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XIAO Ji-jun, GU Cheng-gang, FANG Guo-yong, et al. Theoretical study on binding energies and mechanical properties of TATB-based PBX. *Acta Chim Sinica*, 2005,63(6): 439 – 444.

Dissipative Particle Dynamics Simulation on the Mesoscopic Structure of TATB-based PBX

ZHANG Yan-li[1,2], JI Guang-fu[2], GONG Zi-zheng[3], LI Xiao-feng[2,4], CUI Hong-ling[2,4]

(1. *Institute of High Pressure & High Temperature Physics, Southwest Jiaotong University, Chengdu* 610031, *China*;
2. *Laboratory for Shock Wave & Detonation Physics Research, Institute of Fluid Physics, Mianyang* 621900, *China*;
3. *Beijing Institute of Spacecraft Environment Engineering, Beijing* 100094, *China*;
4. *College of Physical Science and Technology, Sichuan University, Chengdu* 610065, *China*)

Abstract: The mesoscopic structures of TATB (1,3,5-triamino-2,4,6-trinitrobenzene)-based PBXs(polymer bonded explosive) and their time evolutions were investigated using the dissipative particle dynamics(DPD) method. The results show that most of the polymers are condensed to spheres and only several polymer chains extend into TATB, the polymers form reseau structure in TATB. TATB is fixed in the polymers, but can not be wrapped perfectly by the polymers. At the same time, with the increasing of the temperature and the content of the polychlorotrifluoroethylene(PCTFE) monomers in the polymer, more polymers are dispersed in TATB. When the temperature is up to 400 K, the polymers form the alveolate structure, and wrap TATB perfectly.

Key words: physical chemistry; TATB-based PBX; dissipative particle dynamics; mesoscopic structure; Flory-Huggins parameter

读者·作者·编者

向作者致谢

近年,《含能材料》得到了广大作者的大力支持,为表达我们深深的谢意,特向 2007 ~ 2008 两年来发表两篇以上论文的作者(第一作者)赠送 2009 年全年《含能材料》。本刊期望在新的一年能得到广大作者更多的关心！欢迎赐稿！

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二〇〇八年十二月