

研究论文

**HMX/TATB复合材料弹性性能的MD模拟**

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**摘要** 用分子动力学(MD)方法COMPASS力场, 分别在正则系综(NVT)和等温等压系综(NPT)下, 模拟计算了著名常用高能炸药HMX(环四甲撑四硝胺)与著名钝感炸药TATB (1,3,5-三氨基-2,4,6三硝基苯) 所构成的混合体系在室温时的弹性性能和结合能. 结果表明, 在NVT和NPT两种系综下模拟所得结果呈平行一致的趋势; 与纯HMX相比, HMX/TATB复合材料的拉伸模量、体模量和剪切模量均有所下降; 在NVT系综下, 还完成了HMX/TATB混合体系的不同温度的MD模拟. 发现当温度在245~345 K范围时, 体系的刚性和弹性变化很小; 但当温度达到395 K时, 材料的刚性减弱, 柔性增强.

**关键词** [1,3,5-三氨基-2,4,6三硝基苯\(TATB\)](#) [环四甲撑四硝胺\(HMX\)](#) [复合材料](#) [弹性性能](#) [分子动力学](#)

分类号

**Molecular Dynamics Simulation of Elastic Properties of HMX/TATB Composite**

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**Abstract** The elastic properties and binding energy of composite which consists of famous high insensitive explosive TATB (1,3,5-triamino-2,4,6-trinitrobenzene) crystal and the well-known high explosive *b*-HMX (cyclotetramethylene tetranitramine) crystal have been simulated by molecular dynamics (MD) and COMPASS force field in NVT and NPT ensemble by DISCOVER model block in the Materials Studio software package. Their elastic coefficients, moduli and Poisson's ratios were calculated at room temperature. The outcomes obtained from NVT and NPT ensemble show similar parallel trend. The composite was also simulated in NVT ensemble at different temperatures. The results show that at the temperature of 245 to 345 K the elastic properties of HMX/TATB composites remain unchanged. When the temperature rises to 395 K, the rigidity decreases and the flexibility increases.

**Key words** [TATB \(1,3,5-triamino-2,4,6-trinitrobenzene\)](#) [HMX \(cyclotetramethylene tetranitramine\)](#) [composite elastic property](#) [molecular dynamics](#)

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