Molecular Dynamics Simulation on the Crystal Morphology of 2,6-Diamino-3,5-dinitropyridine-1-oxide

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Abstract: In order to understand the mechanism of the effect of solvent on the crystal morphology of explosives, and provide a gist for solvent selection, the attachment energy (AE) models were employed to predict the growth morphology and the main crystal faces of 2,6-diamino-3,5- dinitropyridine-1-oxide(ANPyO) in vacuum. The molecular dynamics (MD) simulation was applied to investigate the interaction of ANPyO crystal faces and *N*,*N*-dimethylformamide (DMF) solvent, and the growth habit of ANPyO in DMF was predicted using the modified AE model. Results indicate that the morphology of ANPyO crystal in vacuum is dominated by the four faces of (1 1 0), (1 0 0), (1 0 −1) and (1 1 −2), and the crystal shape is similar to ellipsoid. The radial distribution function analysis shows that the solvent- crystal face interactions mainly consist of van der Waals forces, coulomb interaction and hydrogen bonds. In DMF, the absolute value of the corrected attachment energies change in the order of (1 1 0)<(1 1 −2)<(1 0 −1)<(1 0 0),which causes the crystal morphology to become very close to a flake and accords well with the experiment results. Furthermore, the analysis of diffusion coefficient of DMF molecules on ANPyO crystal faces shows that diffusion coefficient changes linearly with the absolute value of the corrected attachment energies, and the growth habit is also affected by the diffusion capacity of solvent.

Key words: 2,6- diamino-3,5-dinitropyridine-1-oxide (ANPyO); crystal morphology; molecular dynamics(MD) simulation; diffusion coefficient; modified attachment energy (ME)model

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