Crystal Morphology Prediction of Dihydroxylammonium 5,5′-Bistetrazole-1,1′-diolate Under Different Growth Conditions

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Abstract: To accurately predict the crystal morphologies of dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate (HATO, also known as TKX-50) under different growth conditions, the PCFF force field parameters were systematically validated and modified. The attachment energies of HATO crystal surface were calculated by the molecular simulation method. The crystal morphologies of HATO in vacuum, in seven solvents (water, dimethyl sulfoxide, methanol, ethanol, ethyl acetate, tetrahydrofuran and trichloromethane), and in three additives (sodium laurylsulfonate, sodium dodecyl benzene sulfonate and dextrin) were obtained. Results show that the crystal morphology of HATO in a vacuum is long flaky, consisting of five cryatal faces, (0 2 0), (1 1 −1), (0 1 1), (1 1 0) and (1 0 0), among them, cryatal face (0 2 0) is the most important, occupying the 53.97% of total surface area. In the polar solvents, including dimethyl sulfoxide, methanol, and ethanol, the morphological importance of (0 2 0) cryatal face decreases, the crystal morphology of HATO is improved. In the three additives, the crystal morphology of HATO is still long flaky. The predicted structure of crystal morphology of HATO is in good agreement with the experiments, it can provide theoretical guidance for the crystal morphology control of HATO.

Key words: dihydroxylammonium 5,5′-bistetrazole-1,1′-diolate(HATO); force field parameters; attachment energy; growth condition; crystal face

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《含能材料》“损伤与点火”专栏征稿

含能材料的损伤特征与点火过程有密切的联系,炸药、推进剂的内部损伤及其对力学特性、安全特性和点火行为的影响规律受到了含能材料学界的高度重视,为推动这一重要研究方向的学术交流,本刊特设立“损伤与点火”专栏。专栏主要征集炸药、推进剂等含能材料的损伤观测与多尺度表征技术、含损伤的本构方程、准静态与动态损伤演化规律、损伤与破坏的宏(细)观模式、损伤对起爆、爆炸、爆轰成长以及非冲击起爆行为的影响等方向的原创性研究论文。来稿请注明“损伤与点火”专栏。

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