Stochastic model showing a transition to self-controlled particle-deposition state induced by optical near-fields

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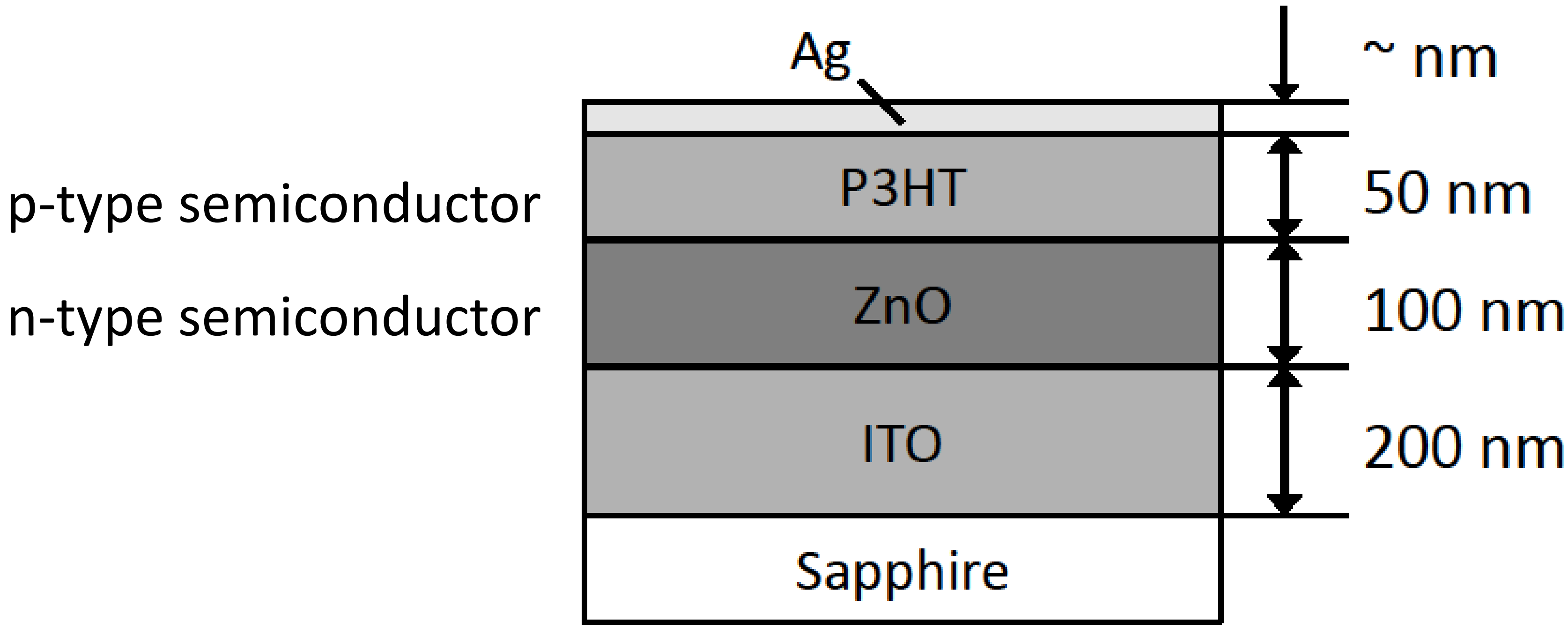
CONTENTS

Introduction

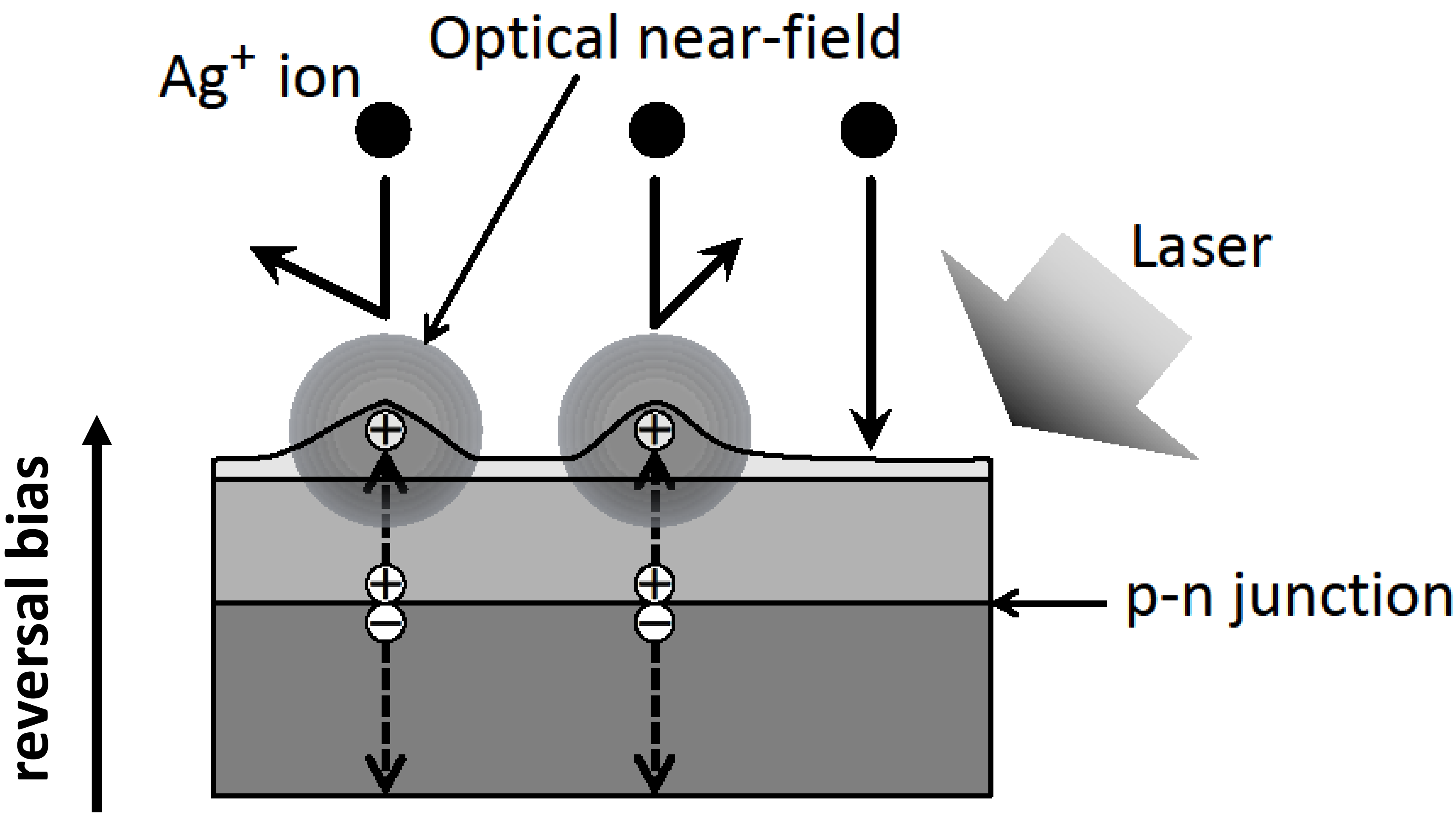
- Nanophotonics, which investigates light-matter interactions on the nanometer scale, has been intensively studied from a variety of aspects ranging from fundamental interests to applications.
- Precision control of the geometrical features are important in realizing valuable functionalities.
- The nanophotonics fabrication-principles and techniques have been providing interesting and important light-assisted, self-controlled nanostructures.
- Stochastic modeling is very useful in order to obtain deeper understanding of the underlying physical process.
- We develop the cellular automaton model (Naruse et al. 2011), which was introduced to simulate self-controlled pattern formation of Ag film (Yukutaka et al. 2010) on the electrode of their photovolatic device.

Introduction



Cross-sectional structure of photovolatic device (Yukuataka et al. 2010)

Introduction



Introduction

- $L \times L$ square lattice $\Lambda_L = \{1, 2, \cdots, L\}^2$
- Discrete time $t \in \mathbf{N}_0 \equiv \{0, 1, 2, \cdots\}$
- $n_t(\mathbf{r})$ = the number of deposited particles at site

  $n_t(\mathbf{r}) \in \mathbf{N}_0$
- $q_t(\mathbf{r})$ = the amount of charge at site

  $q_t(\mathbf{r}) \in \mathbf{R}_+ \equiv \{x \in \mathbf{R} : x \geq 0\}$

$$V(x) = \sum_{r \in \Lambda_L} a \frac{q_t(r)}{|x-r|}$$

- $C_t(\mathbf{r}) = \{\boldsymbol{r'} \in \Lambda_\mathrm{L} : \boldsymbol{r} \text{ and } \boldsymbol{r'} \text{ are connected}\}$
- a = effective coupling constant of a Coulomb potential
- b = strength of illumination of light per site
- E_{th} = threshold energy for deposition on the surface
- $\xi_t = \{(n_t(\mathbf{r}), q_t(\mathbf{r})) : \boldsymbol{r} \in \Lambda_L\}$

$$q_{t+1}(r) = \frac{1}{|C_{t+1}(r)|}\left\{ \sum_{r' \in C_{t+1}(r)} q_t(r') + b|C_{t+1}(r)|\, f(|C_{t+1}(r)|) \right\},$$

Introduction

The main result of our numerical simulation of the model is that, when the lattice size *L* is large but finite, there are two district mesoscopic state.

- Phase A : If Ag clusters on the surface are formed with a proper size *s such that* $(s-s_0)^2 \leq \sigma^2$, then the optical near fields are induced efficiently and hence the total positive charge on the surface increases monotonically in time. It causes strong suppression of further deposition of Ag on the surface and then the deposition will be stopped. As a result, a unique Ag film is formed.

- Phase B : If sizes of Ag clusters on the surface tend to deviate from s_0 *by more than* σ*, the* optical near fields are not induced efficiently. In this case the charges on the surface will be saturated and the suppression of deposition of Ag on the surface remains weak. Hence the deposition process will continue without any self-control and unique Ag film is not formed.

Model process

- 1 : Choose a site x randomly
- 2 : Calculate the repulsive Coulomb potential $V(x)$

  -i). If $V(x) <= Eth$, $x^* = x$

  -ii). If $V(x) > Eth$, $y0 = x$,

  redefine : $x = \{y: |y0-y|=1, V(y) < V(y0)\}$

  back to " 2: "
- 3 : Deposition at x^* ･･･ $nt+1(x^*) = nt(x^*)+1$
- 4 : The charge (depending on the cluster size)

  is added in every site

Model parameter

- $L \times L$:ΛL
- s0 :the characteristic size of the cluster

  ・・・ the efficiency of the optical near-field for charging cluster is maximized
- σ^2:a characteristic size-variation

  ・・・ (s0-s)^2 > σ^2 : low efficiency

→f(s):function of size dependence

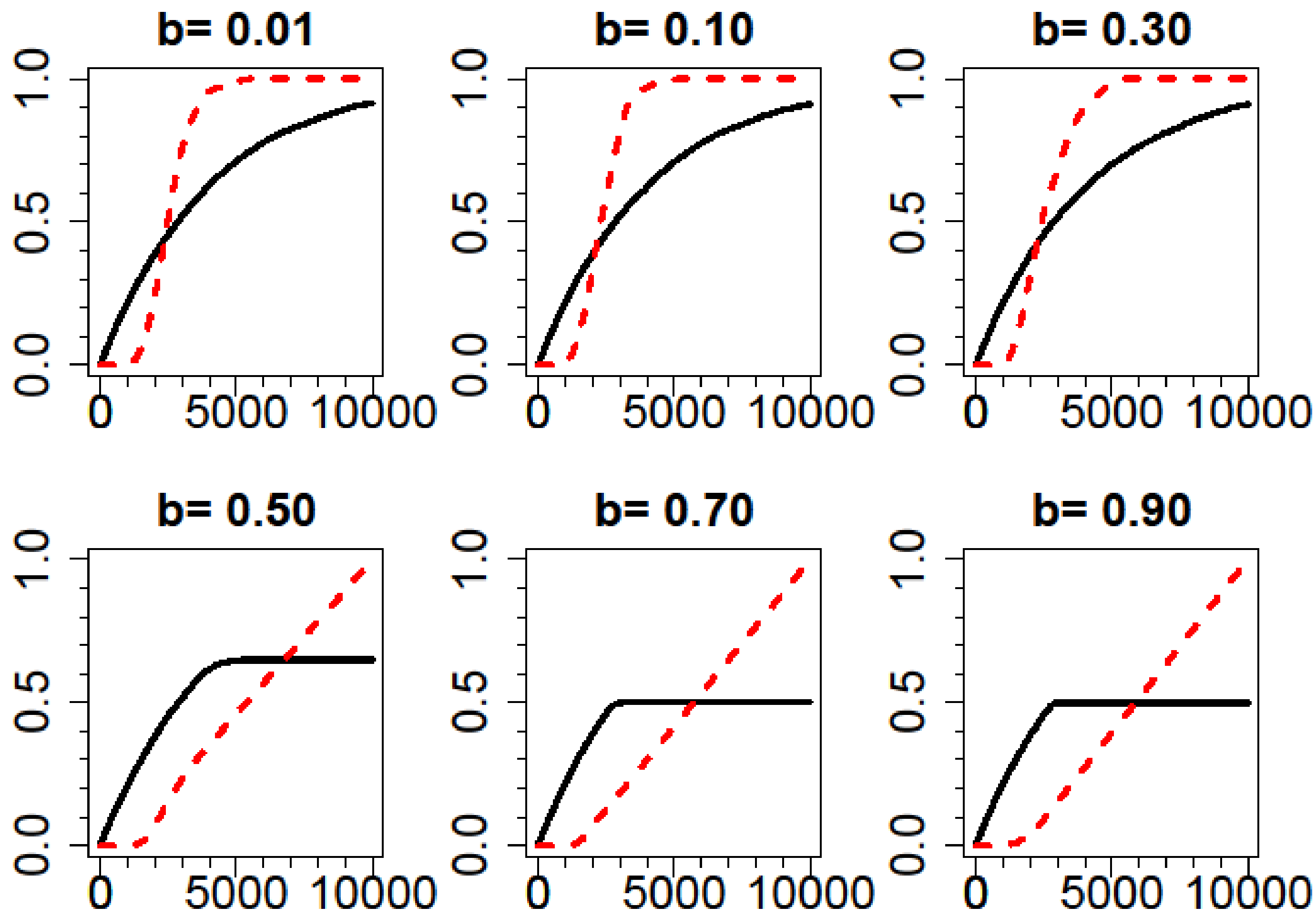
  ・・・ $f(s) = \exp[-(s-s0)^2 / 2\sigma^2]$
- a :effective coupling constant of a Coulomb potential
- b :strength of illumination of light per site
- E_{th} :threshold energy for deposition on the surface

Two stochastic variable

- nt(r):the number of deposited grain
- qt(r):the amount of charge per site

Simulation results

▪Two states :

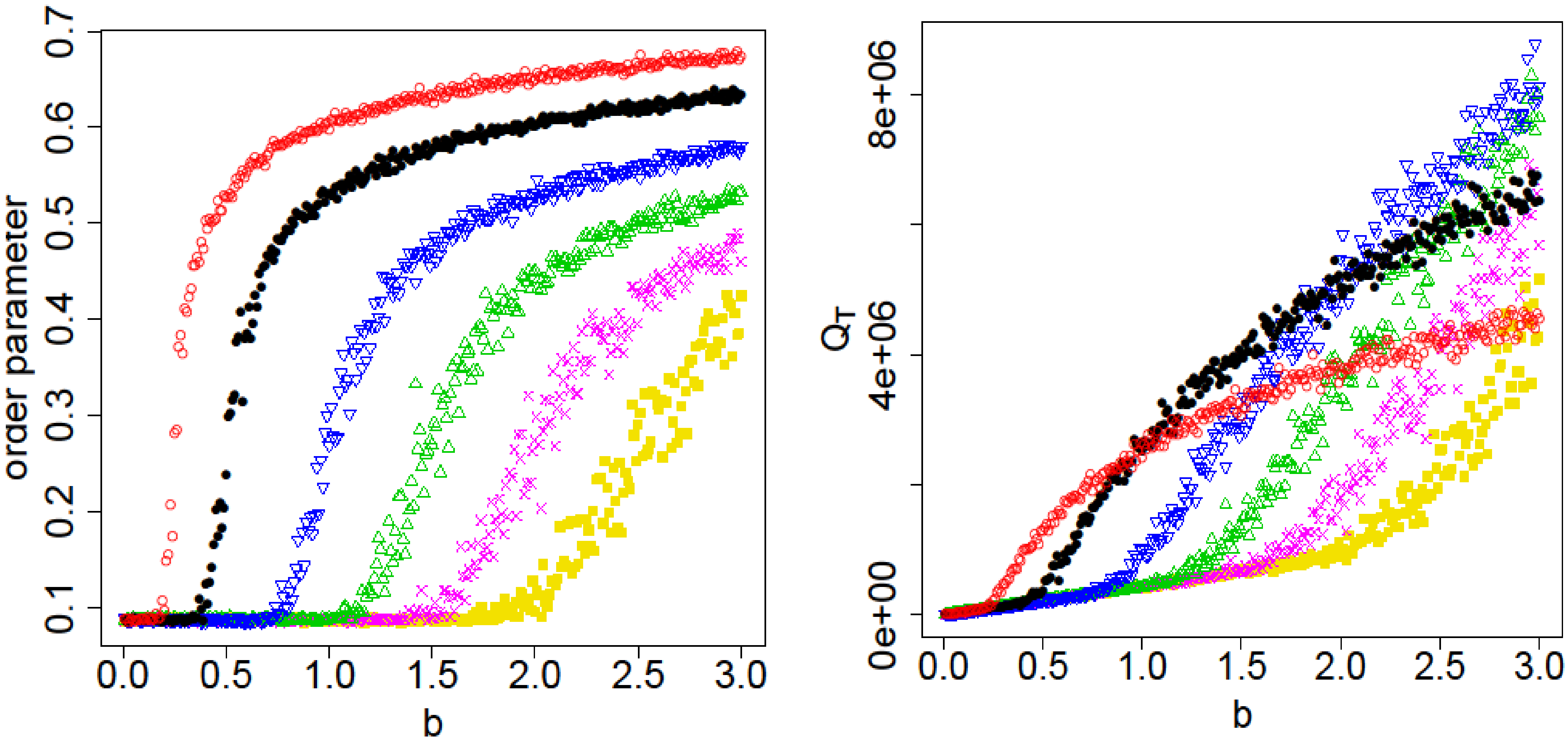


●: the occupation ratio, $R_t = A_t / L^2$

●: normalized total charge, $Q_t^{(T)} = Q_t / Q_T$

Simulation results

・Order parameter and critical exponent :

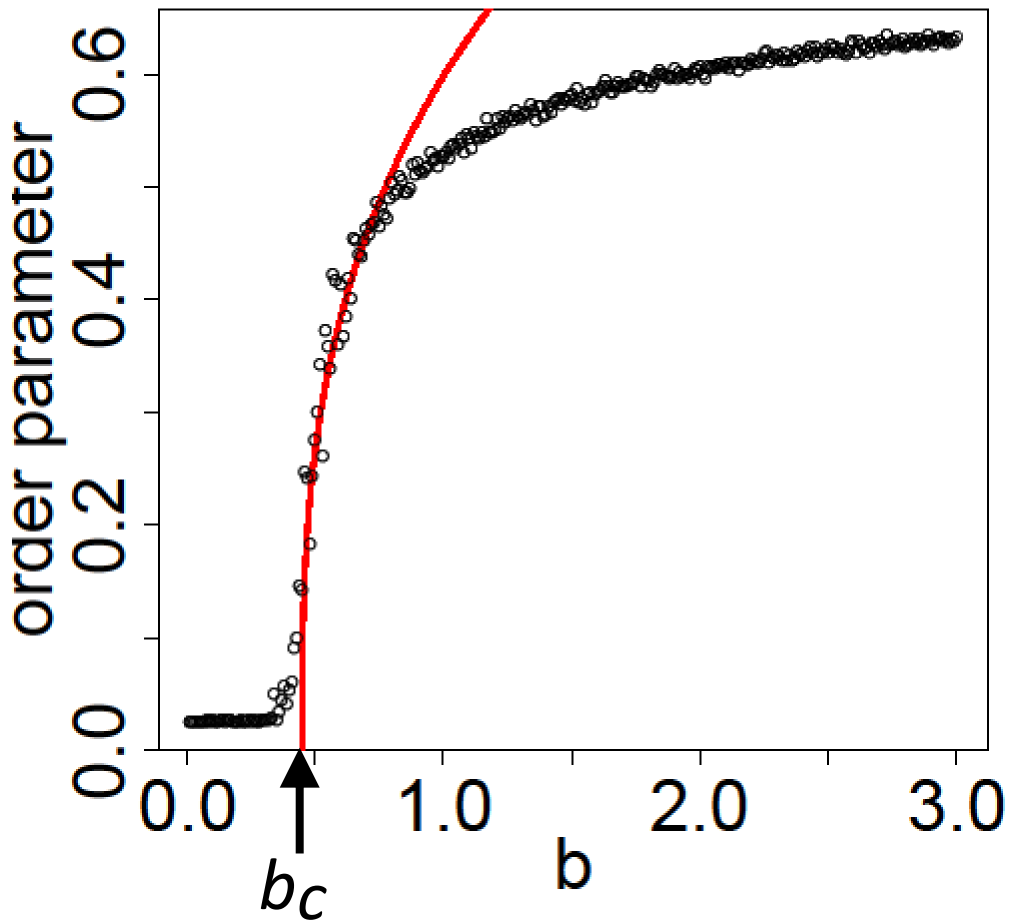


E_{th} = {○ : 5 ● : 10 △ : 20 ▽ : 30 × : 40 ■ : 50 }

Order parameter : $\rho_0 = 1 - R_\infty$

Simulation results

- Order parameter and critical exponent :

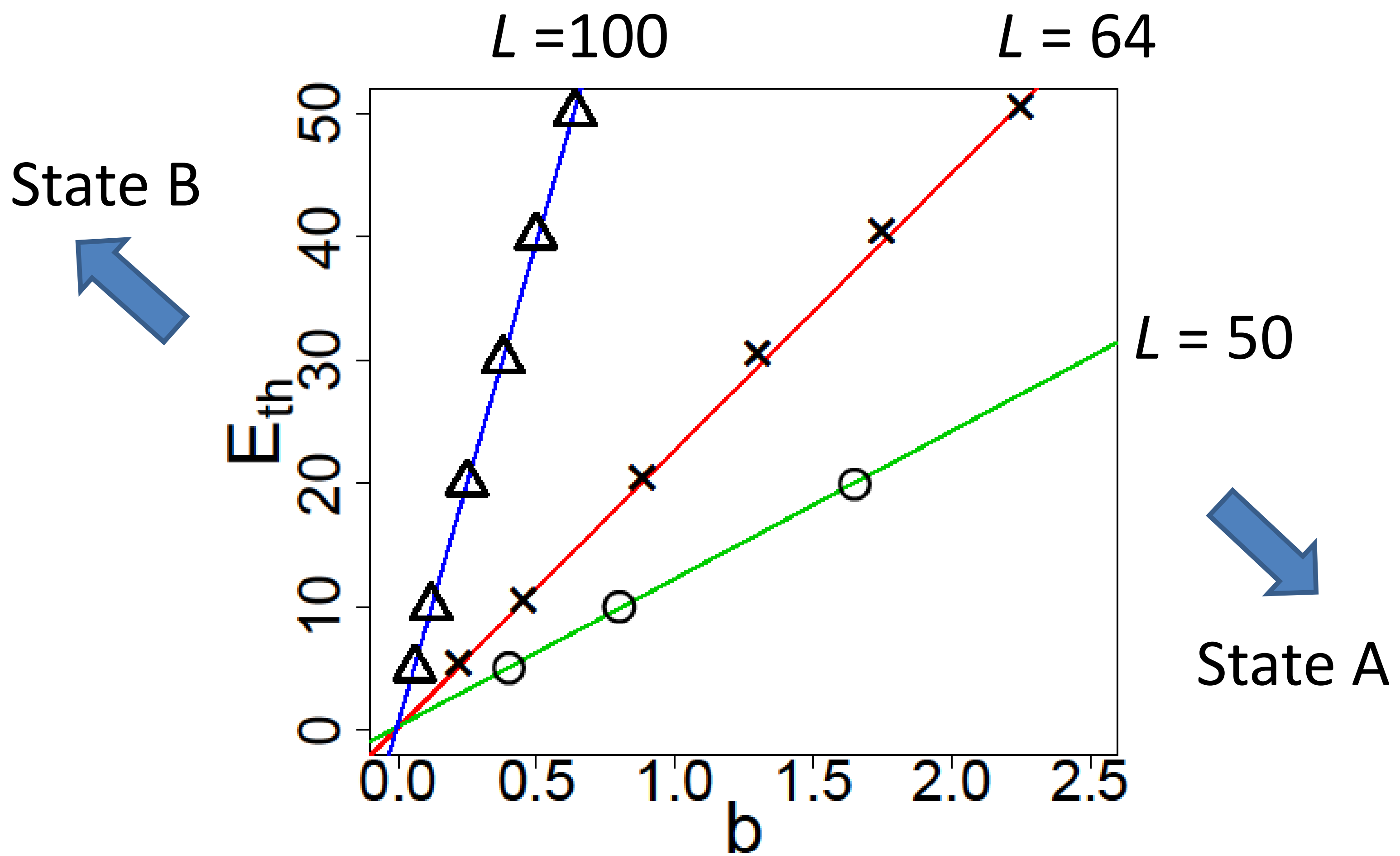


$$\rho_0 \sim (b - b_c)^{\beta} \;, \quad 0 < b - b_c \ll 1$$

$b_c = 0.44$, $\beta = 0.34$ for $E_{th} = 10$

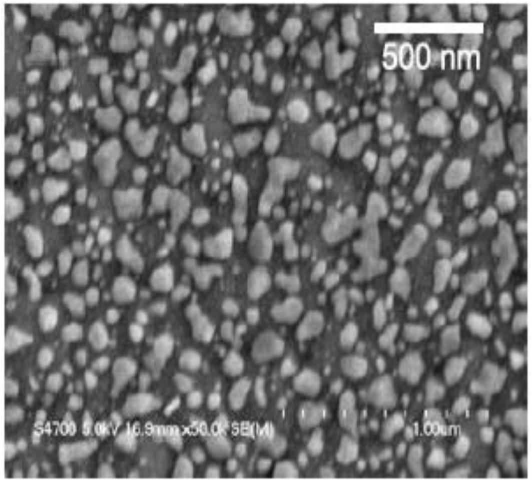
Simulation results

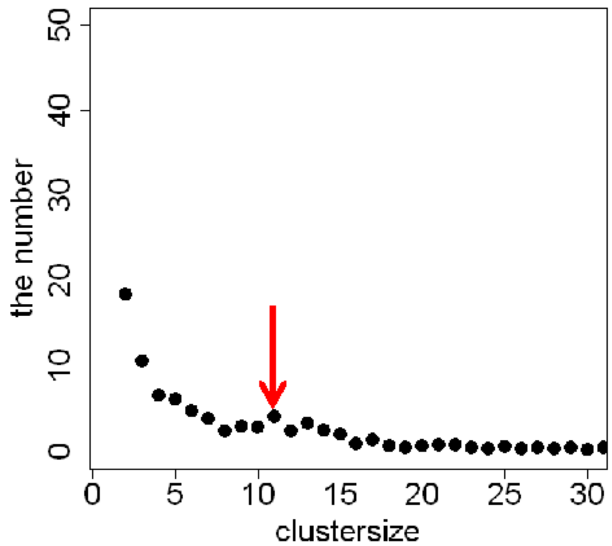
- Critical line between State A and State B :

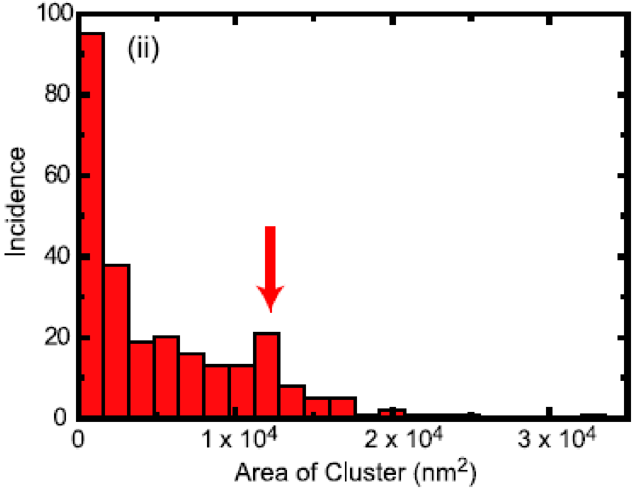


Simulation results

▪ Cluster structures in State A :







Quotation : S.Yukutake , et al , Appl. Phys. B **99** (2010) 415.
: M.Naruse , et al , Appl. Phys. B **105** (2011) 185.