Contribution ID: **22** Type: **Oral Presentation**

Dynamic Modelling on the Crystallization of Mono-sized Cubical Particles under Mechanical Vibrations

Monday, 11 July 2016 11:00 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

The realization of the densest possible geometrical ordering is one of the most fundamental questions in self-assembly of particles. In this work, the crystallization process of single crystal (disorder-order transition) formed by mono-sized cubical particles under three-dimensional (3D) mechanical vibrations is investigated by the dynamical simulation of discrete element method (DEM). The efficiency of crystallization in various vibration conditions and different shaped containers is analyzed and compared. The evolution of macro property such as packing density and micro properties such as coordination number (CN), radial distribution function (RDF), particle orientation and inter-particle forces during vibrated crystallization are characterized. The results show that the perfect single crystal of mono-sized cubical particles can be reproduced if the 3D vibration conditions are properly controlled. The distribution of particles in the crystallization process is also affected by the container walls, where the crystallization of particles initially emerges. In particular, the disorder-to-order transition is demonstrated as an entropy driven process under the entropic effects of particle shape and geometrical confinement of container walls. These findings can be helpful for our general understanding of self-assembly problems.

Primary author: Mr WU, Yongli (Monash University)

Co-authors: Prof. YU, Aibing (Monash University); Prof. AN, Xizhong (Northeastern University)

Presenter: Prof. AN, Xizhong (Northeastern University)

Session Classification: Parallel Track B