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Title: Calculated Simulation of the Crystal Morphology of HMX

作者: 汤焱; 杨利; 乔小晶; 张同来; 齐书元
北京理工大学机电学院, 北京100081

Author(s): TANG Zhan; YANG Li; QIAO Xiao jing; ZHANG Tong lai; QI Shu yuan
School of Mechatronical Engineering, Beijing Institute of Technology, Beijing
100081, China

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摘要: 利用Material Studio中Morphology模块所含的BFDH、Growth Morphology和Equilibrium Morphology 3种方法计算了HMX的晶体形态和结晶习性; 研究了重要晶面的结构、晶体的生长习性和晶面结构与晶形控制剂的关系。结果表明, Growth Morphology和Equilibrium Morphology方法的计算结果与实际比较吻合。

Abstract: The crystal morphology and crystallization behavior of HMX were calculated by using BFDH, Growth Morphology and Equilibrium Morphology contained in Morphology module of Material Studio. The structures of important crystal faces, the growth habit of the crystal and the relationship between the structures of crystal faces and surfactants were studied. The calculated results show that the results obtained by Growth Morphology and Equilibrium Morphology quite coincide with the actual results.

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