Modelling
of
Microstructural Evolutions
in
Structural Materials

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   Target
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   grain growth, spinodal decomposition
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   3-D multiscale, Nanostructural materials

Problems

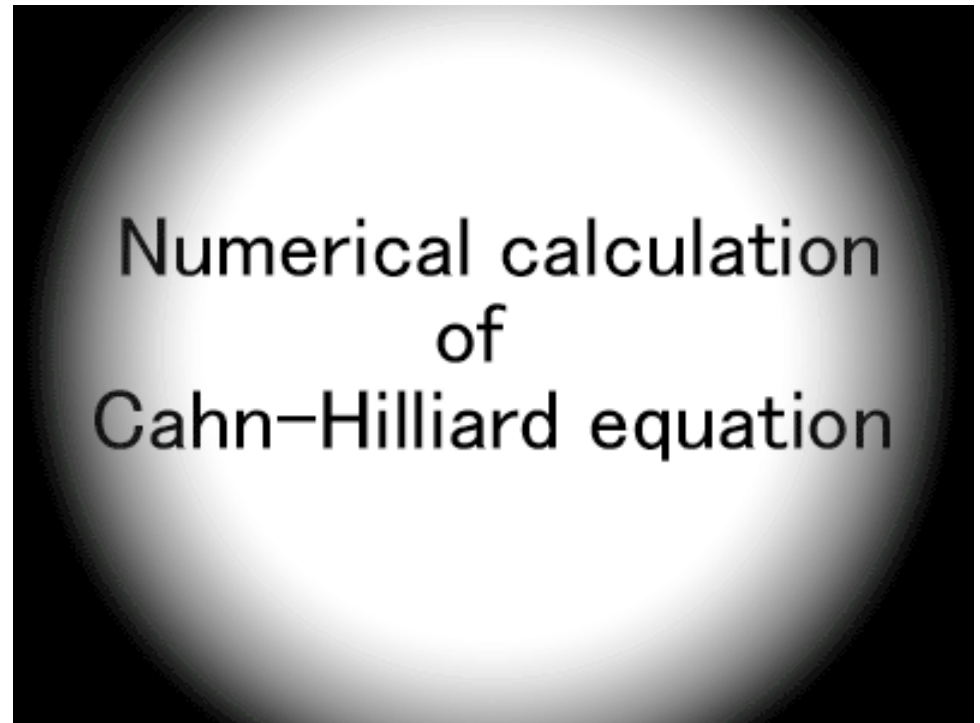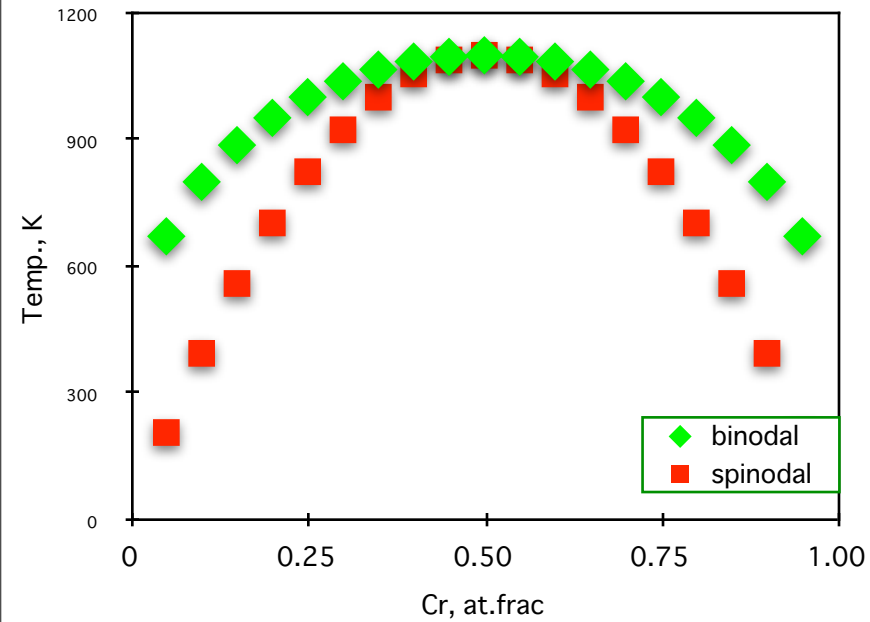## Modelling of microstructural evolutionds in structural steels

- **Synergetic effects**

 grain growth, recrystallization, second phase precipitation, spinodal decomposition, γtoα phase transformation,
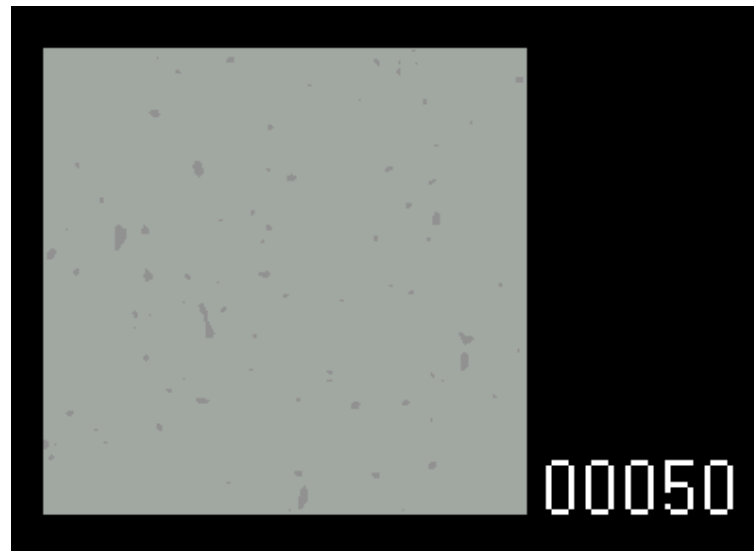
- **Multiscale**

  several nm to several handeredsμm

- **Multicomponent system**

Phase separation

Grain growth

Modelling of microstructural evolution in structural steel

- 1st stage(1985-1995)

  Integrated model based on thermodynamics and

  phase transformation theory

- 2nd stage(1995-2005)

  MC, PF for Grain growth, Spinodal decomposition etc.

- 3rd stage(2005-)

  Multiscale 3-D simulation for microstructural
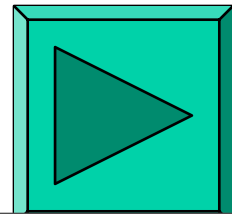
  evolution in structural steel.

Computational Models based on Thermodynamics and Phase Transformation Theory

1. **Theories of Microstructural Evolution**

    Nucleation, Growth and Interface Migration

2. **Integrated Models for Predicting Microstructural Evolution in HSLA steels**

    Grain growth, Precipitation, Phase Transformation

Modelling of microstructural evolution in structural steel

- 1st stage(1985-1995)

  Integrated model based on thermodynamics and

  phase transformation theory

- 2nd stage(1995-2005)

  MC, PF for Grain growth, Spinodal decomposition
  etc.

- 3rd stage(2005-)

  Multiscale 3-D simulation for microstructural

  evolution in structural steel.
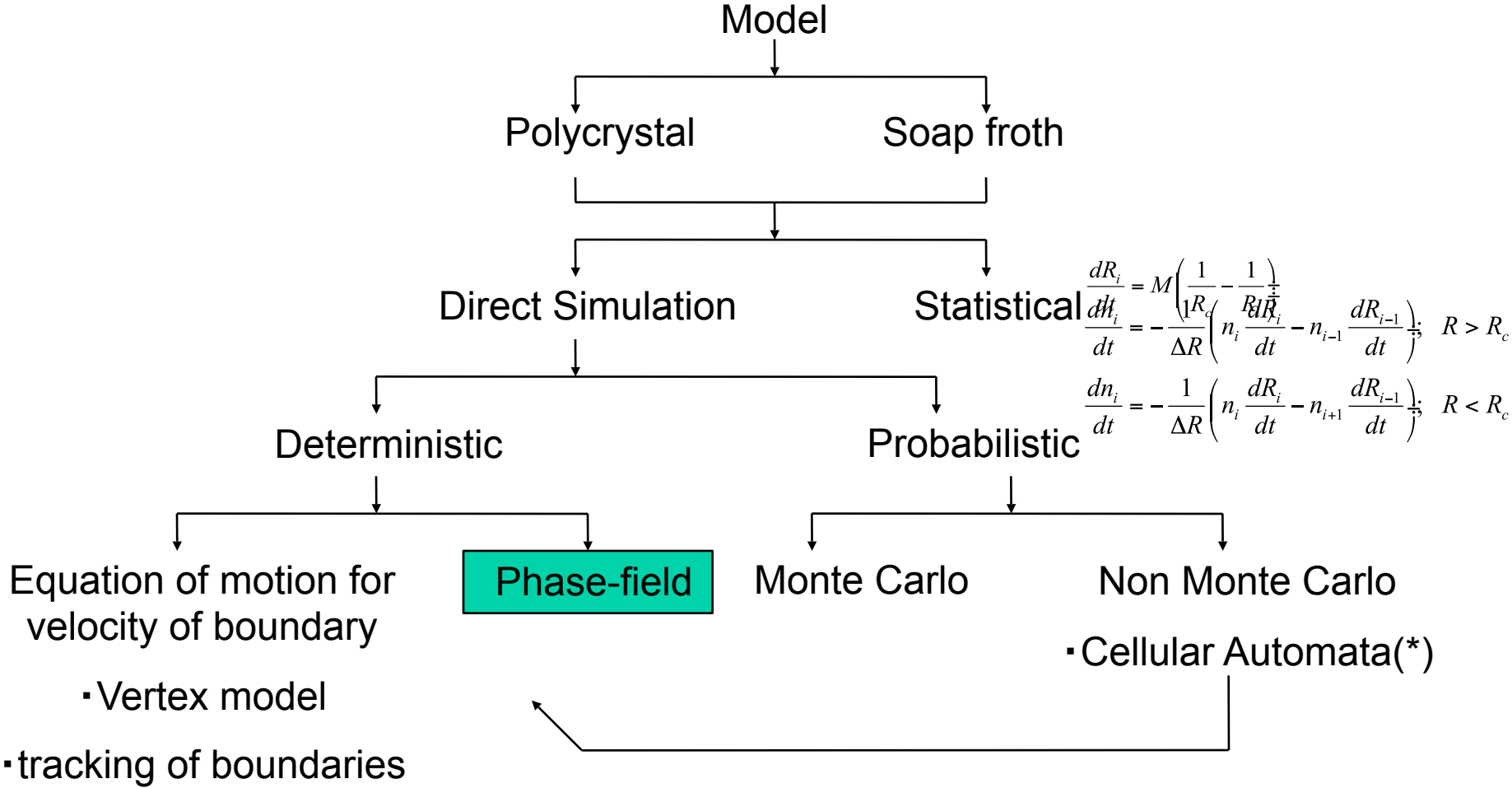
Computer Simulation

- Discrete   model

    Monte Carlo method

- Continuum   model

    Phase field model

Grain Growth

Classification of simulation models

Model

Polycrystal   Soap froth

Direct Simulation   Statistical

$$\frac{dR_i}{dt} = M\left(\frac{1}{R_c} - \frac{1}{R_i}\right)$$

$$\frac{dn_i}{dt} = -\frac{1}{\Delta R}\left(n_i\frac{dR_i}{dt} - n_{i-1}\frac{dR_{i-1}}{dt}\right); \quad R > R_c$$

$$\frac{dn_i}{dt} = -\frac{1}{\Delta R}\left(n_i\frac{dR_i}{dt} - n_{i+1}\frac{dR_{i-1}}{dt}\right); \quad R < R_c$$

Deterministic   Probabilistic

Equation of motion for velocity of boundary   Phase-field   Monte Carlo   Non Monte Carlo

・Cellular Automata(*)

・Vertex model

・tracking of boundaries

Simulation of Grain Growth by

We can write the total free energy of an inhomogeneous system in terms of all the orientation field variables and their gradients as:

$$F = \int \left[f_0\left(\eta_1, \eta_2, \cdots\cdots, \eta_p \right) + \frac{1}{2} \sum_{i=1}^{p} k_i (\nabla \eta_i)^2 \right] dV$$

f_0 : the local free energy density

k_i : the gradient energy coefficients

p : total number of orientation field variable

Since the orientation field variables η_i are non-conserved order parameter, the temporal evolutions of these parameters are written as follows

$$\frac{\partial \eta_i(\vec{x}, t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i(\vec{x}, t)}$$

L_i : Onsager's phenomenological parameters(mobility of a interface)

The Phase field model

Time dependent Ginzburg Landau (TDGL) equation

For conserved fileld variables

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = M\nabla^2\left(\frac{\delta F}{\delta c(\mathbf{r},t)}\right)$$

For nonconserved field variables

$$\frac{\partial \eta(\mathbf{r},t)}{\partial t} = -L\left(\frac{\delta \widetilde{F}}{\delta \eta(\mathbf{r},t)}\right)$$

The free energy functional F

$$\widetilde{F} = \int\left[(F_{chem}(c(\mathbf{r},t),\eta(\mathbf{r},t),T) + F_{elas}(c(\mathbf{r},t),\eta(\mathbf{r},t),T) + F_{int_t}(c(\mathbf{r},t),\eta(\mathbf{r},t),T)\right]d\mathbf{r}$$

Simulation of grain growth

$\eta_1(\mathbf{r}), \eta_2(\mathbf{r}), \cdots \eta_p(\mathbf{r})$; a set of orientation field variables

The total free energy functional

$$F = \int \left[f_0(\eta_1(\mathbf{r}), \eta_2(\mathbf{r}), \cdots, \eta_p(\mathbf{r})) + \sum_{i=1}^{p} \frac{k_i}{2} (\nabla \eta_i(\mathbf{r}))^2 \right] d\mathbf{r}$$

The spatial and temporal evolution of orientation field variables

$$\frac{\partial \eta_i(\mathbf{r},t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i(\mathbf{r},t)} = -L_i \left(\frac{\partial f_0}{\partial c} - k_i \nabla \eta_i \right) \quad i = 1, p$$

The Ginzburg-Landau type free energy density functional

$$f_0(\eta_1, \eta_2, \cdots \eta_p) = \sum_{i=1}^{p} \left(-\alpha \eta_i^2 / 2 + \beta \eta_i^4 \right) + \gamma \sum_{i=1}^{p} \sum_{j \neq i}^{p} \eta_i^2 \eta_j^2$$

α, β, γ are phenomenological parameters.
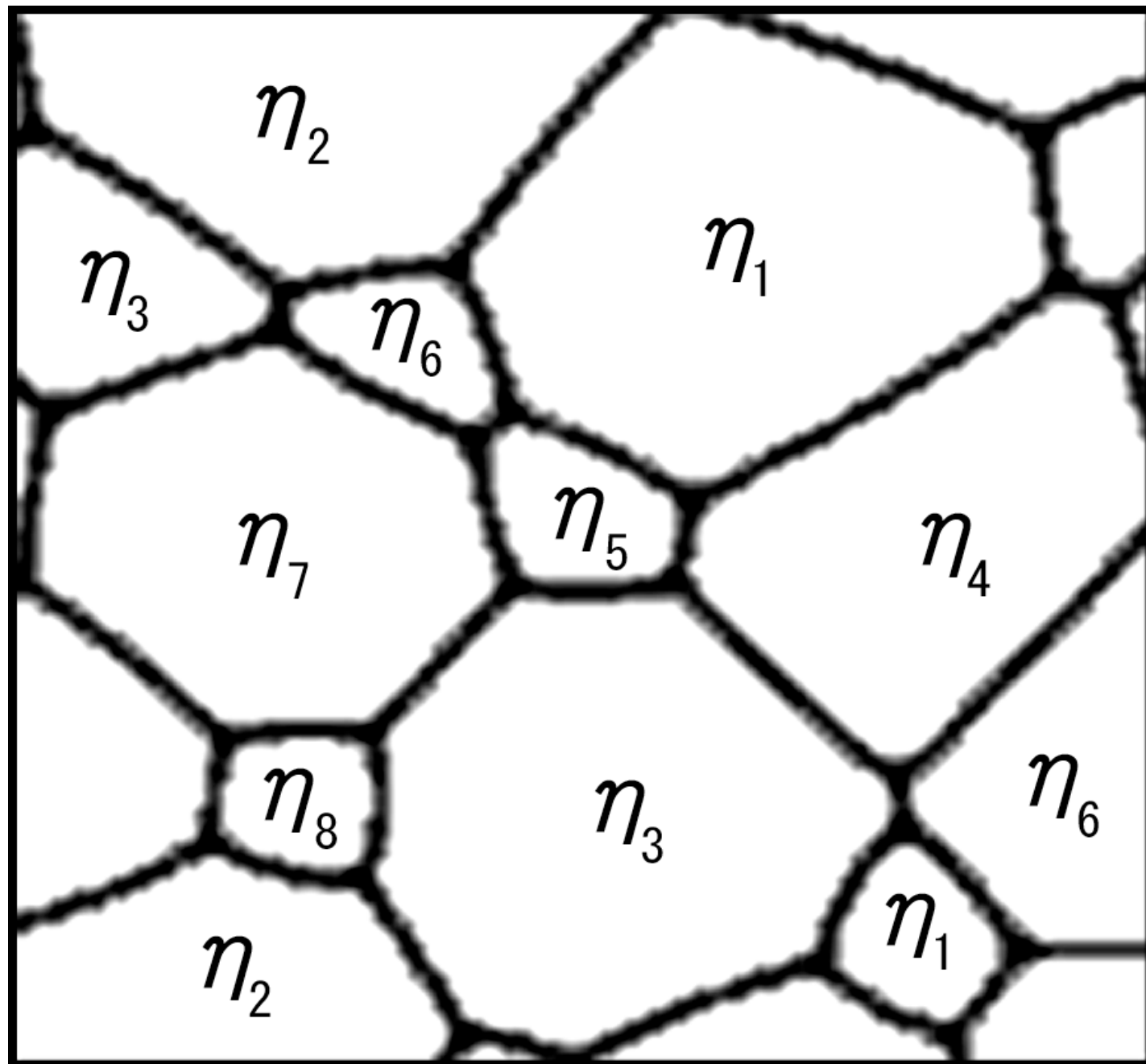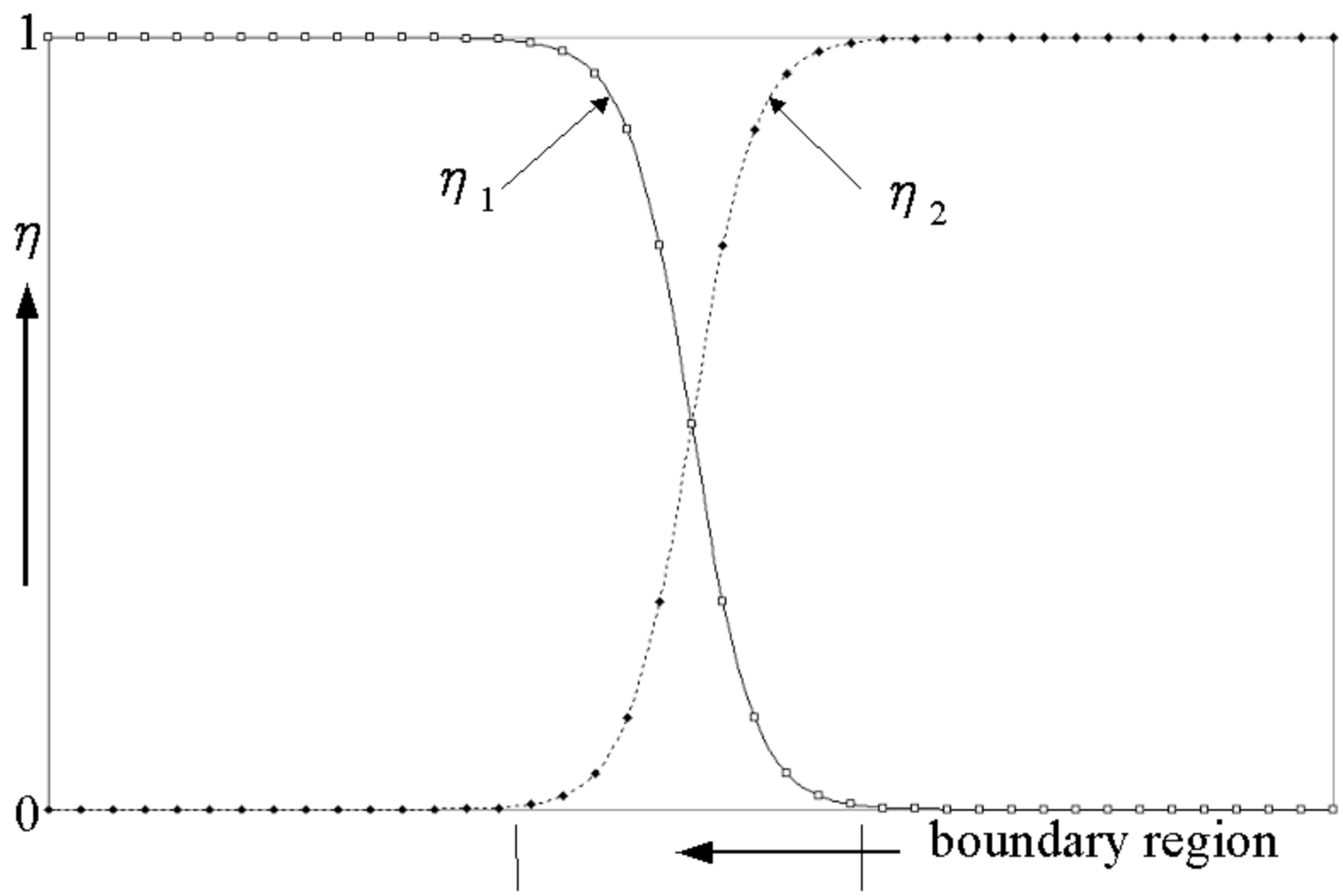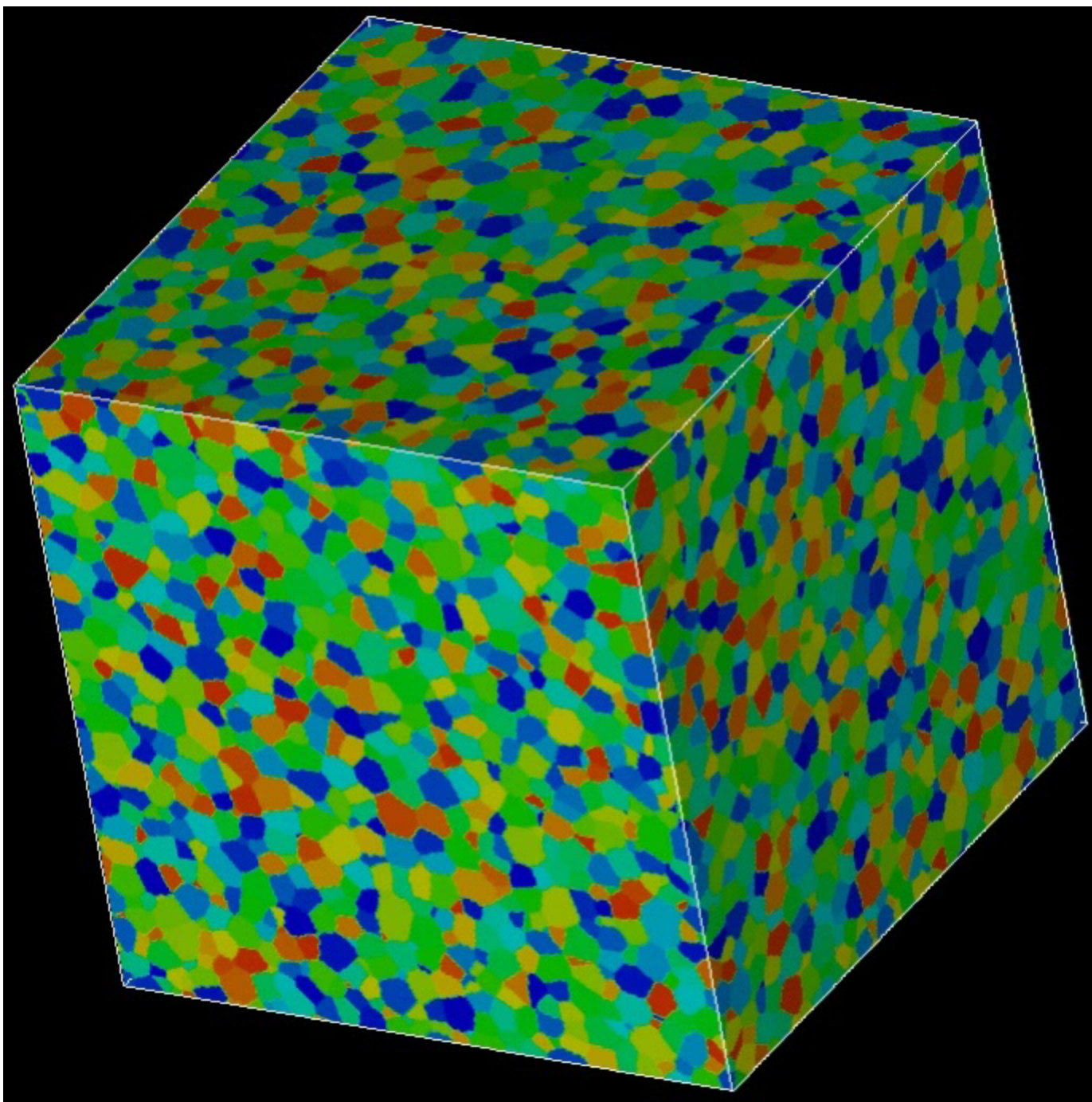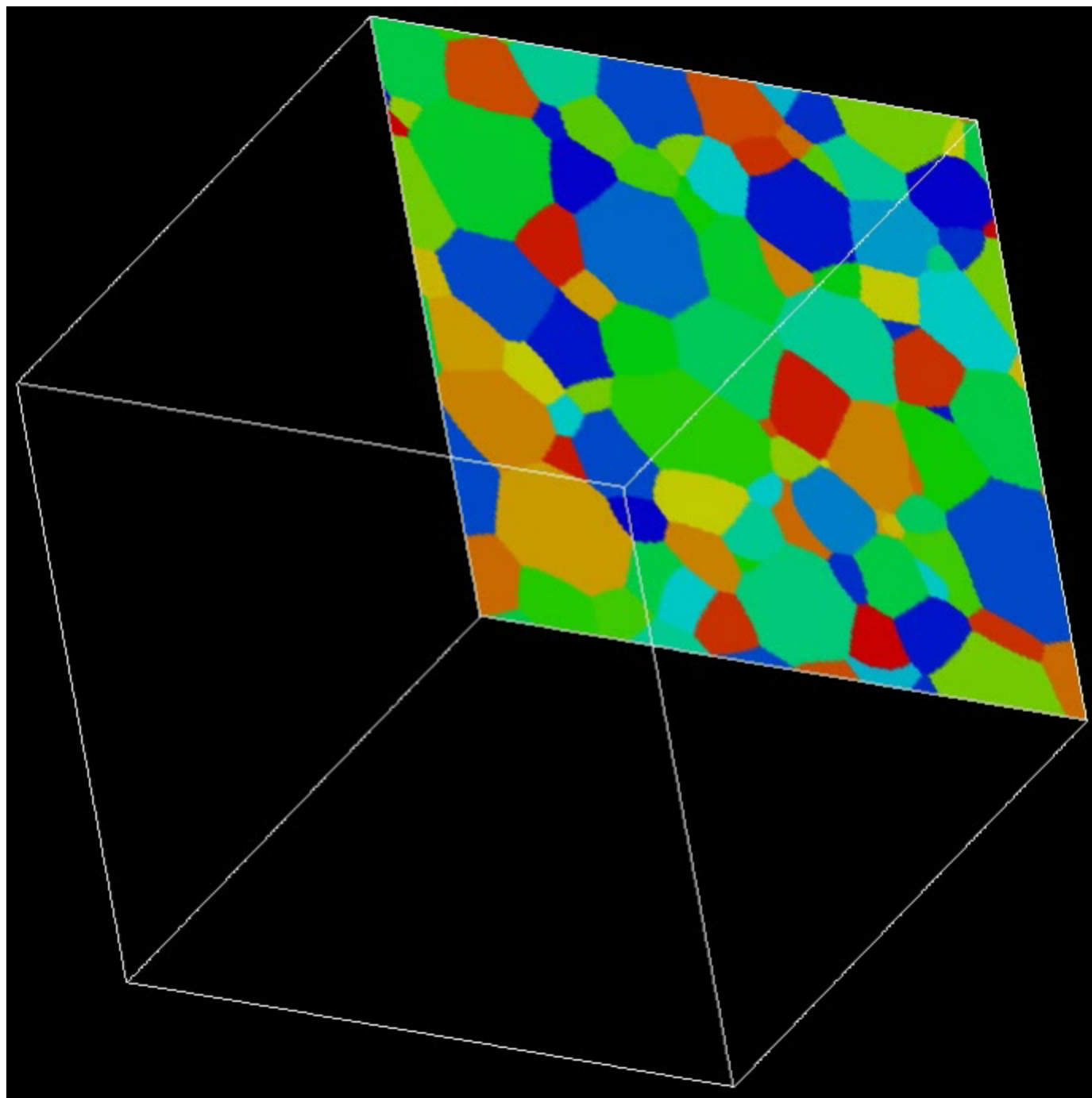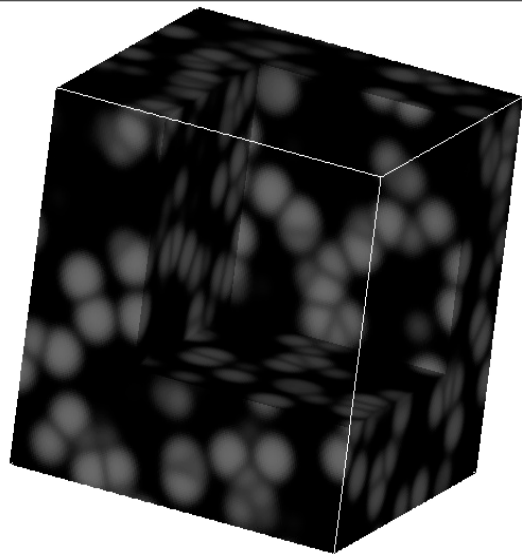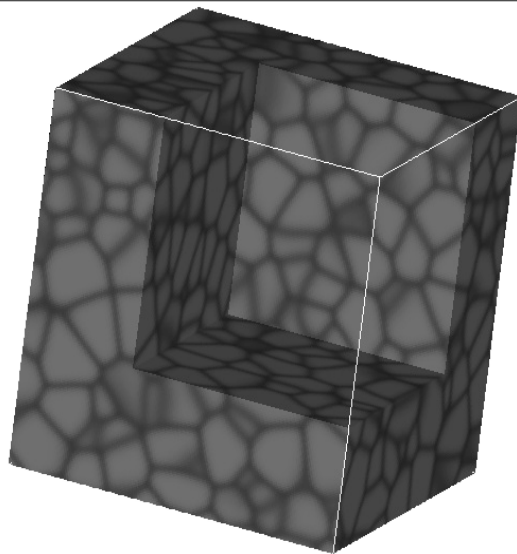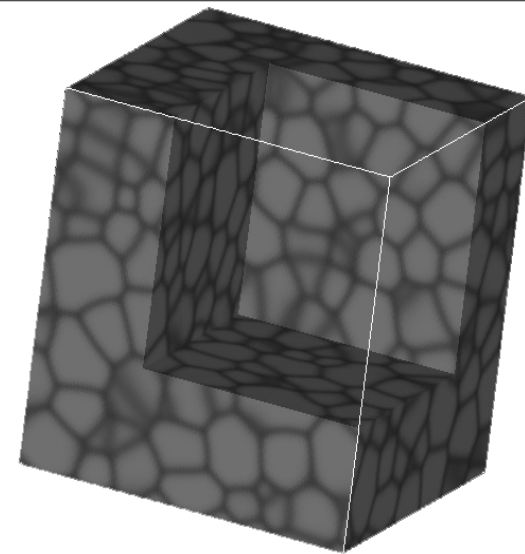
$t=10.0$ $t=20.0$ $t=50.0$
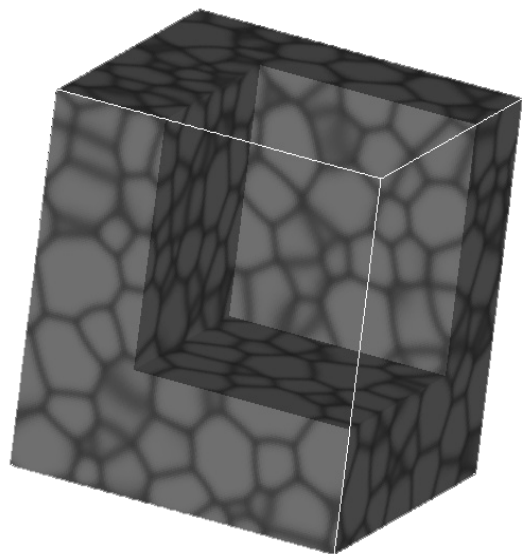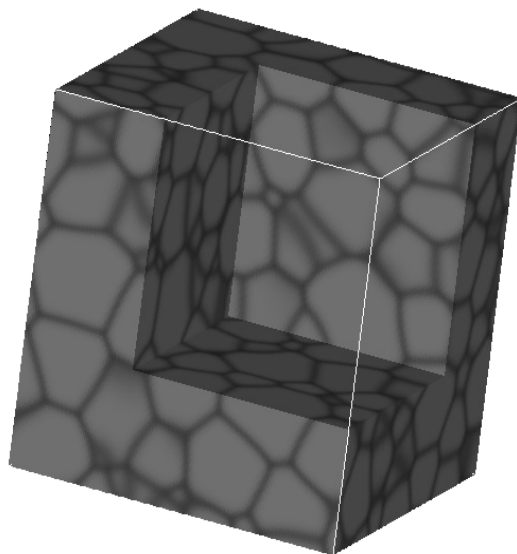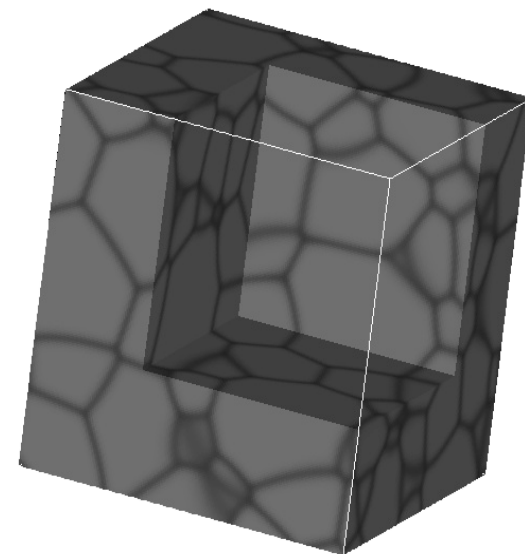
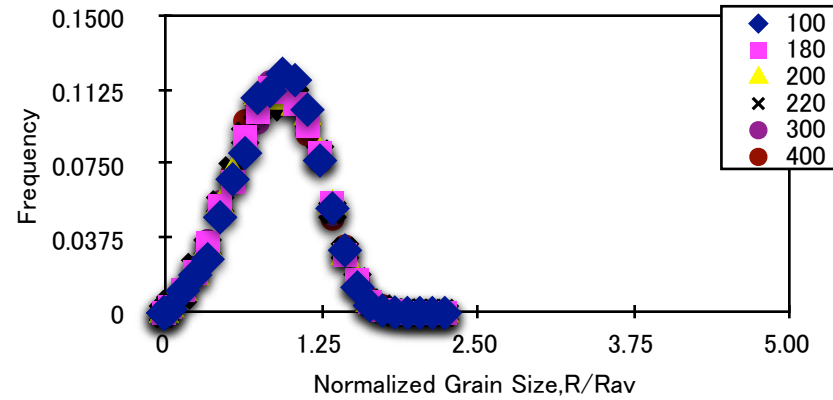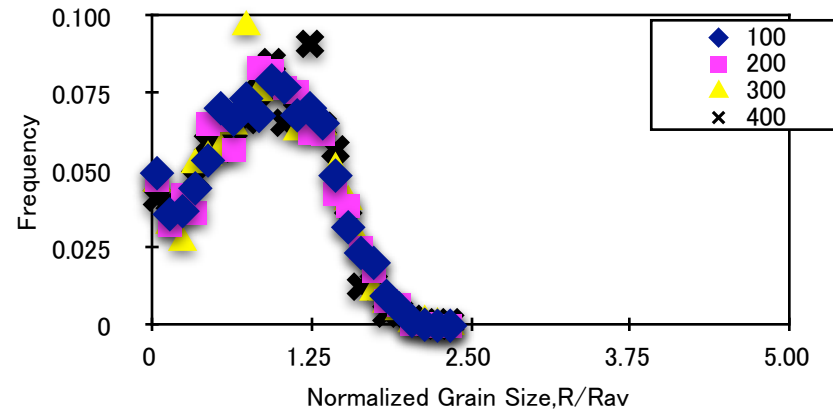$t=100.0$ $t=200.0$ $t=500.0$
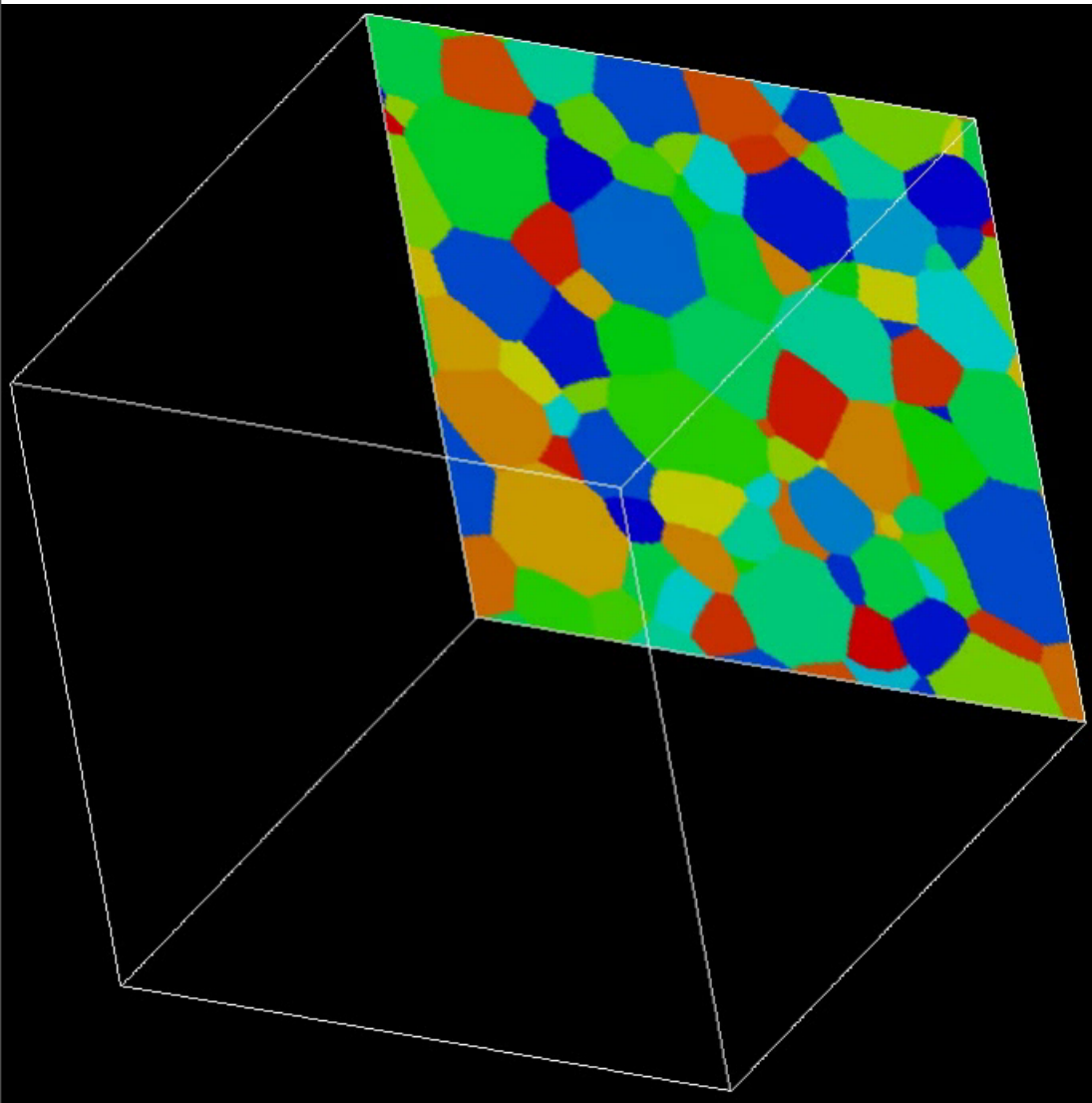
−Isotropic Grain Growth

・3D-simulation
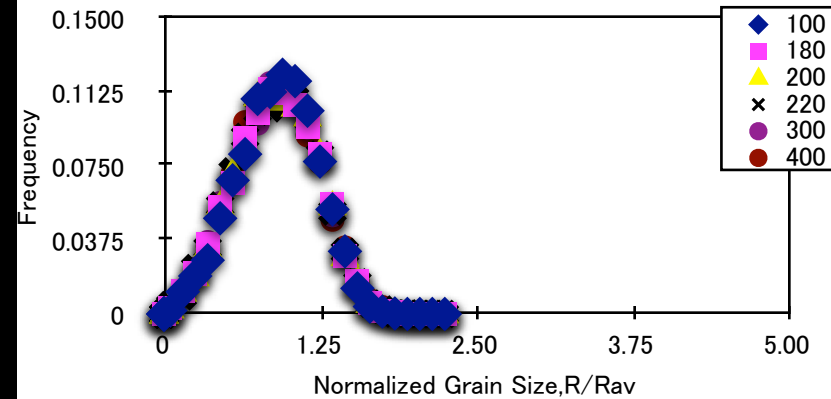
・2D cross section of 3D simulation

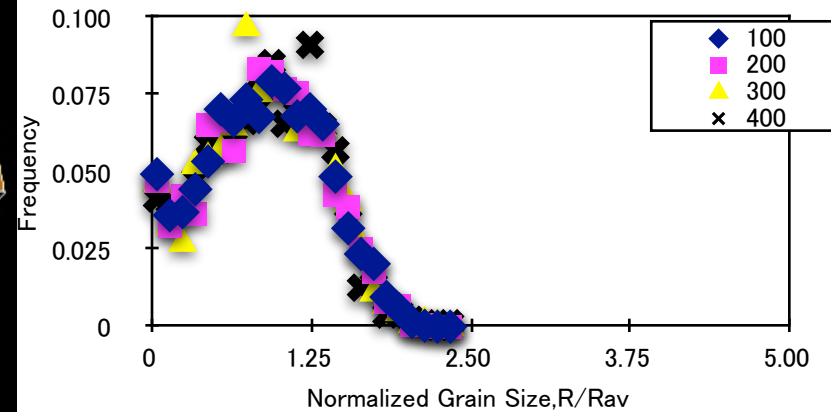Variation in the scaled grain size distribution function

System size : 320^3

–Isotropic Grain Growth
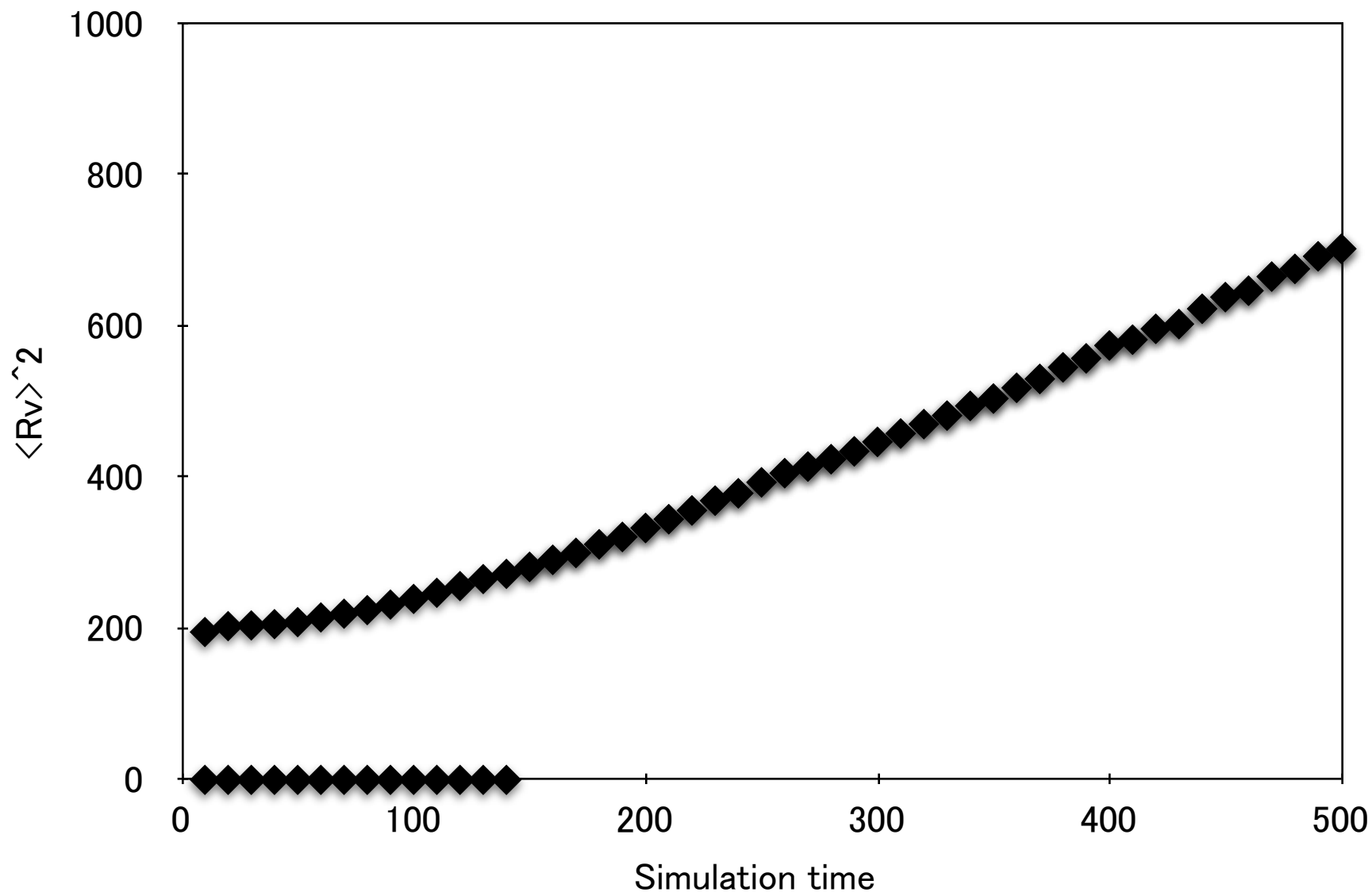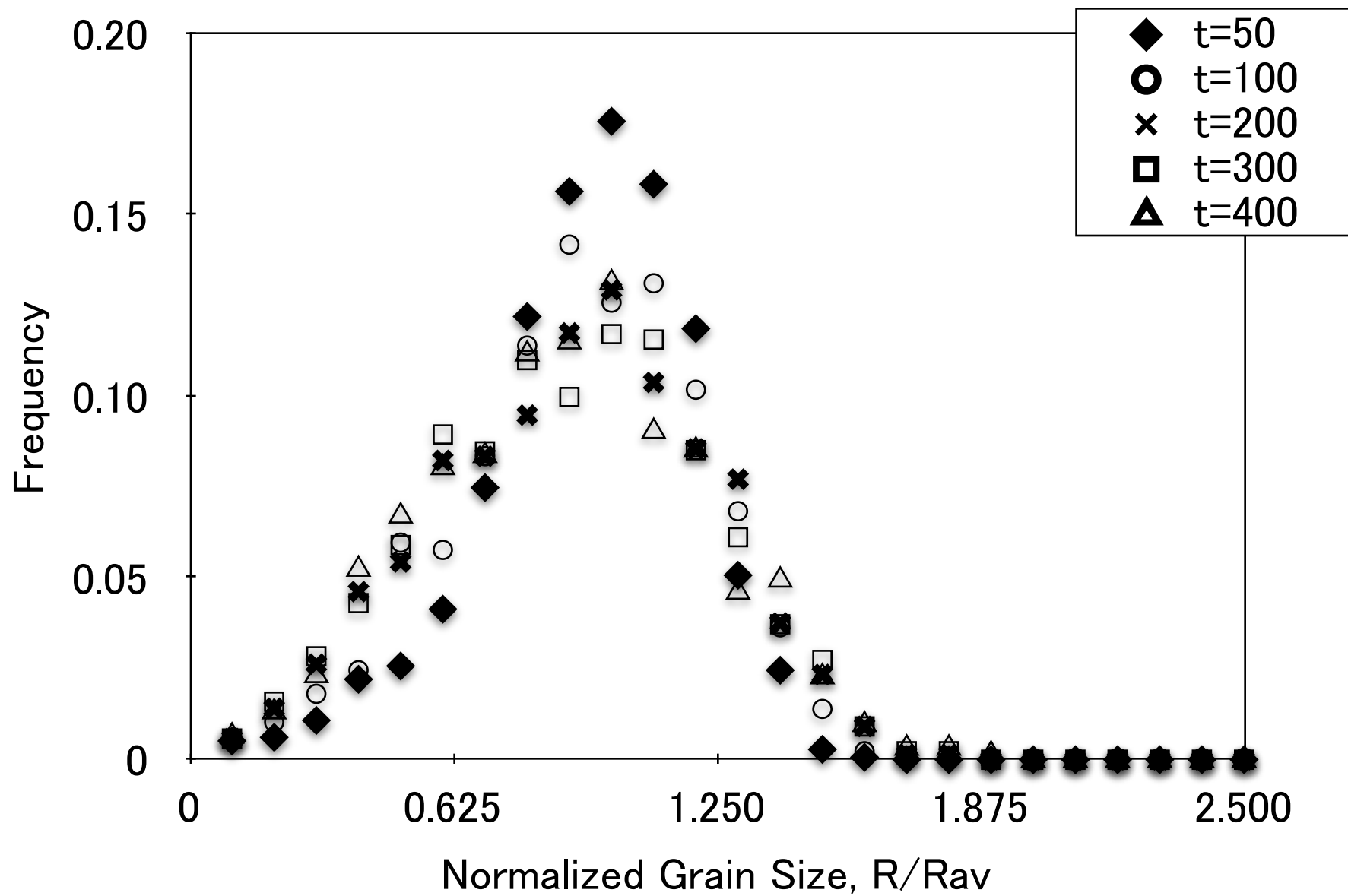

System size : 320^3

・3D-simulation

・2D cross section of 3D simulation

Variation in the scaled grain size distribution function

Figure: Frequency vs. Normalized Grain Size, R/Rav, for t=50, t=100, t=200, t=300, t=400.
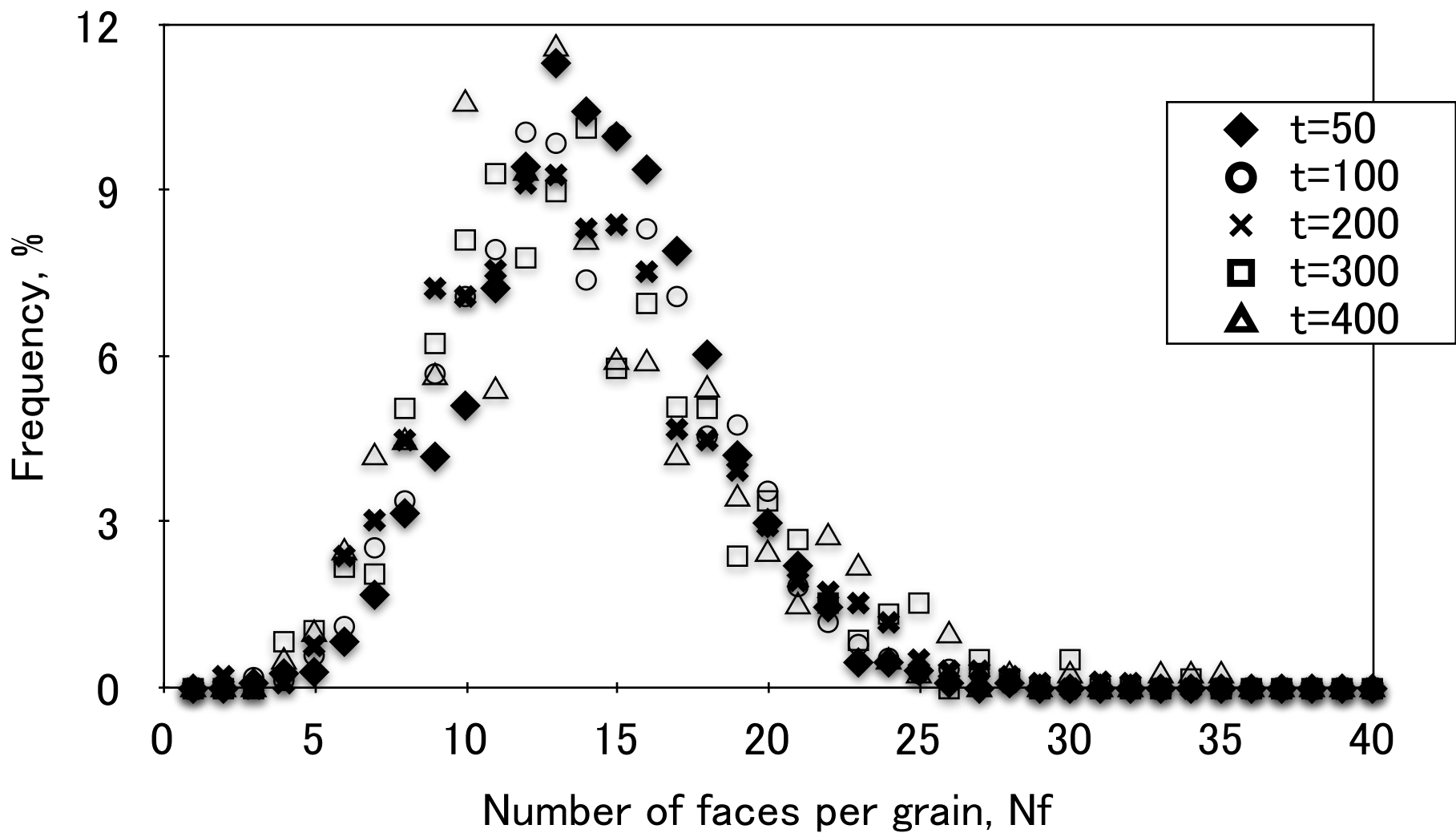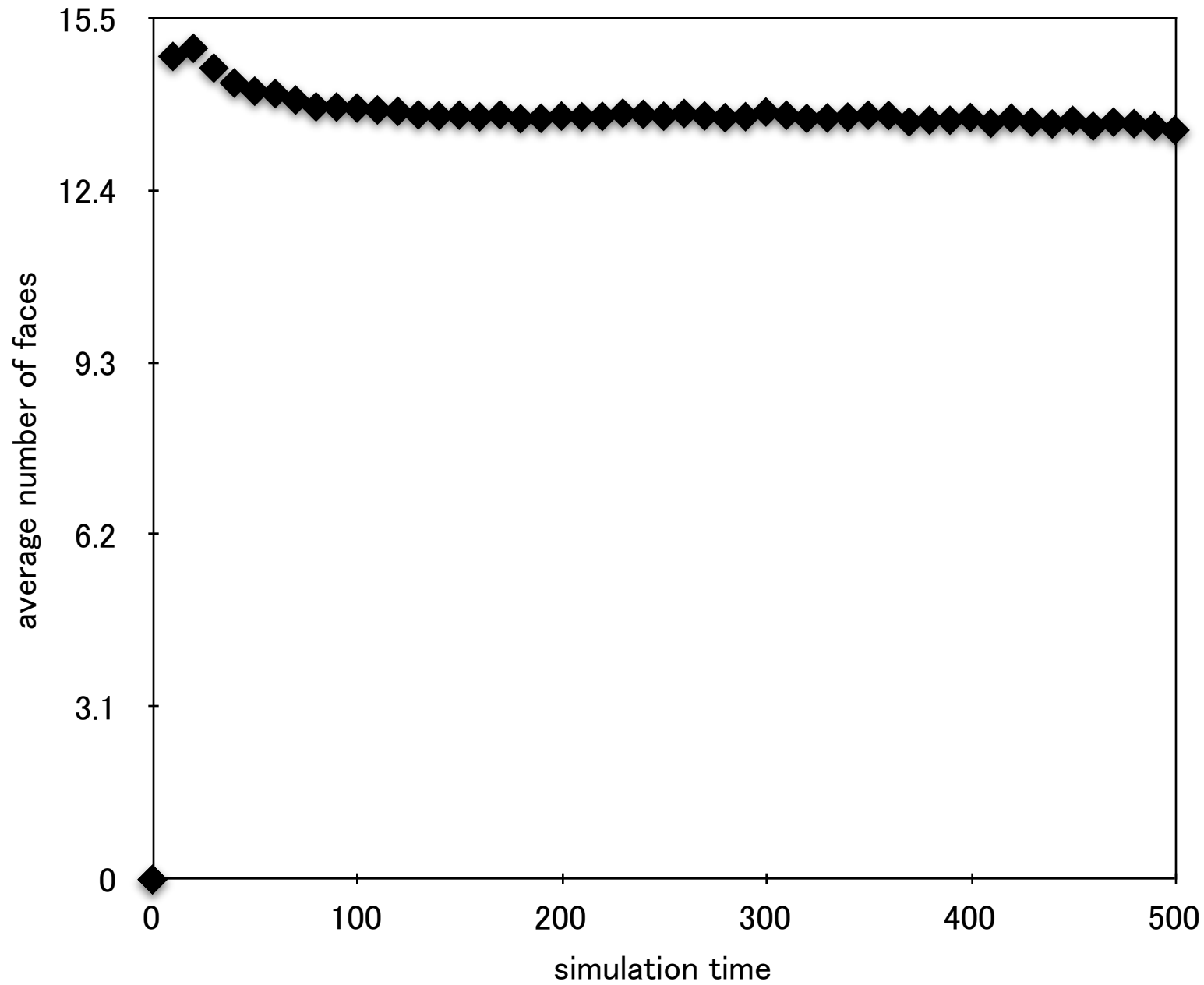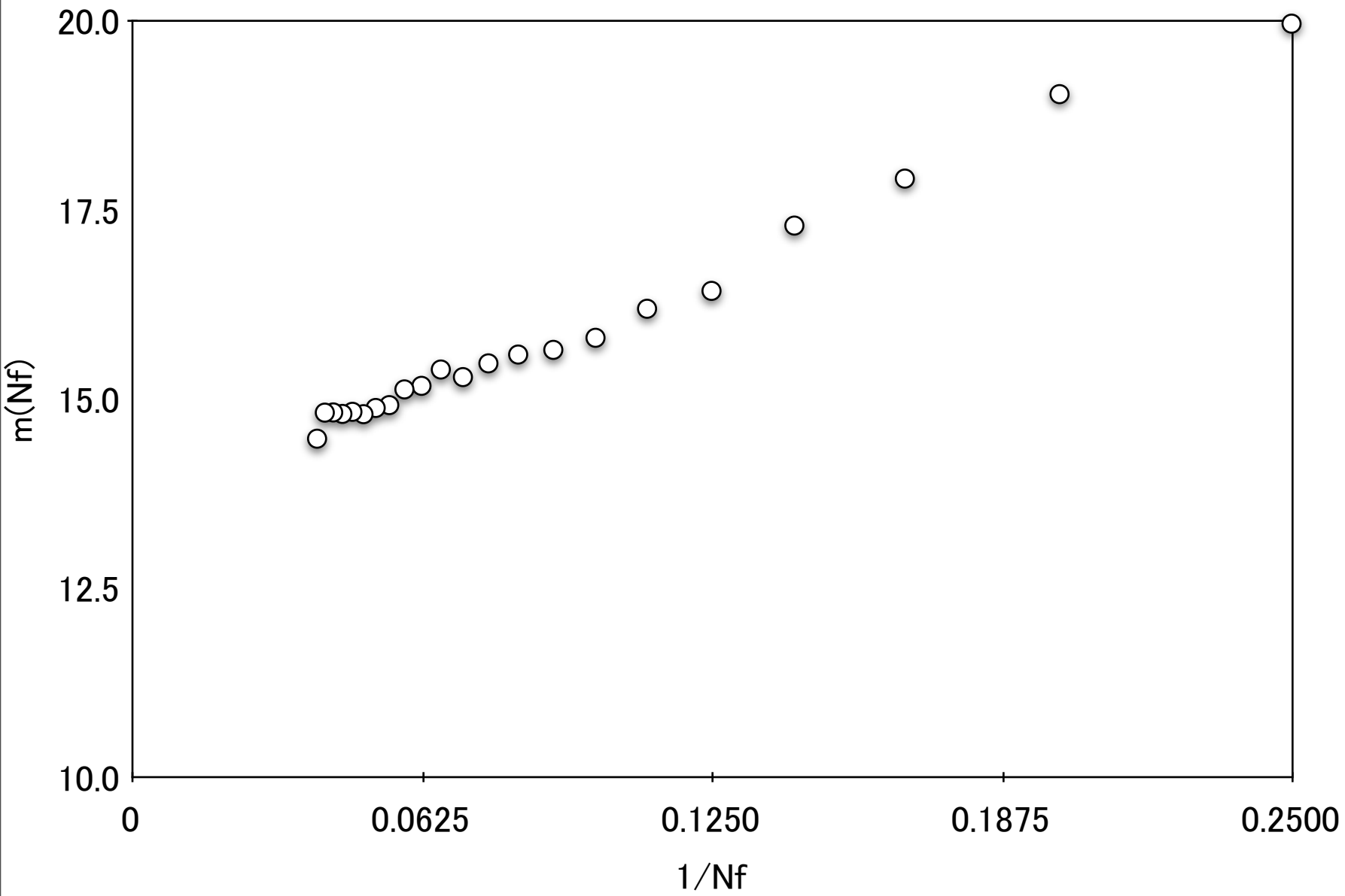
Simulation of Grain Growth
by

The Metropolis Algorithm

Importance Sampling--- Markov process

A configuration {s'} is generated from the knowledge of a configuration {s}.

W({s},{s'}): the conditional probability to select {s'} starting from {s}.
The equilibrium distribution:
$$P_{eq}(\{s\})=\exp[-E(\{s\})/k_BT]/Z.$$

E: internal energy function, k_B : the Boltzmann constant,
T: temperature ,   Z : canonical partition function.

The procedure of the simualtion

- (1). A grain number from 1 to the system size, N, is assigned to each lattice point.

- (2). A number corresponds to an orientation is randomly assigned to each grain.

- (3). The evolution of microstructure is tracked by the change of orientations on each lattice

- (a). One lattice site is selected at random .

- (b). If the lattice site belongs to grain boundary, then a new orientation is generated.

- (c).If one of nearest neighbor lattices has the same orientation as the newly selected grain orientation, a re-orientation trial is attempted.

- (d). The change in energy, ΔE, associated with the change of grain orientation is calculated. The re-orientation trial is accepted if ΔE is less than or equal to zero. If the value ΔE is greater than zero, the re-orientation is accepted with probability,

- $$W = \exp(-\Delta E/k_B T).$$

The change of interfacial energy accompanying re-orientation

. The interfacial energy is a function of the grain misorientation:

$$E_0 = - \sum_{<1J>} M_{s_i s_j},$$

s_i ; grain orientation.
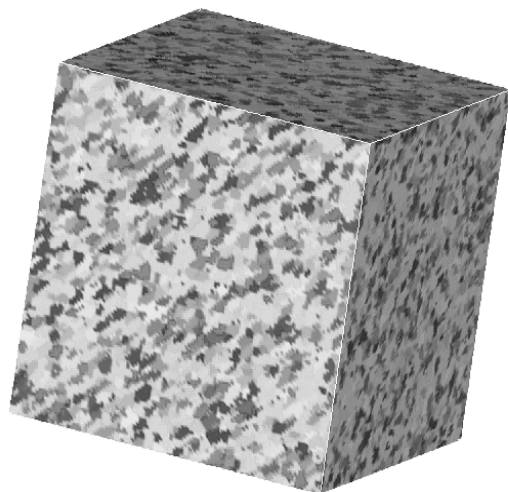
Matrix M_{ij}

$$M_{ij} = J \ (1 - \delta_{ij}) \qquad \text{isotropic}$$

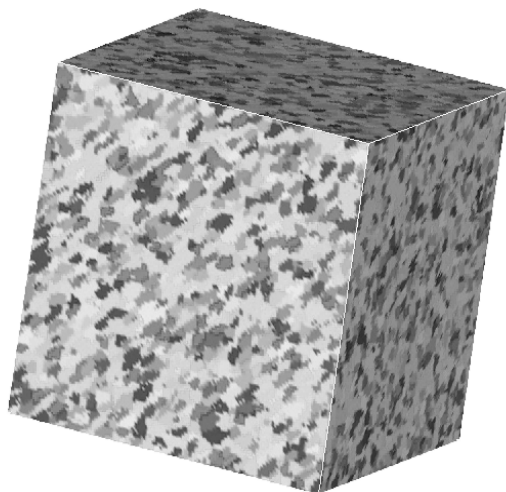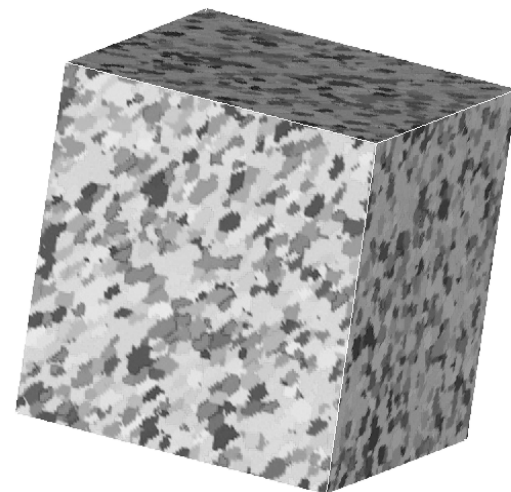$$M_{ij} = J \ (1 - \delta_{ij})[1 - (1 - r)\delta_{i \ i+k}] \qquad \text{anisotropic}$$

Condition of the simulation

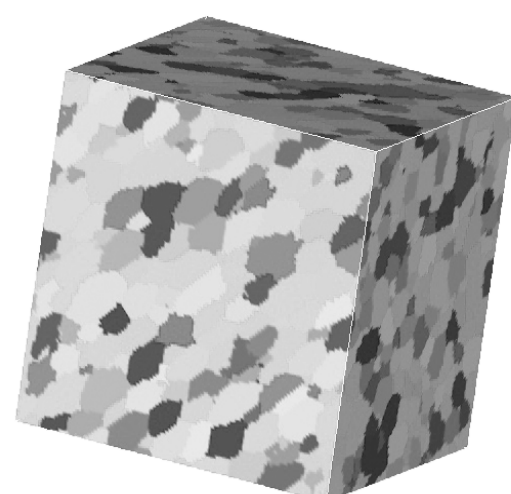- System size: 128^3
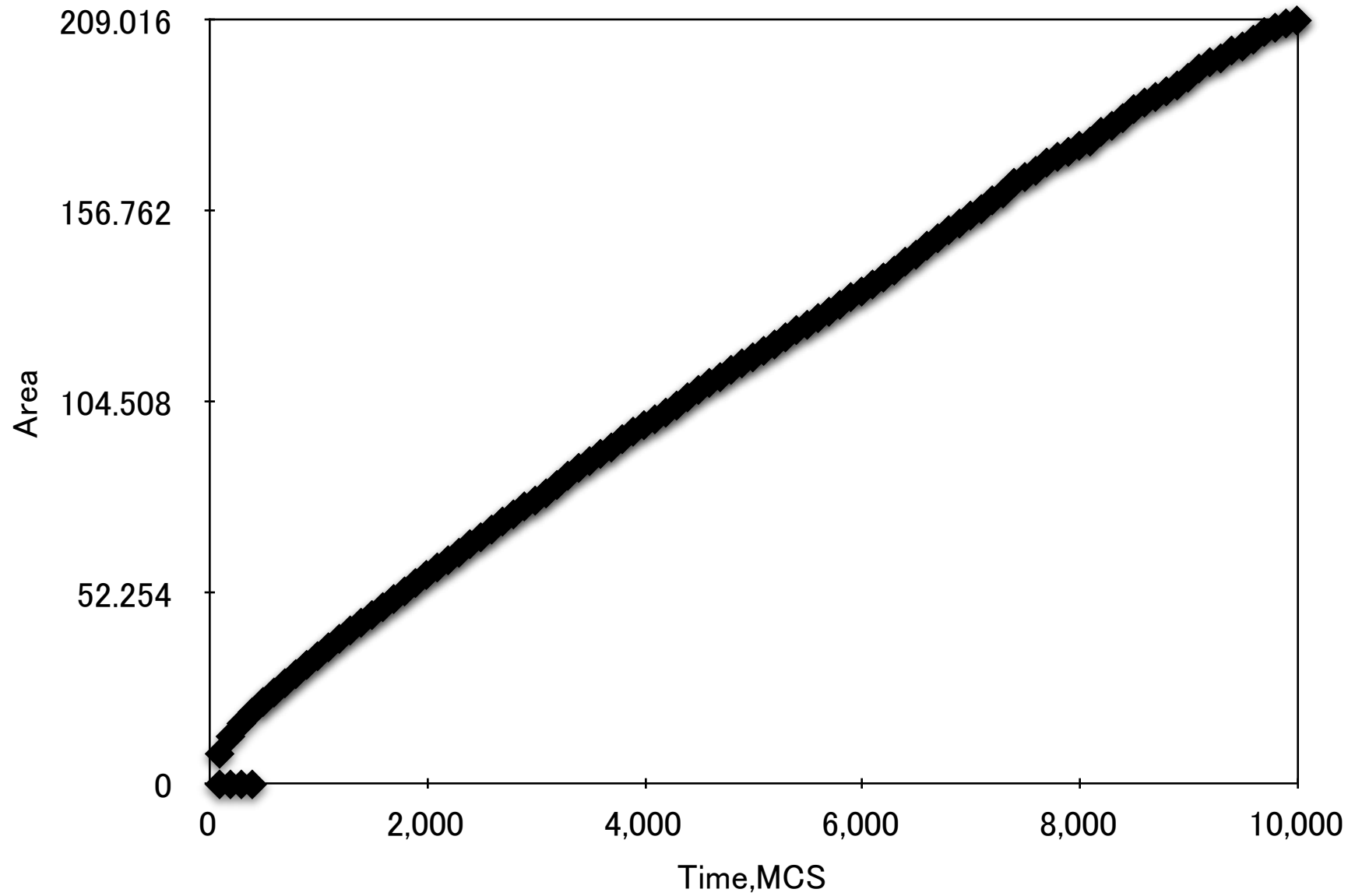- The number of orientation: 16 or 32
- 3-dimensional
- $J/K_BT=0.75$

100 MCS

200 MCS

500 MCS
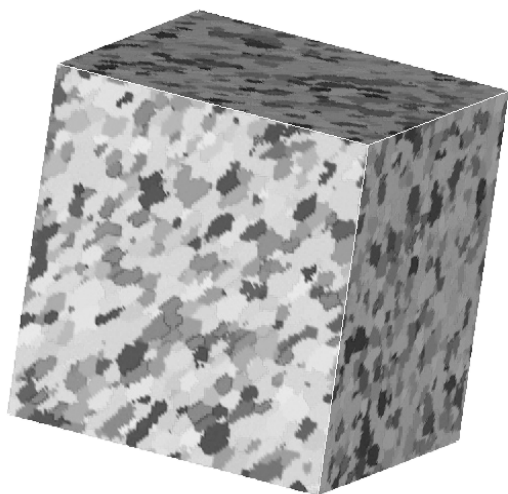
1000 MCS

2000 MCS

5000 MCS

Legend:
◇ 400 MCS
○ 500 MCS
▲ 750 MCS
✕ 1000 MCS

X-axis: Number of faces per grain

Y-axis: Frequency, %
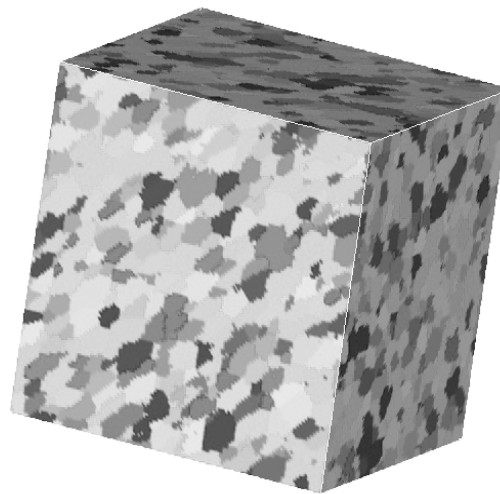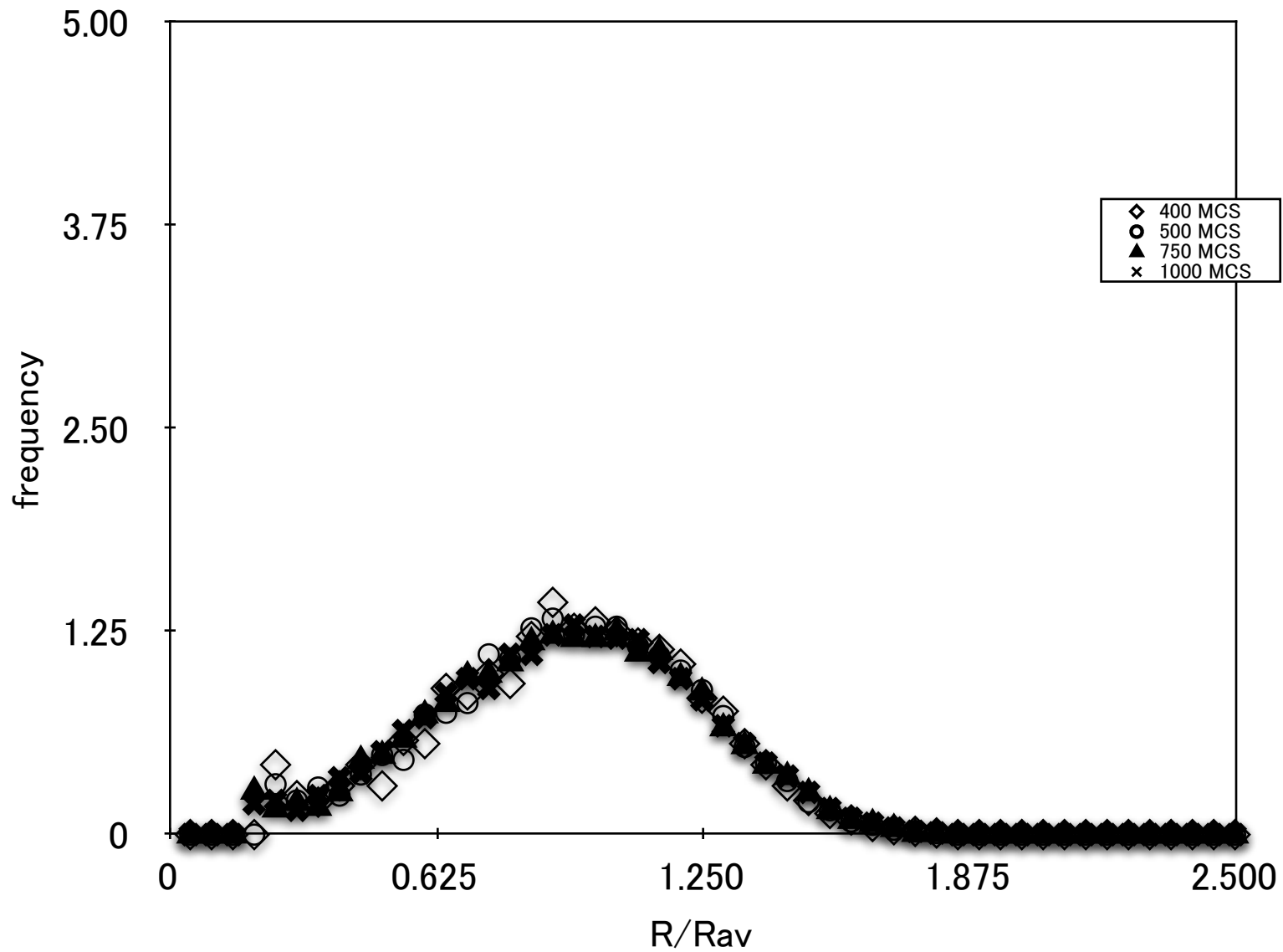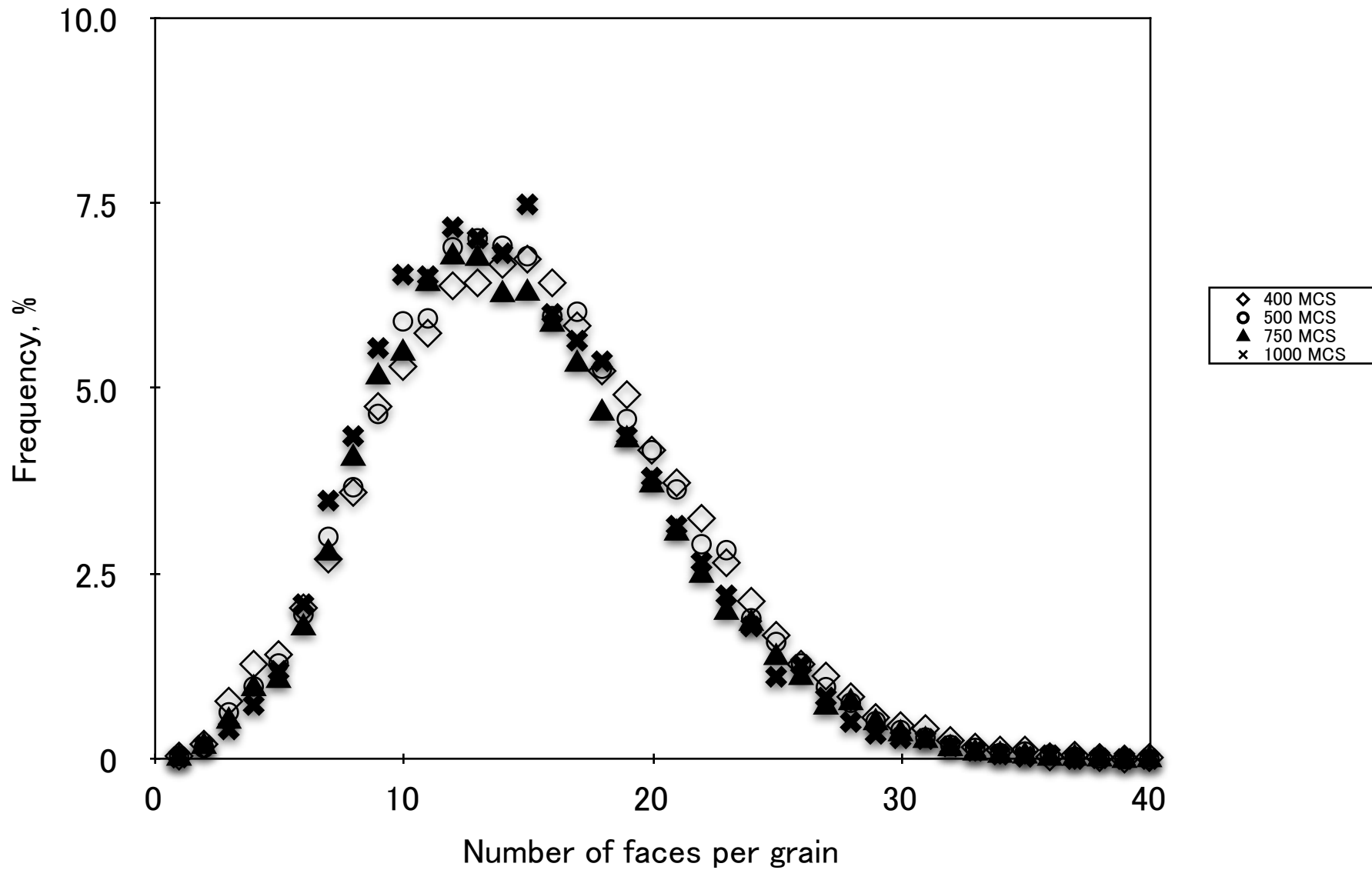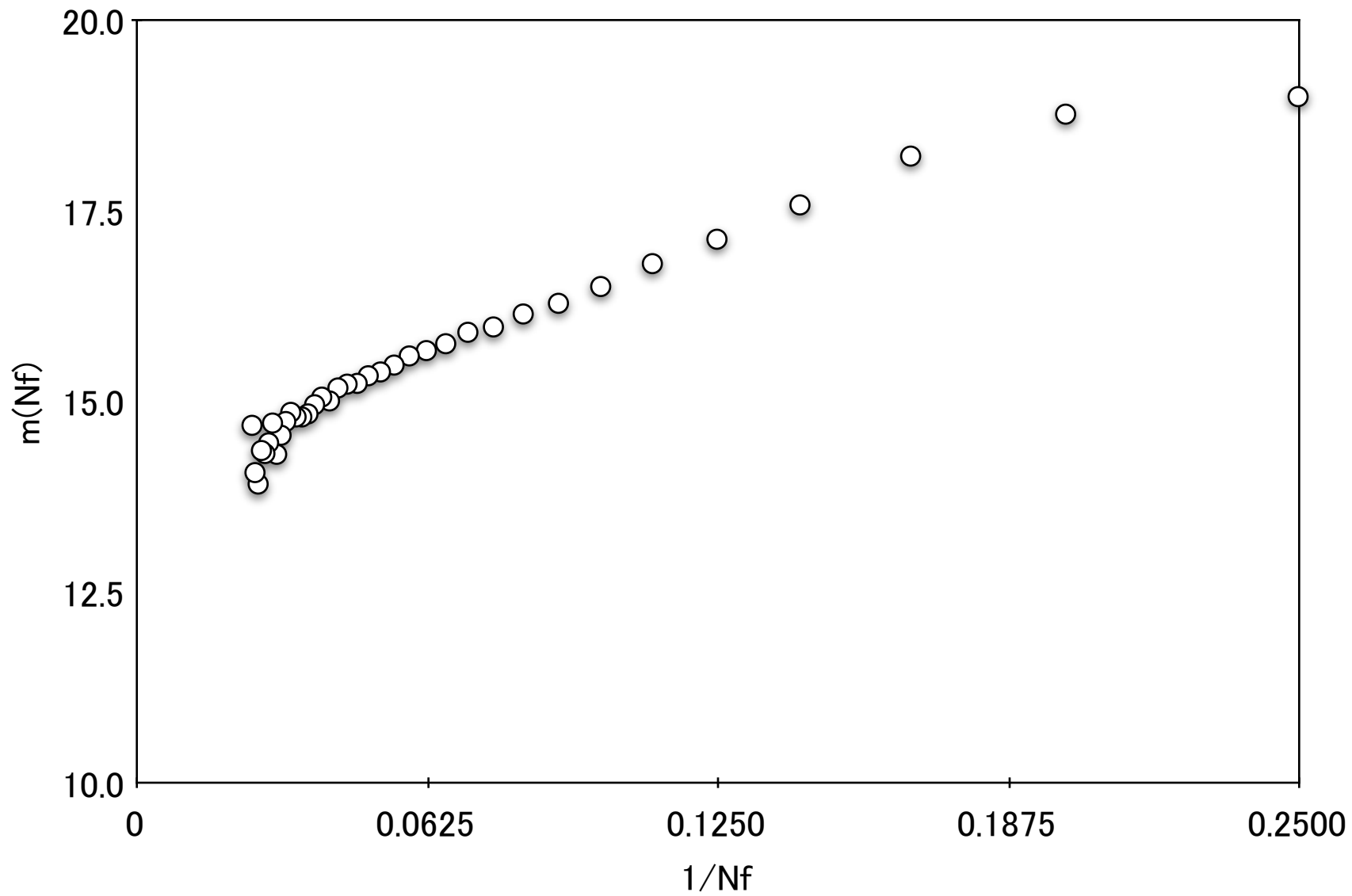
Phase Field vs. Monte Carlo
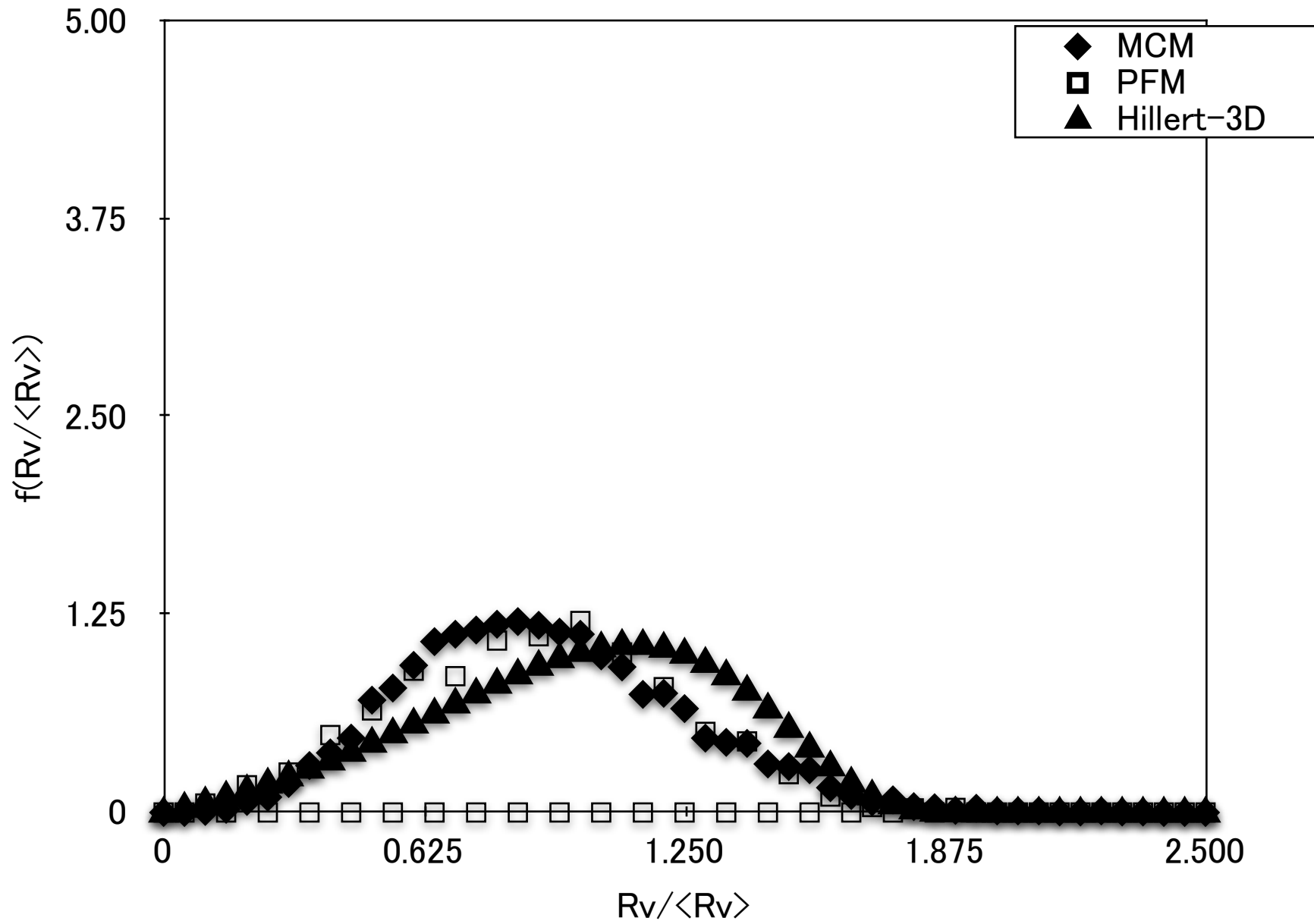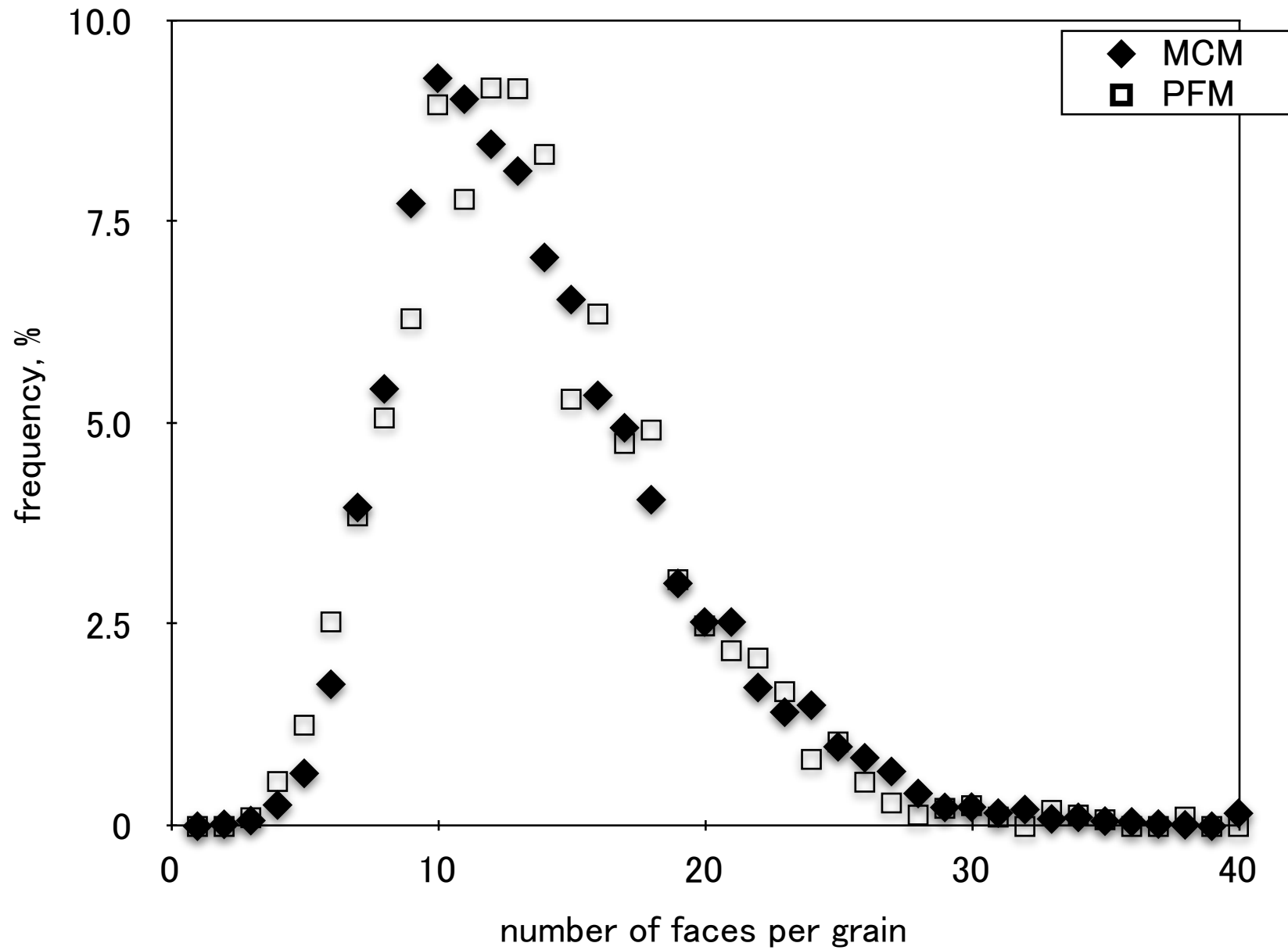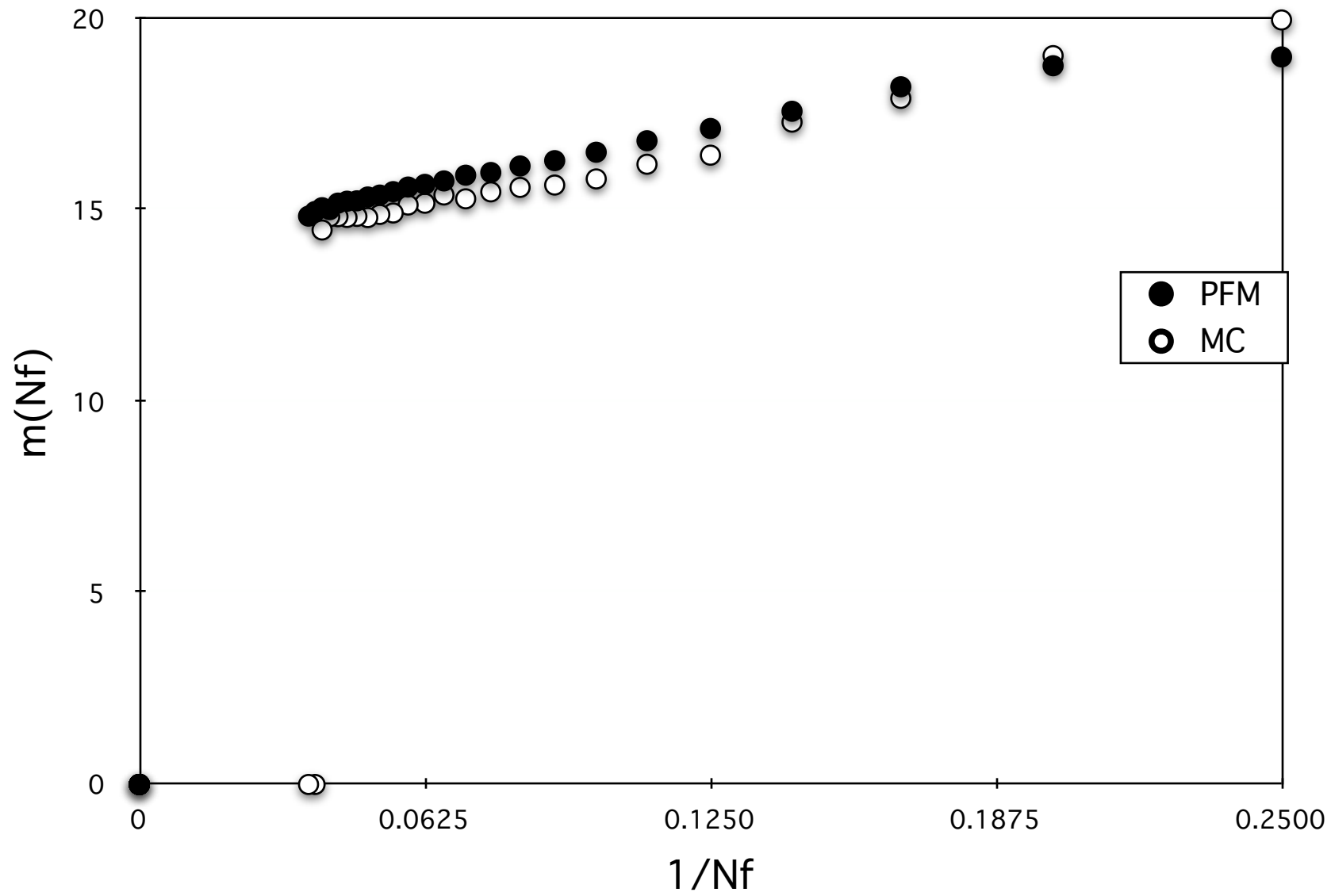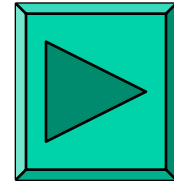
Phase Field vs. Monte Carlo

Problems related to interface migration

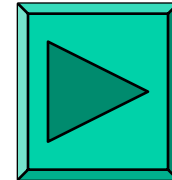**Effect of anisotropy on grain growth**
   Abnormal grain growth

Effect of second phase

Texture control

Solute drag effect

Recrystallization

Phase transforamtion

Spinodal Decomposition

Background

- **Duplex stainless steel**

- ・**high strength, ・good weldability, ・high resistance to stress corrosion cracking → Chemical reactor**

-
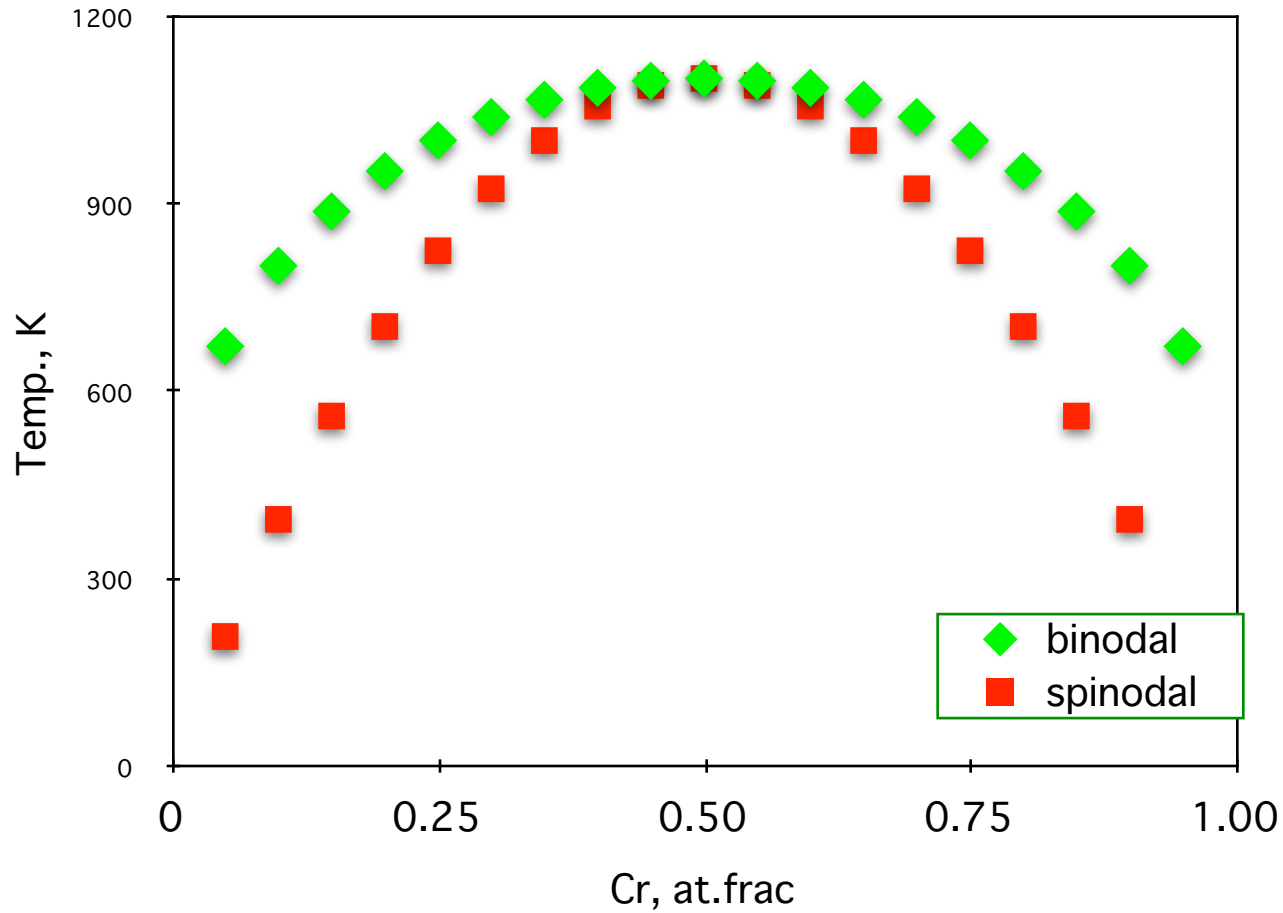
- <u>Problem: 475°C embrittlement</u>

- Hardening due to thermomechanical instability of ferrite phase in duplex stainless steels

- **Prediction of long time stability of**

- **chemical reactor**

Fe-Cr binary alloy

A numerical method for solving Cahn-Hilliard Equation

$$\frac{C(\vec{r}, t + \Delta t) - C(\vec{r}, t)}{\Delta t} = \frac{M}{(\Delta r)^2} \sum_{NN} \left[\frac{\partial f_0}{\partial C} - \frac{K}{(\Delta r)^2} \sum_{NN} C(\bar{r}, t) \right]$$

Second order differential parameter

1D

2D

3D

Second order differential parameter

1D

$$\sum_{NN} F(x,t) = F(x + \Delta x, t) + F(x - \Delta x, t) - 2F(x,t)$$
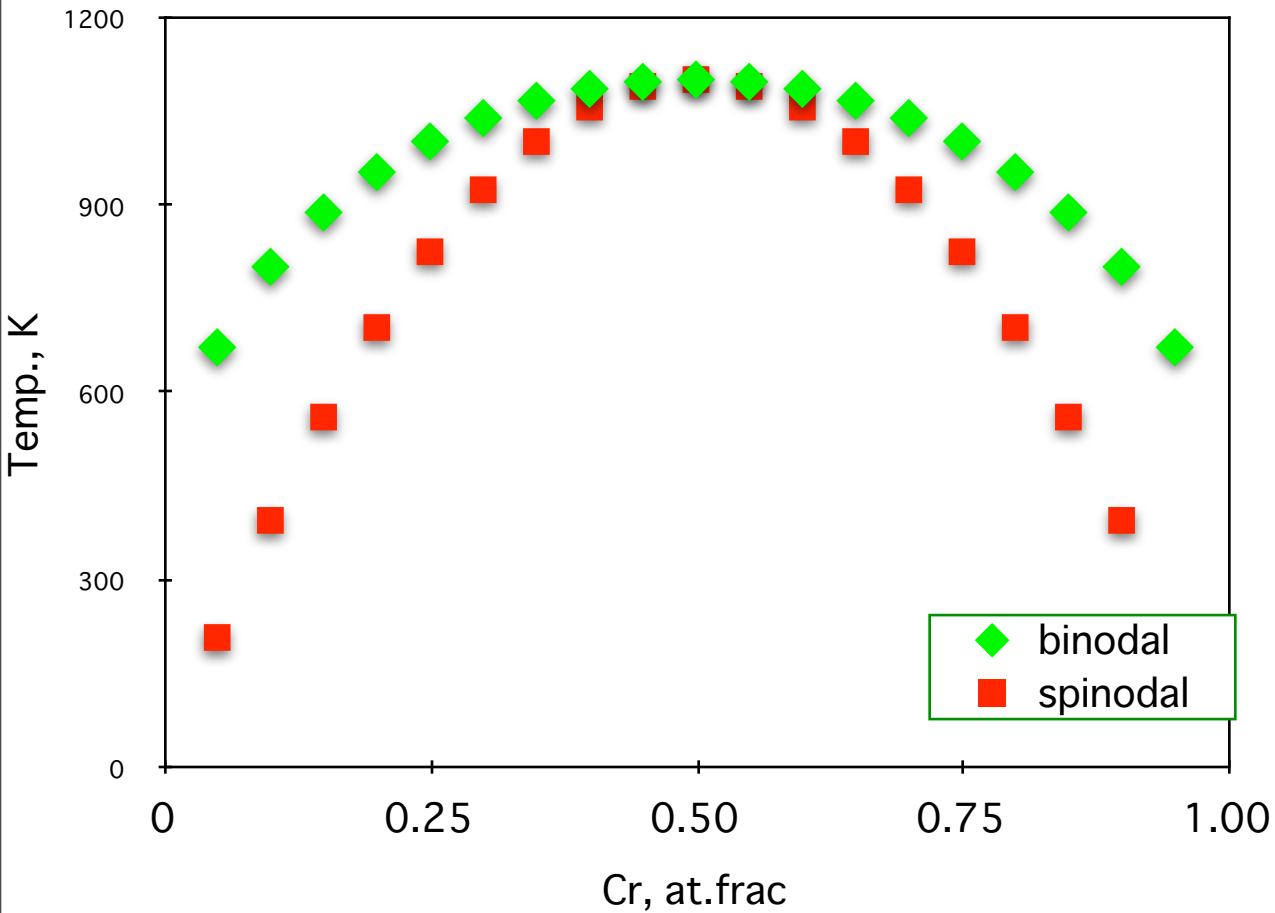
2D

$$\sum_{NN} F(x, y, t) = F(x + \Delta x, y, t) + F(x - \Delta x, y, t)$$
$$+ F(x, y + \Delta y, t) + F(x, y - \Delta y, t)$$
$$- 4F(x, y, t)$$

3D

$$\sum_{NN} F(x, y, z, t) = F(x + \Delta x, y, z, t) + F(x - \Delta x, y, z, t)$$
$$+ F(x, y + \Delta y, z, t) + F(x, y - \Delta y, z, t)$$
$$+ F(x, y, z + \Delta z, t) + F(x, y, z - \Delta z, t)$$
$$- 6F(x, y, z, t)$$

Fe-Cr binary alloy

Chemical free energy
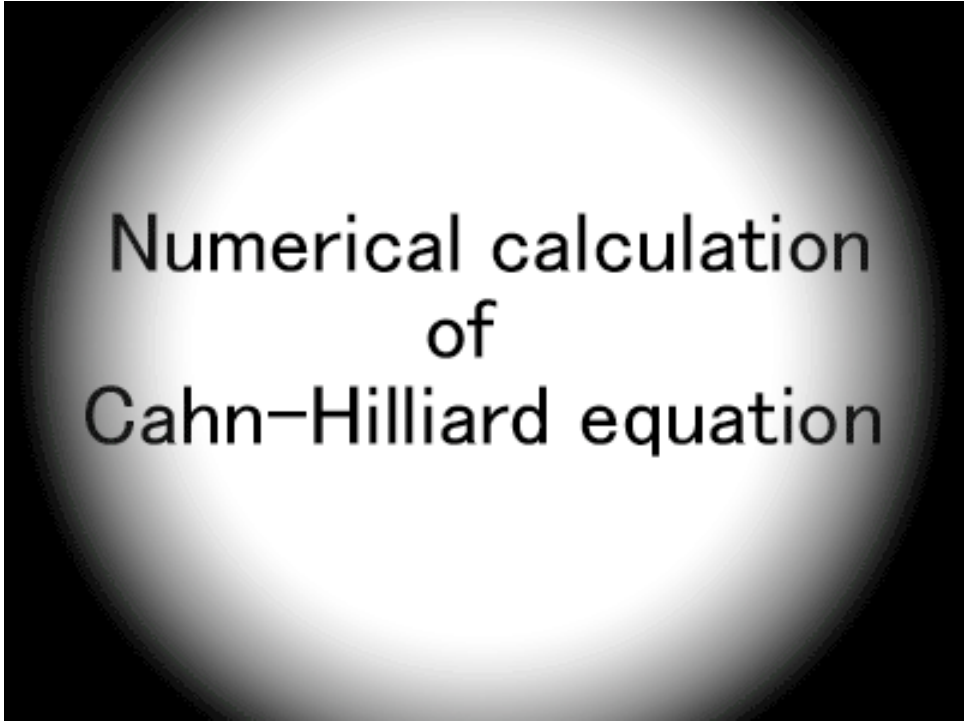
$$f_0 = \Omega x(1-x) + RT[x\ln(x) + (1-x)\ln(1-x)]\}$$

Phase boundary

$$\frac{\partial f_0}{\partial x} = \grave{U}(1 - 2x) + RT\left[lnx - ln(1 - x)\right] = 0$$
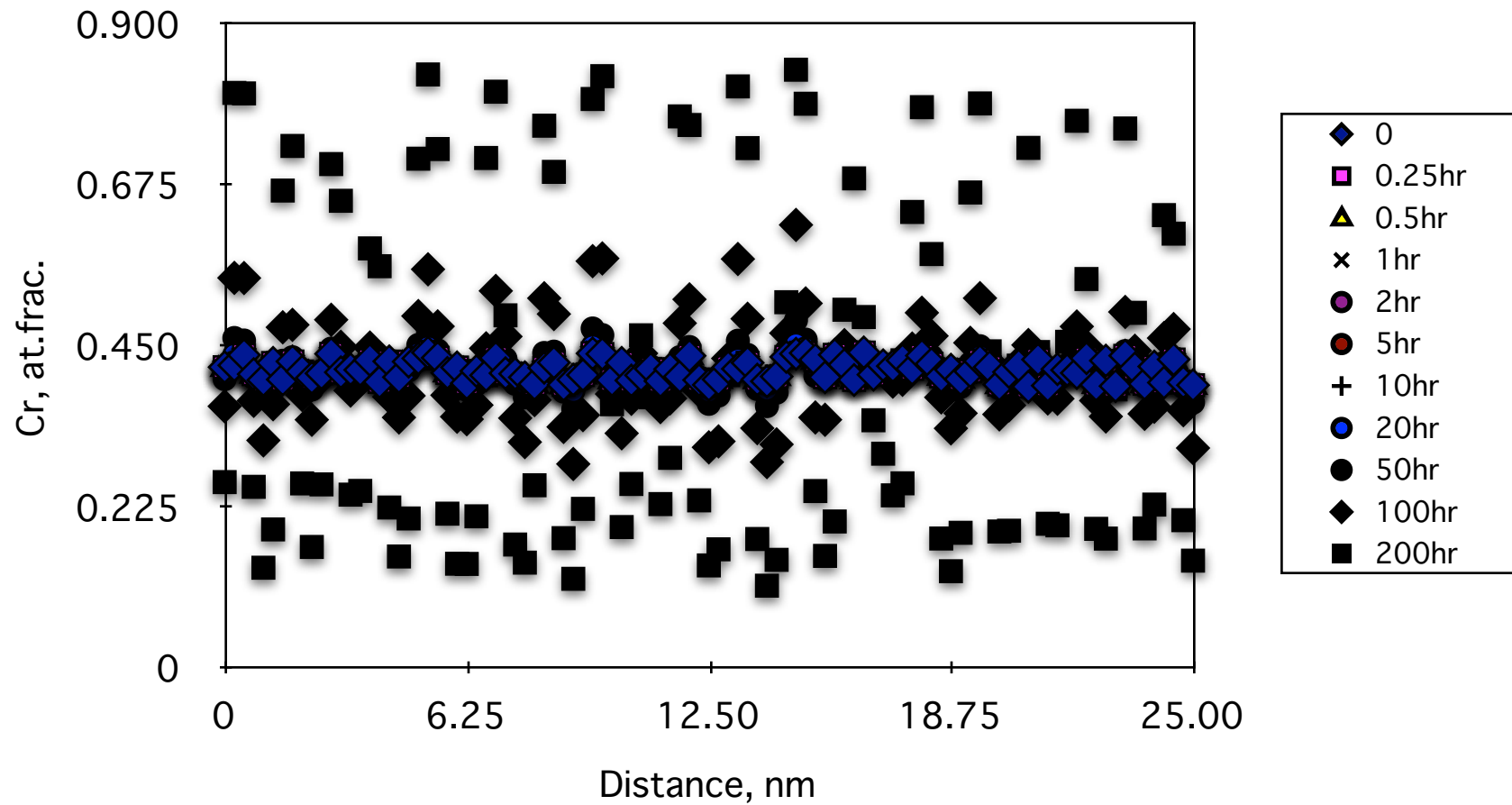
Spinodal

$$\frac{\partial^2 f_0}{\partial x^2} = -2\Omega + RT\left[\frac{1}{x} + \frac{1}{1-x}\right] = 0$$

Proto type simulation(Fe-40wt.%Cr ally）
850K

Fe-40%Cr   binary   alloy

Simulation of Phase Separation

Cahn-Hillirad equation for Fe-X-Y ternary alloys

Cahn-Hillirad equation for Fe-X-Y ternary alloys

$$\frac{\partial c_X}{\partial t} = M_X \left[\nabla^2 \left(\frac{\partial f_0}{\partial c_X} - K_X \nabla^2 c_X - L_{XY} \nabla^2 c_Y \right) \right]$$

$$\frac{\partial c_Y}{\partial t} = M_Y \left[\nabla^2 \left(\frac{\partial f_0}{\partial c_Y} - L_{YX} \nabla^2 c_X - K_Y \nabla^2 c_Y \right) \right]$$

Condition

Aging temperature T:

Composition :

Mobility, M :

Energy gradient coefficient

K :

L :

Condition

Aging temperature T: **800 K**

Composition :

Fe-40at.%Cr-5at.%Mo   Fe-40at.%Mo-5at.%Cr

Mobility, M : $M_{\text{Cr}} = \dfrac{0.01 \times D_{\text{Cr}}}{2\Omega_{\text{FeCr}} - 4RT}$ $M_{\text{Mo}} = \dfrac{0.01 \times D_{\text{Mo}}}{2\Omega_{\text{FeMo}} - 4RT}$

Energy gradient coefficient

K : $K_{\text{Cr}} = \dfrac{1}{2} \times a_0^2 \times \Omega_{\text{FeCr}}$ $K_{\text{Mo}} = \dfrac{1}{2} \times a_0^2 \times \Omega_{\text{FeMo}}$

L : $L_{\text{CrMo}} = L_{\text{MoCr}} = \dfrac{1}{2} \times a_0^2 \left(\Omega_{\text{CrMo}} - \Omega_{\text{FeCr}} - \Omega_{\text{FeMo}} \right)$

Diffusion coeeficient D :

Interaction parameter Ω :

Diffusion coeeficient D :

$$D_{Cr} = 0.19 \exp\left(-\frac{246000}{RT}\right) cm^2 / s$$

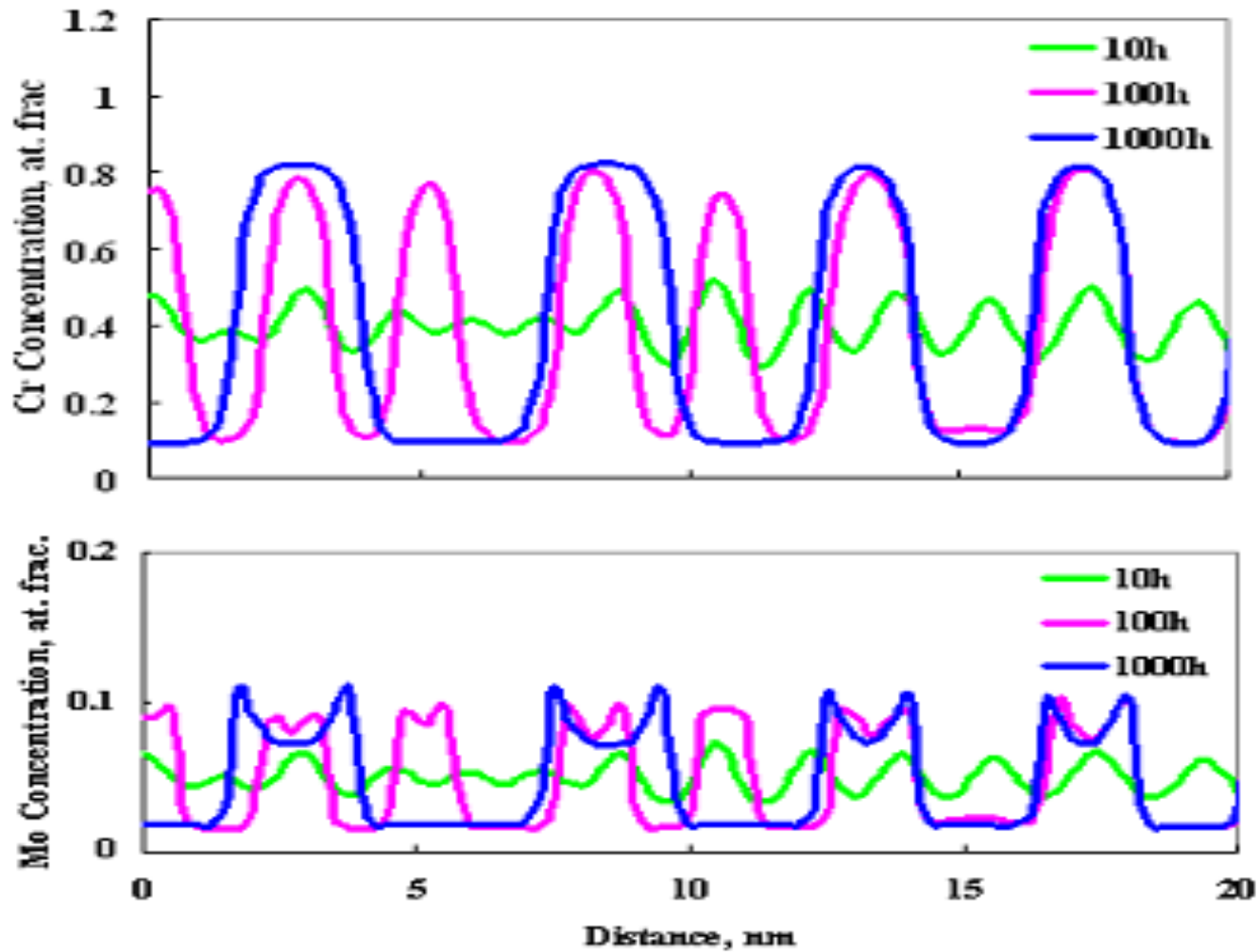$$D_{Mo} = 0.29 \exp\left(-\frac{264000}{RT}\right) cm^2 / s$$

Interaction parameter Ω :

$$\Omega_{FeCr} = 18.6 \text{kJ/mol}$$

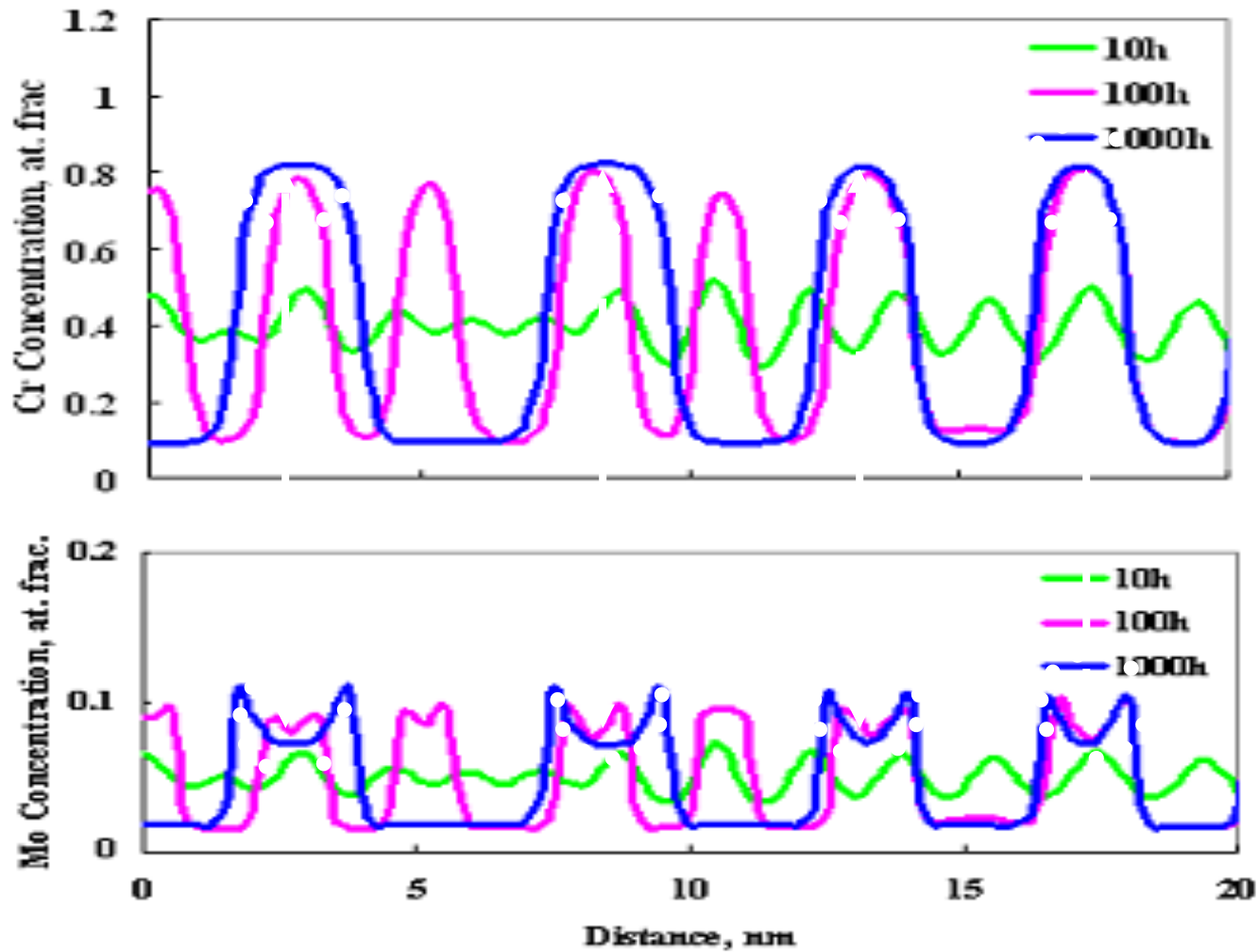$$\Omega_{FeMo} = 18.2 \text{kJ/mol}$$

$$\Omega_{CrMo} = 8.0 \text{kJ/mol}$$

1D simulation
Fe40Cr5Mo(800K)

1D simulation
Fe40Cr5Mo(800K)

2D simulation

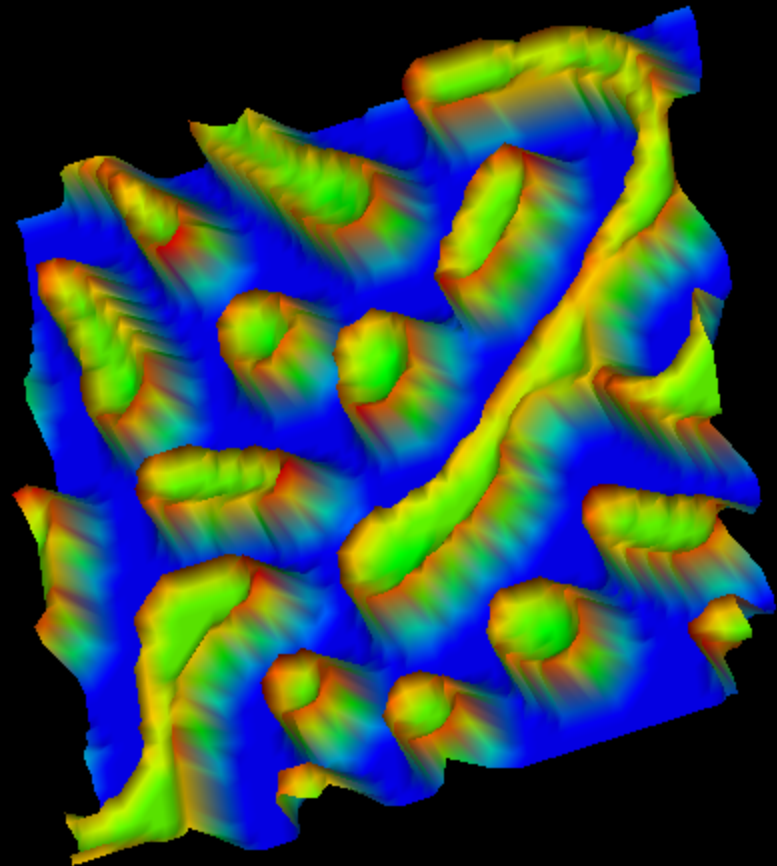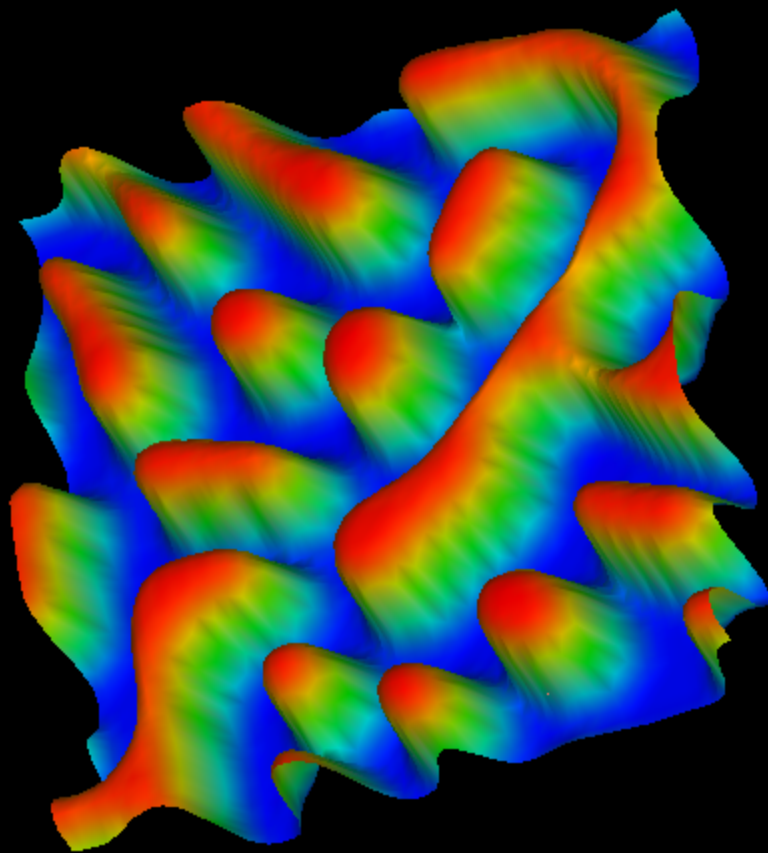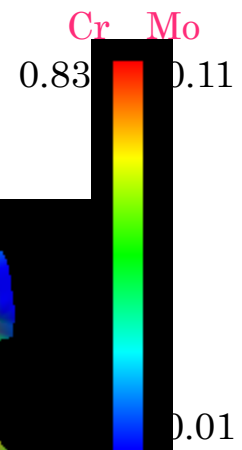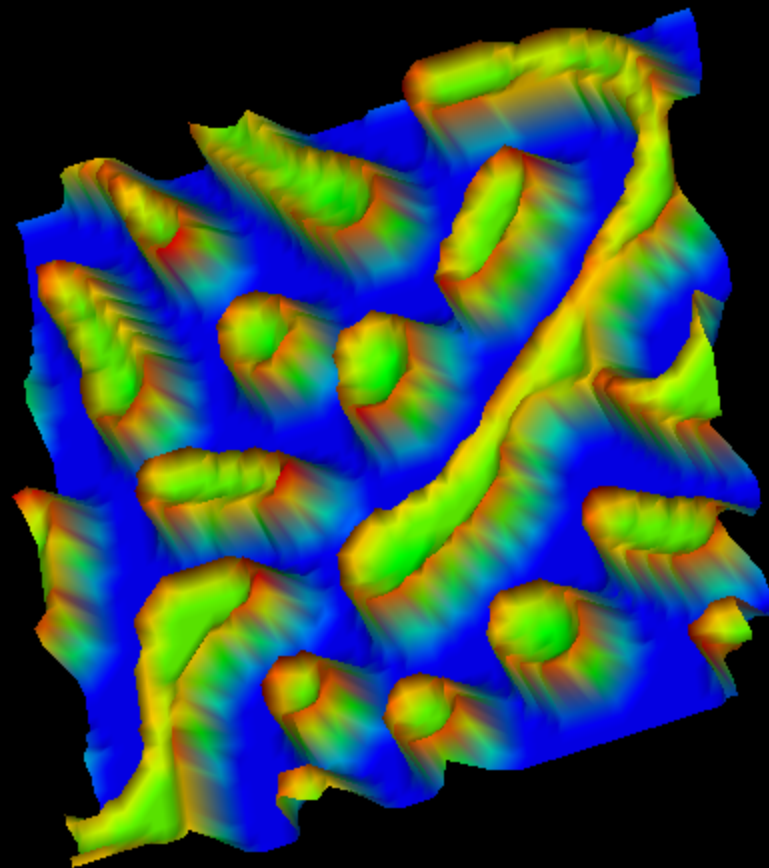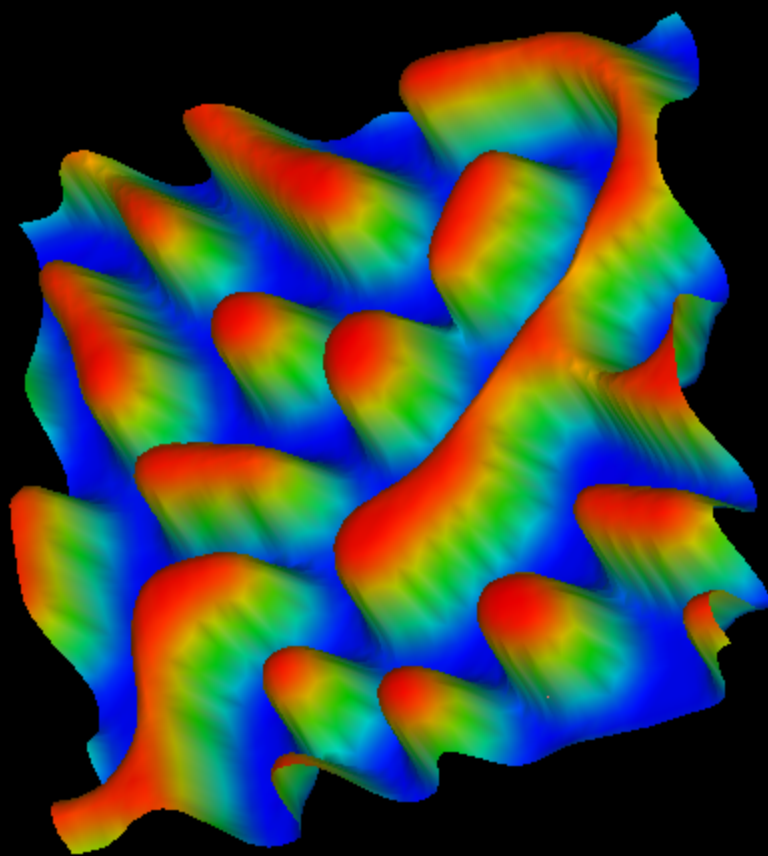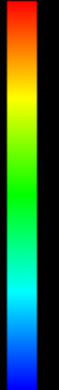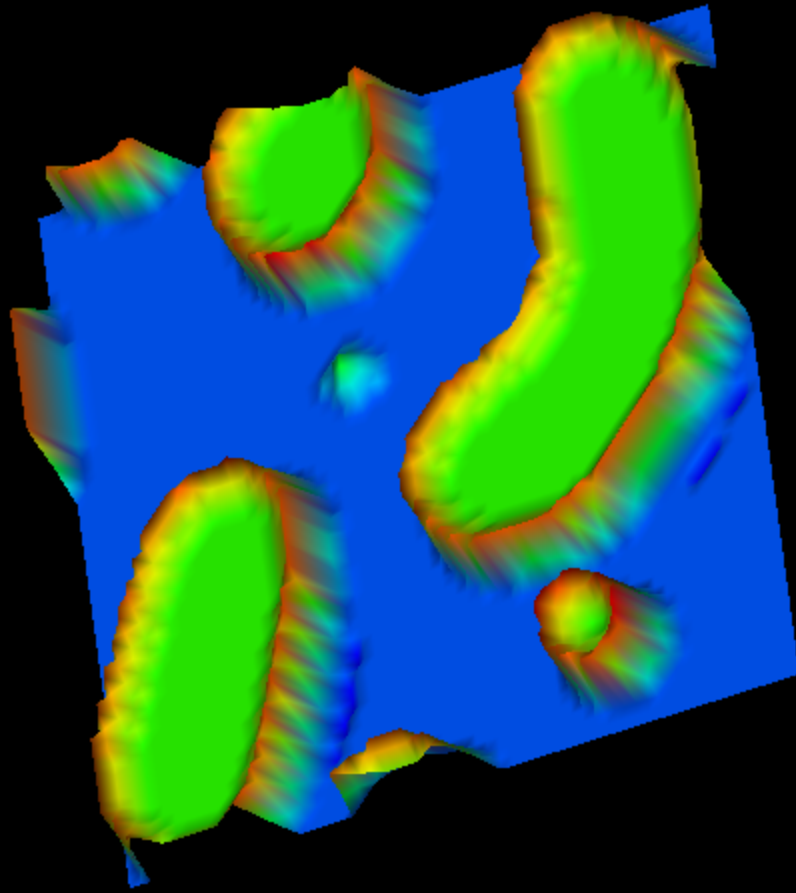100 時間後　　　　　Fe40Cr5Mo

Cr Mo
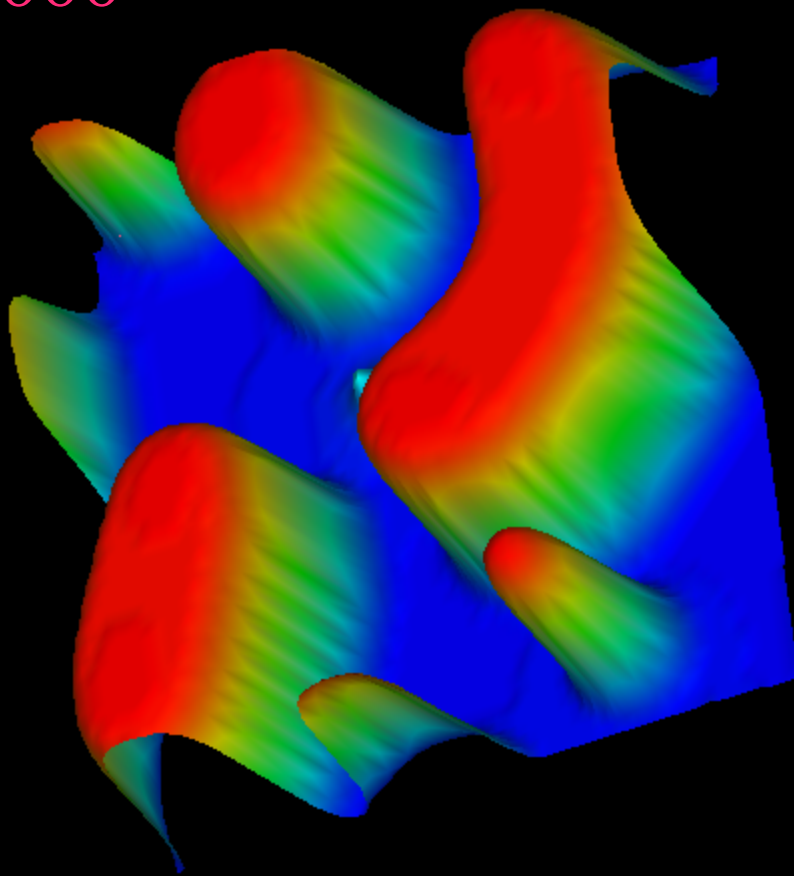
Cr

Mo

10 nm

2D simulation

100 時間後 Fe40Cr5Mo

Cr   Mo
0.83   0.11
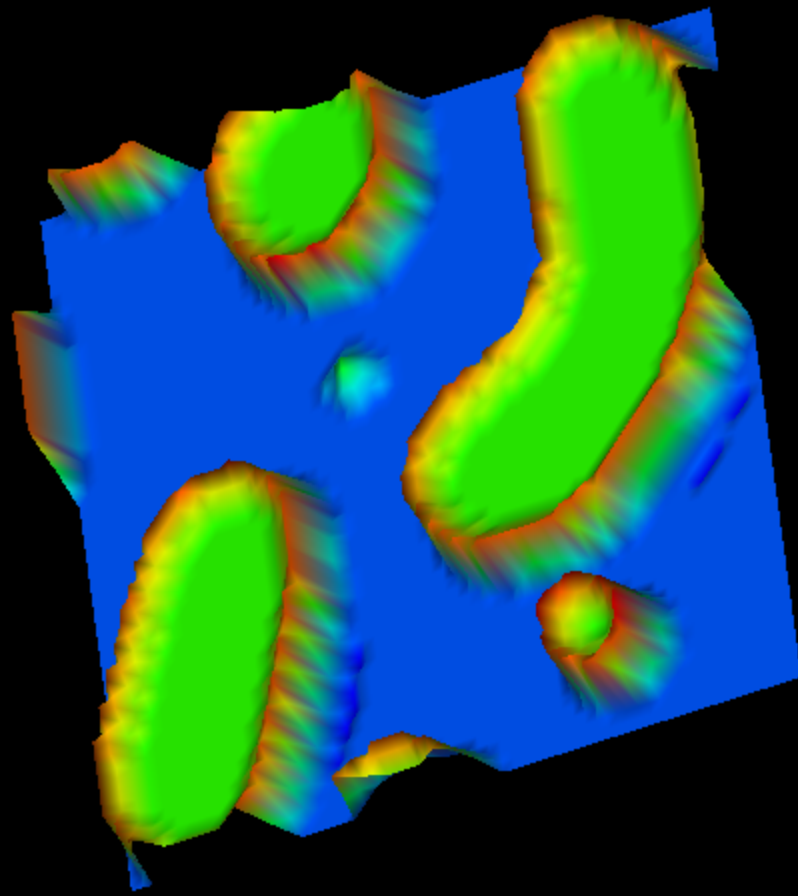
0.01

Cr

Mo

10 nm

2D

1000

Cr   Mo

16 nm

Cr

Mo

Cr   Mo

2D

1000

Cr   Mo

0.82   0.12

0.01
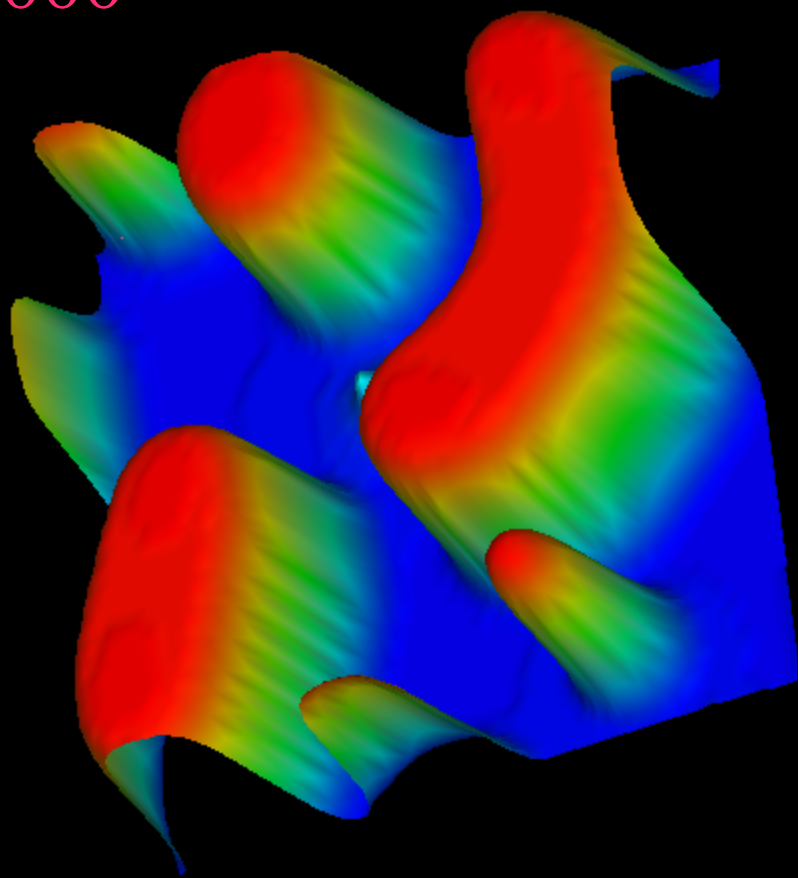
16 nm

Cr

Mo

2D

1000

Cr Mo

Cr Mo
0.82   0.12

0.01
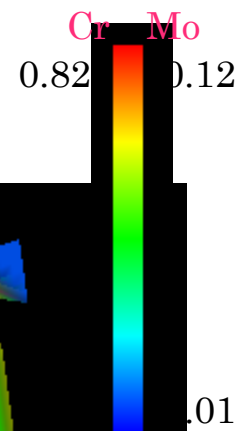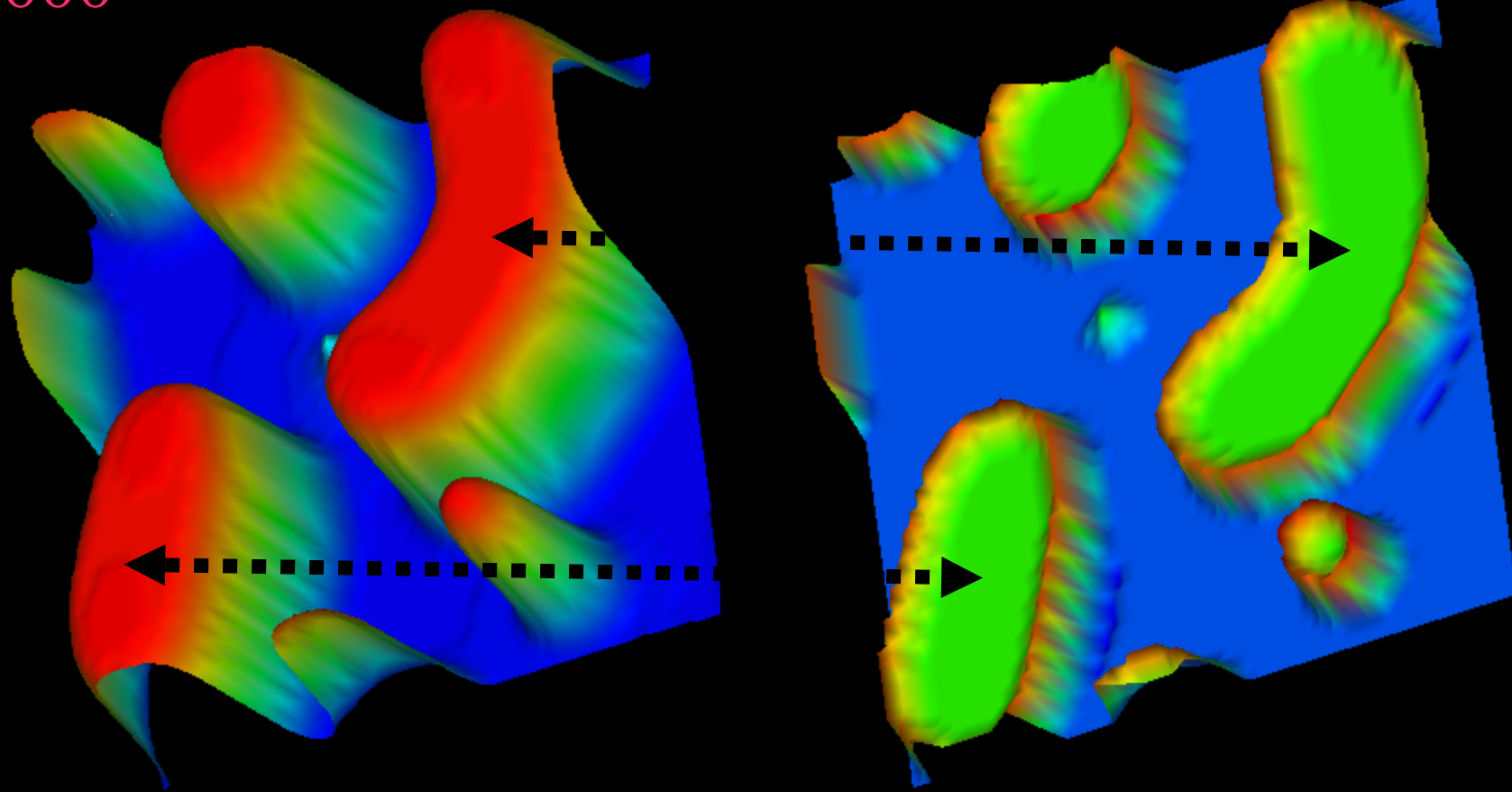
16 nm

Cr

Mo

3D simulation

Fe40Cr5Mo
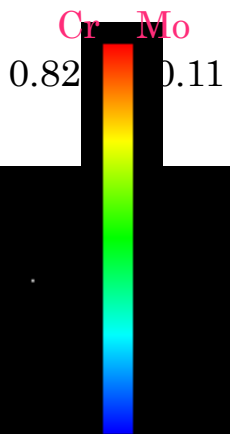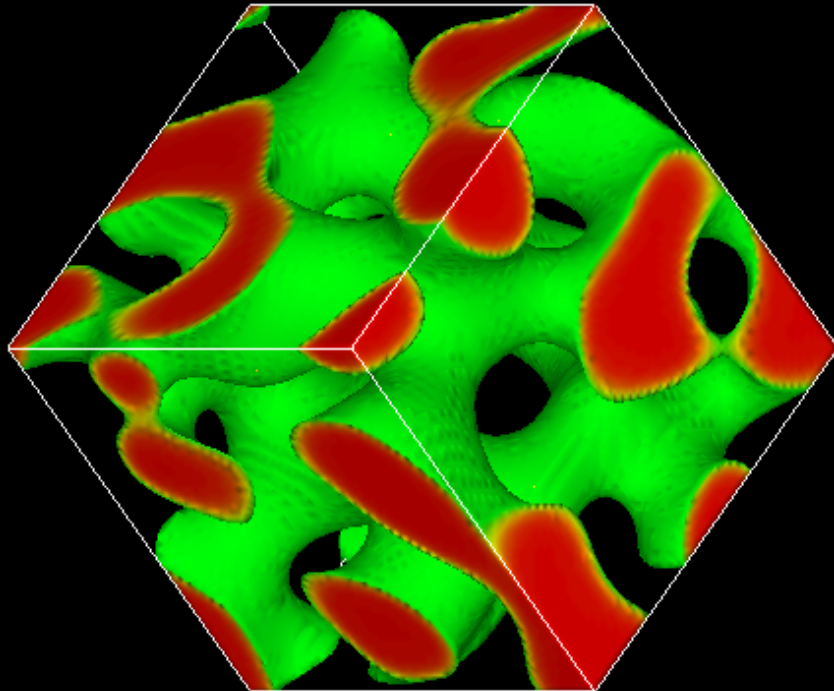
Cr — Mo
0.82 — 0.11

1000

Isosurface of Cr
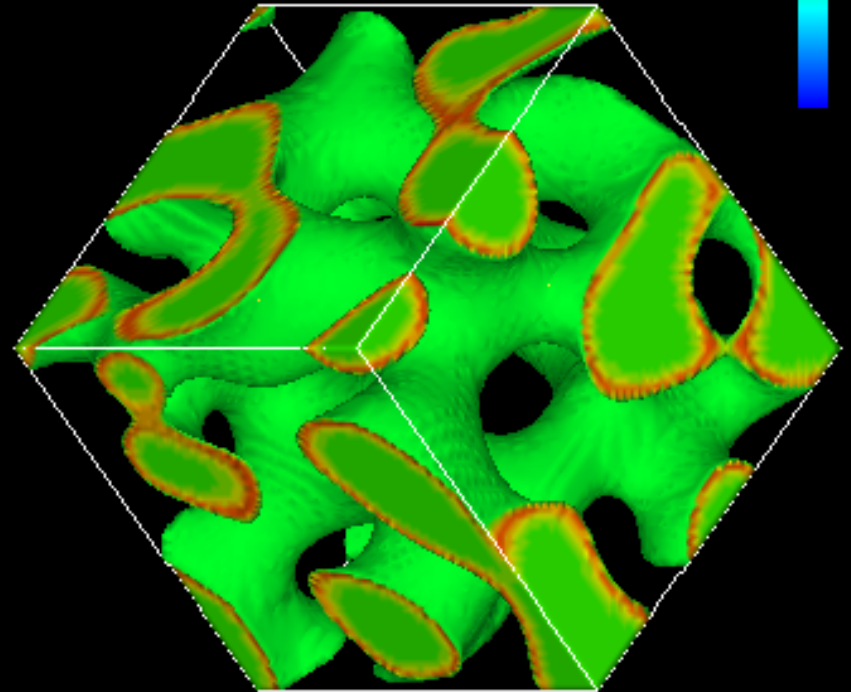
Isosurface of Mo

3D simulation

Fe40Cr5Mo

1000
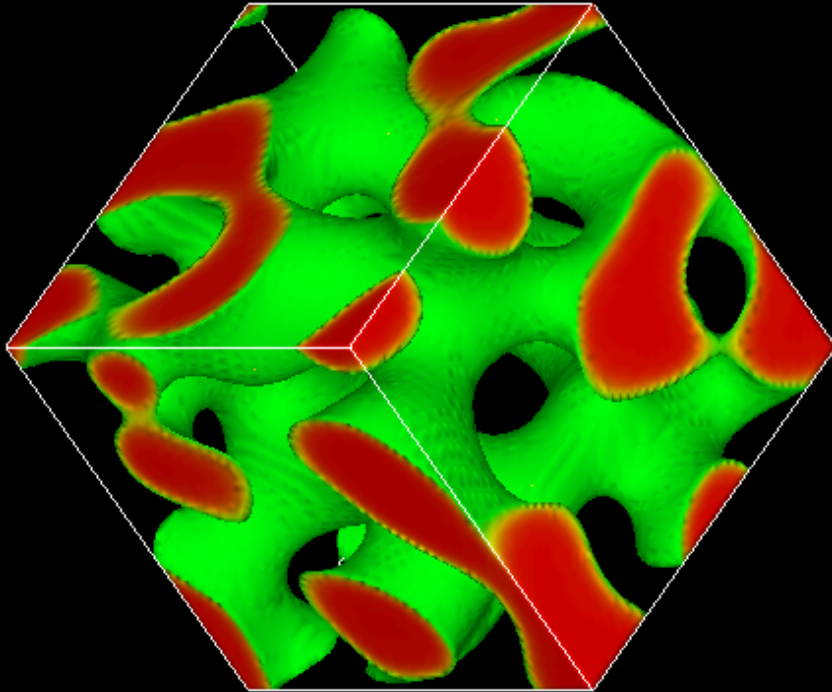
Cr — Mo
0.82   0.11

Isosurface of Cr

Isosurface of Mo

3D

Cr Mo

1000

Cr

Mo

3D

Cr Mo

1000

Cr
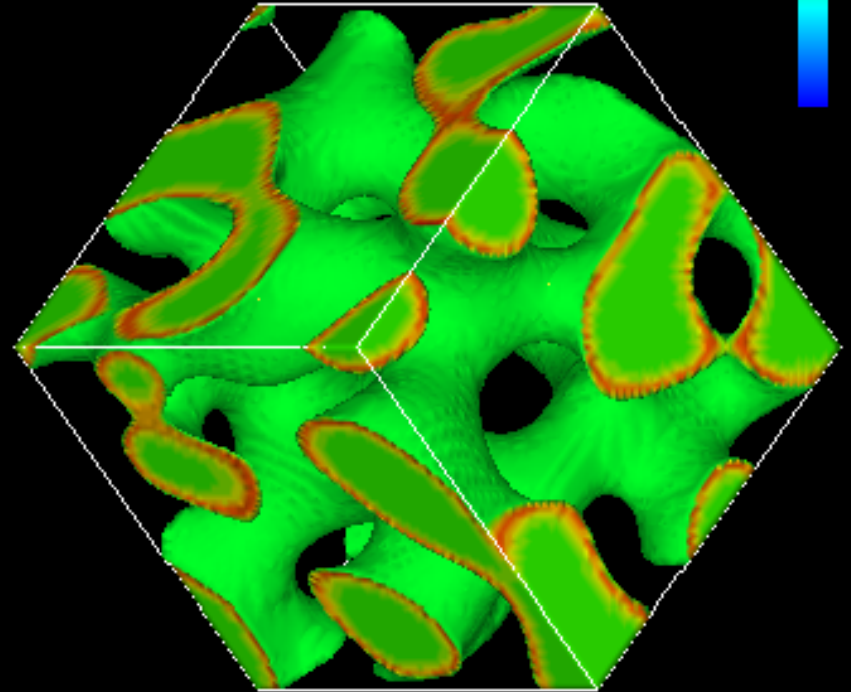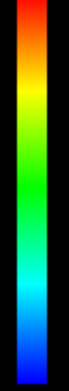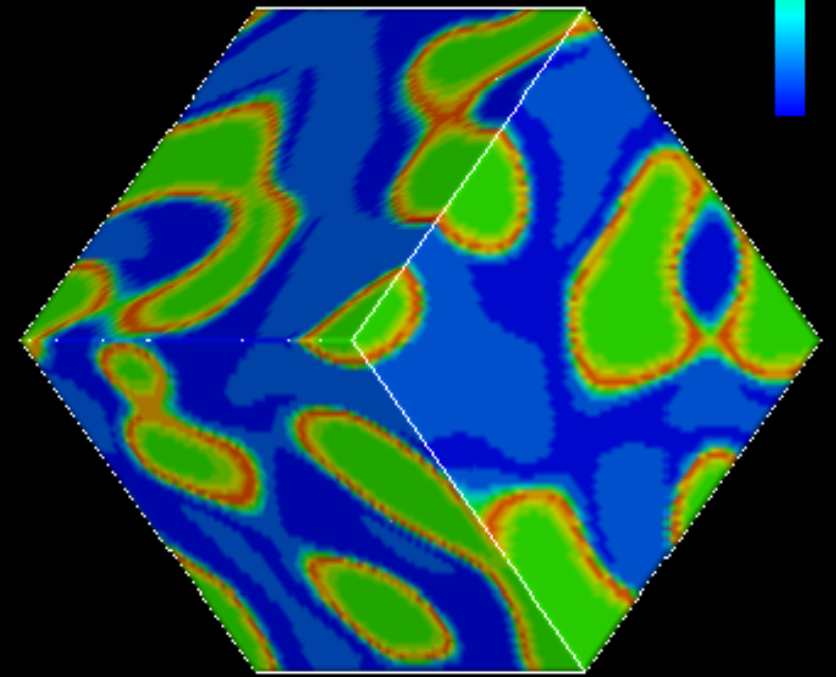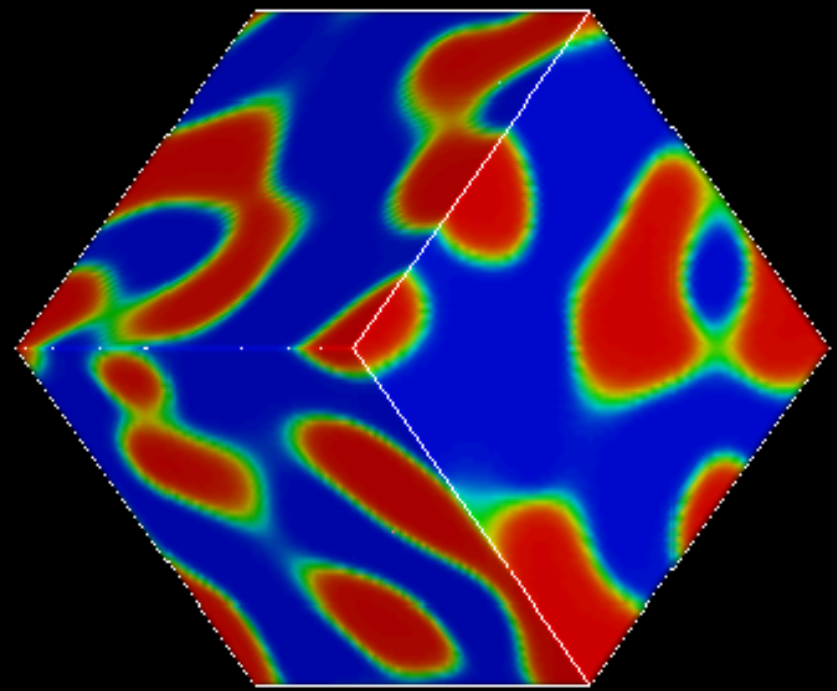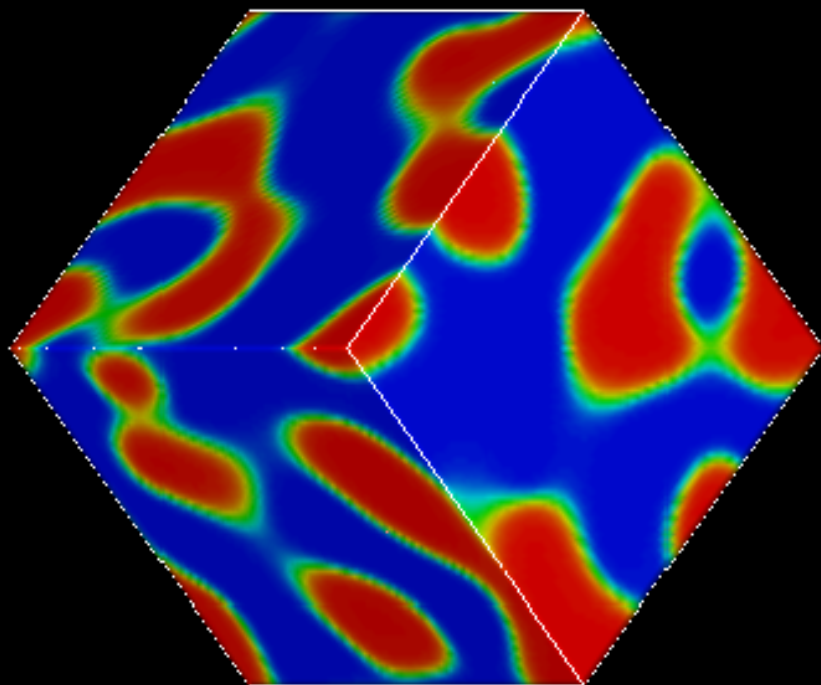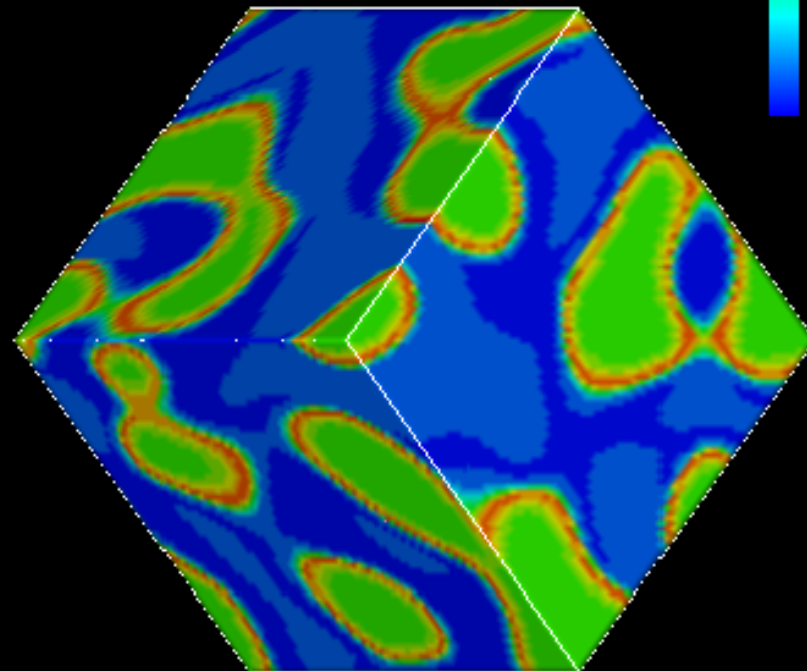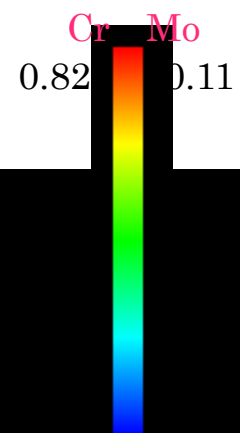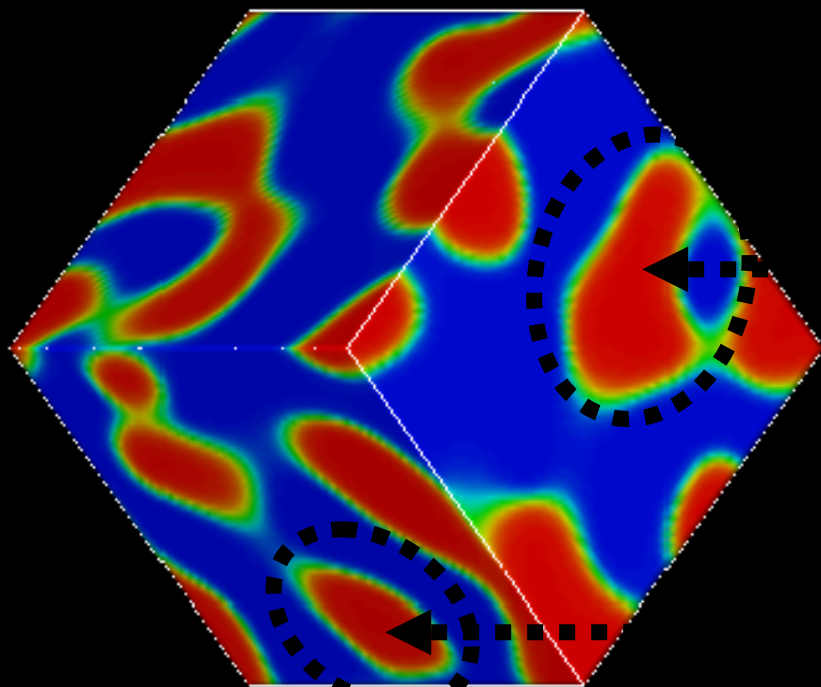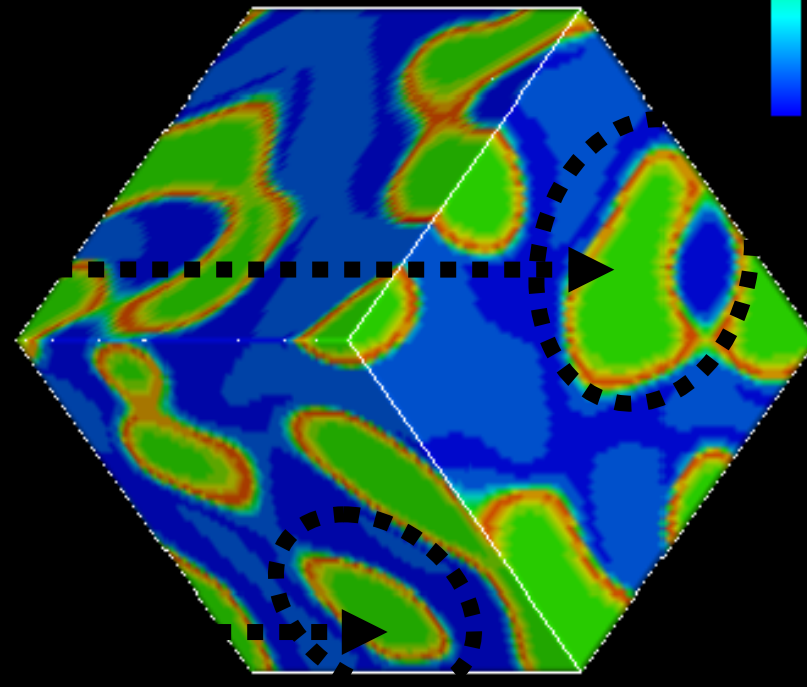
Mo
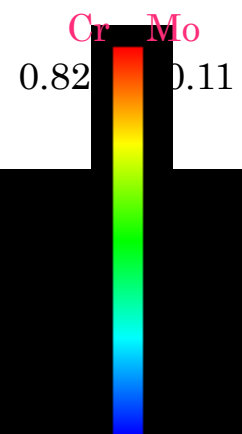
Monte Carlo Simulation

Lenard –Jones Parameter

$$e_{ij}(r) = e_{ij}^0 \left[\left(r_{ij}/r \right)^8 - 2 \left(r_{ij}/r \right)^4 \right]$$

r_{ij} : equilibrium atomic spacing

$-e_{ij}^0$: Interatomic potential at equilibrium atomic spacing

Lenard-Jones potentila

$$e_{ij}(r) = e_{ij}^0 \left[(r_{ij}/r)^8 - 2(r_{ij}/r)^4 \right]$$

Normalized Lenard-Jones parameter

e_{FeFe}	e_{FeCr}/e_{FeFe}	e_{FeMo}/e_{FeFe}	e_{CrCr}/e_{FeFe}	e_{CrMo}/e_{FeFe}	e_{MoMo}/e_{FeFe}
62.0 KJ/mol	0.9537	1.2296	0.9809	1.3001	1.6390

Condition

Fe-40at.%Cr-5at.%Mo	750K
Fe-40at.%Mo-5at.%Cr	800K
	850K

Monte Carlo Simulation

750K

750K

800K

800K

850K

850K

- Fe
- Cr
- Mo
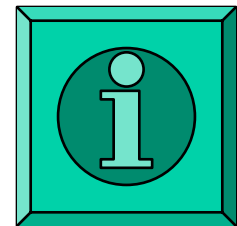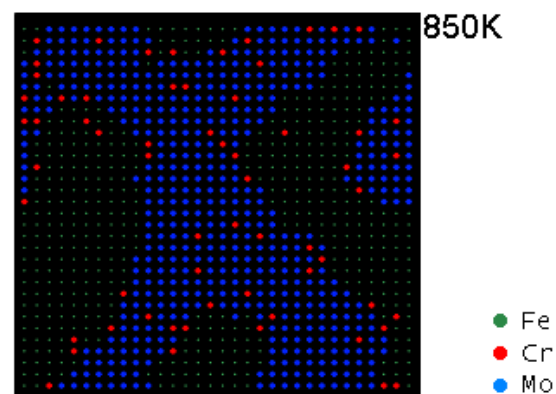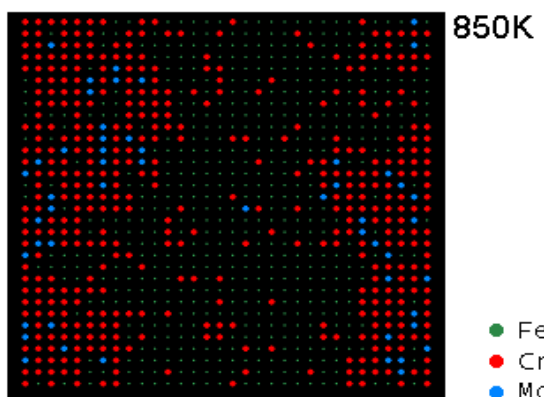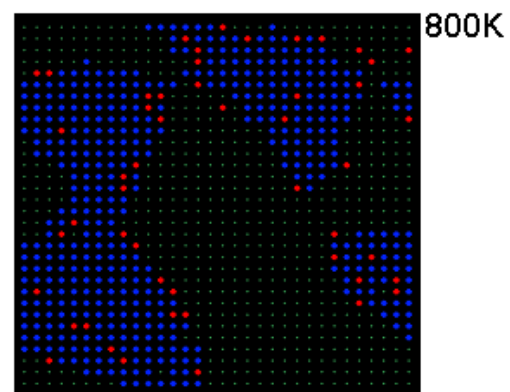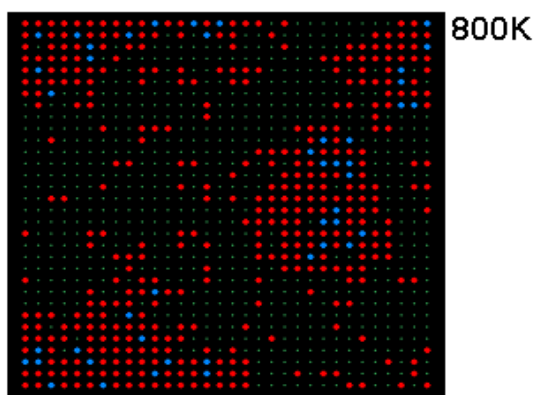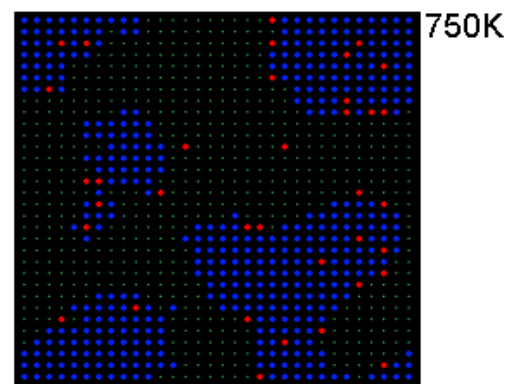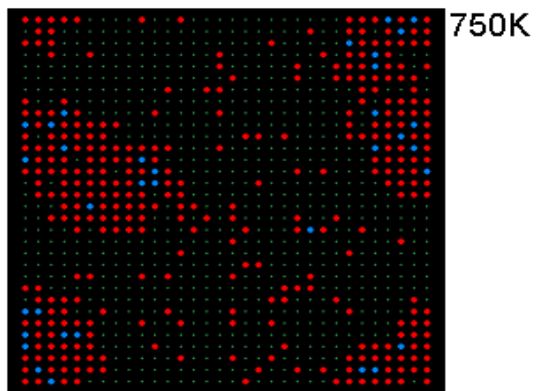
Separation of peaks of Mo

Behavior of element Y along the trajectory of peak top of element X

$$\frac{d\,c_Y}{d\,t}(x_p, t) \cong M_Y \frac{\partial^2 f_0}{\partial c_X \partial c_Y} \frac{\partial^2 c_1}{\partial x^2}$$

Behavior of element Y along the trajectory of peak top of element X

$$\frac{d\,c_Y}{d\,t}(x_p,t) \cong M_Y \frac{\partial^2 f_0}{\partial c_X \partial c_Y} \frac{\partial^2 c_1}{\partial x^2}$$

$$\frac{\partial^2 c_X}{\partial x^2} < 0$$

Regular solution model

$$\mathbf{f}_0 = \mathbf{f_{Fe}c_{Fe}} + \mathbf{f_X c_X} + \mathbf{f_Y c_Y} +$$

$$\Omega_{XY}\mathbf{c_X c_Y} + \Omega_{Fe\,X}\mathbf{c_{Fe}c_X} + \Omega_{Fe\,Y}\mathbf{c_{Fe}c_Y} +$$

$$\mathbf{RT}\left[\mathbf{c_{Fe}}\ln\mathbf{c_{Fe}} + \mathbf{c_X}\ln\mathbf{c_X} + \mathbf{c_Y}\ln\mathbf{c_Y}\right]$$

$$\mathbf{c_{Fe}} + \mathbf{c_X} + \mathbf{c_Y} = 1$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_X^2} = -2\Omega_{\mathbf{Fe\,X}} + \mathbf{RT}\left(\frac{1}{\mathbf{c}_X} + \frac{1}{1 - \mathbf{c}_X - \mathbf{c}_Y}\right) \cdots (1)$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_Y^2} = -2\Omega_{\mathbf{Fe\,Y}} + \mathbf{RT}\left(\frac{1}{\mathbf{c}_Y} + \frac{1}{1 - \mathbf{c}_X - \mathbf{c}_Y}\right) \cdots (2)$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_X \partial \mathbf{c}_Y} = \Omega_{\mathbf{XY}} - \Omega_{\mathbf{Fe\,X}} - \Omega_{\mathbf{Fe\,Y}} + \mathbf{RT}\frac{1}{1 - \mathbf{c}_X - \mathbf{c}_Y} \cdots (3)$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_X^2} = -2\Omega_{\mathbf{Fe\,X}} + \mathbf{RT}\left(\frac{1}{\mathbf{c}_X} + \frac{1}{1-\mathbf{c}_X-\mathbf{c}_Y}\right) \cdots (1)$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_Y^2} = -2\Omega_{\mathbf{Fe\,Y}} + \mathbf{RT}\left(\frac{1}{\mathbf{c}_Y} + \frac{1}{1-\mathbf{c}_X-\mathbf{c}_Y}\right) \cdots (2)$$

$$\frac{\partial^2 \mathbf{f}_0}{\partial \mathbf{c}_X \partial \mathbf{c}_Y} = \Omega_{\mathbf{XY}} - \Omega_{\mathbf{Fe\,X}} - \Omega_{\mathbf{Fe\,Y}} + \mathbf{RT}\frac{1}{1-\mathbf{c}_X-\mathbf{c}_Y} \cdots (3)$$

Modelling of microstructural evolution in structural steel

- 1st stage(1985-1995)

  Integrated model based on thermodynamics and

  phase transformation theory

- 2nd stage(1995-2005)

  MC, PF for Grain growth, Spinodal decomposition
etc.

- 3rd stage(2005-)

  Multiscale 3-D simulation for microstructural

  evolution in structural steel.

Microscopic model

   Thermodynamics model

   Kinetic model

     →Prediction of microstructure

      ＋FEM →

     Prediction of mechanical propertied

Mesoscopic model

   Phase field model

   Monte Carlo method

Neural network

Mathematical method

Dynamics and Microstructure Evolution in Metals during and after the process of Severe Plastic Deformation

Tetsuya Ohashi (Kitami Institute of Technology),

Mitsutoshi Kuroda (Yamagata University),

Yoshiyuki Saito (Waseda University),

Tadanobu Inoue (National Institute of Material Science)

Objectives of this study group are to clarify underlying mechanisms for the development of fine-grained microstructures and to understand the mechanical response of metal polycrystals with high-density lattice defects by using numerical techniques of macro- and meso-mechanics. In the macroscopic analyses, strain histories in materials processed by ARB or ECAP are quantitatively evaluated. The crystal plasticity analyses are performed to understand the characteristics and particularities of dislocation accumulations under different deformation modes. Macroscopic mechanical responses of nano-structured metals are also predicted by crystal plasticity analyses. Thermodynamic stability of ultrafine grained structures is discussed with phase field simulations.

item	2000	2005	2010	2015	needs

Modelling
 Equilibrium state
  Calphad
 Dynamics
  Microstructural evolution
 Properties

 Ab-initio
 MD,MC
 PFM
 FEM
 Empirical

Database

 ThermodynamicsDB
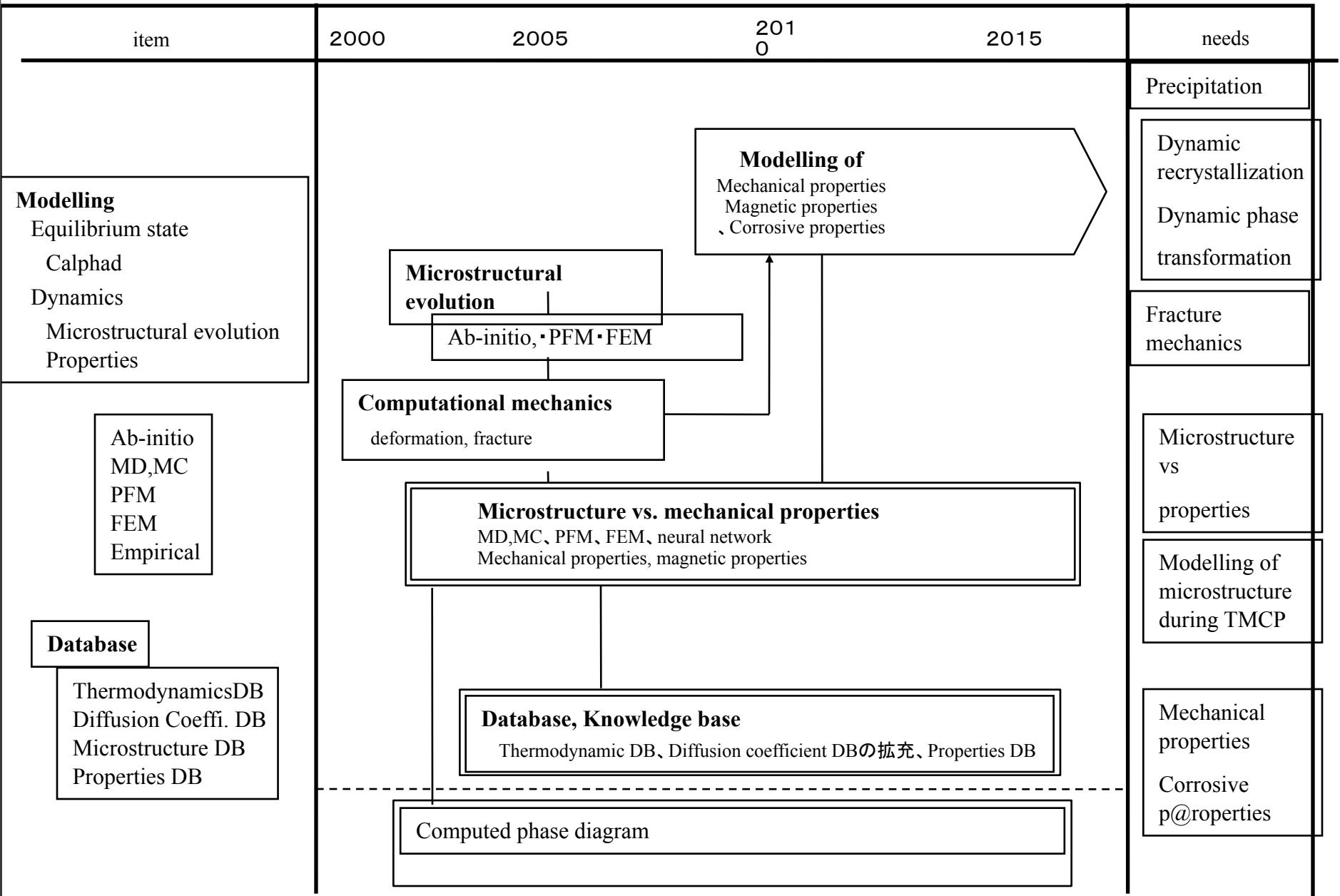 Diffusion Coeffi. DB
 Microstructure DB
 Properties DB

Modelling of
Mechanical properties
 Magnetic properties
、Corrosive properties

Microstructural evolution

Ab-initio,・PFM・FEM

Computational mechanics

deformation, fracture

Microstructure vs. mechanical properties
MD,MC、PFM、FEM、neural network
Mechanical properties, magnetic properties

Database, Knowledge base

Thermodynamic DB、Diffusion coefficient DBの拡充、Properties DB

Computed phase diagram

Precipitation

Dynamic recrystallization

Dynamic phase transformation

Fracture mechanics

Microstructure vs properties

Modelling of microstructure during TMCP

Mechanical properties

Corrosive p@roperties

Multiscale 3D-model

Microstructure

    Phase field+MC and FEM

Properties

    FEM

    Neural network