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研究论文

分子动力学模拟浓度和温度对**TATB/PCTFE PBX**力学性能的影响

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摘要 为探讨高聚物粘结炸药(Polymer Bonded Explosive, PBX)的力学性能随温度和高聚物浓度而变化的规律, 用分子动力学(MD)方法和compass力场, 对著名高能炸药1,3,5-三氨基-2,4,6-三硝基苯(TATB)与常用高聚物粘结剂聚三氟氯乙烯(PCTFE)所构成的TATB/PCTFE PBX进行模拟计算. 结果表明, 在一定范围内, 随高聚物浓度的增加, PBX的弹性系数和模量减小, 表明其刚性减小、弹性增加; 而随温度的升高, PBX的刚性减小、弹性增强. 还发现PBX的结合能随浓度增高而增大, 随温度升高而减小.

关键词 高聚物粘结炸药(PBX) 分子动力学(MD) 力学性能 结合能 温度 粘结剂浓度

分类号

Effects of Concentration and Temperature on Mechanical Properties of TATB/PCTFE PBX by Molecular Dynamics Simulation

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Abstract In order to explore effects of polymer concentration and temperature on mechanical properties of polymer bonded explosive (PBX), molecular dynamics method and compass force field were adopted to simulate 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) coated with polychlorotrifluoroethylene, TATB/ PCTFE PBX. The mechanical properties, *i.e.* elastic coefficients, tensile modulus, bulk modulus, shear modulus and poisson's ratio, and binding energy of PBX were obtained. It was found that to a certain extent with the increase of polymer concentration or temperature, the elastic coefficients and moduli were decreased, to show the rigidity of PBX reduction and its elasticity enhancement. The results also show that binding energies between TATB and polymer were increased with the enhancement of polymer concentration, but decreased with the temperature enhancement gradually.

Key words TATB-based polychlorotrifluoroethylene bonded explosive molecular dynamics mechanical property binding energy temperature polymer concentration

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