A Molecular Approach on Nucleation of Ammonium Perchlorate from Aqueous Solution

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Nucleation is a very important step for crystal growth. It predominantly determines the crystal size and shape during crystallization. In specialty, since the size of propellants affects burning rate and packing density, the efforts to control and predict nucleation have to be necessarily paid. To investigate the nucleation of ammonium perchlorate (AP) from an aqueous solution, molecular dynamics (MD) simulation was employed. The emerging nuclei were monitored in real time by radial distribution functions (RDFs). It showed that dispersive ions were transformed into crystalline clusters. The configuration of ammonium and perchlorate ions exhibited an alternating pattern due to their opposite ionic charges. Compared with the nucleation from a bulk solution, a great deal of nuclei appeared on crystal faces and followed by construction of a crystalline structure. Fundamentally, It showed that two-dimensional nucleation on crystal faces is energetically favorable than three-dimensional nucleation from a solution.