MONTE CARLO SIMULATION OF COLLOIDAL EPITEXY ON SQUSRE PATTERN

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Introduction

An effect of gravity that reduced defects in colloidal crystals was shown in 1997 by Zhu *et al.* [1]. On the basis of Space Shuttle experiments using a hard-sphere (HS) suspension, they concluded that a sediment was a random hexagonal close pack (rhcp) structure under microgravity while it was mixture of rhcp and face-centered cubic (fcc) crystals under normal gravity. Kegek and Dhont [2] also obtained results supporting this trend. Their result was, however, that the structure under normal gravity was fauled-twinned fcc instead of rhcp/fcc mixture.

The present author and coworkers [3] observed the defect disappearance in HS crystals under gravity in a case of fcc (001) stacking by Monte Carlo (MC) simulations. By close looks they found a glide mechanism of a Shockley partial dislocation for shrinking of an intrinsic stacking fault [4]. Their works are related to the colloidal epitaxy [5], where a colloidal crystal is grown on a patterned substrate. While in our simulation the (001) stacking was forced by a stress from the simulation box of a periodic boundary condition (PBC), experimentally a stress with the same symmetry is provided by the pattern on a substrate. While van Blaaderen *et al.* [5] proposed the use of a fcc (001) pattern, Lin *et al.* [6] employed a squared pattern. The use of a square pattern have an advantage that the lattice constant can be adjusted by matching on the lattice lines instead of on the lattice points.

In this paper we present results of simulation of a colloidal epitexy on a square pattern. We will report some details of MC simulations, a part of which we presented previously [7]. Previously we reported that in the case of a square pattern the defect disappearance occurred at lower g^* ($\equiv mg\sigma/k_\mathrm{B}T$ with m being the mass of a particle, g the acceleration due to gravity, σ the HS diameter, $k_\mathrm{B}T$ the temperature multiplied by Boltzmann's constant) than in the case of a flat bottom wall. During such g^* the relaxation of lowering of the center of gravity was of a single relaxation, indicating that the stacking fault was not fixed temporally at a metastable configuration. In this paper we observe at higher g^* than such one.

Simulation

N=6656 HSs were confined in a simulation box of $L_x = L_y = 12.55\sigma$ with PBC and a pattered wall at $z = 0$ and a flat wall at $z = L_z$ ($=200\sigma$). Grooves of width 0.707106781σ were made along transverse and longitudinal directions with separation between the neighboring groove centers 1.045106781σ on the bottom wall. The diagonal length of the squares of the intersection of the grooves results in 0.9999999997σ. Hence, the particle does not fall on to the bottom of the groove. In this paper, we present results of a simulation with g^* increased by $\Delta g^* = 0.1$ at every $\Delta t=2\times10^5$ MC cycle (MCC) to avoid the trapping of the system into a metastable state such as a polycrystalline state [3]. Here, one MCC is defined such that it contains N MC moves. Among varieties of combination of Δg^* and Δt we restrict ourselves to this condition including one we reported in Ref. [7] because details have not been presented anywhere. The maximum displacement of particle is the same as previous simulations we performed [3][4][7].

Results and discussions

The following was as previously reported [7]: Evolutions of the center of gravity during g^*=0.7 and lower than this value were of a single relaxation. The relaxation during such gravitational number, g^*, was not completed. We observed snapshots indicating disappearance of stacking fault in one of side views and incomplete disappearance in the other side view (in the other series of simulations the defect disappearance

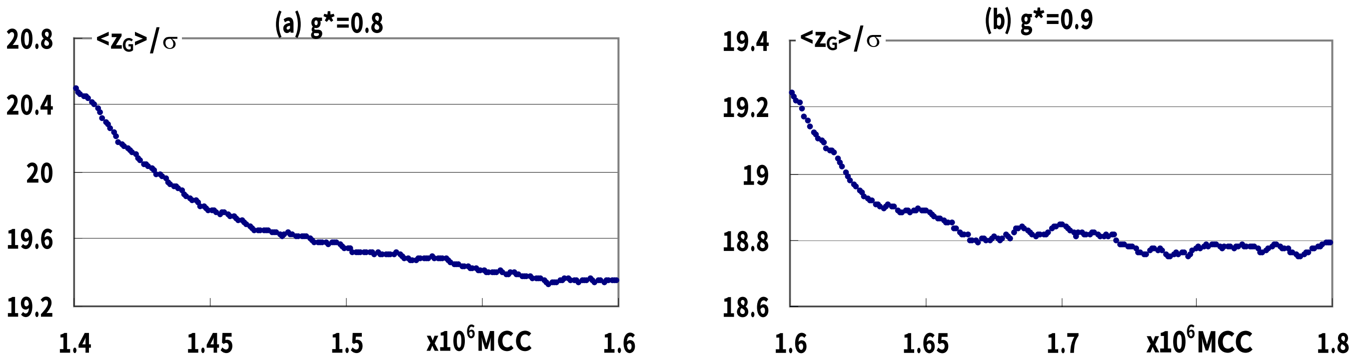

Fig.1: Evolution of the center of gravity at g^*= (a)0.8 and (b)0.9 for the series of simulations of Ref [7].

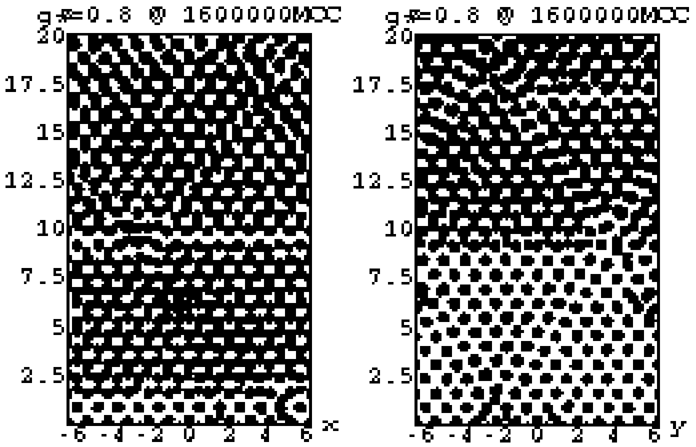

Fig. 2: Projected snapshots at 1.6×10^6MCC (g^*=0.8) of the series of simulations of Ref. [7].

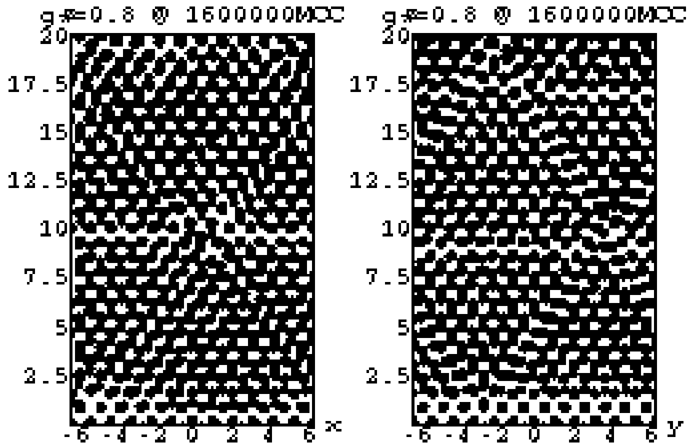

Fig. 3: Projected snapshots at 1.6×10^6MCC (g^*=0.8) of a series of simulations other than that of Ref. [7].

during g^*=0.7 was not so dramatic as that reported in Ref. [7]; it seemed that the upward move of the upper boundary of a less-defective crystal was pinned at two layer thick by a certain sessile structure).

Evolutions of the center of gravity during g^*=0.8 and 0.9 of a series of the simulation we reported in Ref. [7] are shown in Fig.1. During g^*=0.8 though there are parts which can be regarded as short plateaus indicating matastabe states (at 1.49th and 1.53th MCCs), over all shape is seemingly as indicating a single relaxation. During g^*=0.9 the former half portion exhibits a single relaxation and the latter half portion does having reached at the full relaxation. Evolutions of the center of gravity during g*=0.8 and 0.9 of other series of simulations are almost the same as Fig. 1. While evolution of the center of gravity during g^*=1.1 of the series of simulations we reported in Ref. [7] exhibited more rapid lowering, we observe a multiple relaxation, resembling Fig. 1 (b) and more pronounced, for other series.

In Fig. 2 we show snapshots of the series of simulations of Ref. [7]. The lower half portion is almost the same as that of the snapshot at g^*=0.7 (Ref. [7]). Also that at larger g^* is almost the same. This indicates that the upward motion of the upper boundary of the less-defective region is pinned at twelve-layer thick by a certain sessile structure of a complex of the defects. We observe also the pinning of the region of two-layer thick, in which the defect disappeared in the both side views. Fig. 3 are snapshots of a series of simulations other than Ref. [7]. The pinning of the region of two-layer thick, in which the defect disappeared in the both side views, is also observed. We cannot necessarily say that in the colloidal epitaxy using a square pattern the defect appearance smoothly occurs.

Concluding remarks

Conclusions of Ref. [7] have been partially rewritten: The square pattern on the bottom wall can, but not necessarily, lower g^* at which defect disappearance occurs. During such g^* the evolution of the center of gravity is of a single relaxation. That is, the stacking disorder shrinks without temporally trapping by a metastable state. At lager g^* a multiple relaxation can occur, as so for the case of flat bottom wall. Pinning of the upward motion of the upper boundary of the less-defective crystal region occurs.

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