

Full Papers

TATB/氟聚合物PBX力学性能、结合能和爆炸性能的模拟计算

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摘要 对著名钝感炸药1,3,5-三氨基-2,4,6-三硝基苯(TATB), 及其与系列常用含氟聚合物(聚偏二氟乙烯PVDF、氟树脂F₂₃₁₁、氟橡胶F₂₃₁₄和聚三氟氯乙烯PCTFE)所组成的四种高聚物粘结炸药(polymer bonded explosive, PBX), 用分子动力学方法进行了模拟计算, 求得它们的力学性能和结合能。发现当聚合物均取10个链节时, 以F₂₃₁₄对主体炸药TATB的力学性能影响较大, 而以F₂₃₁₁与TATB的结合能最大。通过计算求得该四种TATB/氟聚合物PBX的爆热和爆速, 对比纯TATB, 发现爆热大小排序为TATB>TATB/PVDF>TATB/F₂₃₁₁>TATB/F₂₃₁₄>TATB/PCTFE, 而爆速大小排序则为TATB/PVDF<TATB/F₂₃₁₁<TATB/F₂₃₁₄<TATB/PCTFE<TATB。可见在进行PBX配方设计、优选高聚物粘结剂时, 应综合考虑粘结剂对主体炸药多种性能的不同影响。

关键词 [高聚物粘结炸药, 分子动力学, 力学性能, 结合能, 爆炸性能](#)

分类号

Simulative Calculation of Mechanical Property, Binding Energy and Detonation Property of TATB/Fluorine-polymer PBX

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Abstract Molecular dynamics (MD) method was used to simulate 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) coated with fluorine containing polymers. The mechanical properties and binding energies of PBXs were obtained. It was found that when the number of chain monomers of fluorine containing polymers was the same, the elasticity of TATB/F₂₃₁₄ was increased more greatly than others and the binding energy of TATB/F₂₃₁₁ was the largest among four PBXs. Detonation heat and velocity of such four PBXs were calculated according to theoretical and empirical formulas. The results show that the order of detonation heat is TATB>TATB/PVDF>TATB/F₂₃₁₁>TATB/F₂₃₁₄>TATB/PCTFE while the order of detonation velocity is TATB/PVDF<TATB/F₂₃₁₁<TATB/F₂₃₁₄<TATB/PCTFE<TATB.

Key words [polymer bonded explosive](#) [molecular dynamics](#) [mechanical property](#) [binding energy](#) [detonation property](#)

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