization (such as introducing desensitizer to reduce defect density), process improvement (controlling crystal morphology) and safety protection design (calculating buffer layer thickness).

2.1. Mechanical Sensitivity

2.1.1. Impact Sensitivity

Impact sensitivity testing determines the threshold energy required to initiate chemical reactions through controlled mechanical impacts, employing a variable-mass drop hammer released from adjustable heights to vertically strike specimens positioned on an anvil. The sensitivity value is quantified using the characteristic drop height (H50) at which 50% explosion probability occurs, determined by observing combustion, decomposition, or detonation responses. Since Kast's pioneering impact sensitivity apparatus in 1906, this methodology has undergone a century of technological evolution. Early mechanical systems, exemplified by Soviet-era instruments, were constrained by low automation and reliability. Post-1990s domestic advancements included motorized pulley systems for automated hammer lifting developed at Nanjing University of Science and Technology [10]. In contrast, with the rapid development of international technology, German BAM impactor adopts electromagnetic frame structure to accurately control the release of the drop hammer, French equipment realizes the high load test of 4 meters drop height and 30 kg drop hammer, and American O-M instrument optimizes the operation safety through electromagnetic control [11]. These designs laid a technical foundation for modern impact sensitivity testing.

Since the 21st century, domestic testing methods have been further standardized, and an adaptive testing system covering materials with different sensitivities has been formed by "12-type tool method" to count the firing rate or calculate the H50 value, combined with the flexible configuration of 0.5–10 kg drop hammer and 0–1000 mm drop height. Abroad, there are also instruments tests by the US Bureau of Mines and tests by the German Federal Institute for Materials Testing (BAM) [12]. And other methods. At the same time, equipment innovation advances synchronously. The equipment developed by Xi 'an Zeming and other enterprises integrates wireless remote control, automatic positioning and air extraction protection system or introduces computer control to realize data networking management, which significantly improves the efficiency and safety of the experiment.

The advancement of instrumentation has significantly accelerated research progress in impact sensitivity testing of energetic materials. Guo Xiaode et al [13]. employed the ZJ-1 impact sensitivity apparatus (Nanjing Senweikong Electromechanical Co., Ltd.) to evaluate surface-modified ultrafine ammonium perchlorate (AP) using three carbon-based materials, comparing pre- and post-composite friction sensitivities across characteristic drop heights of 20–50 cm. Concurrently, Ba Shuhong et al [14]. utilized the CGY-1 tester to demonstrate graphite's efficacy in reducing pyrotechnic composition sensitivity, observing stabilized thermal reactions and diminished hotspot formation. Liu Musen et al [15]. further investigated temperature-dependent sensitivity variations in pyrotechnic mixtures using the same CGY-1 system. Zhang Pu et al [16]. implemented the characteristic drop height method (WL-1 tester, 2 kg drop weight, 25 cm drop height, 30 mg sample mass) to assess impact sensitivity of aqueous-phase synthesized ultrafine spherical CL-20 crystals. Subsequently, Zhang Maolin et al [17]. applied explosive probability methodology (10 kg drop weight, 25 cm height) to quantify stability parameters for novel energetic materials under modified synthesis conditions. These systematic investigations collectively refine experimental protocols while advancing the development of high-performance, low-sensitivity energetic material systems.

With the development of science and technology, the evaluation of impact sensitivity has extended from macro-test to micro-mechanism. The relationship between crystal defects and hot spots is revealed by synchrotron radiation X-ray tomography, or the relationship between molecular structure and sensitivity is predicted by molecular dynamics simulation. At present, the development trend focuses on multi-stimulus coupling test (such as mechanical-thermal-electrostatic interaction), environmental adaptability assessment (temperature, humidity and radiation effects) and unification of international standards (mutual recognition of ISO and GJB), while the breakthrough of intelligent response materials and high-energy and low-sensitivity molecular design (such as LLM-105 and TKX-50) will promote energetic materials to leap to a new paradigm of "actively regulating sensitivity" and become a military industry.

2.1.2. Friction Sensitivity

The concept of friction sensitivity originated from the systematic study of insensitive ammunition abroad in 1980s, and its core goal is to solve the problem of accidental explosion of explosives caused by external stimuli such as mechanical friction and thermal shock in storage, transportation and actual combat environment [18]. With the beginning of modern war, the wide application of TNT embodies the balance advantage of high detonation velocity and low sensitivity, while high-energy explosives such as RDX have excellent performance but are limited by cost and sensitivity, which further highlights the importance of friction sensitivity regulation [19].

On the theoretical level, the research proves that friction is one of the core mechanisms that trigger the explosion of explosives, which promotes the development of standardized methods and supporting evaluation systems for friction sensitivity testing in academic circles. Many test methods have been developed, such as explosion probability method, step method, Brusden method, two-ignition explosion method, slide test method and so on [20].

The structure of the friction sensitivity tester is mainly composed of an impact end (pendulum or sliding column system), an impacted end (sample clamping device) and a recording end (sensor and data acquisition system) [21]. The classical test method adopts the friction pendulum mode, which releases the gravitational potential energy by the pendulum rotating around the vertical axis, so that the pendulum exerts friction on the sample (solid particles or slurry medicine) at a specific angle and positive pressure, and simulates the mechanical stimulation in actual working conditions by controlling the displacement (1.50-2.00 mm). In the test, the sample is placed between two smooth interfaces (such as ceramic/metal materials), and the relative sliding is caused by the impact of pendulum. After repeated tests, the friction sensitivity is quantified by the explosion probability (such as sound pressure increment ⩾2dB, optical characteristics or combustion residue) [22-23]. Traditional sensory criteria are gradually replaced by multi-modal sensing technology (such as sound pressure sensor, high-speed camera and spectral analysis) because of their strong subjectivity, which can accurately identify the critical thresholds of decomposition, combustion and explosion. Commonly used instruments include Ke Zlov friction pendulum, BAM friction sensitivity instrument, ABL friction sensitivity instrument and ROTO friction instrument. With the development of science and technology, more and more new instruments are developing continuously, such as Shao Mingwang of Beijing Institute of Technology [24]. A friction sensitivity tester with continuously adjustable pressure is developed, which greatly improves the testing efficiency. Xidian university Shang Jiawei and others [25]. A new digital automatic friction sensitivity testing system is developed, which greatly improves the intelligence of testing.

The renewal of equipment promotes the development of friction sensitivity experiment. Such as Guo Xiaode et al [16]. employed the MGY-1 friction sensitivity tester to evaluate modified materials, while Zhang Pu et al [16]. conducted multiple experimental trials using the explosion probability method with a WM-1 tester under standardized parameters (66 ° pendulum angle, 2.45 MPa gauge pressure, 20 mg sample mass). Zhang Maolin et al [17]. implemented enhanced precision through controlled conditions (900 ±1 ° pendulum angle, 3.92 ±0.07 MPa gauge pressure). Systematic evaluation of measurement uncertainties was achieved by Chen Minglei et al [26]. using BM-B testers combined with probabilistic detonation analysis. These methodological refinements have collectively established comprehensive technical specifications for friction sensitivity characterization in energetic materials, facilitating the strategic transition toward synergistic "high-energy/low-sensitivity" performance optimization in military applications.

2.2. Thermal Sensitivity

The test method of thermal sensitivity of energetic materials is mainly characterized based on the critical conditions and response time characteristics of rapid thermal explosion under external thermal stimulation. According to the national military standards GJB772A-1997 and GJB770B-2005, the commonly used methods include explosion point test, thermal explosion critical temperature measurement and baking sensitivity experiment. Among them, the test of explosion point is realized by constant temperature method: the sample is placed in a specific heat source medium, and the lowest temperature (explosion point) and the corresponding delay period (the interval between the start of thermal action and violent reaction) are measured. The typical index is the explosion temperature of 5 s or 5 min delay period, and its physical essence follows the thermal spontaneous combustion theory. When the heat accumulation rate of the system exceeds the heat dissipation rate, the thermal explosion is triggered. The critical temperature of thermal explosion is measured by programmed temperature rise method, and the critical temperature threshold of the sample from self-accelerated decomposition to explosion is determined by linear temperature rise. Burning sensitivity test simulates the actual thermal environment (such as burning bomb device), and measures the critical temperature of material burning or explosion at a set temperature rise rate, reflecting the response characteristics under dynamic thermal load. These methods need to strictly control the parameters such as sample size, particle size and heat transfer conditions, because the thermal explosion process is affected by the coupling of many factors such as sample heat conduction, reaction kinetics and autocatalytic effect. For the same energetic material, the higher the temperature of heat source medium, the shorter the delay period. The energetic materials with the same delay period and lower explosion point have higher thermal sensitivity. In engineering, the explosion point of standardized delay period is usually used as the core evaluation index of thermal sensitivity, and its value is closely related to the activation energy of materials and Arrhenius kinetic parameters [27].

The commonly used test methods are differential scanning calorimetry (DSC) and differential thermal analysis (DTA), but the samples measured by the above methods are small and not representative, and the test results are greatly affected by the temperature rise, and the use is limited, so the compatibility with liquid energetic materials is not good. In recent years, researchers have developed an adiabatic accelerating rate calorimeter (ARC) method to characterize thermal sensitivity. Its equipment can better simulate the environmental conditions of the substance, and at the same time, it has a wide range of applications and a large amount of samples, which greatly promotes the development of thermal sensitivity testing [28-29]. Its principle and structure are shown in the literature [30-32]. Many researchers have also developed sensitivity measurement by using this equipment and method. Such as Liu Ying et al.'s [28] adiabatic accelerating rate calorimeter was used to measure six kinds of energetic materials, and the relationship between thermal explosion delay and temperature was analyzed, and its thermal sensitivity was evaluated. Concurrently, Liu Zuliang et al[33]. The stability and thermal safety of expanded ammonium nitrate explosive were studied by this method, which provided a scheme for the safe use of explosive.

3. Simulation

In the sensitivity study of energetic materials, the traditional experimental testing methods are restricted by sample preparation process, test conditions and danger irreversibility, which leads to low testing efficiency, high cost and significant data fluctuation, especially for new complex energetic compounds. Therefore, through multi-scale numerical simulation techniques such as quantum chemical calculation, molecular dynamics simulation and finite element analysis, the structure-activity relationship between molecular structural parameters and sensitivity performance can be deeply analyzed, which breaks through the temporal and spatial limitations of experimental observation and realizes the visual reconstruction of the initiation process of energetic materials and the dynamic capture of key mechanisms [34]. The integration of numerical simulation and virtual experiment technology can not only predict the energy release law and sensitivity thresholds of materials under extreme conditions such as high pressure, high temperature and interface effect, but also significantly reduce the experimental risk and resource consumption, which shows important value in the fields of molecular design of high-energy materials, optimization of detonation process and safety assessment.

Simulation plays an important role in the sensitivity test of energetic materials. Hong Huiling [35] conducted molecular dynamics simulations using the Tait and Sun equations of state to evaluate polymer-bonded explosives, providing theoretical insights for optimizing their processing parameters. D.Furman et al [36]. employed the ReaxFF force field to investigate thermal sensitivity and decomposition mechanisms of condensed-phase nitro-explosives under varying temperatures. Liu Dongmei et al [37]. revealed a proportional correlation between temperature and sensitivity of PENT (pentaerythritol tetranitrate) through temperature-dependent molecular dynamics simulations. Prana et al [38]. developed a quantitative structure-property relationship (QSPR) model demonstrating strong agreement with experimental sensitivity data. Rice et al [39]. established predictive frameworks for impact sensitivity using parameters such as midpoint electrostatic potentials. These computational approaches systematically elucidate the effects of molecular configurations, crystalline defects, and interfacial interactions on sensitivity thresholds, enabling rational design of high-energy/low-sensitivity materials. By predicting critical thresholds under diverse conditions, simulation technologies significantly mitigate safety risks associated with accidental detonation during experimental testing while advancing theoretical foundations for energetic material safety.

4. Conclusion And Prospect

This paper introduces the testing mechanism, testing methods and equipment of the most commonly used sensitivity tests of energetic materials (i.e. mechanical sensitivity and thermal sensitivity), and briefly introduces the sensitivity testing research done by some researchers, and also introduces the application of simulation in sensitivity testing. The above contents provide some reference for the development of energetic materials.

Study on Sensitivity Characteristics of Energetic Materials Through the deep integration of experimental test and numerical simulation, the energy release mechanism and safety boundary of materials under external stimulation are systematically revealed. Although traditional experimental methods can provide critical thresholds such as impact sensitivity and friction sensitivity, their high cost, low efficiency and irreversible risks limit the rapid development of new energetic materials. However, the multi-scale simulation technology evolved from microscopic molecular structure and mesoscopic defects to the whole chain analysis of macroscopic detonation process, which realized the visualization of hot spot formation mechanism and the accurate prediction of sensitivity structure-activity relationship. Future research needs to further strengthen the collaborative verification mechanism of experiments and simulations, develop a cross-scale dynamic coupling model, and improve the accuracy of sensitivity prediction under extreme conditions; At the same time, combined with artificial intelligence technology, an intelligent platform of molecular design-sensitivity prediction-safety evaluation of energetic materials is constructed to promote the directional development of high-energy insensitive materials. In addition, it is necessary to establish a standardized testing system and database covering complex environments to provide theoretical support and technical support for the safety management and control of energetic materials throughout their life cycle, and finally realize the collaborative optimization of energy density and safety performance.

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