Effect of External Fields on Microstructures: A Modeling Perspective

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Outline

- Motivation
- Quaternary System Phase Microstructure: Inhomogeneous Elastic Properties
- Intermediate Phase Growth: Externally Applied Electric Fields

What can we do with OOF:

Study the effect of externally applied tractions and electric fields on the kinetics and the final microstructure formed.

Motivation

- Diffuse Interface Model used to study phase microstructure evolution in a III-V system with site occupancy restriction.
  - What is the effect of self-stress?
  - What is the effect of externally applied tractions?
  - Can we consider elastic inhomogeneity?
- Diffuse Interface Model is used to study the behavior of an existing intermediate phase during current flow.
  - What effect does the direction of current have?
  - How do stress considerations play a role?
- Our Numerical Engine uses the Multigrid Method to solve equations.
- We do not have the versatility as OOF.
- We can compare our results with that by OOF

1. III-V Phase Microstructure Evolution

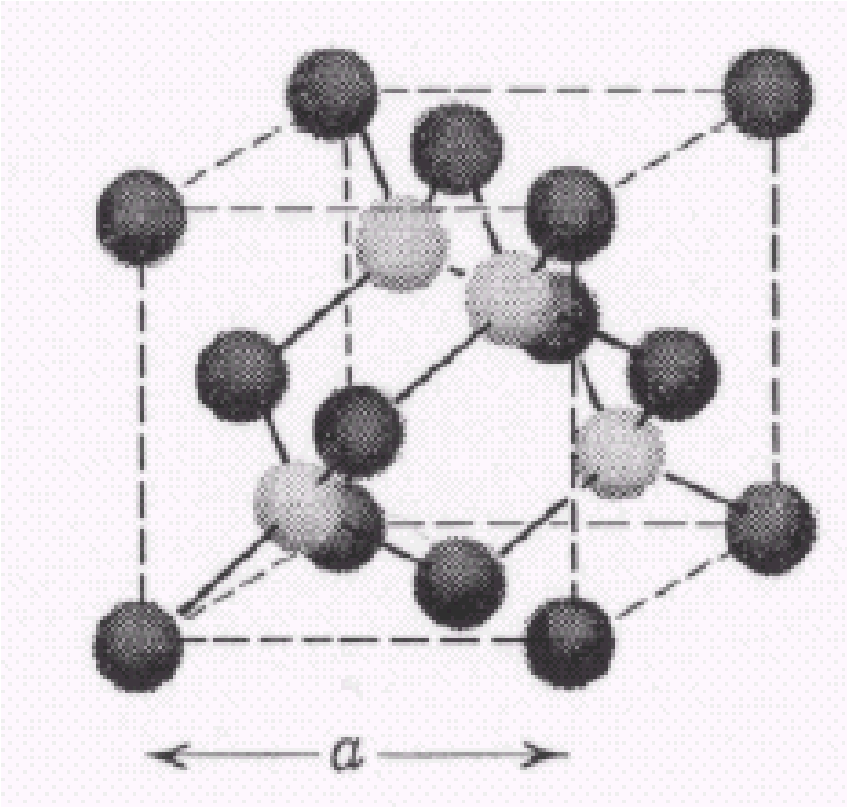
- Model the microstructural evolution of a III-V pseudo-binary system which has a miscibility gap.

- Model Physical System:
  - $In_xGa_{1-x}As_ySb_{1-y}$
  - Group III: In, Ga
  - Group V: As, Sb
  - Mixture of 4 binary compounds

    InAs, InSb

    GaAs, GaSb

- The quaternary solid solutions crystallize in Zinc-Blend structure which consists of two interpenetrating binary sublattices.



Free Energy Functional

$$F(x,y,\Phi) = \int_V \{f^{chem}(x,y,\Phi) + f^{elas}(x,y,\Phi,u) - \mu_A(x-x_o) - \mu_C(y-y_o) + \kappa_{xx}/2\,\Delta x + \kappa_{yy}/2\,\Delta y + \kappa_{\Phi\Phi}/2\,\Delta\Phi\}\, d^3z + \int_S [f_S(x,y) - t.u]d^2z$$

κ_{xx}, κ_{yy}, $\kappa_{\Phi\Phi}$ - Cahn-Hilliard gradient energy coefficients associated to the x, y and Φ fields.

Regular Solution Model for $A_xB_{1-x}C_yD_{1-y}$ system

$$f^{chem}(\Phi, x, y) = xy\,\mu^0_{AC}(\Phi) + x(1-y)\,\mu^0_{AD}(\Phi) + y(1-x)\,\mu^0_{BC}(\Phi) + (1-x)(1-y)\,\mu^0_{BD}(\Phi) + \rho_o kT[x\ln x + (1-x)\ln(1-x) + y\ln(y) + (1-y)\ln(1-y)] + x(1-x)[y\,\omega_{BC-AC}(\Phi) + (1-y)\,\omega_{AD-BD}(\Phi)] + y(1-y)[x\,\omega_{AD-AC}(\Phi) + (1-x)\,\omega_{BC-BD}(\Phi)]$$

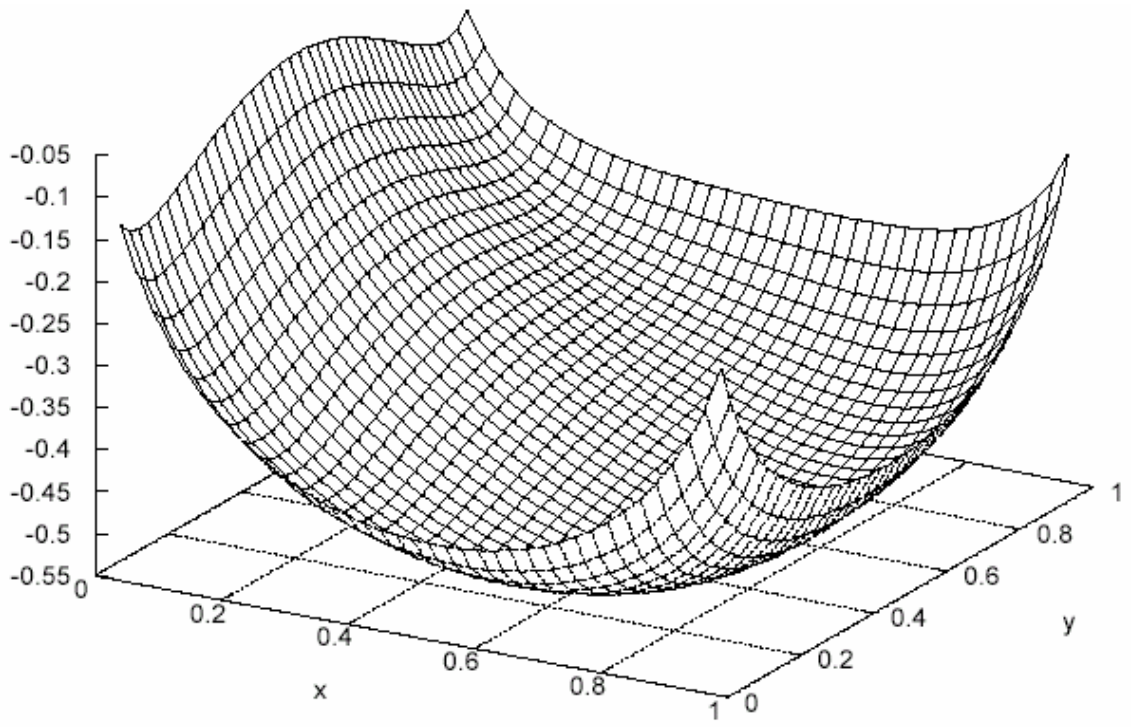
Elastic Energy for $A_xB_{1-x}C_yD_{1-y}$ system

$$f^{elas}(\Phi, x, y, u) = 1/2\; T_{ij}(\Phi, x, y, u)(E_{ij}(u) - e(\Phi, x, y)\delta_{ij})$$

$e(\Phi, x, y)$ - eigenstrain in the system

Free Energy Surface

Free energy surface across the ‘x’ and ‘y’ composition at T = 773 K for a $In_xGa_{1-x}As_ySb_{1-y}$ system.



Thermodynamics

$In_xGa_{1-x}As_ySb_{1-y}$ system

Chemical Spinodal

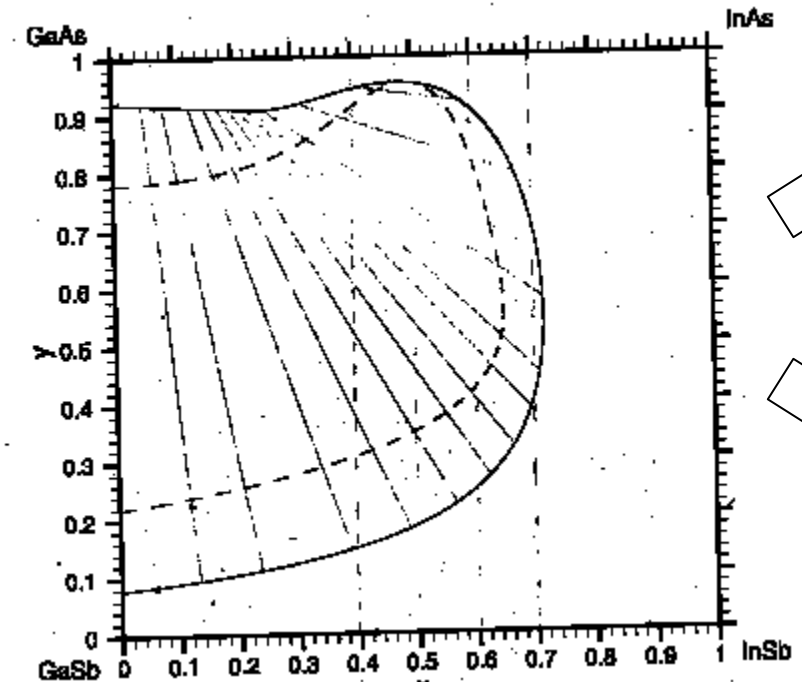
$$\left(\frac{\partial^2 f^{chem}}{\partial^2 x}\right)\bullet\left(\frac{\partial^2 f^{chem}}{\partial^2 y}\right)-\left(\frac{\partial^2 f^{chem}}{\partial x \partial y}\right)^2 = 0$$

Miscibility Boundary

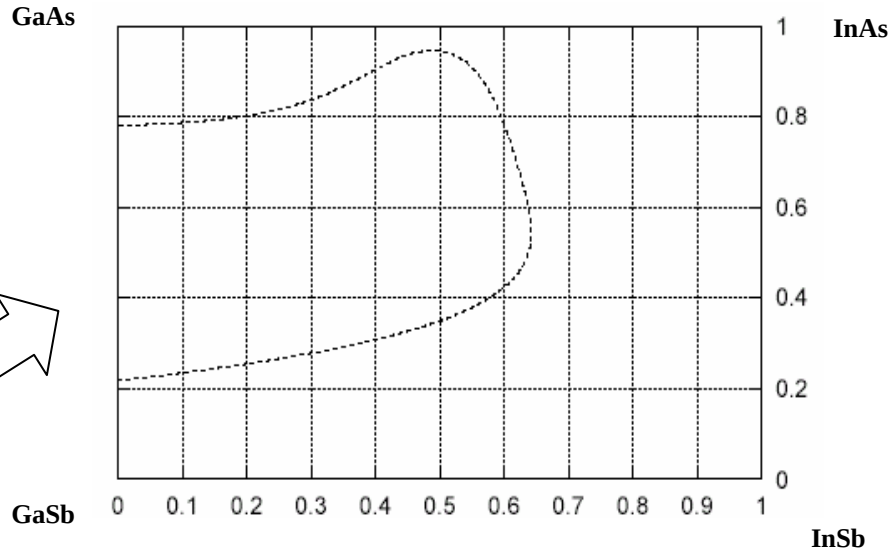
$$\mu_{AC}^{\alpha} = \mu_{AC}^{\beta} \qquad \mu_{AD}^{\alpha} = \mu_{AD}^{\beta}$$

$$\mu_{BC}^{\alpha} = \mu_{BC}^{\beta} \qquad \mu_{BD}^{\alpha} = \mu_{BD}^{\beta}$$

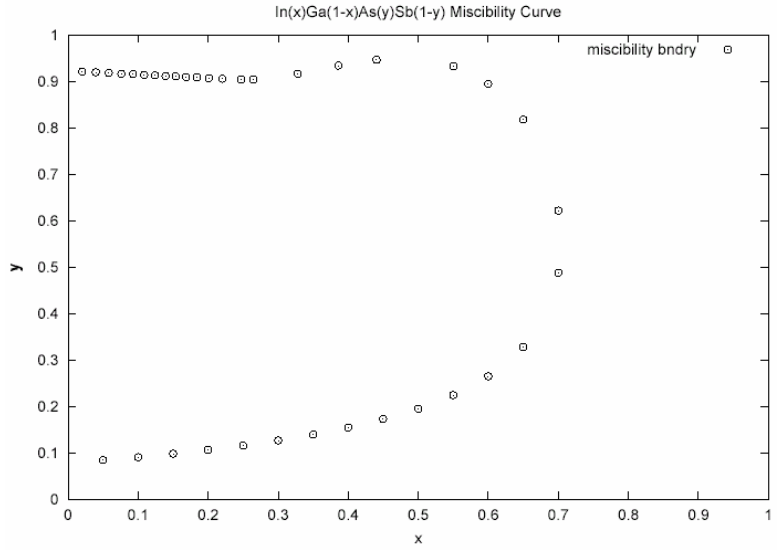
Calculated Phase Diagram



Calculated Spinodal Boundary



Calculated Miscibility Boundary



Evolution Equations for the Order Parameters

-order parameters evolve so that the total free energy decreases

Evolution Equations for the order parameters

$$\frac{\partial x}{\partial t} = \nabla \bullet \left(M_{xx} \nabla \left(\frac{\delta F}{\delta x} \right) + M_{xy} \nabla \left(\frac{\delta F}{\delta y} \right) \right)$$

$$\frac{\partial x}{\partial t} = \nabla \bullet \left(M_{yx} \nabla \left(\frac{\delta F}{\delta x} \right) + M_{yy} \nabla \left(\frac{\delta F}{\delta y} \right) \right)$$

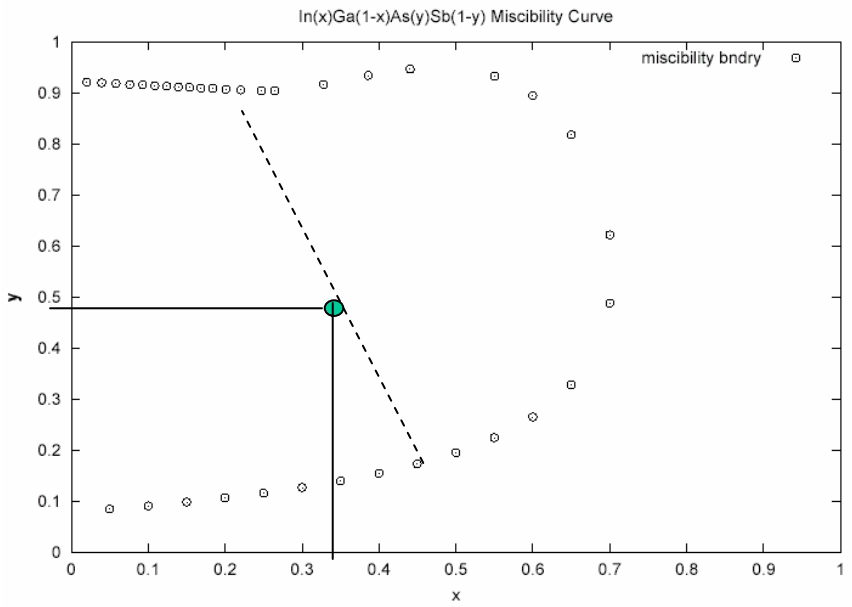
$$\mu_x \equiv \frac{\delta F}{\delta x} = \frac{\partial f^{chem}}{\partial x} + \frac{\partial f^{elas}}{\partial x} - \kappa_{xx} \nabla^2 x$$

$$\mu_y \equiv \frac{\delta F}{\delta y} = \frac{\partial f^{chem}}{\partial y} + \frac{\partial f^{elas}}{\partial y} - \kappa_{yy} \nabla^2 y$$

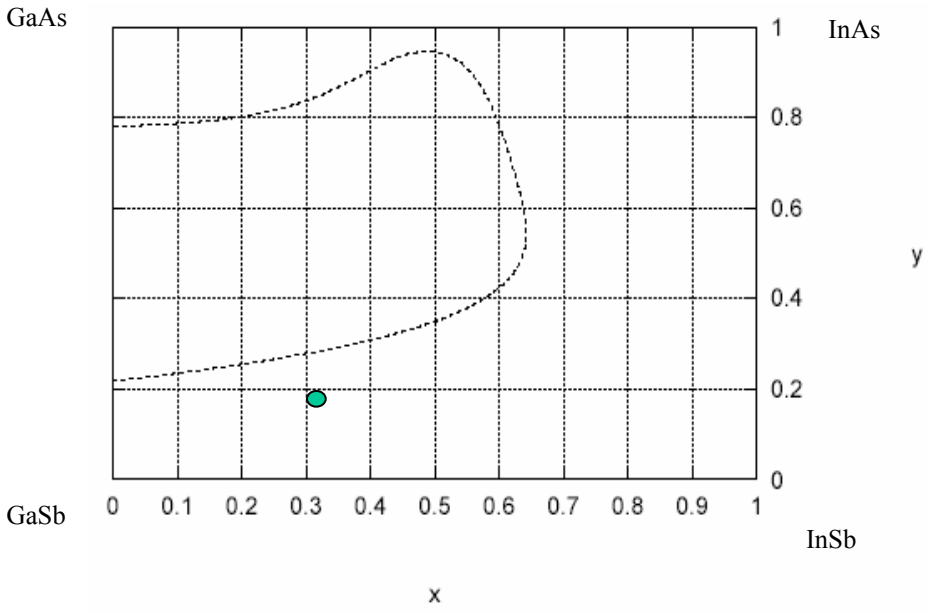
Simulation 1: Initial Conditions

(X,Y) = (0.3,0.4)

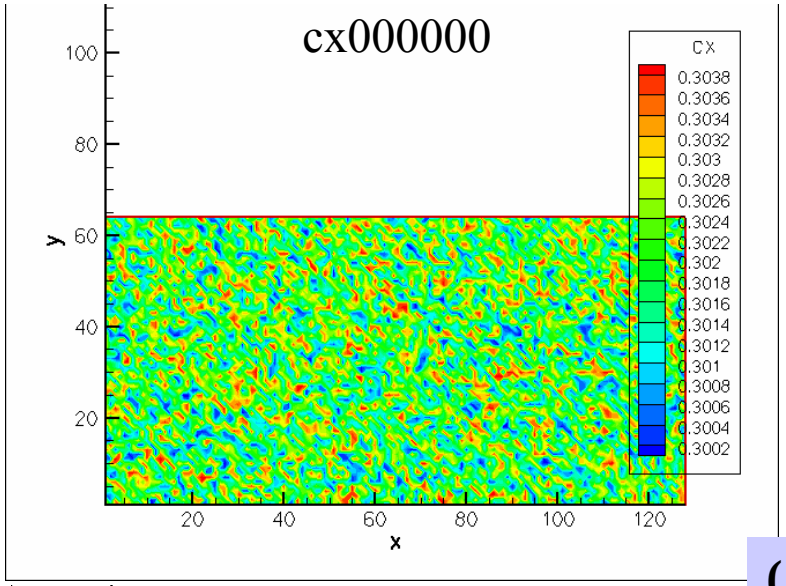
Miscibility Boundary

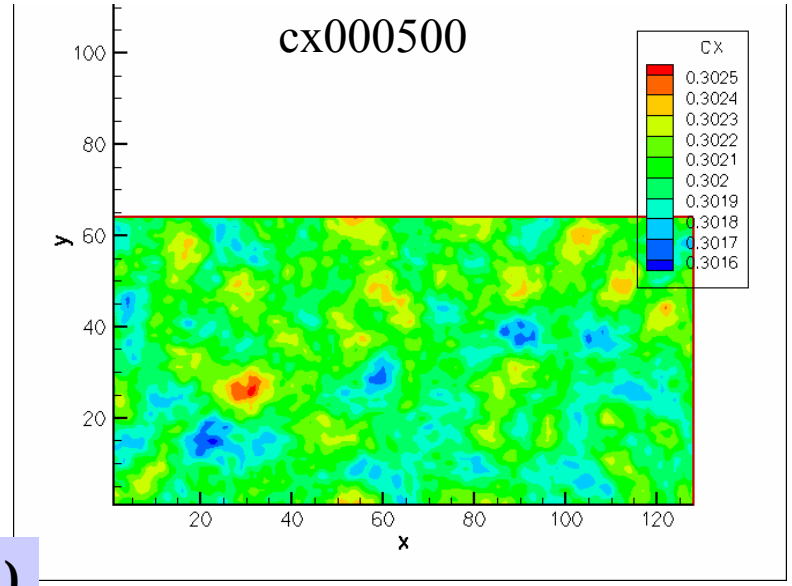


Spinodal Boundary

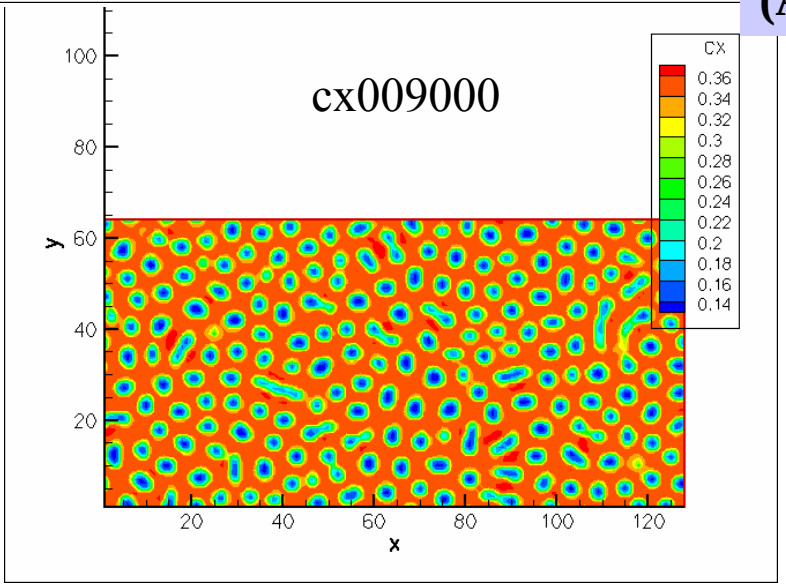


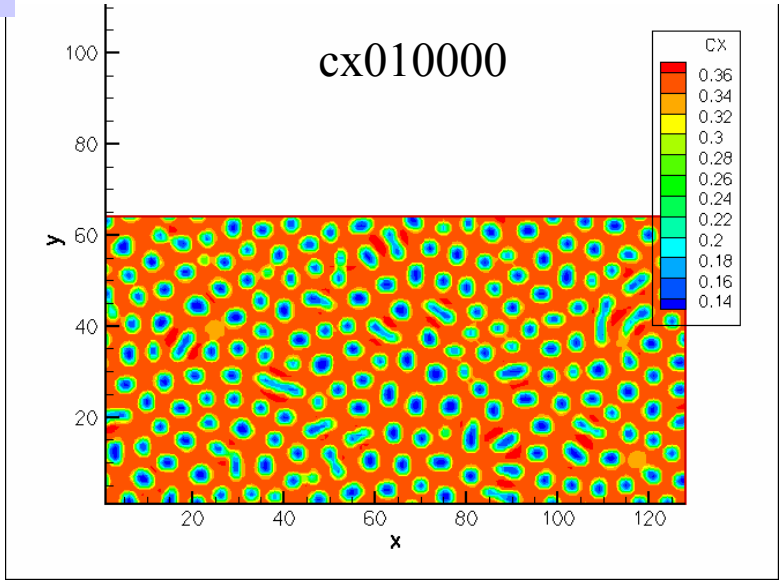
Simulation 1: Results for X



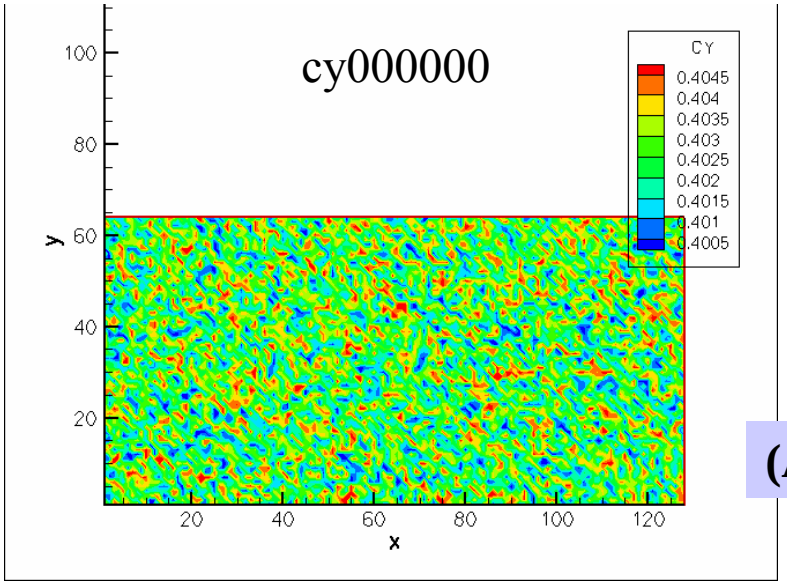


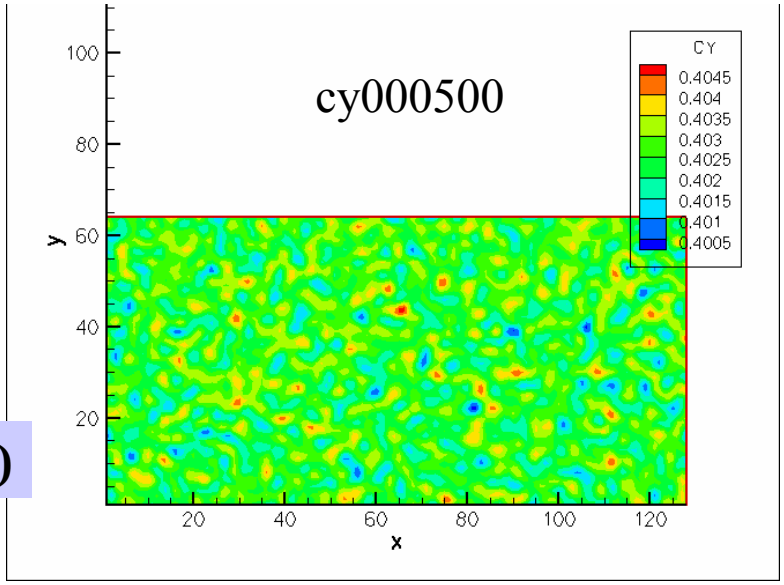
$(A_xB_{1-x}C_yD_{1-y})$



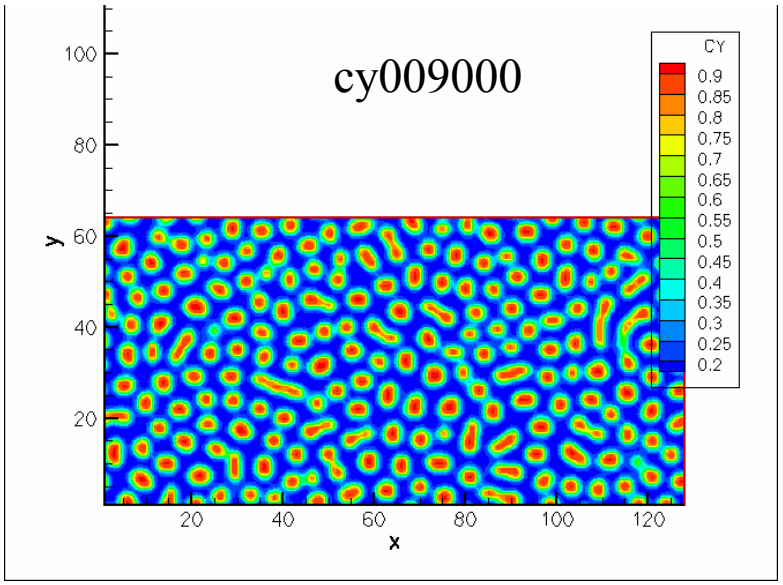


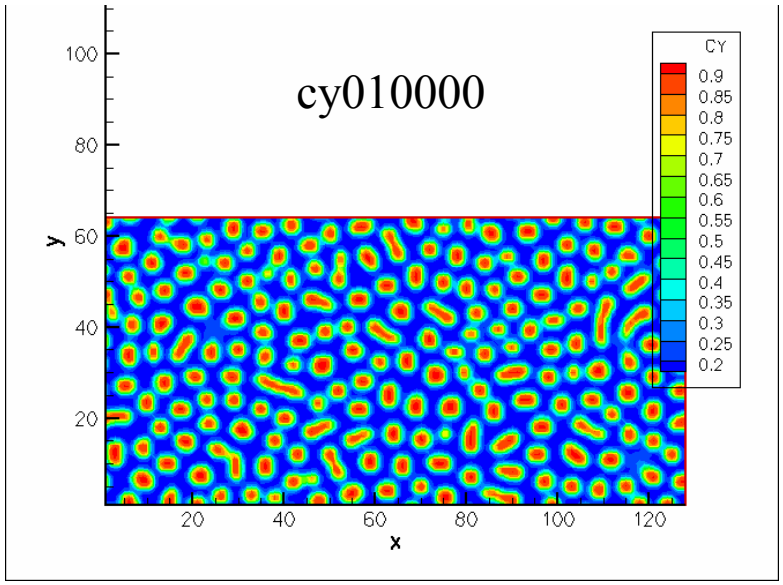
Simulation 1: Results for Y





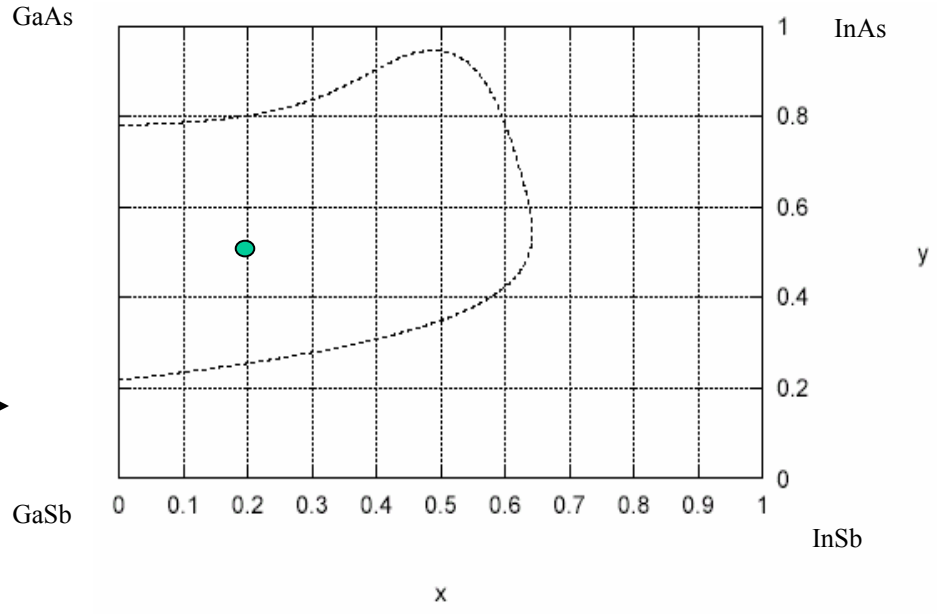
$(A_xB_{1-x}C_yD_{1-y})$

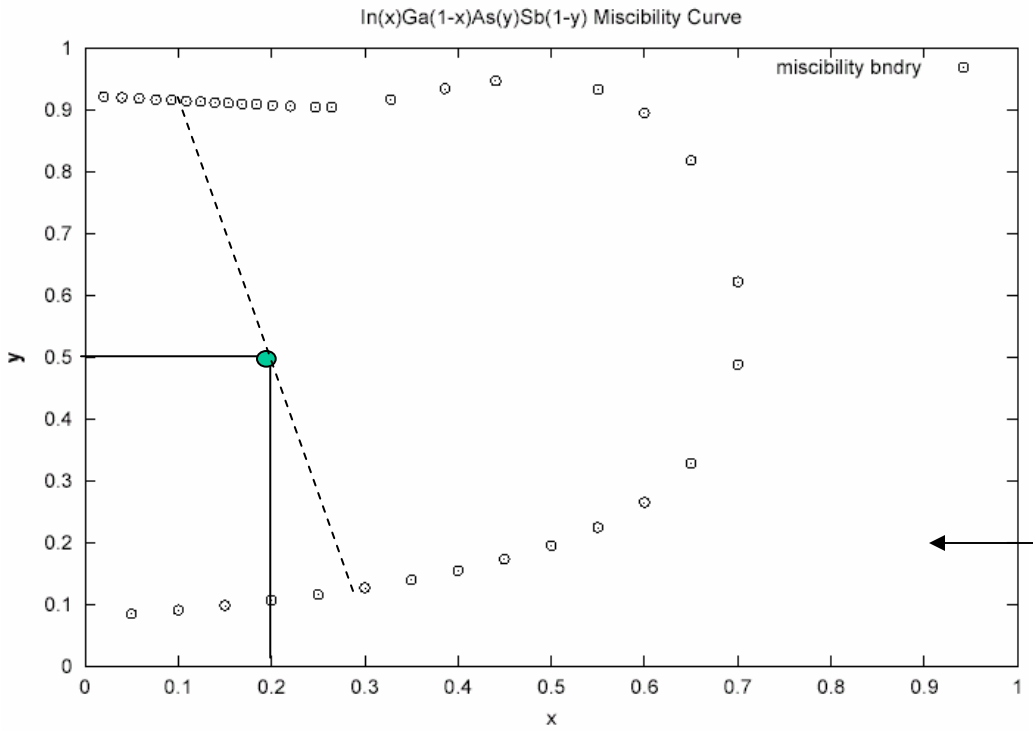




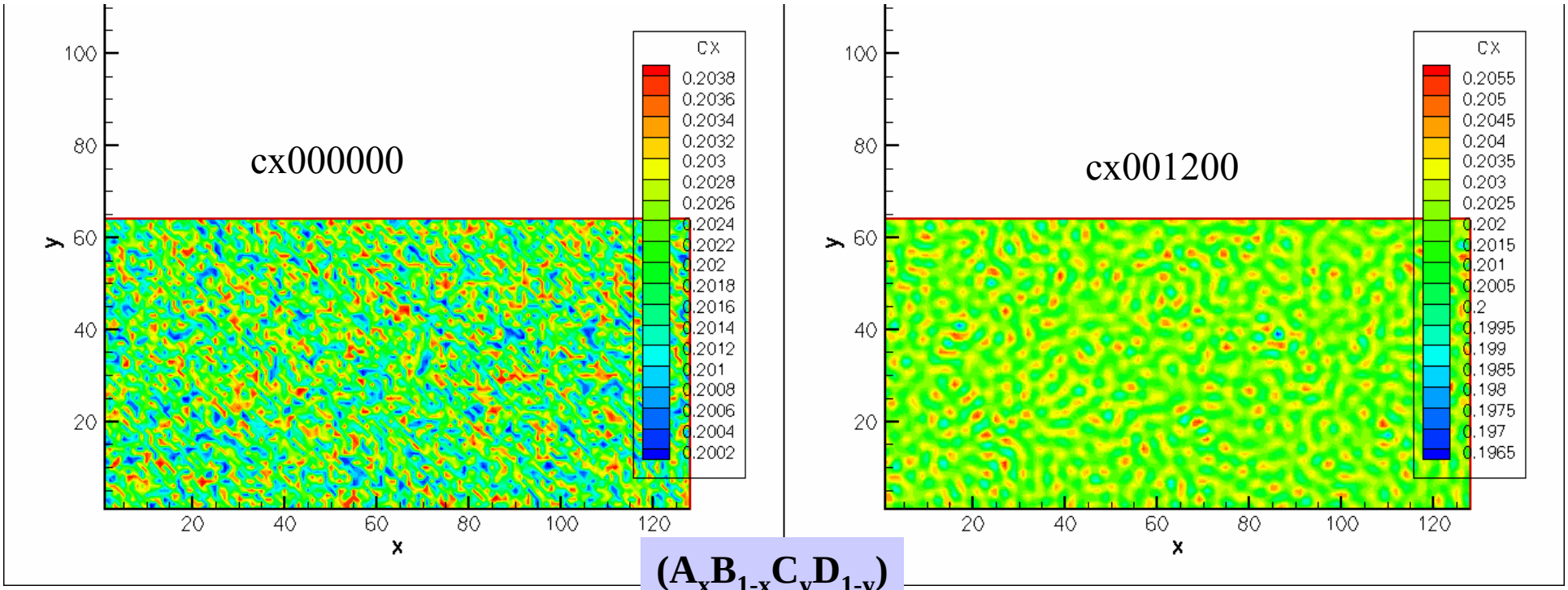
(X,Y) - (0.2, 0.5)

Spinodal Boundary →





← Miscibility Boundary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0.2036
0.2034
0.2032
0.203
0.2028
0.2026
0.2024
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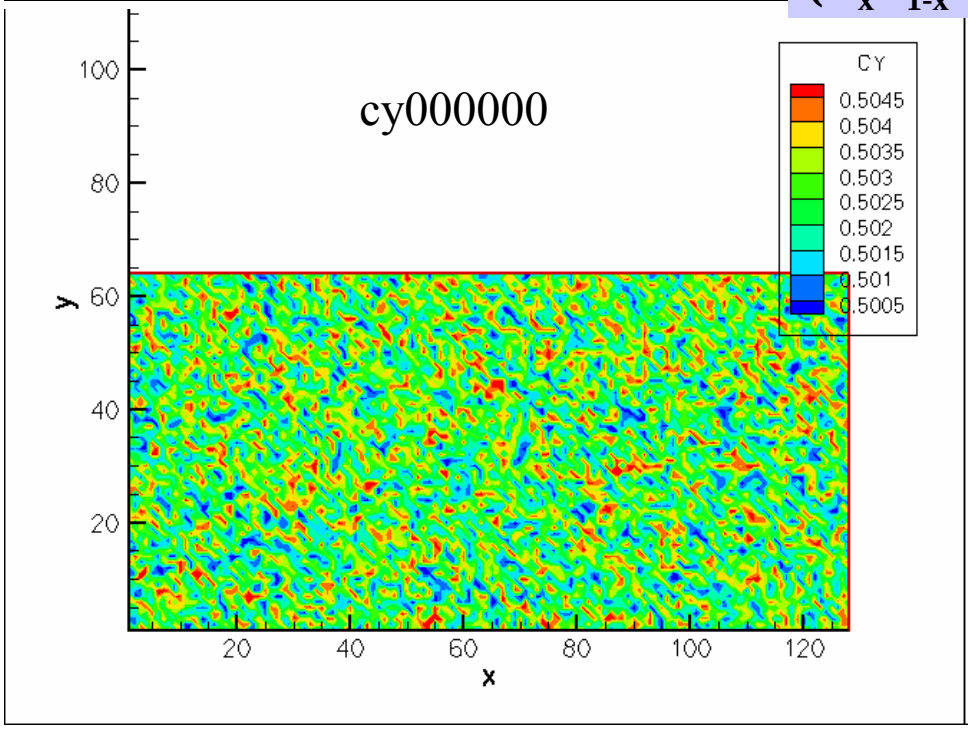
0.202
0.2018
0.2016
0.2014
0.2012
0.201
0.2008
0.2006
0.2004
0.2002
y
x

cx001200
CX
0.2055
0.205
0.2045
0.204
0.2035
0.203
0.2025
0.202
0.2015
0.201
0.2005
0.2
0.1995
0.199
0.1985
0.198
0.1975
0.197
0.1965
y
x

$(A_xB_{1-x}C_yD_{1-y})$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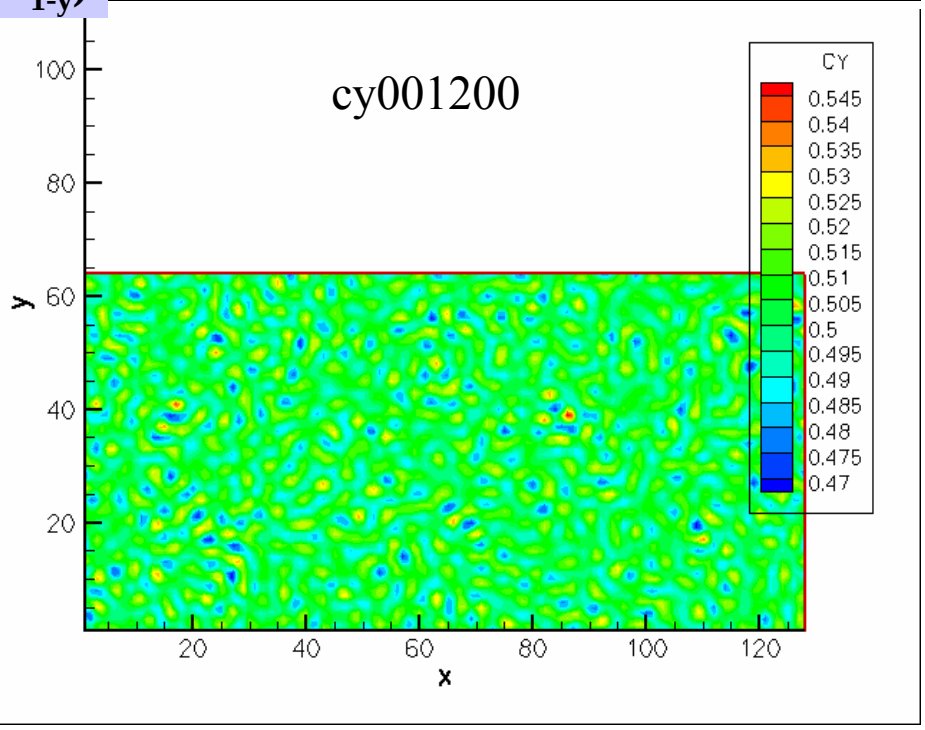
y
x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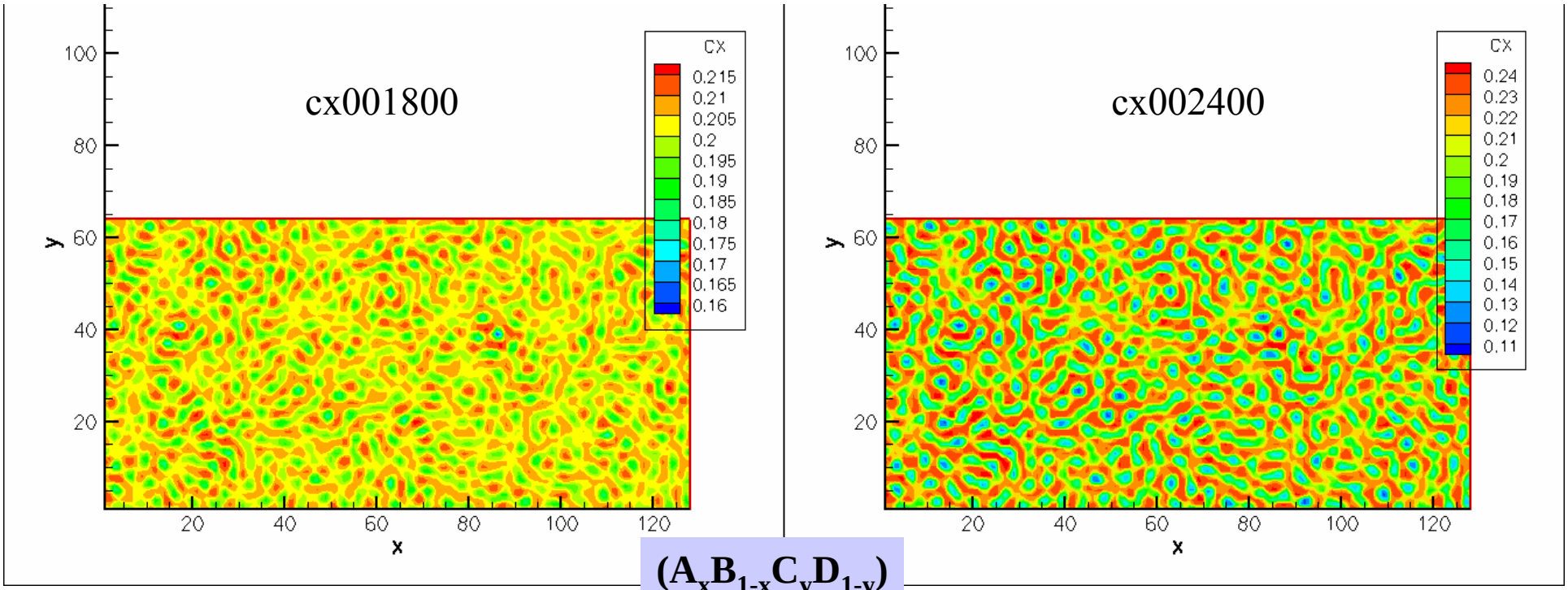
y
x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0.16
y
x
20
40
60
80
100
120

cx002400
CX
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0.21
0.2
0.19
0.18
0.17
0.16
0.15
0.14
0.13
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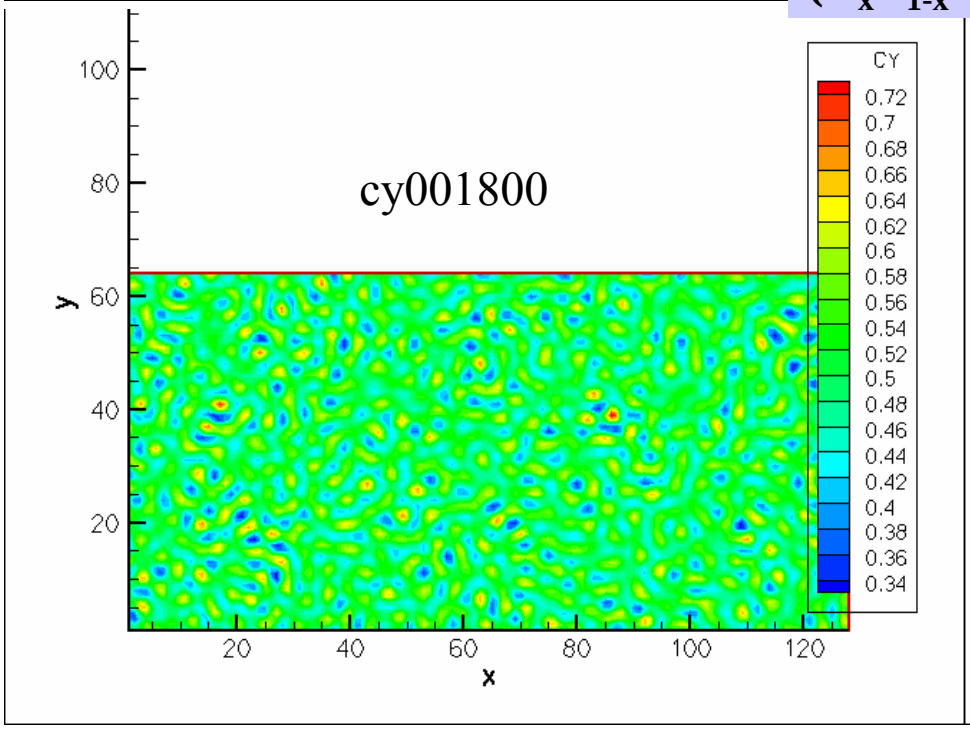
0.11
y
x
20
40
60
80
100
120

$(A_xB_{1-x}C_yD_{1-y})$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0.5
0.48
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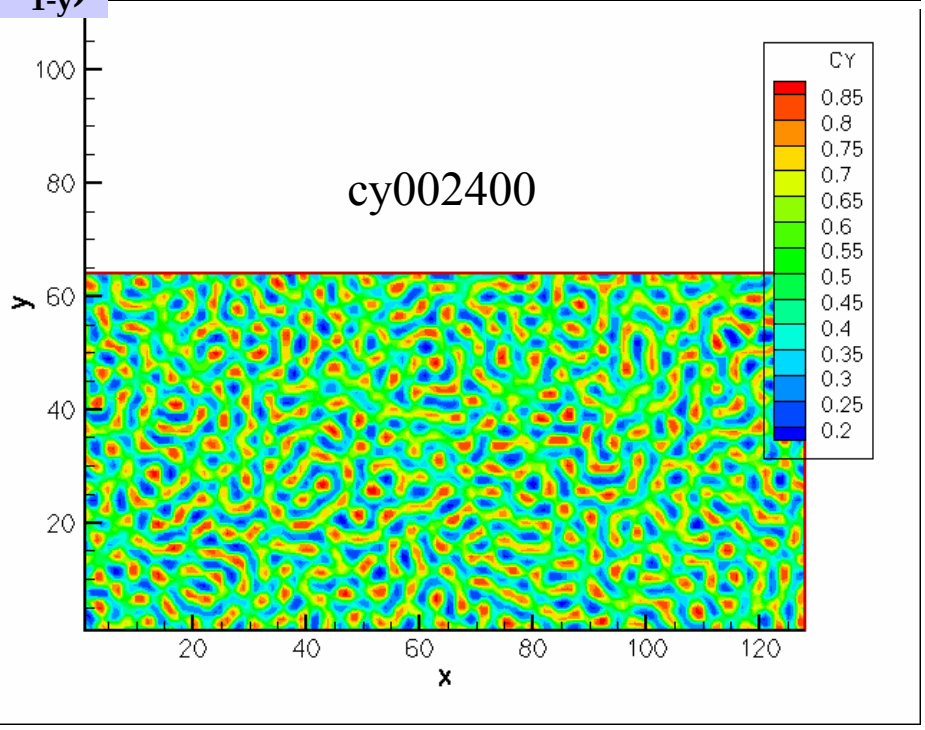
0.34
y
x
20
40
60
80
100
120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0.7
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0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
y
x
20
40
60
80
100
120

2. Intermediate Phase growth

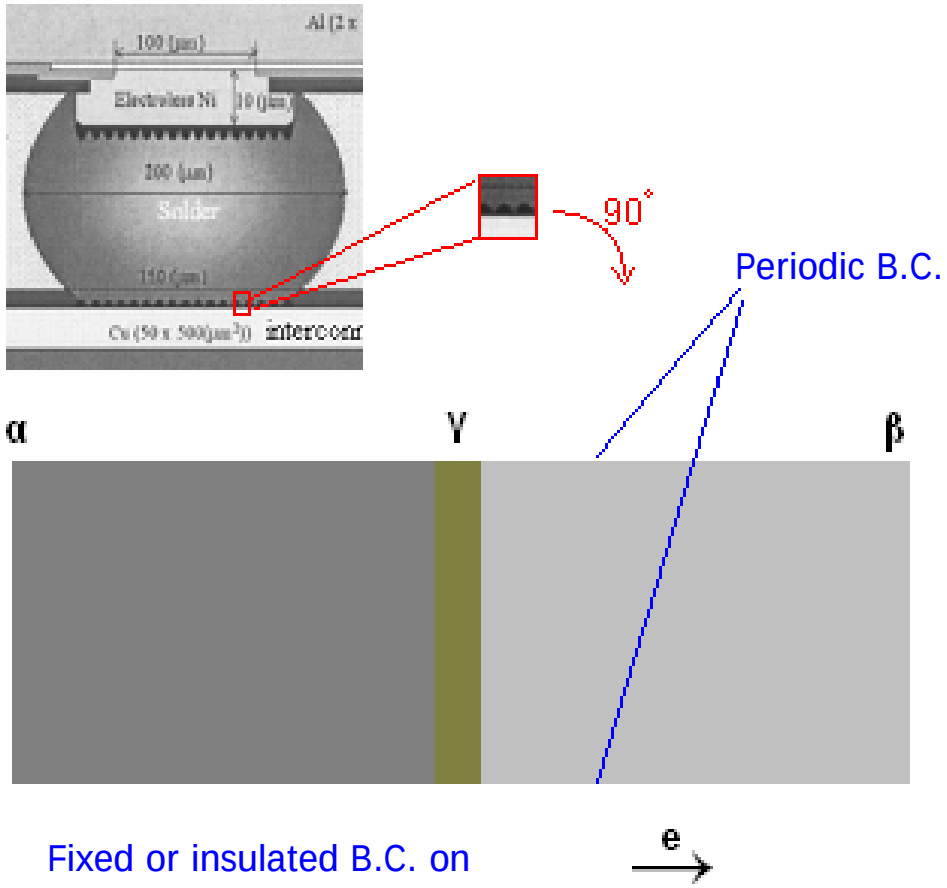
- Diffusion couple
  - Binary, multiphase

- Independent variables:

  Diffusion:
  - c (composition)
  - ϕ (crystal structure)

  Electromigration:
  - ψ (electric potential)

  Elasticity:
  - u (elastic displacement)



Free Energy Density

- Free energy density of the system(Joule/mol)

$$f(\phi,c) = f_{ch}(\phi,c) + f_{elec}(\phi,c,\varphi) + f_{elas}(\phi,c,u) + \frac{\kappa_c}{2}|\nabla c|^2 + \frac{\kappa_\varphi}{2}|\nabla \phi|^2$$

  - Chemical free energy
  - Electrostatic energy
  - Elastic energy
  - Gradient energy

Electrostatic Energy

- Effective charge
  - $Z_i = Z_v + Z_m$ (i=A,B)

Valence charge

Momentum transfer

Dominant contribution

Effecitive charge of Al: -20/-30

- Electrostatic energy

$$f_{elec} = N_0 e(cZ_B + (1-c)Z_A)\psi$$

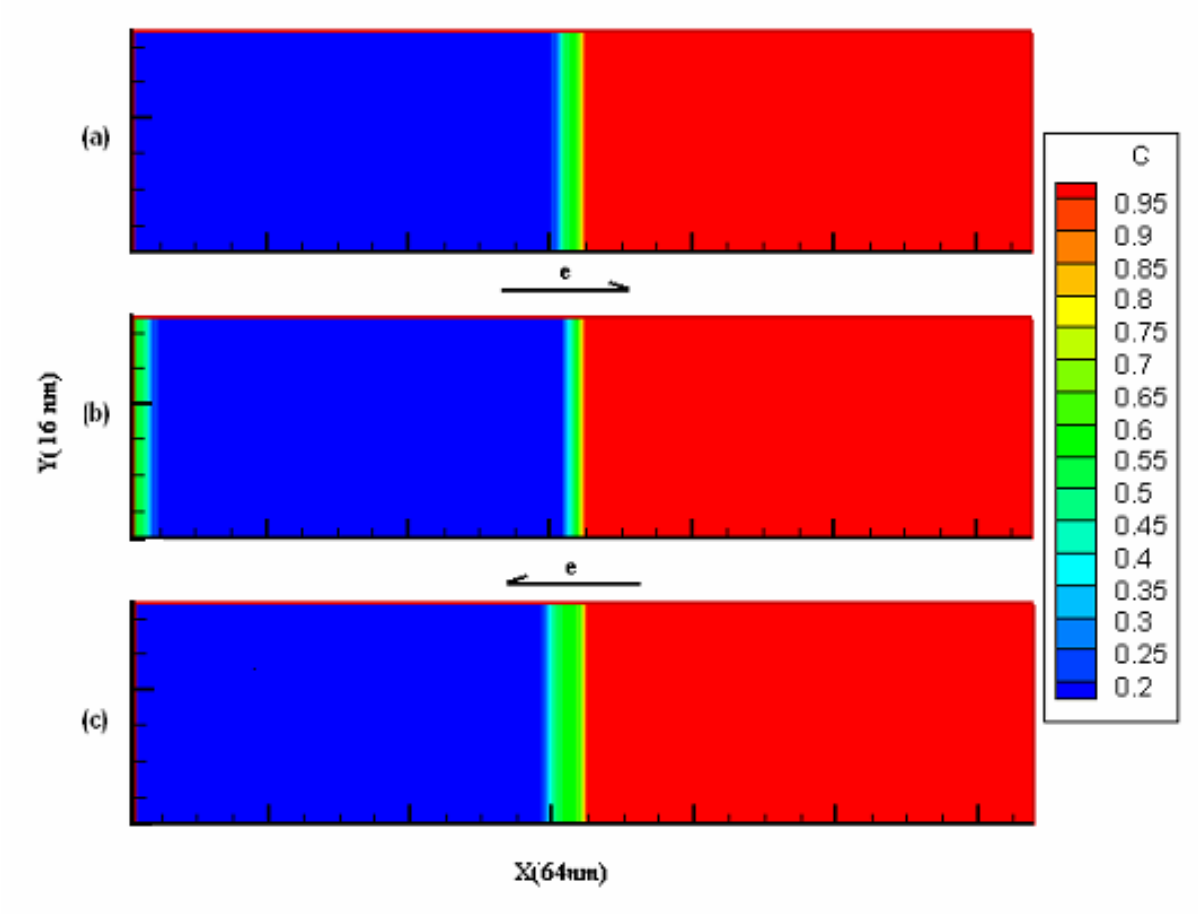
ψ : the electric potential

N_0 : Avogadro's number

$Z_i (i=A,B)$: the effective charges

Intermediate Phase Growth

- Polarity effect in Al/Zn diffusion sample



What can we do with OOF?

- Compare our results
- OOF is more versatile
- More accurate material property information can be used
- OOF can take information from real microstructures
- Perform Virtual Experiments
- Is it applicable to study dynamic processes?
- What other external long range fields can be included?