Poster Presentations

[MS45-P01] Bulk Single Crystal Growth and Mechanical Properties of RDX Explosive Crystal.

Xiaoqing Zhou, Qi Zhang , Hongzhen Li*

Institute of Chemical Materials, China Academy of Engineering Physics, P.O. BOX 919-311, Mianyang, Sichuan, China, 621900.
E-mail: zhxq_a@163.com

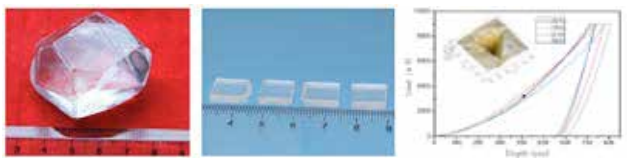
The investigations on explosive molecular crystals have attracted extensive attention because such research is essential to comprehend the structure-performance relationship of explosives. Comparison with nonhomogeneous explosives, single crystals are homogeneous and relatively defect free, which can simplify the complexities associated with extrinsic factors . Therefore, single crystals play an important role in study of explosive properties, such as mechanical properties, which are crucial to understanding the mechanism of detonation initiation of explosives. [1] However, the studies of growth, characteristic and mechanical properties of explosive crystals are poorly because of the difficulty in preparing samples, and the complex nature of the crystal structures themselves. Thus it can be seen that the research on the growth, processing and related material properties of bulk single crystals without defects is a challenging task for materials scientists and crystal engineers.

Cyclotrimethylene trinitramine (RDX) is an important modern nitramine molecular explosive widely used in military. Although some studies on the processes used to prepare suitable RDX crystals and the influence of solvents on the crystal morphology are available in the open literature,[2-3] the growth, cutting, polishing and characterization of bulk RDX single crystals have not been fully investigated. Moreover, there is rare crystalline deformation research of RDX,[4] but by which the elastic constants is provided to correlate the strength of the lattice interactions with detonation properties.

In these years the single crystal growth of RDX and the study of the intrinsic properties based on the single crystal are proceeding in our lab.

A good optical transparent and uniform large size single crystal of RDX has been successfully grown by slowly solvent evaporation. Powder X-ray diffraction (XRD) was done to confirm the phase of the grown crystals. Crystalline perfection of the as-grown crystals was investigated using the high resolution X-ray diffraction (HRXRD) technique. The nanoindentation technique has been employed to relate the mechanical properties of RDX single crystals with their internal structure. Nanoindentation and nano-scratch were performed on (210), (021), (001) and (102) faces to assess the mechanical anisotropy.

The results of XRD show that the grown crystals are α-RDX. The single sharp diffraction curve with very low FWHM indicates that the crystalline perfection is extremely good. And the results of nanoindentation and nano-scratch tests illuminate the anisotropy in crystal packing and interactions is reflected in the mechanical behavior on (210), (021), (001) and (102) faces.



[1] J.J. Haycraft, L. L. Stevens and C. J. Eckhardt,(2006). *J. Chem. Phys.* **124**, 024712 .
[2] P.J. Halfpenny, K.J. Roberts, J.N. Sherwood,(1984). *J. Cryst. Growth.* **69**, 73-81.
[3] J.H. ter Horst, R.M. Geertman, A.E. van der Heijden, et al., (1999). *J. Cryst. Growth.* **198/199**, 773-779.
[4] W.L. Elban, R.W. Armstrong, K.C. Yoo,et al., (1989). *J. Mater. Sci.* **24**, 1273-1280.
[5] K. J. Ramos, D. E. Hooks, D. F. Bahr, (2009). *Phil.Mag.* **89**, 2381-2402.

Keywords: single crystal, growth, mechanical properties