[MS45-P02] The Effects of Tailor-Made Additives on Explosive Crystal Morphology

Qi Zhang, Xiaoqing Zhou, Hongzhen Li

Institute of Chemical Materials, China Academy of Engineering Physics, P.O. BOX 919-311, Mianyang, Sichuan, China, 621900.
E-mail: jackzhang531@gmail.com

The wide application of explosives has prompted vigorous efforts to understand and improve their safety. A large number of evidence show that the safety of explosives can be related to their chemical as well as physical characteristics.[1] Among the physical factors, crystallographic properties of explosives, such as crystal size, morphology, purity, internal, and external defects, play important roles in the safety of explosives.
[2] For instance, explosives with sharp edges render the materials to be more sensitive to mechanical stimuli.[3] So it is not strange to explore new approaches for modifying the crystal morphology to cubic or spherical shape.
[4] However, crystal morphology modification are limited to optimizing the macro crystallization conditions, such as solvent composition, temperature, stirring rate and so on, and the process utilizing the molecular level technique is rarely mentioned, which is also helpful to understand the rules about crystal habits on the microscale. Therefore, the use of more reproducible and predictable techniques in a high level of molecular control would be more beneficial and are in high demand. Tailor-made additives, which are defined as having the similar chemical structures as the corresponding substrate molecules, have previously been presented as a promising way to control crystallization dynamics in solution. So crystallization with tailor-made additives is known as a efficient crystal engineering technique for controlling crystal morphology and is used intensively in design of pharmaceuticals and inorganic particles with desired properties, as altering the growth rate, size and shape.[5] Inspired by these, We attempt to apply this strategy as a mean to predictably control crystal morphology of some classic explosives. According to the principle of tailor-made additives action, we choose some additives having the similar structures with model compounds and accomplish the morphology modification of HMX(cyclotetramethlyene tetranitramine, a classical nitramine explosive), FOX-7 (1,1-diamnio-2,2-dintroethene, a novel high energy material). The investigation of tailor-made additives for HMX show that guanidines have an obvious effect on the crystal morphology, which induce inerratic polyhedra into long and slender needle. Interestingly, crystal knit by the needle is obtained when cyclic ethers are used as the additives. And we also discovery some difference of the crystal properties between these particles with new shapes and the normal one. Moreover, we develop a new approach to control the morphology of FOX-7. The use of tailor-made additives with amide or urea functional group provides a possibility to affect the particulate shape of FOX-7 in evaporative crystallization. The prismatic, lamellar, and cylindric crystals are provided at the presence of the additives, which is a dramatic change compared with the common one. Thus it can be seen that crystal engineering by tailor-made additives provides an opportunity to control explosive crystal characteristics including morphology and physical property
.

[1] H. Czerski, W. G. Proud, J. Appl. Phys. 2007, 102, 235
[2] J. Oxley, J. Smith, R. Buco, J. Energ. Mater. 2007, 25, 141.
[3] R. Sivabalan, G. M. Gore, U. R. Nair, J. Hazard. Mater. 2007, 139, 199.
[4] X. Song, Y. Wang, C. An, X. Guo, F. Li, J. Hazard. Mater. 2008, 159, 222.
[5] I. Weissbuch, L. Addadi, M. Lahav, L. Leiserowitz, Science, 253, 637.

Keywords: morphology modification, additives, explosives,