2017. 11. 13

Plan on Nanophotonics by Atsushi Mori

1. Two lectures will be given on Colloidal Photonic Crystal in 08:40-10:10 and 10:25-11:55 on Dec. 6 (Wed.) at the seminar roon on the 4^{th} floor of frontier bulidling. The lectures will be started from a histrical review on the colloidal crystals and cover the recent topics on the collodal photonic crystals. A reference introduced on the back side of this leaf can be downloaded freely.

2. A 20-30min presentation including questions, comments, and discussions should be given by every student. A student has two options: English presentation materials (written) and/or an English presentaion (oral). A one-papge report in an electric form should be submitted. The theme can be in a field of colloidal sciences and/or phtonic crystals in a wide sense. Arrangement on the date (from late December to early January) will be made after the lectures on Dec. 6.

URL:
http://cms.db.tokushima-u.ac.jp/DAV/person/S10802/education/NanoPhoto-17/index.html

crystals

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Review

Computer Simulations of Crystal Growth Using a Hard-Sphere Model

Atsushi Mori

Graduate School of Science and Technology, Tokushima University, Tokushima 770-8506, Japan; atsushimori@tokushima-u.ac.jp

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Abstract: A review of computer simulation studies on crystal growth in hard-sphere systems is presented. A historical view on the crystallization of hard spheres, including colloidal crystallization, is given in the first section. Crystal phase transition in a system comprising particles without bonding is difficult to understand. In the early days, therefore, many researchers did not accept such crystalline structures as crystals that should be studied in the field of crystal growth. In the last few decades, however, colloidal crystallization has drawn attention because in situ observations of crystallization process has become possible. Next, simulation studies of the crystal/fluid interface of hard spheres are also reviewed. Although colloidal crystallization has now been recognized in the crystal growth field, the stability of the crystal–fluid coexistence state has still not been satisfactorily understood based on a bond-breaking picture, because of an infinite diffuseness of the interfaces in non-bonding systems derived from this picture. Studies of sedimentary colloidal crystallization and colloidal epitaxy using the hard-sphere model are lastly reviewed. An advantage of the colloidal epitaxy is also presented; it is shown that a template not only fixes the crystal growth direction, but also improves the colloidal crystallization. A new technique for reducing defects in colloidal crystals through the gravity effect is also proposed.

Keywords: hard spheres; crystal/fluid interface; colloidal crystals; sedimentation; colloidal epitaxy

1. Introduction

Bonds are commonly formed between various entities in solid materials. In contrast, a class of matter called "soft matter" does not have any bonding. A colloidal system is a typical example of soft matter. The presence of large entities is one of the characteristics of soft matter. Therefore, because of their large size, such entities have slow motion; unlike atomic systems, in situ observation of the crystal growth process at the particle level is possible in colloidal systems.

To get insight into the particle-level mechanism in atomic systems, researchers have to rely on computer simulations. One cannot only follow the rapid motion of atoms in reality and simultaneously look at the atoms in crystal growth processes. These difficulties are not faced with computer simulations such as molecular dynamics (MD) and Monte Carlo (MC) simulations. However, these simulation methods have a limitation in total computation time. For example, a simulation for atomic systems can be conducted for several microseconds at most. In contrast, because colloidal particles have slower motion than atoms, the simulation of colloidal particles can be performed for several days. In other words, simulations corresponding to real situations are possible for soft matter.

This paper is a review on computer simulations using a hard-sphere (HS) model for crystal growth. Information about the structure of the crystal/melt interface at the particle level is necessary to understand phenomena and develop techniques. For example, the relationship between the interface structure and the growth mode, and the colloidal crystallization defect behavior that depends on the