

Method for surface coating of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine with submicron 1,3,5-triamino-2,4,6-trinitrobenzene

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To improve the safety of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), a submicron energetic material, 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), was introduced to coat HMX by a novel method. This novel method contained the reaction crystallisation and the solvent–non-solvent method. X-ray diffraction, scanning electron microscope, and optical microscopy analyses showed that a homogeneous layer of TATB particles with submicron scale had been successfully coated on the surface of HMX particle. Differential scanning calorimetry and thermogravimetry indicated that the coated HMX only had an exothermic peak at 279.4 °C, and the phase transition temperature reached 213.5 °C and increased by 20.2 °C compared with the pure HMX. The content of the coating TATB was determined to be 6.2 wt.% through high-performance liquid chromatograph. Relative to the mechanically mixed HMX/TATB, the drop height (H_{50}) was increased from 23.0 to 74.1 cm, and the friction probability was reduced from 4 to 0% for the coated HMX.

1. Introduction: Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) is extensively used in initiating explosive material and solid-fuel rocket propellant due to its advantage such as stable performance, rapid explosion rate, and high energy. However, HMX is very sensitive to impact and friction stimuli and easy to explode under unintended initiations to cause casualties and property damage. Therefore, for many applications, HMX must be taken pretreatment to decrease sensitivity [1]. It has been reported that crystal size, shape, morphology, crystal size distribution, internal and external defects, and the microstructure inside the crystal strongly affect the sensitivity of high explosives [2, 3]. Therefore, much interest has been generated on control of the crystal size, morphology, and defects of HMX to lower its sensitivity toward the external stimuli [4, 5]. In addition, surface coating has been developed as another important technology to reduce the sensitivity of explosives by embedding the less sensitive materials [6]. Numerous studies have shown that proper surface modification or coating of nitramine explosives is also a kind of method to improve their comprehensive performance [7, 8].

The types and properties of coating materials and the performance of the coated particles have a close relationship with coating effects. Therefore, selecting appropriate coating materials is particularly important according to the property of coated material. Up to now, the kind of coating material mainly includes insensitive agent, polymer, plasticiser, and organic salts [9–13]. However, numerous studies have shown introducing non-energetic materials could decrease the explosion performance of coated HMX; therefore, many studies have tried using insensitive energetic materials to coat HMX [14–17]. 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) is a kind of insensitive high explosive, with the performances of excellent heat resistance, low mechanical sensitivity, and high crystal density, which has been widely applied in atomic bomb and polymer bonded explosive [18]. Research [19] shows that introducing a small amount TATB in propellant formulation to replace the high sensitivity of HMX, 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), and Ammonium perchlorate (AP) not only ensures the amount of energy needed, but also reduces the sensitivity of the propellant. In addition, using TATB to coat HMX can obviously reduce its impact sensitivity, the friction sensitivity, and the

shock wave sensitivity [17]. Furthermore, acid–base coordination theory [20, 21] points out that chemical physics effect exists in the surface between coating material and coated material. TATB and HMX can form strong N–O...H hydrogen bonding between –NH₂ (TATB) and –NO₂ (HMX) [22]. Those factors make TATB to be the ideal coating material for HMX.

The traditional synthetic method is that amination of trichlorotri-nitrobenzene (TCTNB) in HMX-toluene slurry makes TATB coated HMX crystals in situ in a ultrasound equipment. Hofmann and Rudolf [23] patented this method for preparing HMX/TATB complex. However, this patent fails to give the specific dosage of TATB, and also has no relevant data on the passivation effects. Nandi *et al.* [24] detailedly studied both coated methods of the conventional amination and the sonochemical amination. Sonochemical amination formed uniform coating on the surface of HMX crystals compared with the conventional method. However, the impact sensitivity of the coated HMX was much higher than the original HMX. The author predicted the result may be caused by the porous and rough surface of the coated materials. Therefore, in this work, we try to find a novel method to obtain a compact and smooth coated surface to effectively decrease the sensitivity of HMX.

This paper first describes the novel method to crystallise submicron TATB onto the HMX crystal surface. Second, the microstructure and performance of the coated HMX are characterised. In addition, the binding energies between TATB and HMX crystal faces are calculated by molecular dynamics (MD) simulation. Finally, a possible recrystallisation process is brought forward based on experimental and theoretical investigations.

2. Theoretical and Experimental section: Using the Compass force field [25], the theoretical calculations were run with the Forcite module of the software package Materials Studio 3.0 [26]. The HMX neutron diffraction experiment was the data source of the unit cell model of HMX [27]. The HMX crystal was cleaved parallel to the (h k l) crystal face with a depth of three unit cell. Crystal faces were determined based on the X-ray diffraction (XRD) measurements, namely, these crystal faces with stronger absorption signal. Thereafter, a crystal slice was constructed, which

was a periodic superstructure of 3×3 unit cells, and optimised using the molecular mechanics (MM). The initial structure of TATB molecule was taken from the unit cell of TATB crystal [28]. Along c -axis, TATB molecule was adsorbed on the $(h\ k\ l)$ crystal face of HMX. To get rid of the effect of additional free boundaries on the structure, 40 Å thickness vacuum slab was built in above TATB molecule. The crystal slice was constrained during the MM optimisation and MD simulation processes. Using the Anderson constant temperature method, the MD simulation was performed on an canonical ensemble (NVT) ensemble at the temperature of 298 K. The time step was 1 fs and the period was 200 ps. The van der Waals and Coulomb interactions were calculated by employing the atom-based and Ewald method, respectively. Moreover, the final structure of MD simulation was used as the balance structure of the HMX/TATB model. Through the theoretical simulations, we could evaluate the binding energy E_b of TATB molecule and HMX crystal face to explain the coating mechanism. E_b can be calculated using the following relationship:

$$E_b = -(E_{\text{tot}} - E_{\text{surf}} - E_{\text{TATB}}) \quad (1)$$

where E_{tot} is the total energy of TATB molecule and the surface, E_{surf} is the energy of the surface without TATB molecule, and E_{TATB} is the energy of TATB molecule without the surface.

TATB and HMX were made by the Institute of Chemical Materials, Chinese Academy of Engineering Physics. The sodium hydroxide (NaOH), nitric acid, and dimethyl sulphoxide (DMSO) were supplied by Chengdu Kelon Chemical Reagent Factory. Water used in the experiment is deionised.

In this work, the coating process included three steps. First, 2 ml nitric acid solution (2 mol/l) and 6.659 g HMX were dissolved in 200 ml dimethyl sulphoxide to obtain an acid solution. Second, 0.645 g TATB was dissolved in another 300 ml dimethyl sulphoxide which was added 1 ml NaOH (2 mol/l) in advance to obtain a brownish transparent solution. With constant stirring, it was added in a large amount of deionised water drop by drop to obtain a yellow milky liquid. Finally, coating of HMX with TATB: the acid solution was added into the yellow milky liquid inch by inch with constant stirring and the coated HMX precipitation was obtained. The coated HMX precipitation was separated from the mother liquor using a centrifuge. After that, it was washed by lots of ultrapure water till the filtrate became neutral. Finally, it was dried by freeze drying.

XRD data were measured by XRD apparatus (X'pert PRO PANalytical, Netherlands) using Cu $K\alpha$ radiation ($\lambda = 1.540598$ Å) scanning from 10° to 80° . The microstructure was studied by type tungsten filament scanning electron microscope (SEM) (Evo 18 Carl Zeiss SMT Pte Ltd., Germany). Optical microscopy (OM) image was observed by multi-function microscope with matching

refractive index (BX51-P, Japan Olympus Company). A high-performance liquid chromatograph (HPLC) was used to measure the component (Agilent 1260, America Agilent Company). The HPLC system consisted of dual G1312A pumps, a standard automatic G1313A sampler, a diode-array detector, and Zorbax Extend C-18 column (5 μm , 4.6 mm \times 250 mm). The injection volume was 5 μl . Moreover, the analytic process used the gradient mode: mobile phase A was water; mobile phase B was methanol; flow rate was 0.8 ml/min, ratio of A to B 0–17 min, 70:30–36:64; 17–20 min, 36:64–70:30; and 20–25 min, 70:30. The detection wave of length was 230 nm. In the dry air atmosphere, differential scanning calorimetry (DSC) and thermogravimetry (TG) and were analysed using a simultaneous thermal analyser (SDT Q600 TA, USA). From ambient temperature to 500 $^\circ\text{C}$, the linear heating rate was 10 $^\circ\text{C}/\text{min}$. Impact sensitivity was tested and evaluated by the drop hammer apparatus (ML-1, De Kong Corporation) with National Army Standard of China (GJB772A-97). The sample mass was 30 ± 1 mg and the drop hammer weight was 2 kg. Friction sensitivity was measured by pendulum friction apparatus (MGY-1, 213 Research Institute of China) with National Army Standard of China (GJB772A-97). The sample mass was 20 ± 1 mg. The pendulum weight was 1.5 kg. The gage pressure was 3.92 Mpa. Moreover, the swaying angle was 90° .

3. Results and discussion: XRD is used to analyse the phases and components of coated HMX, and the results are shown in Fig. 1. The curve of coated sample shows the coated sample contains TATB with a main diffraction peak at $2\theta = 28.32^\circ$ of TATB ((powder diffraction file) PDF# 44-1627); the main phase of the coated sample is still β -HMX (PDF# 45-1539), for the molar ratio of TATB and HMX added in prepared process is 1:9. The main exhibiting faces of the coated HMX are (011), (020), ($\bar{1}02$), (120), and ($\bar{1}32$), which will be used to calculate the binding energies of TATB molecule and HMX crystal faces.

Fig. 2 shows the SEM picture of HMX crystals coated with TATB (see Fig. 2a) and the morphology of the coating surface (see Fig. 2b).

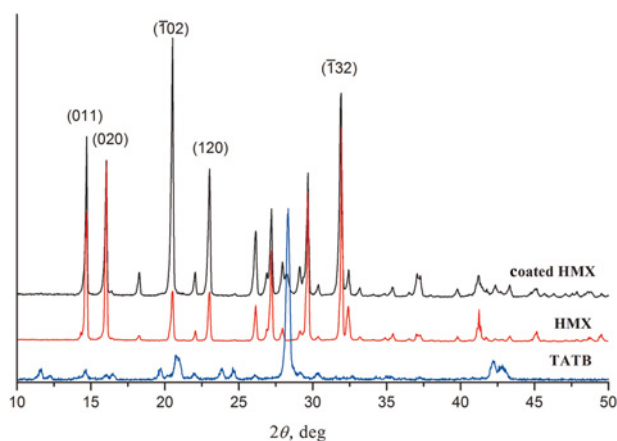


Fig. 1 XRD spectra of coated sample, HMX, and TATB

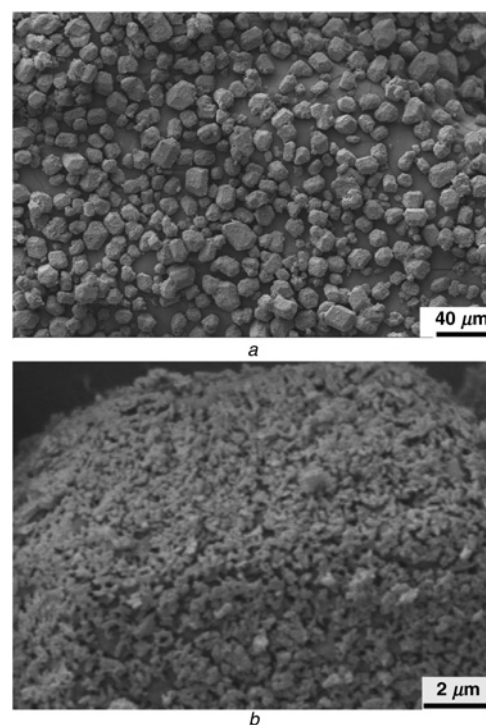


Fig. 2 SEM photographs

a Coated HMX samples

b Magnified coating surface

It can be seen from Fig. 2a that the samples with the size of about 7–20 μm are evenly covered by many small particles. In addition, there are little particles shedding in the blank area suggesting that the small particles firmly affix to the surface of HMX crystal. Fig. 2b reveals that the most of small particles on the coated surface are irregular rod-like crystals with submicron scale, and the coated surface is compact and smooth. To investigate the kind of the surface particles, analysis of the coated sample is carried out by OM with matching refractive index. Fig. 3 provides the OM images of HMX particles (Fig. 3a), coated HMX particles (Fig. 3b), and TATB particles (Fig. 3c) with matching refractive index. With the matching refractive index, a defect inside the HMX particle generally looks like a dark area or a dark point on an image of OM. Fig. 3a qualitatively confirms that pure HMX particles show less dark areas. Fig. 3b suggests that there is a layer of dark area inside the OM image of coated HMX particle. From Fig. 3c, we can find that all pure TATB particles with smaller size show dark areas inside the OM image. From Figs. 1–3, it can be drawn that the surface of HMX particle has been uniformly coated by a layer TATB particles. HPLC technology is used to determine the content of TATB in coated sample. The result shows that

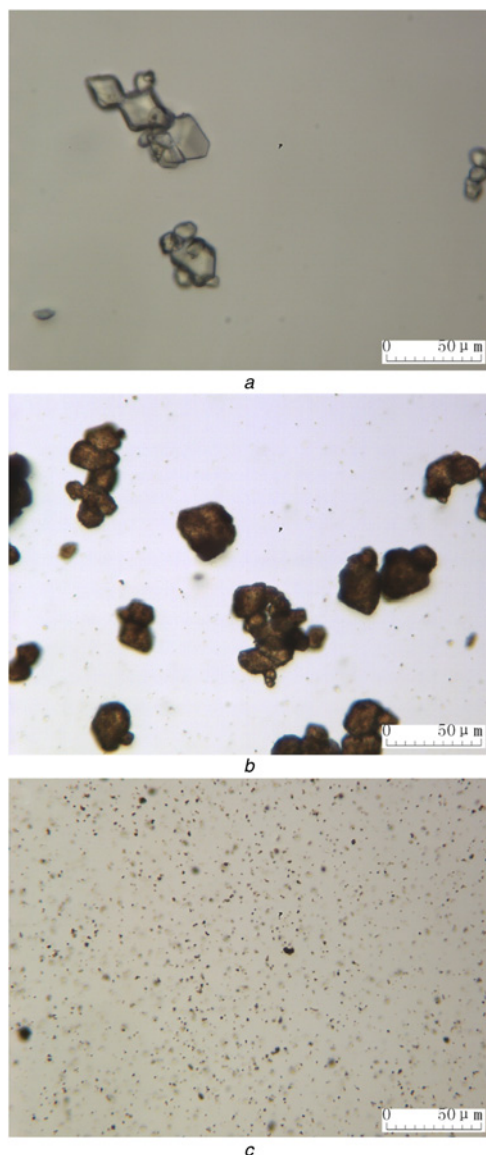


Fig. 3 OM images
a HMX particles
b Coated HMX particles
c TATB particles

the content of TATB is 6.2 wt.%, lower than the added amount of 8.45 wt.%. Owing to low content, TATB cannot affect the explosive performance of coated sample.

For contrasting the differences of thermal decomposition characteristics of HMX, TATB, mechanically mixed, and coated sample, we have carried out DSC and TG analyses. For comparison, the mole ratio of TATB and HMX is also 1:9 in mechanically mixed sample. The DSC and TG curves are both shown in Fig. 4 and the experimental data are shown in Table 1.

The exothermic peaks of TATB and HMX are at 385.8 and 282.0 $^{\circ}\text{C}$, severally. However, the coated and mechanically mixed samples both only have an exothermic peak, respectively, at 279.4 and 280.3 $^{\circ}\text{C}$. Moreover, the TATB exothermic peak is disappeared (see Fig. 4a). The melting and decomposition temperatures of the coated sample have no significant change compared with the pure HMX and mechanically mixed HMX/TATB. The changeless decomposition temperature makes it clear that the thermal decomposition behaviour of HMX keeps intact in the coated samples. The TG curves in Fig. 4b reveal that the coated and mechanically mixed samples have one stage decomposition, which is similar to the curve of the pure HMX. A rapid weight loss (>97%) and only one exothermic peak suggest that TATB has been decomposed with the decomposition of HMX before 300 $^{\circ}\text{C}$, which may be due to the decomposition of large amount of HMX to induce the decomposition of TATB.

It is worth attention that the endothermic peak of coated HMX is at 213.5 $^{\circ}\text{C}$ which is the phase transition temperature $\beta \rightarrow \delta$ of HMX. There is a significant shift of 20.2 $^{\circ}\text{C}$ toward higher temperature compared with the pure HMX and 16.8 $^{\circ}\text{C}$ with mechanically mixed HMX/TATB. As known to all, particle size significantly

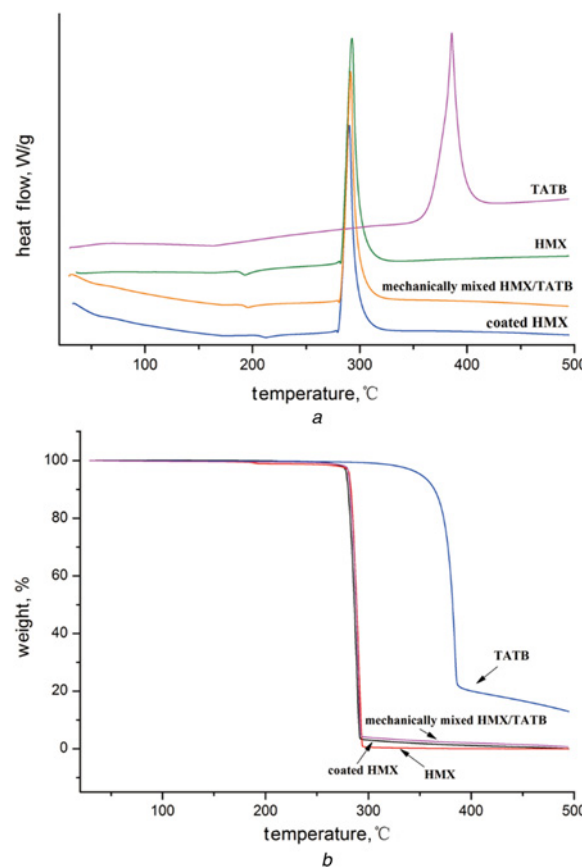


Fig. 4 DSC and TG curves
a DSC curves of TATB, HMX, mechanically mixed HMX/TATB, and coated HMX
b TG curves of TATB, HMX, mechanically mixed HMX/TATB, and coated HMX

Table 1 DSC experiments results of TATB, HMX, mechanically mixed HMX/TATB and coated HMX

| Samples | Phase transition temperature, °C | Melting temperature, °C | Decomposition temperature, °C |
|-----------------------------|----------------------------------|-------------------------|-------------------------------|
| TATB | — | — | 385.8 |
| HMX | 193.2 | 282.0 | 292.7 |
| mechanically mixed HMX/TATB | 196.3 | 280.3 | 291.4 |
| coated HMX | 213.5 | 279.4 | 290.3 |

influences phase transition of HMX crystal [29]. To rule out the effect of particle size, the particle size of HMX in mechanical mixing is near to that of HMX in coated sample. It indicates that the TATB particles coated on the surface of HMX can delay the phase transition of HMX ($\beta \rightarrow \delta$) and consequently reduce the initiation sensitivity, because Brill and Reese [30] consider the formation of δ -HMX is the first step of decomposition HMX, which has been confirmed in the subsequent studies [31].

The chemical and physical properties of materials have a strong impact on the impact sensitivity. In Table 2, the test results for friction and impact sensitivities are listed. In these results, the drop height H_{50} and standard deviation (S) are used to express the impact sensitivity. The explosion probability (P) and its confidence interval (P_i, P_u) are used to express the friction sensitivity. The data of Table 2 show that H_{50} and P of mechanically mixed HMX/TATB are 20.0 cm and 4%, respectively, whereas for the coated HMX with TATB, the values are 74.1 cm and 0%. The result indicates that the impact and friction sensitivities of HMX through TATB coating are significantly decreased. Researches deem that TATB with a graphite-like crystalline structure plays a buffer and lubrication role when external forces are acted on the coated sample [14]. This impact can reduce the formation probability of hot spots [32, 33]. Besides, judging from the SEM, submicron TATB with larger surface area can cover larger area of HMX surface, and binds with HMX surface more closely, which makes the sensitivity of coated product further lower.

To explain the coating mechanism, we have calculated the binding energies between TATB molecule and different HMX faces. On the basis of the XRD spectrum of coated sample, five crystal faces with stronger absorption signal, (011), (020), ($\bar{1}02$), (120), and ($\bar{1}32$), are chosen to calculate the binding energies. Taking ($\bar{1}02$) face as an example, Fig. 5 shows the unit cell and interface structures. The calculation results of binding energies are shown in Table 3. Usually, molecular interactions mainly include hydrogen bonding, van der Waals, and electrostatic interactions. As the hydrogen bonding is contained within the electrostatic and van der Waals interactions when applying Compass force field, the binding energies in Table 3 only include van der Waals and electrostatic interactions. Judging from Table 3, the binding energies between TATB molecule and the different crystal faces of HMX are different, mainly due to the difference in surface chemistry and the step structure of the crystal face, but the energy change is small, making TATB be evenly coated on main crystal faces of

Table 2 Mechanical sensitivities of mechanically mixed HMX/TATB and coated HMX

| Samples | Impact sensitivity | | Friction sensitivity | |
|-----------------------------|--------------------|------|----------------------|--------------|
| | H_{50} , cm | S | P , % | $[P_i, P_u]$ |
| mechanically mixed HMX/TATB | 20.0 | 0.19 | 4 | [0.00, 0.02] |
| coated HMX | 74.1 | 0.21 | 0 | [0.00, 0.14] |

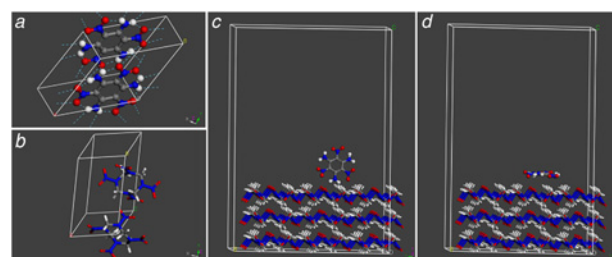


Fig. 5 Units cells and interface structures

a TATB unit cell

b HMX unit cell

c Interface structure of (102) crystal face with TATB molecule before MD simulation

d Interface structure of (102) crystal face with TATB molecule after MD simulation

HMX. The hydrogen bonds are formed between the oxygen atoms in $-\text{NO}_2$ group from HMX and hydrogen atoms in $-\text{NH}_2$ group from TATB. Hydrogen-bonding lengths tabulated in Table 3 indicate the hydrogen-bonding interactions are relatively strong. There is no hydrogen bond for ($\bar{1}02$) crystal face, and the main interaction is van der Waals force. This can also be illustrated from the interface structures shown in Fig. 5. The relative orientation of TATB molecule to the ($\bar{1}02$) face changes from the perpendicularity to prostration after MD simulation.

By the recrystallisation method, the coating material TATB is precipitated from the nitric acid solution and forms particles with submicron scale. In fact, there are two different recrystallisation methods in the whole coating process. Recrystallisation of HMX occurs in the third step when adding the acid solution into the yellow milky liquid, and the applying method is solvent–non-solvent method. DMSO is the solvent and water added in the second step is the non-solvent. Adding water in the second step and adding the acid solution in the third steps both result in the recrystallisation of TATB, and they involve reaction crystallisation process. On the basis of literature [34, 35], earlier work at our laboratory has studied the reaction process in detail. It is clear that TATB is dissolved at high pH, but precipitated at low pH. This is because that TATB has been changed to another complex in the solution of DMSO/NaOH; adding water or acidification is a reaction recrystallisation process. The generated TATB is insoluble in the solution of DMSO/NaOH, which rapidly develops high supersaturation level and then induces rapid crystallisation with a very high nucleation rate, leading to the generation of ultrafine TATB crystals [36]. This is why the yellow milky liquid can be obtained by adding water in the second step. In the yellow milky liquid, a small number of ultrafine TATB can form well-dispersed solid particles in aqueous solution at a high stirring speed. HMX and the rest of TATB crystallise at the same time during adding the acid solution into the yellow milky liquid, but the nucleation and growth speed of HMX crystal is faster than TATB owing to higher supersaturation level of HMX. Owing to strong interactions between TATB

Table 3 Binding energies (E_b) and the hydrogen-bonding lengths (D) of coated HMX with TATB

| (h k l) | E_b , kJ/mol | van der Waals, kJ/mol | Electrostatic, kJ/mol | D , Å |
|-----------------|----------------|-----------------------|-----------------------|---------|
| (011) | 19.297 | 11.090 | 8.207 | 1.919 |
| (020) | 20.363 | 9.620 | 10.743 | 2.076 |
| (102) | 24.186 | 15.226 | 8.960 | — |
| (120) | 23.255 | 11.739 | 11.516 | 1.953 |
| ($\bar{1}32$) | 23.235 | 11.493 | 11.532 | 2.047 |
| | | | | 1.945 |

molecule and HMX crystal face and high surface energy of ultrafine TATB, TATB particles will be adsorbed (or adhered) onto the surface of grown HMX particle and continue to grow. Besides, according to the crystallisation mechanism, primary nucleation is the main nucleation mode in the precipitation and reaction crystallisation process. Besides, a small quantity of HMX may grow with ultrafine TATB as the crystal nucleus. Clearly, additional theoretical and experimental approaches are needed to solve this coating mechanism. The details will be reported in follow-up studies.

4. Conclusion: By combining the reaction crystallisation and the solvent–non-solvent method, a novel method is developed for the surface coating of HMX with submicron TATB to improve stability while maintaining explosion performance. Through this method, the rod-like submicron TATB particles with submicron scale have been uniformly coated on the surface of HMX crystal. The TATB content in the coated HMX is 6.2 wt.% determined by HPLC technology. The coated HMX only has an exothermic peak at 279.4 °C, because large amount of heat releasing by the HMX decomposition induces the decomposition of TATB before 300 °C. The phase transition temperature of coated HMX reaches 213.5 °C and increases by 20.2 °C compared with pure HMX, and this will largely decrease the initiation sensitivity of coated HMX. However, the thermal decomposition behaviour of coated HMX remains unchanged. Meanwhile, the friction and impact sensitivities of coated HMX decreased observably. The drop height (H_{50}) is increased from 23.0 to 74.1 cm, and the friction probability is reduced from 4 to 0% compared with the mechanically mixed HMX/TATB. The strong interactions between TATB molecule and HMX crystal faces and the high surface energy of TATB particles with submicron scale enable TATB to coat on the HMX crystal face tightly.

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