Simuations Using Hard Spheres: Fandamentals to Model Colloids

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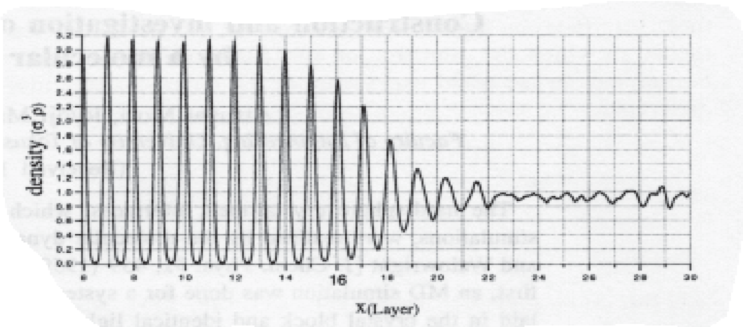

Fig. 1. A density profile of crystal-fluid interface of hard spheres. In this figure, x-direction is taken to be nornal to the interface. [Mori *et al.*, Phys. Rev. E **51** (1995) R3831.]

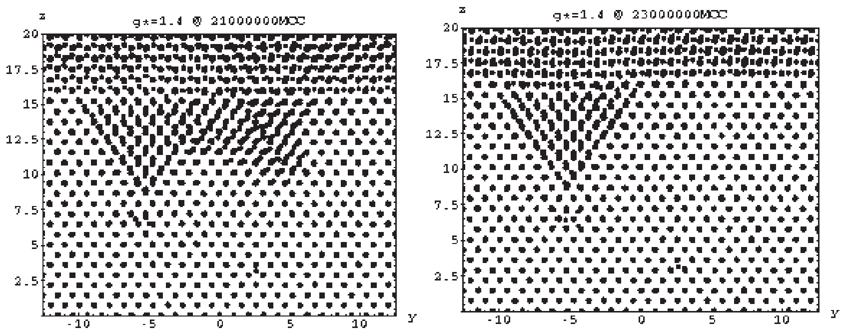

Fig. 2. Snapshot demonstrating gravitational tempering in collodal epitaxy. For first 2×10^7 Monte Carli cycles (MCCs) we grew a hard-sphere crystal under a gravitational condition of $g^*=mg\sigma/k_BT=1.6$, then g^* was decresed to 1.4. We show yz-projections at 2.1 and 2.3×10^7th MCCs. [Mori and Suzuki, submitted.]

Content:

In soft matters, no bonds are formed between their entities. A typical example is a colloid. Despite of absence of bonding between collidal particles, at a high particle density the collidal system crstallizes. Nowadays, we understand that such kinds of phase transisions are driven entropically. Hard shere is an idealized model of a colloidal particle. In 1995, coworkers and I sucesfully perfoemed a molecular dynamics simulation of crystal-fluid interface of hard sphres; this is the first relization of the two phase coexistence in the hard-sphre system. A density profile is shown in Fig. 1.

Recently, cowokers and I have developed a method to reduce defects in a collodal crystal base on results of Monte Carlo simuations. After growing a collidal crystal at a relatively high gravitational condition, one can erase some defects by slightly weaken the strength of gravity and maintaing for a perioid of time. We call this method gravitational tempring. Snapshots are shown in Fig. 2.

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