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Molecular dynamics study on the effect of temperature on the properties of TATB and PBX

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Abstract: *In order to study the effect of temperature on the properties of PBX explosive, three models of TATB pure crystal, JB-9014 coated and mixed structure were established by using material studio (MS) software. Molecular dynamics calculations were carried out at different temperatures (255k, 275k, 295k, 315K, 335k and 355k) using compass II force field. The initiation bond length, bonding diatomic energy, cohesive energy density and mechanical properties of different structures were obtained and compared. The results show that compared with TATB pure crystal, the two PBX structures have less change in the initiation bond length, and the density of bonding diatomic energy and cohesive energy is significantly reduced, and the sensitivity is higher. The results of mechanical properties show that the two PBX structures have less rigidity, stronger elasticity and better ductility compared with TATB pure crystal, which is conducive to the processing and transportation of explosives. In addition, with the increase of temperature, the sensitivity of the two PBX structures increases, the stability becomes worse, and the influence on the mechanical properties tends to be complex.*

Keywords: *Physical chemistry; TATB explosive; Material Studio; Molecular dynamics; mechanical property*

1. Introduction

The development of energy-containing materials to date has been a great achievement, the current widely used CL-20, HMX, FOX-7, TATB and other monolithic explosives are the results of modern scientific research, they are loved because of high energy density, as missile weapons, blasting charges are commonly used. But with the turbulent world situation, the requirements of weapons and equipment are getting higher and higher, these monomers either because of high sensitivity or because of poor ductility and other shortcomings cannot meet the demand. In order to improve the performance of monolithic explosives, domestic and foreign developers have focused on polymer-bonded explosives (PBX).

Polymer bonded explosive is a hybrid explosive, made by mixing one or more monomeric explosives and fluoropolymer, which not only inherits the high energy density of traditional monomeric explosives, but also improves the ductility, making the explosive easier to prepare for synthesis and easier to consume the external stimulus energy applied to it during loading and transportation, avoiding the generation of hot spots.

TATB explosive (1,3,5-triamino-2,4,6 trinitrobenzene) is a kind of aromatic explosives, because of its low impact sensitivity, high decomposition temperature, to light, heat, friction, impact and shock waves and other external stimuli performance blunt, also known as "wood explosives"[1-6], It is the main component of various high-energy insensitive explosives and is widely used in weapon explosives [7,8]. The molecular formula of TATB is $C_6 H_6 N_6 O_6$, and its cell space group is P_1, TATB molecule is highly symmetric and belongs to D_{3h} point group, and the cell contains two TATB molecules, as shown in Figure 1 *(a)(b)(c).* From its cell structure, it can be seen that TATB exhibits a layered structure like graphite, with strong anisotropy. Hydrogen bonds exist between molecules in the same layer and within each molecule, while the layers are connected to each other by van der Waals forces, as shown in Figure 1.(c). The hydrogen bonding within the layers and the π-π bonding of the benzene ring of the TATB molecule along one direction lead to the extremely high stability of the TATB cell. Because of its low susceptibility and high energy density, the study of TATB-based PBX explosives has become a concern for domestic and foreign researchers. Xiao Heming's team in China has studied TATB-based PBX explosives [9.10] in depth and found that the addition of a small amount of fluoropolymer can effectively improve the mechanical properties of TATB. Bower J K et al [11] studied three polymers (Kel-F 800, phenoxy PKHJ

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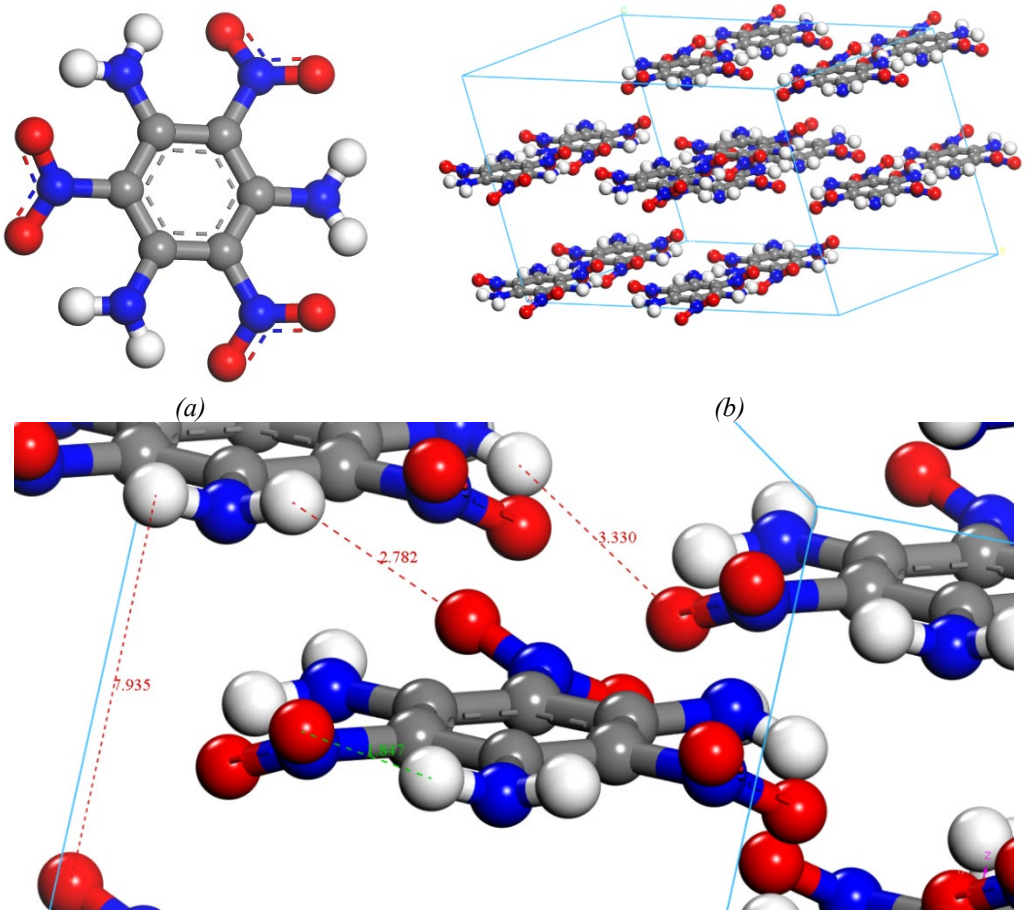
and Kraton G 1650) on the properties of TATB explosives after adsorption on their surfaces, and found that the three polymers changed the tensile and compressive capacities of the explosives to different degrees.



(a), 2×2×2 cell structure (b), hydrogen bonding and van der Waals forces (c) (where white atoms are H atoms, gray atoms are C atoms, red atoms are O atoms, and blue atoms are N atoms)

Figure 1: Molecular structure of TATB

As a TATB-based PBX explosive developed in China, it is necessary to simulate the performance of JB-9014 explosive. Based on this, the pure crystal model of TATB, the adsorption-cladding model of JB-9014[12,13] and the AC (Amorphous Cell) hybrid model of JB-9014[14,15] are constructed in this chapter, and the molecular dynamics simulations at different temperatures are carried out by COMPASSII force field. The results were analyzed, and the binding energy, bond length, bond density and mechanical properties of different models were compared, and the characteristics of different models with temperature were studied.

2. Model construction and calculation conditions setting

2.1. Model construction

The initial crystal structure of TATB was obtained from the X-ray diffraction data of Cady and Larson [16], which was expanded into a 2 × 5 × 4 supercell model along the ABC direction to obtain a pure crystal model of TATB containing 80 TATB molecules with 1920 atoms and a density of 1.938 g/cm^3. A vacuum layer of 3 Å was added to the (001) face of the pure crystal model of TATB One F2314 molecule was placed and two TATB molecules were deleted to obtain the adsorption cladding model of JB-9014, containing 78 TATB molecules and one F_{2314} molecule, with a total of 1934 atoms and a density of 1.861 g/cm^3 .The Amorphous Cell module in Materials Studio software was used to calculate the density of TATB:F_{2314} =95: 5 mass ratio and a density of 1.898 g/cm^3 , the AC synthesis model of JB-9014 explosive was obtained, containing 78 TATB molecules and a F_{2314} molecule, with a total of 1934 atoms. The three

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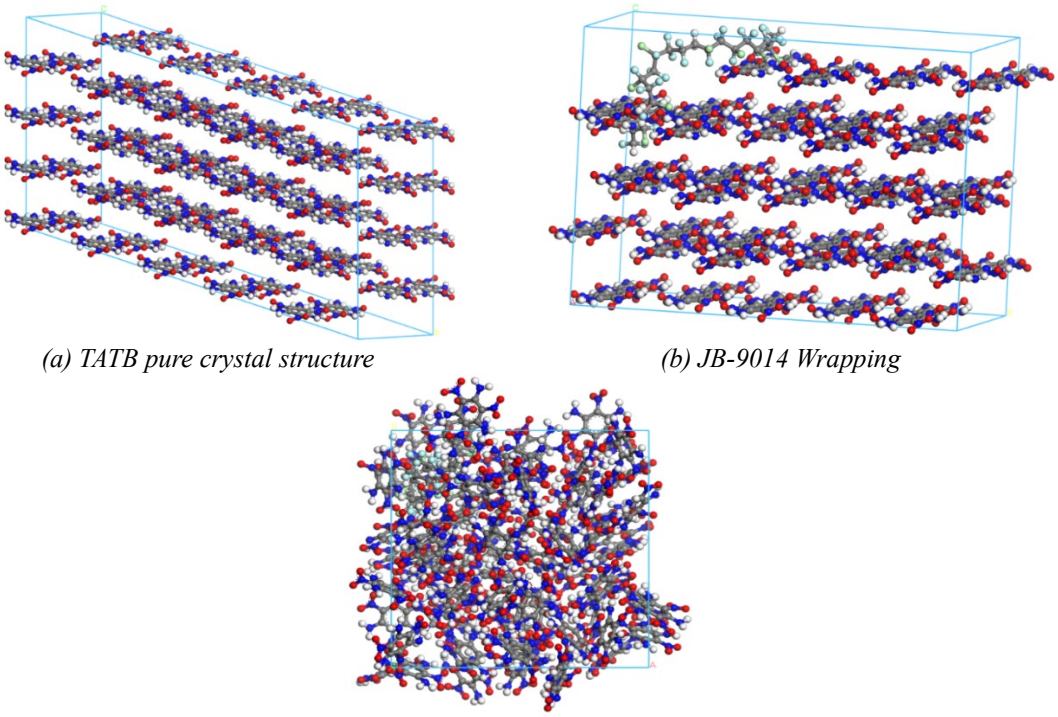
structures were noted as TATB pure crystal, JB-9014 encapsulated, and JB-9014 mixed, and Figure 2. shows the schematic diagrams of the three model structures.



(a) TATB pure crystal structure *(b) JB-9014 Wrapping*

(c) JB-9014 Mixing

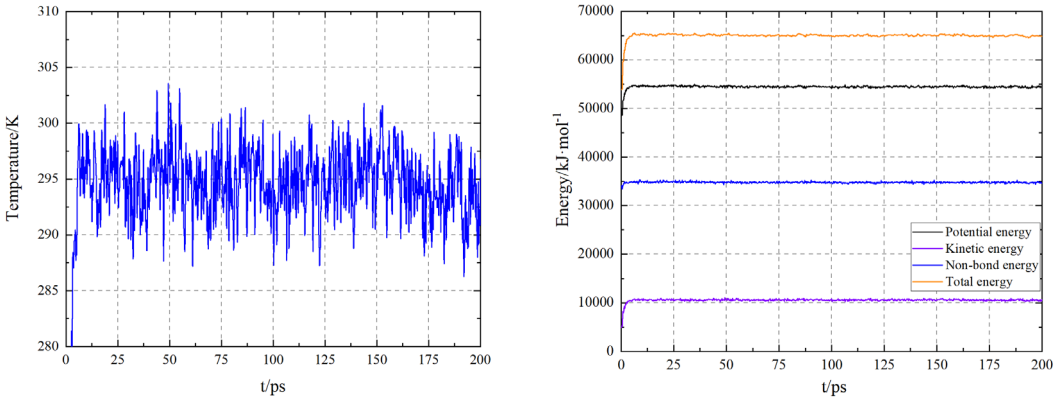
Figure 2: Pure crystal structure of TATB and two configurations of JB-9014

2.2. Calculation condition setting

Firstly, the initial models of the three structures were geometrically optimized to converge their energies. The optimized structures were then subjected to molecular dynamics calculations using a constant temperature and pressure system, NPT, in which an Andersen thermostat was selected to set the temperature to 255, 275, 295, 315, 335 and 355 K. The Parrinello pressure control method was selected to control the pressure at 0.0001GPa, i.e., atmospheric pressure, and the Ewald method and the The Ewald and Atom-based methods were used to calculate the electrostatic force and van der Waals force, respectively. The total calculation time was set to 200ps and the unit step was 1fs.

3. Analysis of results

3.1. Equilibrium discriminations



(a)Temperature change curve *(b) Energy change curve*

Figure 3: Temperature and energy change curves of TATB pure crystals at 295K

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The criterion for judging the equilibrium of the hybrid system is that the changes in temperature and energy are less than 10%, and the calculation results after the system reaches the equilibrium state have analytical significance. Taking the calculation of TATB pure crystal at 295K temperature as an example (as shown in Figure 3), the temperature rises 10ps before the simulation, and then fluctuates between 283~308K, with the fluctuation range within 29.5K, i.e., the change is less than 10%, so it can be considered to be in equilibrium; all four energies rise 10ps before the simulation, and then fluctuate with a small change, so it can be considered to be in equilibrium state. The changes of temperature and energy are within 10%, so the system can be considered to be in equilibrium, and the calculation results have analytical value.

3.2. Binding energy

The binding energy reflects the strength of the intermolecular forces in the system, and the larger the binding energy, the stronger the intermolecular forces and the more stable the system. For the JB-9014 explosive cladding and mixing two configurations, the size of the binding energy between the TATB molecules and F_{2314} molecules can reflect the strength of the stability of the two structures, the binding energy calculation formula is

$$E_b = -E_{inter} = -(E_{total} - E_{TATB} - E_{F2314}) \tag{1}$$

where E_b is the binding energy between TATB molecules and F_{2314} molecules (kJ·mol^{-1}); E_{inter} is the intermolecular force in the structure (kJ·mol^{-1}); E_{total} is the total energy of the structure at equilibrium (kJ·mol^{-1}); E_{TATB} is the total energy of the structure after removing all F_{2314} molecules (kJ·mol^{-1}); and E_{F2314} is the total energy of the structure after removing all TATB molecules (kJ·mol^{-1}).

According to the results of molecular dynamics calculations, the total energy and the energy of each component of the two structures of JB-9014 cladding and mixing at equilibrium were obtained, and the binding energies at different temperatures were calculated by equation 1 as shown in Figure 4.

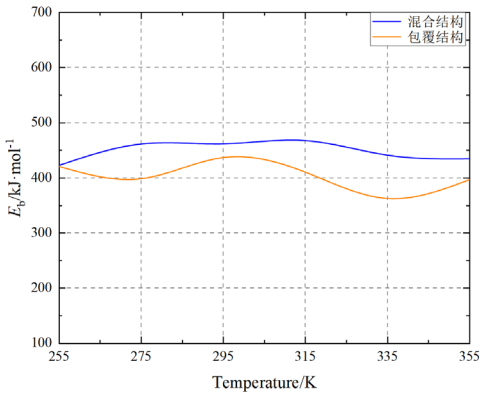

Figure 4: Trend of binding energy of different models

From Figure 4, it can be seen that the binding energy of the JB-9014 hybrid structure is larger than that of the cladding structure at the same temperature, which indicates that the configuration of the JB-9014 hybrid structure is more stable compared with that of the cladding structure. In addition, for the JB-9014 hybrid structure, the binding energy does not change much with the increase of temperature, which indicates that the hybrid structure is not very sensitive to temperature. For the JB-9014 cladding structure, the binding energy fluctuates more with the increase of temperature compared with the hybrid structure, which indicates that the cladding structure is more sensitive to temperature and less stable.

3.3. Initiating key bond length

The susceptibility is an important property for energy-containing materials, and it is an important property to measure the stability of energy-containing materials and their applicability to weapons explosives. In China, Xiao Heming [17] has proposed that the susceptibility of energy-containing materials is related to their initiation bond length and cohesive energy density through a long-term study of energy-containing materials, and has successfully predicted the susceptibility of various energy-containing materials. The initiation bond is the smallest and most fragile bond in energy-containing materials, which is the first to break upon external stimulation and react with other molecules to cause

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the explosion or decomposition of the overall structure. The bond length of the initiating bond reflects the strength of the initiating bond, the longer the bond length indicates that the weaker the force between the two atoms connecting the initiating bond, the lower the bond energy, conversely, the shorter the bond length, the stronger the force of the initiating bond, the greater the bond energy, the more stable the structure. JB-9014 explosive main explosive is TATB, Jiang Wencan [18] by first principles and combined with vdW-DF2 correction method to study the TATB explosive crystal The phonon spectrum and specific heat capacity of TATB explosives were studied by first nature principle and combined with vdW-DF2 correction method, and it was pointed out that the initiating bond of thermal decomposition of TATB is likely to be C-N (NO2); A. David Stephen[19] used density flooding (B3P86/6-311G**) to study the charge density of TATB, and predicted that C-NO2 is the weakest bond by the topological analysis of the bond. Therefore, the initiating bond of JB-9014 explosive studied in this paper is C-NO2 bond, as shown in Table 1 for the average bond lengths of the initiating bonds of TATB pure crystal, JB-9014 clad and hybrid structures at different temperatures, and Figure 5 shows the bond length distribution of the initiating bonds of JB-9014 hybrid structure at 315 K. (Unit: Å)

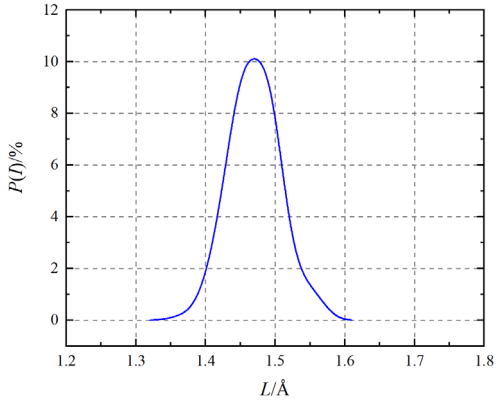

Figure 5: Bond length distribution of JB-9014 Mixing structure with initiating bonds at 315K

Table 1: Average bond lengths of TATB pure crystals, JB-9014 Wrapping and Mixing structure trigger bonds at different temperatures

Models	255K	275K	295K	315K	335K	355K
TATB	1.470	1.471	1.471	1.472	1.472	1.473
JB-9014 Wrapping	1.469	1.470	1.471	1.471	1.472	1.472
JB-9014 Mixing	1.467	1.468	1.469	1.469	1.471	1.471

As can be seen from Table 1, the bond lengths of the initiating bonds of all three configurations increase with increasing temperature at different temperatures for the same configuration, indicating that the higher the temperature, the smaller the bond energy of the initiating bonds, the more likely the initiating bonds are to break, and the higher the susceptibility of the system, which is consistent with the experimental conclusion of thermal susceptibility of energy-containing materials. The average bond lengths of the three structures at the same temperature and in different configurations were smaller (0.001 Å), and the relationship between the bond lengths of the initiating bonds was $L_{TATB} > L_{JB\text{-}9014Wrapping} > L_{JB\text{-}9014Mixing}$. The average bond lengths of TATB were the largest, followed by those of the clad structure, and the average bond lengths of the hybrid structure were the smallest, which indicated that both the clad and hybrid treatments reduced the bond lengths of the initiating bonds of TATB to a certain extent, thus making its susceptibility The average bond length of the hybrid structure was the smallest. In addition, the average bond length of the hybrid structure is the smallest, so the bond of the cladding structure is more likely to break under less stimulation than the hybrid structure, and the susceptibility is higher and less stable.

3.4. Bond-linked diatomic action energy

The larger the bond energy of the initiating bond, the more energy is absorbed to break the initiating bond, and the stronger and more stable the initiating bond is. At the same time, a larger initiation bond energy indicates a lower susceptibility of the energy-containing material, a better safety performance and a more stable overall structure.

For JB-9014 with TATB as the main explosive, the initiating bond is the C-NO_2 bond in TATB, and the calculation formula for the bonding diatomic action energy is

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$$E_{C\text{-}NO_2} = \frac{E_{total} - E_1}{n} \tag{2}$$

where $E_{C\text{-}NO2}$ is the bond energy of the initiating bond C-NO_2 (kJ·mol^{-1}); E_{total} is the total energy of the whole system when the structure reaches equilibrium (kJ·mol^{-1}); E_1 is the total energy of the whole system after fixing all the C and N atoms in the initiating bonds in the structure (kJ·mol^{-1}); n is the number of initiating bonds contained in the structure.

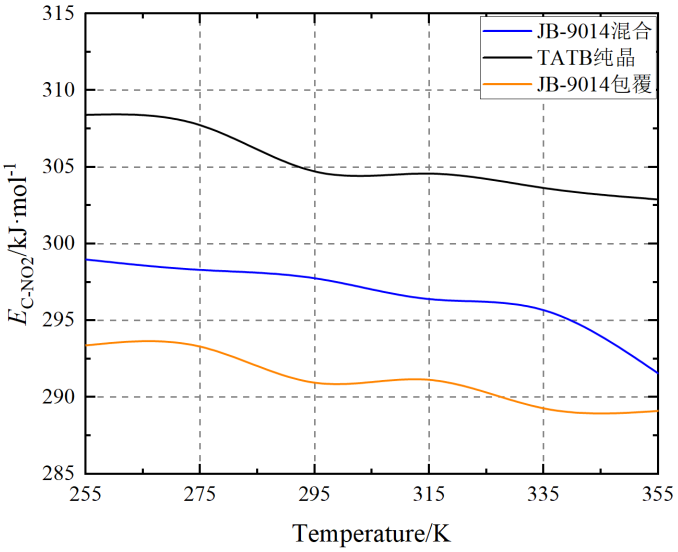

Figure 6: Trend of the initiating bond bond-linked diatomic energy for different models

From Figure 6, it can be seen that the initiating bond bond-linked diatomic energy of the system decreases with the increase of temperature at the same configuration, which indicates that the initiating bond strength of the system is decreasing, the sensibility of the system is increasing, and the stability becomes worse, which is consistent with the experimental understanding. In addition, comparing different configurations at the same temperature, the initiating bond linkage diatomic energy of the TATB pure crystal structure is the largest, the mixed structure is the second largest, and the cladding structure is the smallest, which means that the treated explosives are more likely to be decomposed or exploded by external stimuli than the TATB pure crystal structure, and the susceptibility becomes higher and the stability becomes worse.

3.5. Cohesive energy density

Cohesive energy density (CED), refers to the energy required to overcome the intermolecular forces of vaporization of 1 mol of condensate in a unit volume, calculated as

$$\mathrm{CED} = \frac{\mathrm{H_V} - RT}{\mathrm{V_m}} \tag{3}$$

where CED is the cohesive energy density, kJ·cm^{-3}; H_V is the molar heat of evaporation, kJ·mol^{-1}; RT is the work of expansion done when the substance is vaporized, kJ·mol^{-1}; V_m is the molar volume, cm^3 ·mol^{-1}.

The cohesive energy density is mainly composed of van der Waals force (vdW) and electrostatic force (electrostatic), which is a kind of non-bond force (non-bond) in nature and can reflect the strength of intermolecular forces in the system. The higher the cohesive energy density, the greater the van der Waals and electrostatic forces that need to be overcome when the energy-containing material changes from solid to gaseous state, the stronger the intermolecular forces in the system, and the more stable the system. As shown in Table 2, the cohesive energy density, van der Waals force and electrostatic force of TATB pure crystal, JB-9014 cladding and hybrid structure at different temperatures are shown. (Unit: kJ·cm^{-3})

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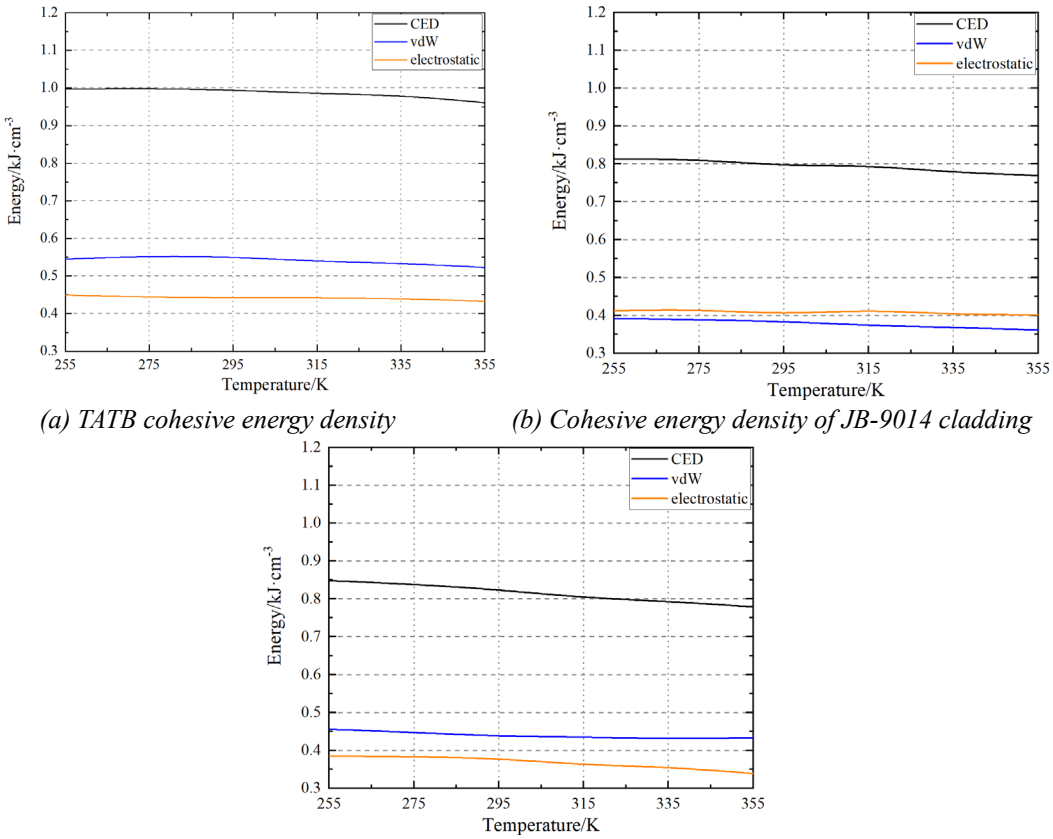
Table 2: Cohesive energy density, van der Waals force and electrostatic force of the three structures at different temperatures

Structure	Parameters	255K	275K	295K	315K	335K	355K
TATB	CED	0.997	0.999	0.995	0.985	0.981	0.961
	vdW	0.545	0.553	0.551	0.539	0.534	0.523
	electrostatic	0.449	0.444	0.442	0.442	0.440	0.433
JB-9014 Wrapping	CED	0.813	0.812	0.794	0.796	0.777	0.769
	vdW	0.392	0.388	0.384	0.373	0.368	0.361
	electrostatic	0.412	0.416	0.402	0.415	0.402	0.401
JB-9014 Mixing	CED	0.848	0.838	0.824	0.803	0.793	0.779
	vdW	0.456	0.447	0.437	0.435	0.430	0.433
	electrostatic	0.385	0.383	0.379	0.361	0.356	0.339



(a) TATB cohesive energy density

(b) Cohesive energy density of JB-9014 cladding

(c) Cohesive energy density of JB-9014 blend

Figure 7: Trends of cohesive energy density for different models

From Table 2 and Figure 7, it can be observed that at the same temperature for different structures, the pure TATB crystal corresponds to the largest cohesive energy density, the mixed structure is the second and the cladding structure is the smallest, which indicates that a smaller energy stimulus can make the cladding structure react, so the mixed structure requires more energy to sublimate from the condensed to the gaseous state compared to the cladding structure, and the susceptibility is smaller and more stable. At different temperatures of the same structure, the cohesive energy density, van der Waals force and electrostatic force of all three structures decrease with increasing temperature, indicating that the increase in temperature leads to a decrease in the energy required to sublimate the system from the condensed to the gaseous state, an increase in susceptibility and a decrease in stability, which is consistent with the experimental understanding.

3.6. Mechanical properties

Improving mechanical properties is one of the objectives of the development of polymer-bonded explosives, and mechanical properties are also important properties of energy-containing materials, which are directly related to their processing, transportation and storage.

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The mechanical property parameters of interest in the study of energy-bearing materials include bulk modulus K, shear modulus G, tensile modulus E, Poisson's ratio γ and Cauchy's pressure C12 -C44 . The bulk modulus K reflects the fracture strength and incompressibility of energy-bearing materials. Shear modulus G reflects the shear resistance of the energy-containing material, the larger the shear modulus, the less likely the energy-containing material is to be deformed. Tensile modulus E reflects the hardness of the energy-containing material, the larger the tensile modulus, the more rigid the energy-containing material. Poisson's ratio γ reflects the degree of expansion of the energy-bearing material in the one-way pressure, perpendicular to the direction of pressure. The Cauchy pressure C12 -C44 reflects the ductility of the energy-containing material, the larger the Cauchy pressure the better the ductility of the energy-containing material.

The basic parameters of the above mechanical properties all satisfy the generalized Hooke's law[20], according to this law:

$$E = \frac{9KG}{3K+G}, \quad \gamma = \frac{3K-2G}{2(3K+G)} \tag{4}$$

In this paper, static mechanical analysis is performed based on the equilibrium trajectories, and the mechanical parameters of different models are calculated as shown in Table 3, Table 4, Table 5 and Figure 8. It can be seen that the mechanical parameters of the energy-containing materials all decrease to different degrees with the increase of temperature, showing a softening trend. the *E*, *K* and *G* of the pure crystal structure of TATB are larger than those of the cladding and hybrid structure, which indicates that the rigidity of TATB decreases and the elasticity increases after the cladding and hybrid treatment, which means that it is easier to exhaust the energy of external stimuli applied to its surface during loading and transportation, which can reduce the occurrence of hot spots This can reduce the possibility of hot spots; the Corsi pressure (C_{12} -C_{44}) is smaller than the cladding and hybrid structure indicating that the treated TATB is more ductile and more conducive to the processing of explosives. In addition, the *E*, *K*, and *G* values of the hybrid structure are smaller than those of the clad structure, indicating that it is less rigid and more elastic, which is more conducive to the processing of explosives.

Table 3: Mechanical property parameters of TATB pure crystal structure at different temperatures

Temperature	255K	275K	295K	315K	335K	355K
E	8.179	7.746	7.096	7.140	6.960	6.830
K	2.823	2.535	2.694	2.347	2.238	2.484
G	7.594	6.856	7.173	6.346	6.066	6.645
C_{12} -C_{44}	0.345	0.352	0.332	0.352	0.355	0.338
γ	-0.464	0.047	-0.061	-0.344	-0.499	-0.269

Table 4: Mechanical property parameters of JB-9014 cladding structure at different temperatures

Temperature	255K	275K	295K	315K	335K	355K
E	6.561	6.754	6.119	6.124	4.747	4.969
K	2.035	1.979	1.846	1.990	1.785	2.028
G	5.532	5.408	5.032	5.386	4.758	5.356
C12 -C44	0.359	0.367	0.363	0.353	0.333	0.320
γ	1.641	1.521	1.672	1.951	0.821	0.860

Table 5: Mechanical property parameters of JB-9014 hybrid structure at different temperatures

Temperature	255K	275K	295K	315K	335K	355K
E	6.088	4.910	4.927	4.676	4.550	4.704
K	1.886	1.873	1.635	1.648	1.559	1.609
G	5.129	4.985	4.416	4.424	4.197	4.334
C12 -C44	0.360	0.331	0.351	0.342	0.346	0.346
γ	2.721	1.946	2.211	3.421	1.701	1.917

Note: Except for Poisson's ratio γ , all other units are GPa

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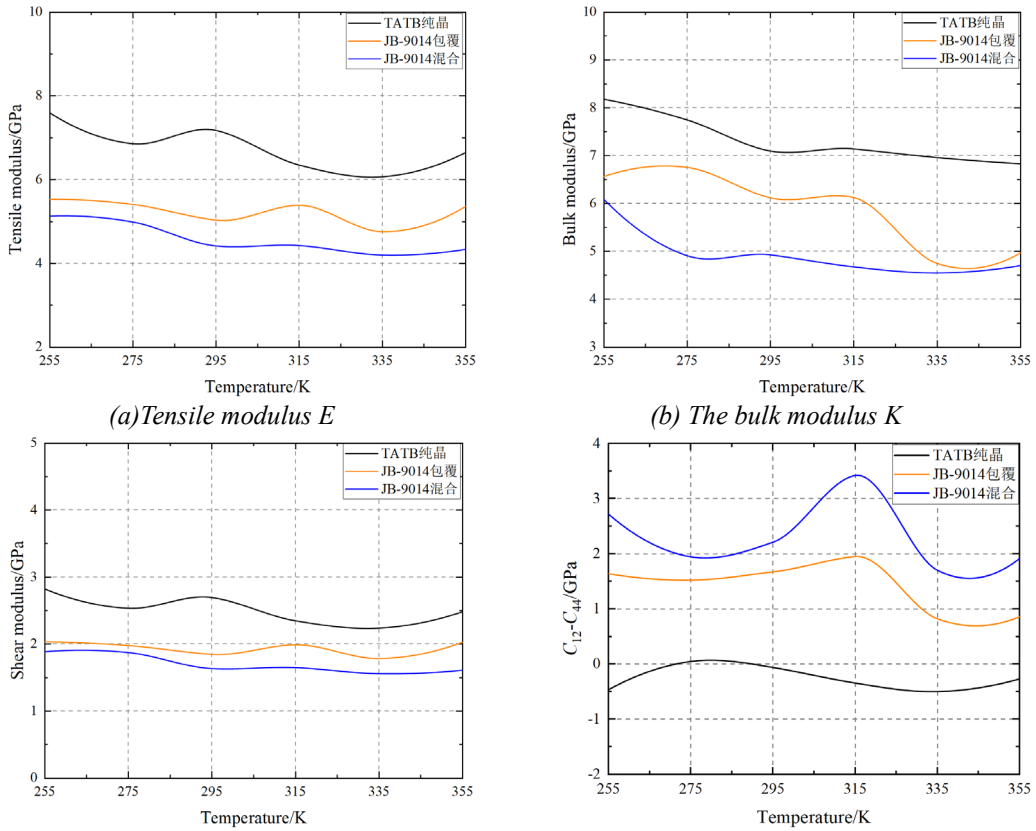

(a)Tensile modulus E *(b) The bulk modulus K*

(c) Shear modulus G *(d) Corsi pressure C_{12} -C_{44}*

Figure 8: Trend of mechanical property parameters of different models

4. Conclusion

In this chapter, three models of TATB pure crystal, JB-9014 cladding and hybrid structure were constructed, and COMPASSII force field was selected to perform molecular dynamics calculations on the three models under NPT system synthesis, and the following conclusions were obtained by analyzing and comparing the binding energy, initiating bond bond length, initiating bond linkage diatomic action energy, cohesion energy density and mechanical properties.

(1) The binding energy of JB-9014 hybrid structure is larger than that of the cladding structure at the same temperature, i.e., the configuration of the hybrid structure is more stable compared with that of the cladding structure. With the increase of temperature, the binding energy of the cladding structure fluctuates more, and the change of the binding energy of the hybrid structure is relatively flat.

(2) The average bond lengths of the initiation bonds of the clad and hybrid structures at the same temperature are smaller than those of the TATB pure crystal structure, but the difference is small (0.001 Å), and the bond length of the hybrid structure is the smallest. With the increase of temperature, the bond lengths of all three configurations increase, the stability becomes worse and the susceptibility increases.

(3) The bonding diatomic energy and cohesive energy density of both the cladding structure and the hybrid structure are smaller than those of the TATB pure crystal structure, and the bonding diatomic energy and cohesive energy density of the cladding structure are smaller than those of the hybrid structure at the same temperature, and the stability is worse than that of the hybrid structure, and the sensibility is higher.

(4) The cladding structure and hybrid structure have better ductility, lower rigidity and resistance to deformation compared to TATB pure crystal, which is beneficial to the processing of explosive materials.

In a comprehensive view, TATB pure crystal after cladding and mixing with F_{2314} treatment to obtain two JB-9014 explosive model, the initiation bond bond length changes little, the bond even double atomic energy and cohesion energy density becomes smaller, the system is stimulated by the decomposition or explosion threshold is reduced, the sensitivity increases, the stability becomes worse; after treatment

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compared to the TATB pure crystal structure its rigidity is reduced, the elasticity increases, while due to the increase in Corsi pressure , the explosive has a better ductility, more conducive to its processing. In addition, the hybrid structure has lower susceptibility and better ductility than the cladding structure, and its binding energy, initiation bond length, bonding diatomic energy, cohesive energy density and mechanical properties change less with temperature and are more stable, so the hybrid structure can be used as the next step to study the base model of gas adsorption on the explosive surface.

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