Simulation and Calculation for Binding Energy and Mechanical Properties of ε-CL-20/Energetic Polymer Binder Mixed System

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Abstract: To design the formulation of energetic polymer bonded explosives, the energetic binder with different hard and soft segments proportions of 3-azidomethyl-3-methyl oxetane(AMMO): 3,3-diazidomethyl oxetane(BAMO) was added into the high energy density compound hexanitrohexaazaisowurtzitane (ε-CL-20) used as main body of formulation, forming PBX. The binding energy, the interaction modes between the energetic binder and ε-CL-20 and the mechanical properties of ε-CL-20/energetic binder mixed systems were simulated by molecular dynamic (MD) method. The enthalpies of formation of the energetic binders with different hard and soft segments proportions were calculated by a group additive method. Results show that the compatibility and stability of PBXs predicted by binding energy decrease in the order of ε-CL-20/PBAMO(9)-*g*-PAMMO(2)>ε-CL-20/PBAMO(5)-*g*-PAMMO(7)> ε-CL-20/PAMMO (17)>ε-CL-20/PBAMO (12), PBAMO interacts with ε-CL-20 mainly in van der Waals force. PAMMO interacts with ε-CL-20 in van der waals force, electrostatic interaction and other forces. The energetic binders can effectively reduce the rigidity of ε-CL-20, wherein the thermoplastic elastomer can enhance the ductility of ε-CL-20 effectively. The unit mass enthalpy of formation of energetic binder increases gradually with the increase of BAMO content.

Key words: hexanitrohexaazaisowurtzitane (CL-20); polymer bonded explosives (PBX); energetic binder; binding energy; mechanical properties
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