Kinetic Monte Carlo Simulation of Two-dimensional Semiconductor Quantum Dots Growth

by

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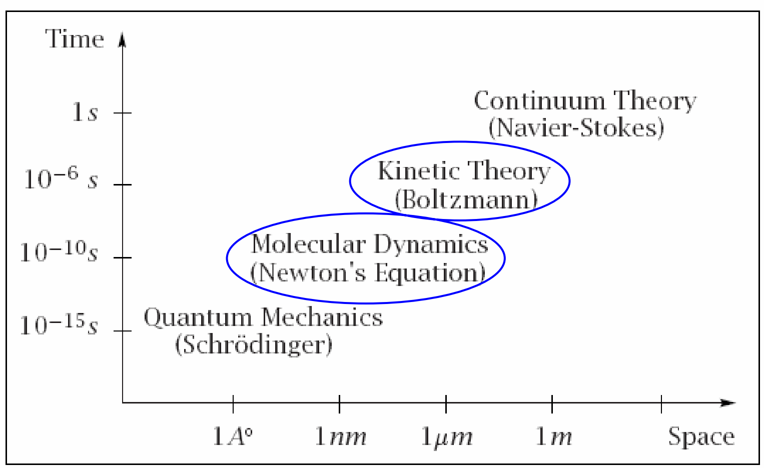
Outline

- **Crystal (QDs) Growth Back Ground**
  - Simulation Method
  - Application of QDs Growth
  - QDs Epitaxial Growth
- **Kinetic Monte Carlo (KMC) Two-dimensional (2D) QDs Growth**
  - KMC 2D Growth Model
  - Growth Parameters Dependence of QDs Shape and Distribution
    - Temperature —— T
    - Surface coverage —— c
    - Flux rate —— F
    - Interruption time —— t_i
  - Substrate Orientation Dependence of QDs Ordering
    - Strain Energy Distribution
    - QDs Patterns with Different Substrate Directions
    - QDs Patterns with Different Growth Parameters

- **Kinetic Monte Carlo (KMC)**
  - Stochastic techniques
  - Random numbers and probability statistics

- **Molecular Dynamics (MD)**
  - Newton’s second law
  - Interactions between molecules



Different laws of physics used to describe materials at different scales

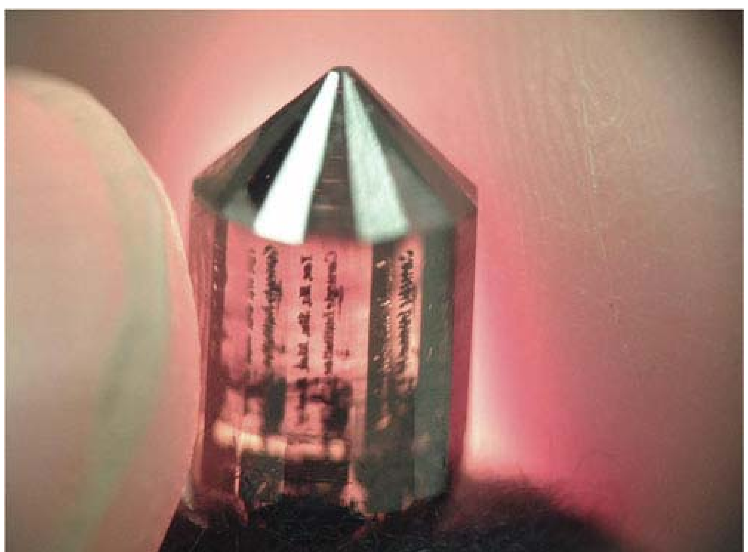
Crystal (QDs) Growth - Examples

Very Large Diamonds Produced Very Fast

ScienceDaily

May 16, 2005 Carnegie Institution

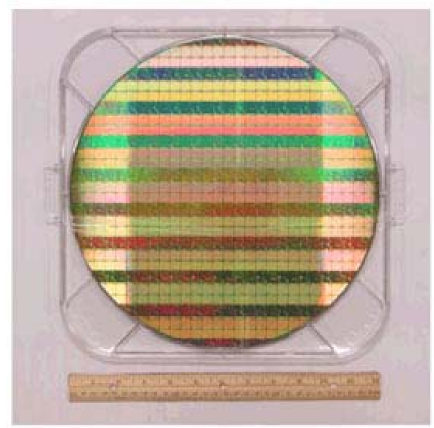
Washington, D.C. -- Researchers at the Carnegie Institution's Geophysical Laboratory have produced 10-carat, half-inch thick single-crystal diamonds at rapid growth rates (100 micrometers per hour) using a chemical vapor deposition (CVD) process.



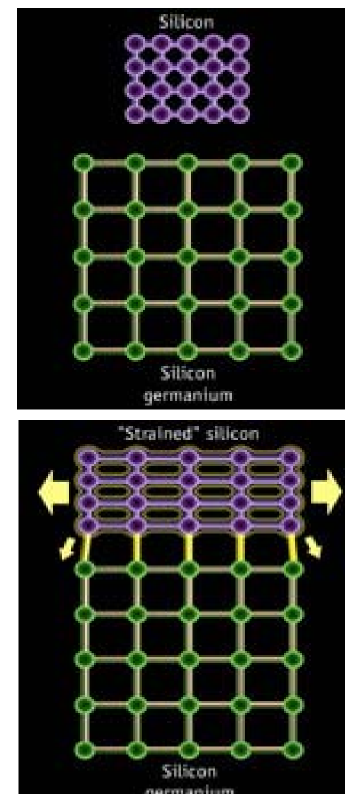
AMD, IBM announce breakthrough in strained silicon transistor

December 13, 2004

AMD and IBM today announced that they have developed a new and unique strained silicon transistor technology aimed at improving processor performance and power efficiency. The breakthrough process results in up to a 24 percent transistor speed increase, at the same power levels, compared to similar transistors produced without the technology.



52 Mbit SRAM Chips on 300 mm Wafer
120 billion transistors on one wafer

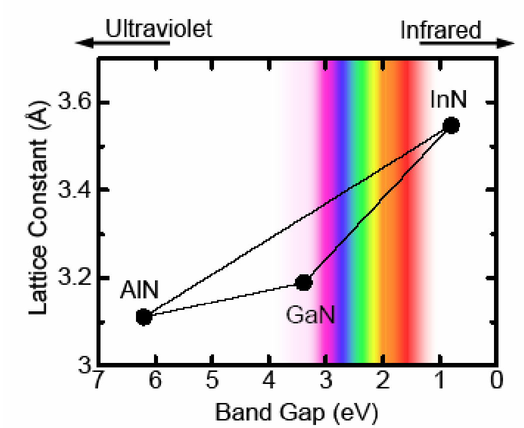


QDs for Light Emitting Diodes

First white LED using quantum dots created

July 15, 2003 Sandia National Laboratories

"Highly efficient, low-cost quantum dot-based lighting would represent a revolution in lighting technology through nanoscience."



Economy **E**nergy **E**nvironment

Comparing with traditional light devices:

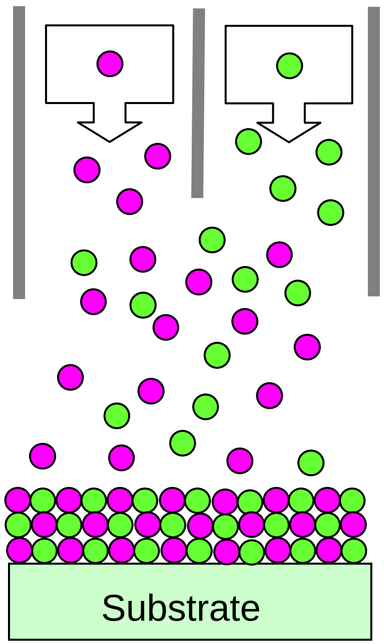
- ✓ Energy saving
- ✓ Longer life time

Comparing with traditional LEDs:

- ✓ Color adjustable
- ✓ Nontoxic
- ✓ Cheaper

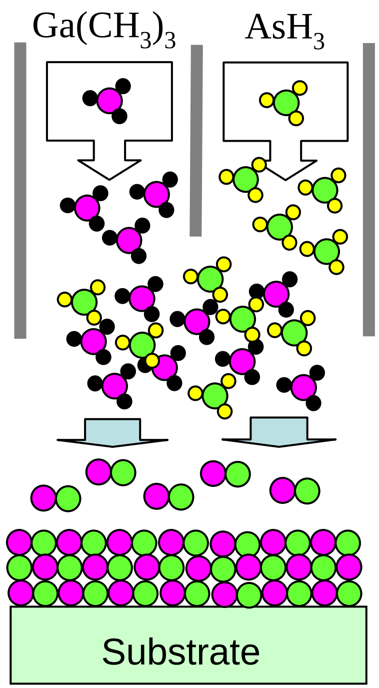
QDs Epitaxial Growth

Physical Vapor Deposition

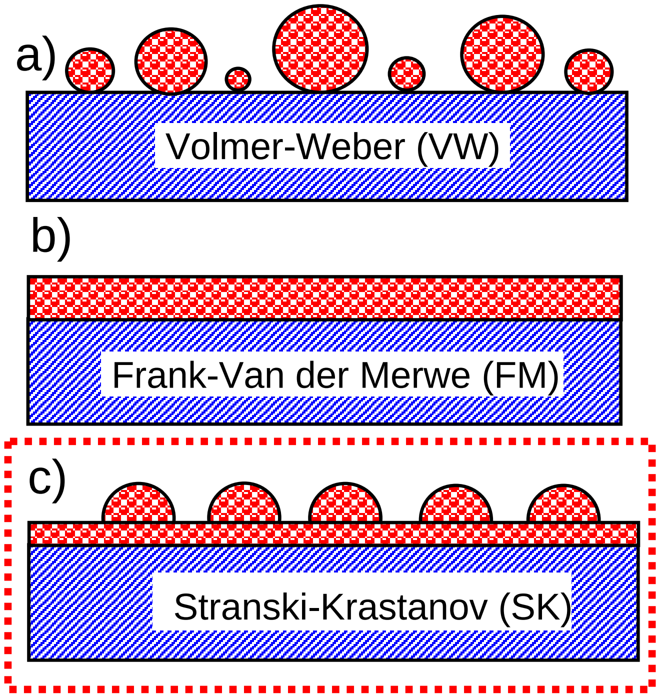


Chemical Vapor Deposition

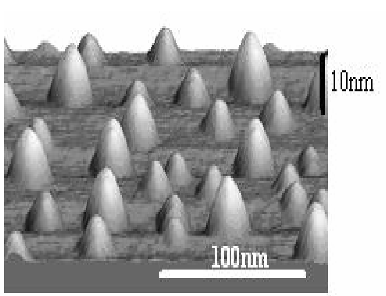
$Ga(CH_3)_3 + AsH_3 \rightarrow GaAs + 3CH_4$

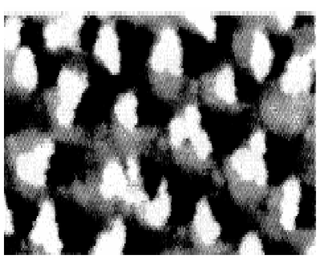


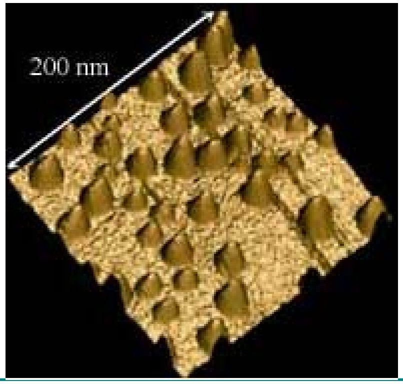
Epitaxial Growth Modes:

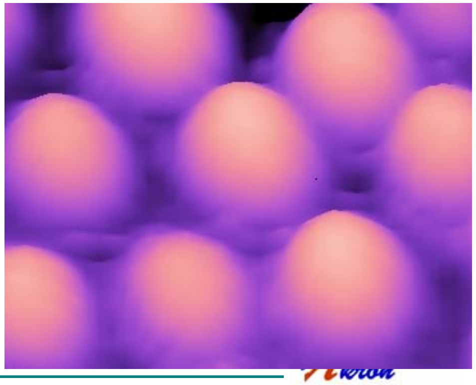


SK Mode QDs Pictures









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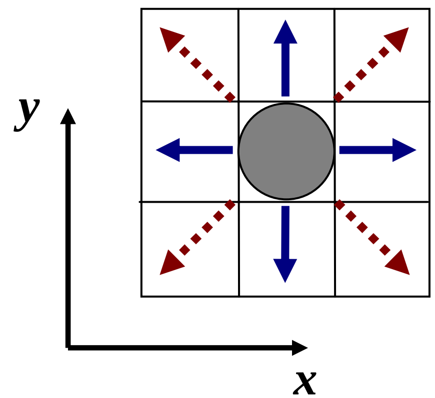
Hopping probability



$$p = \nu_0 \exp\left(-\frac{E_s + E_n - E_{str}(x,y)}{k_B T} \right)$$

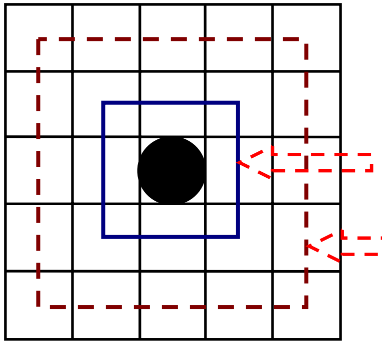
ν_0 — Attempt frequency

E_s, E_n — Bonding energies to the surface and to the neighboring atoms

$E_{str}(x,y)$ — Strain energy field

T — Temperature

k_B — Boltzmann's constant



$$E_n = (n - gn')E_b + (m - gm')\alpha E_b$$

E_b — Bonding energies of a single nearest neighbor

α, g — Reduction factor for next nearest neighbors

n, m — # of nearest and next nearest atoms in original positions ($n \leq 4$, $m \leq 4$)

n', m' — # of nearest and next nearest atoms in new positions ($n' \leq 4$, $m' \leq 4$)

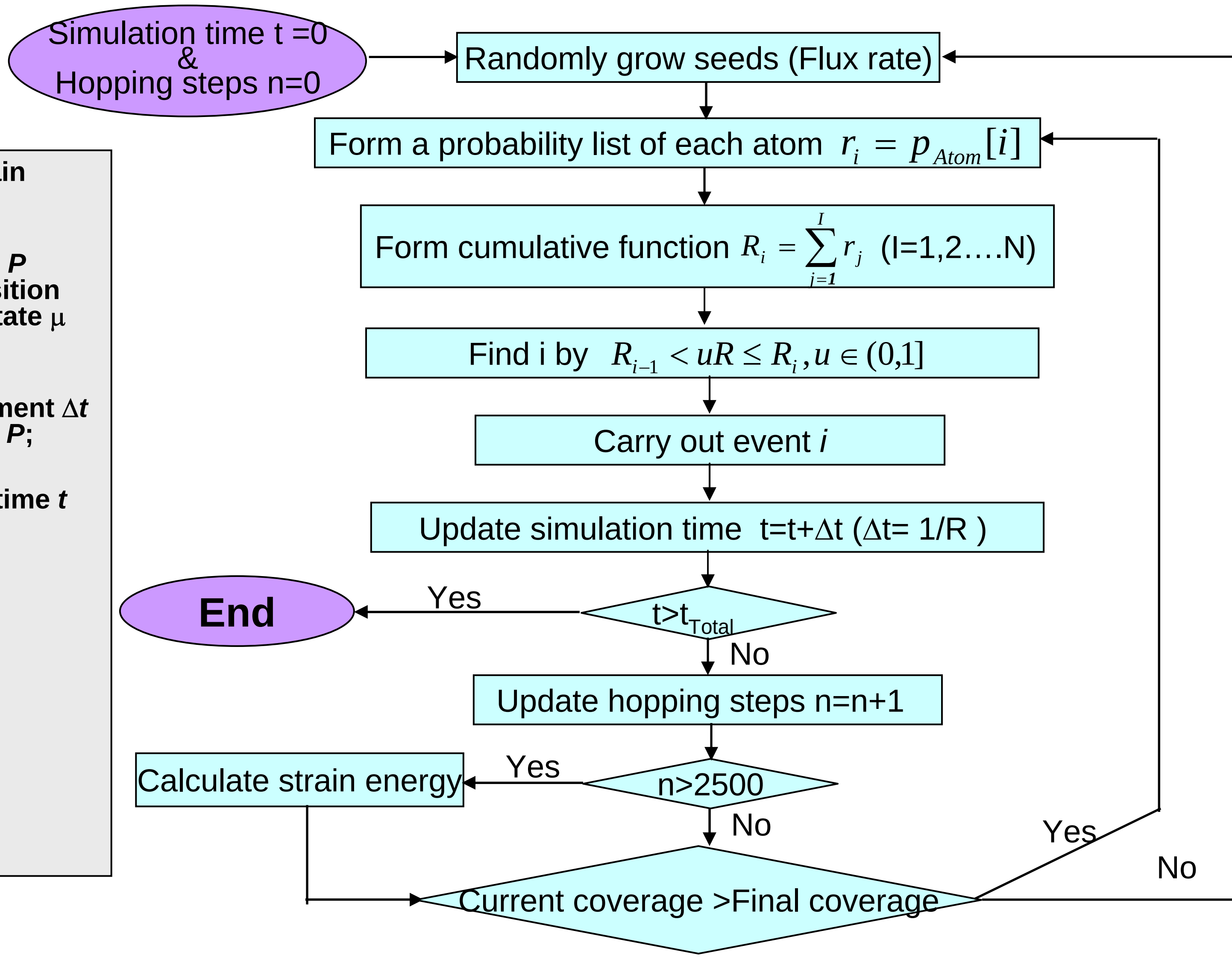
Flow Chart of 2D KMC QDs Growth Model

KMC algorithm --- three main parts

1) Calculate the probability *P* (μ→ν) for the transition from the current state μ to a new state ν;

2) Calculate the time increment Δ*t* by using the value *P*;

3) Increase the simulation time *t* by Δ*t* to mimic the elapsed step.



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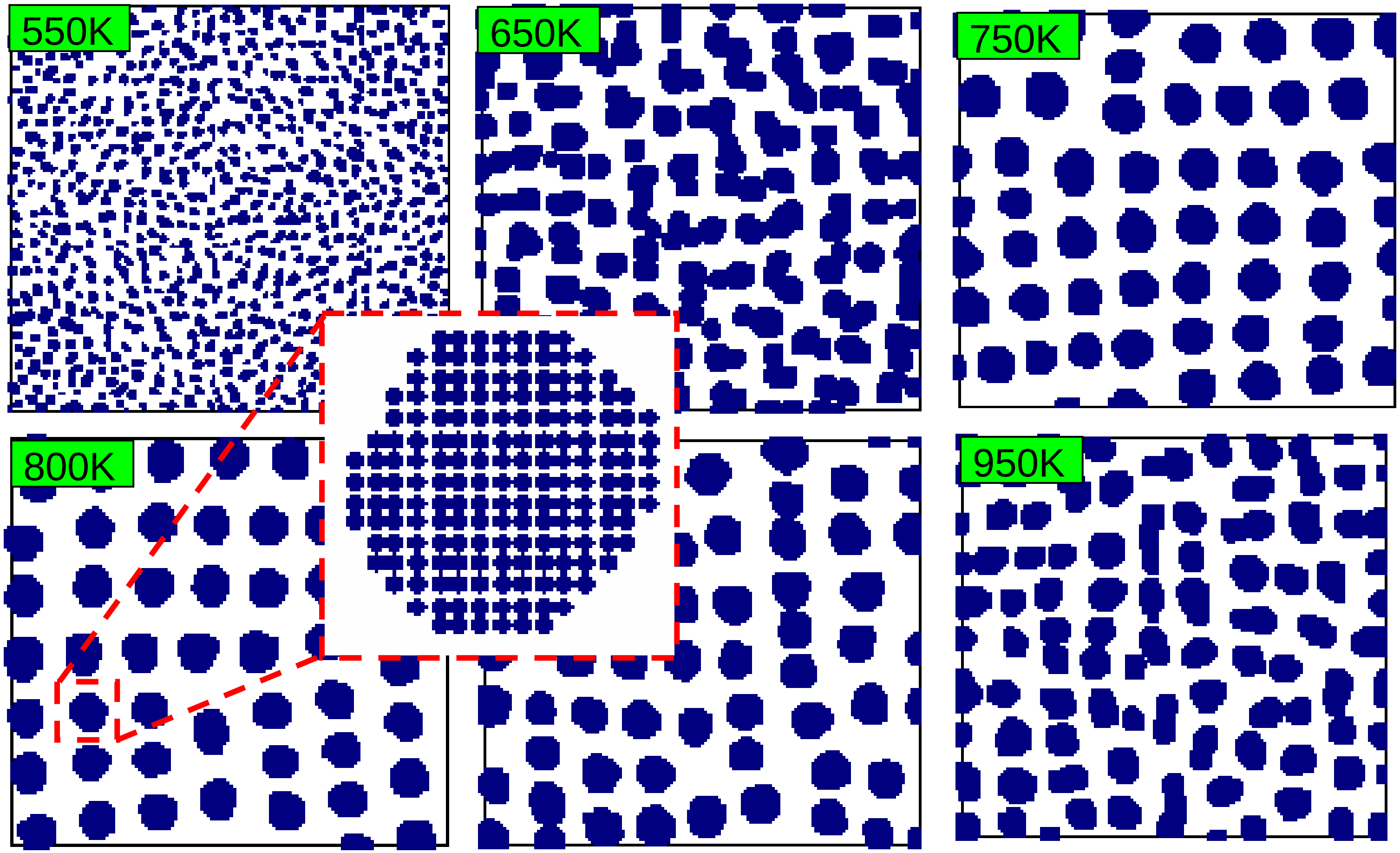
Growth Parameters — Temperature T

Four Growth Parameters:

Temperature	— T
Surface coverage	— c
Flux rate	— F
Interruption time	— t_i

$$p = \nu_0 \exp\left(-\frac{E_s + E_n - E_{str}(x, y)}{k_B T} \right)$$

Growth Parameters — Temperature T

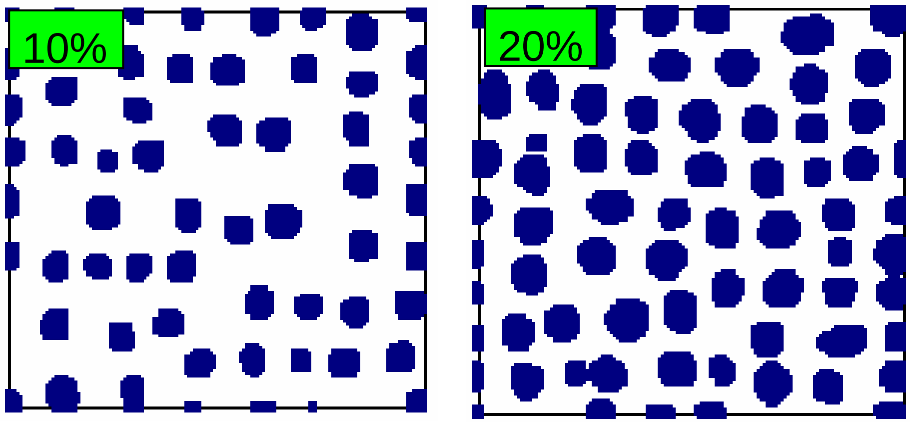


Growth of InAs/GaAs. Flux rate F=1.0Ml/s, coverage c=20% and interruption time t_i=200s on a 200×200 grid.

Optimal T centered at 750-800K

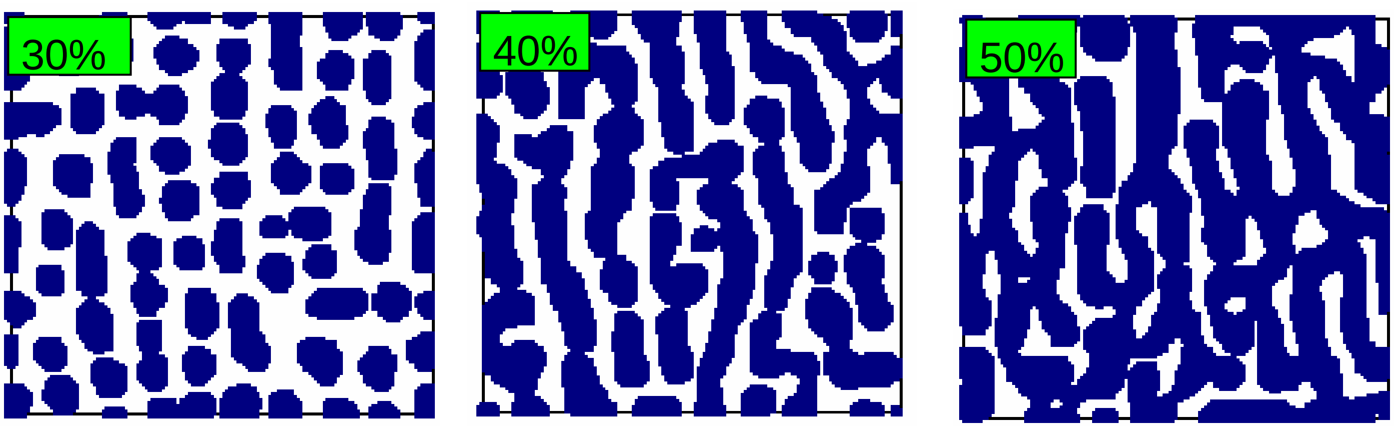
(Pan, Zhu, and Chung, JNN, 2004)

Growth Parameters — Surface Coverage *c*



Four Growth Parameters:

- Temperature — *T*
- Surface coverage — *c*
- Flux rate — *F*
- Interruption time — t_i



Growth of InAs/GaAs. Temperature T=700K, flux rate F=1.0Ml/s, interruption time t_i=200s on a 200×200 grid .

Optimal *c* centered at 20%

(Pan, Zhu, and Chung, JNN, 2004)

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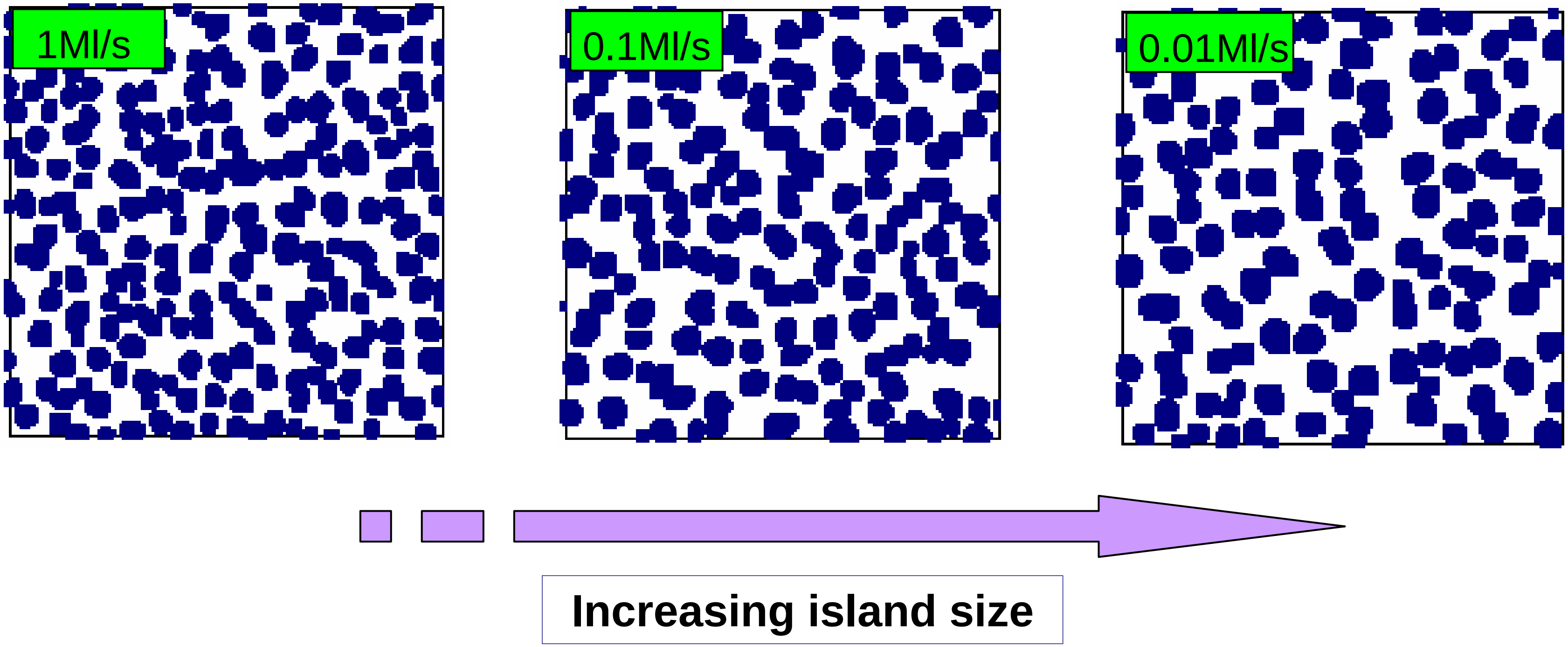
Growth Parameters — Flux Rate F



Growth of InAs/GaAs. Temperature T=700K, coverage c=20% and interruption time t_i=200s on a 200×200 grid.

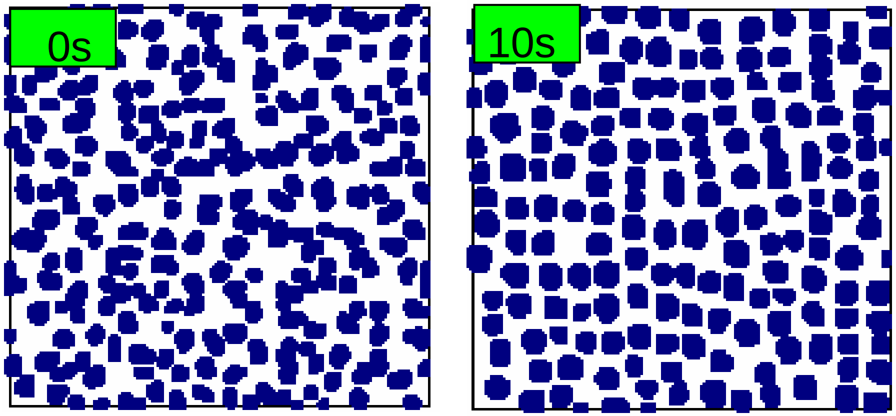
Deposition stops after 0.2s on the left, 2s in the middle, and 20s on the right. Strain energy field is not included for simplicity.

Four Growth Parameters:

- Temperature — T
- Surface coverage — c
- Flux rate — F
- Interruption time — t_i

(Pan, Zhu, and Chung, JNN, 2004)

Growth Parameters — Interruption Time t_i



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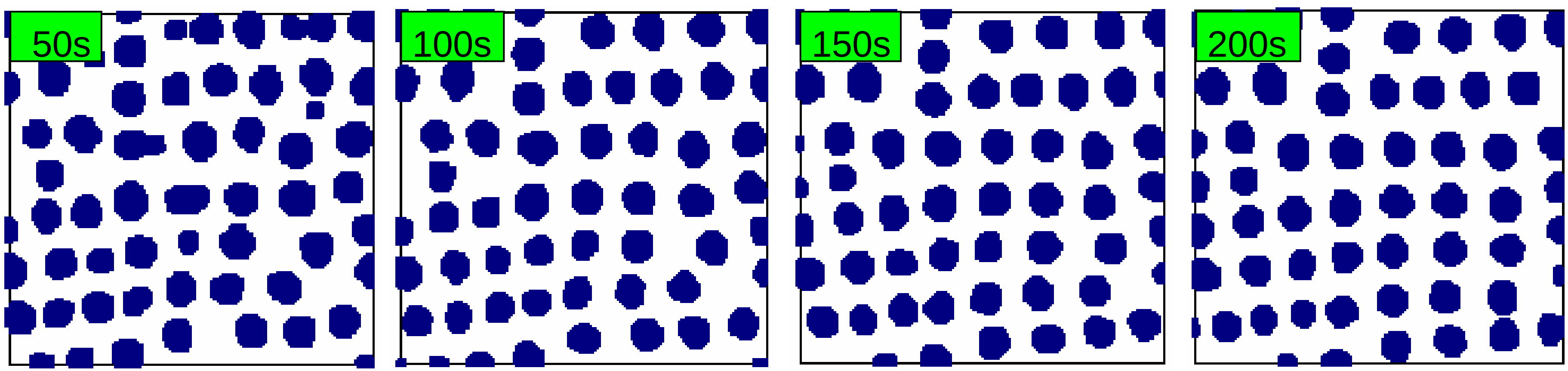

Growth of InAs/GaAs. Temperature T=750K, flux rate F=1.0Ml/s, coverage c=20% on a 200×200 grid

Equilibrium

(Pan, Zhu, and Chung, JNN, 2004)

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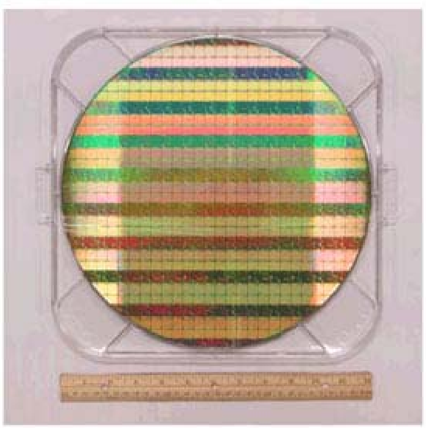

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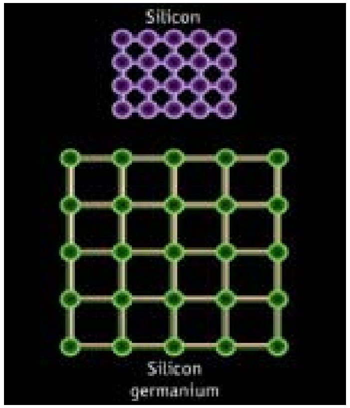
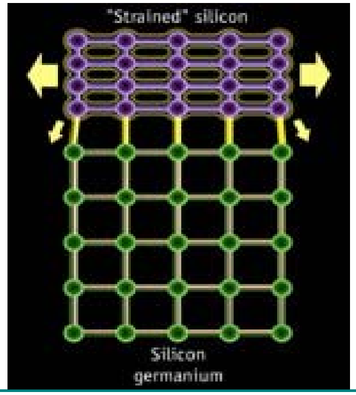
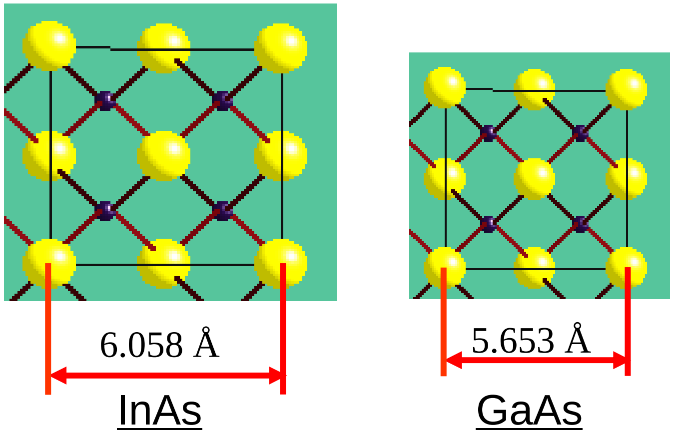
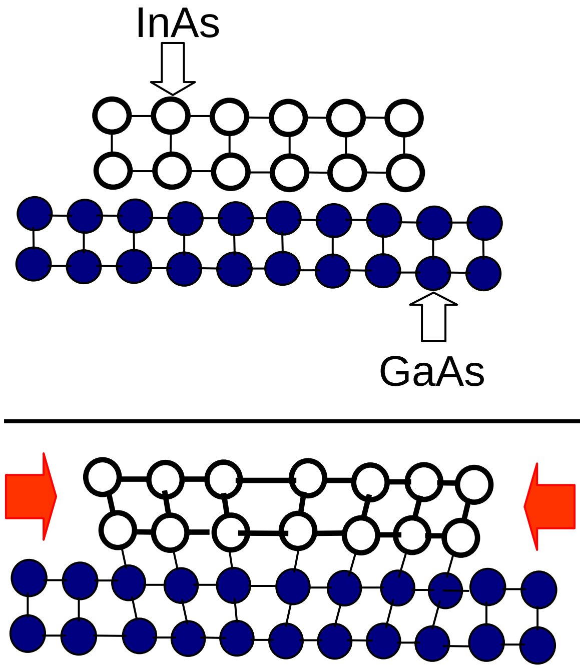








InAs growth on GaAs substrate

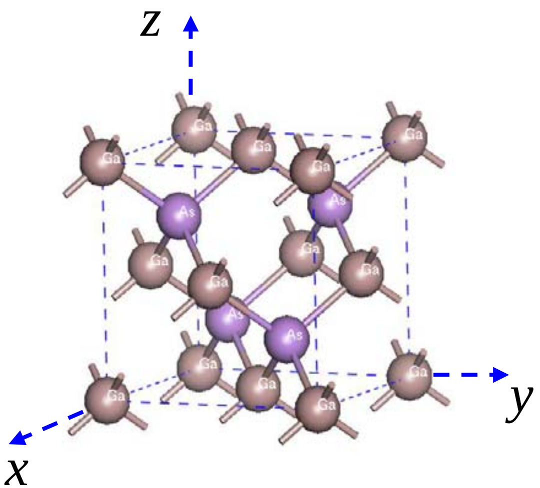
Maximum mistfit strain: 7%

Strain Energy Distribution

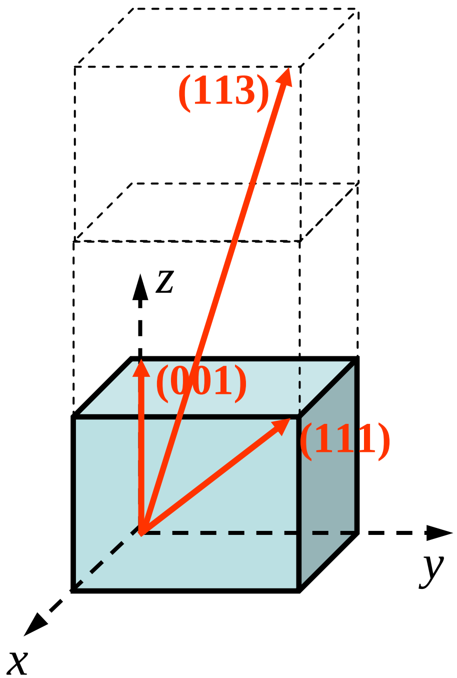
$$p = \nu_0 \exp\left(-\frac{E_s + E_n - E_{str}}{k_B T}\right)$$

$$E_{str}(\mathbf{y}) = \frac{1}{2} C_{ijkl} \iint_A \gamma_{ij}(\mathbf{y};\mathbf{x})\gamma_{kl}(\mathbf{y};\mathbf{x})dA(\mathbf{x})$$

C_{ijkl} — elastic moduli



Unit crystal of GaAs



Elastic moduli of GaAs (001)

$$C = \begin{bmatrix} 118.8 & 53.8 & 53.8 & 0 & 0 & 0 \\ 53.8 & 118.8 & 53.8 & 0 & 0 & 0 \\ 53.8 & 53.8 & 118.8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 59.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 59.4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 59.4 \end{bmatrix} \text{GPa}$$

Elastic moduli of GaAs (111)

$$C = \begin{bmatrix} 145 & 45 & 36 & 0 & 12.73 & 0 \\ 45 & 145 & 36 & 0 & -12.73 & 0 \\ 36 & 36 & 154 & 0 & 0 & 0 \\ 0 & 0 & 0 & 41 & 0 & -12.73 \\ 12.73 & -12.73 & 0 & 0 & 41 & 0 \\ 0 & 0 & 0 & -12.73 & 0 & 50 \end{bmatrix} \text{GPa}$$

Elastic moduli of GaAs (113)

$$C = \begin{bmatrix} 152.81 & 31.79 & 41.79 & 0 & -4.72 & 0 \\ 31.79 & 145.7 & 48.91 & 0 & -10.38 & 0 \\ 41.79 & 48.91 & 135.70 & 0 & 15.09 & 0 \\ 0 & 0 & 0 & 54.51 & 0 & -10.38 \\ -4.72 & -10.38 & 15.09 & 0 & 47.39 & 0 \\ 0 & 0 & 0 & -10.38 & 0 & 37.39 \end{bmatrix} \text{GPa}$$

Isotropic condition

$(C_{11}-C_{12})/2=C_{44}$

C_{12}=53.8GPa

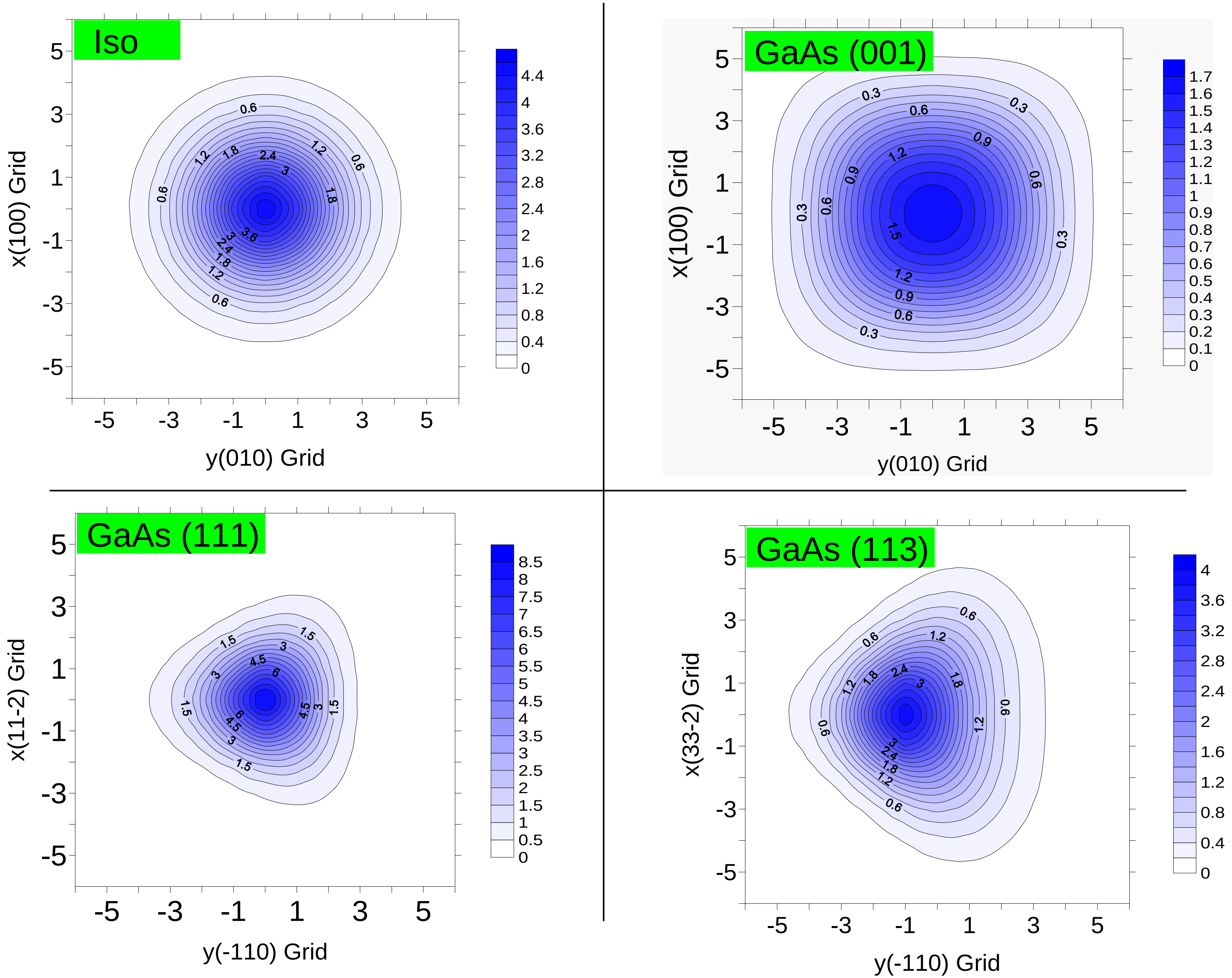
C_{44}=59.4GPa

⇨ C_{11}=172.6GPa ⇨

Elastic moduli of Iso (001)

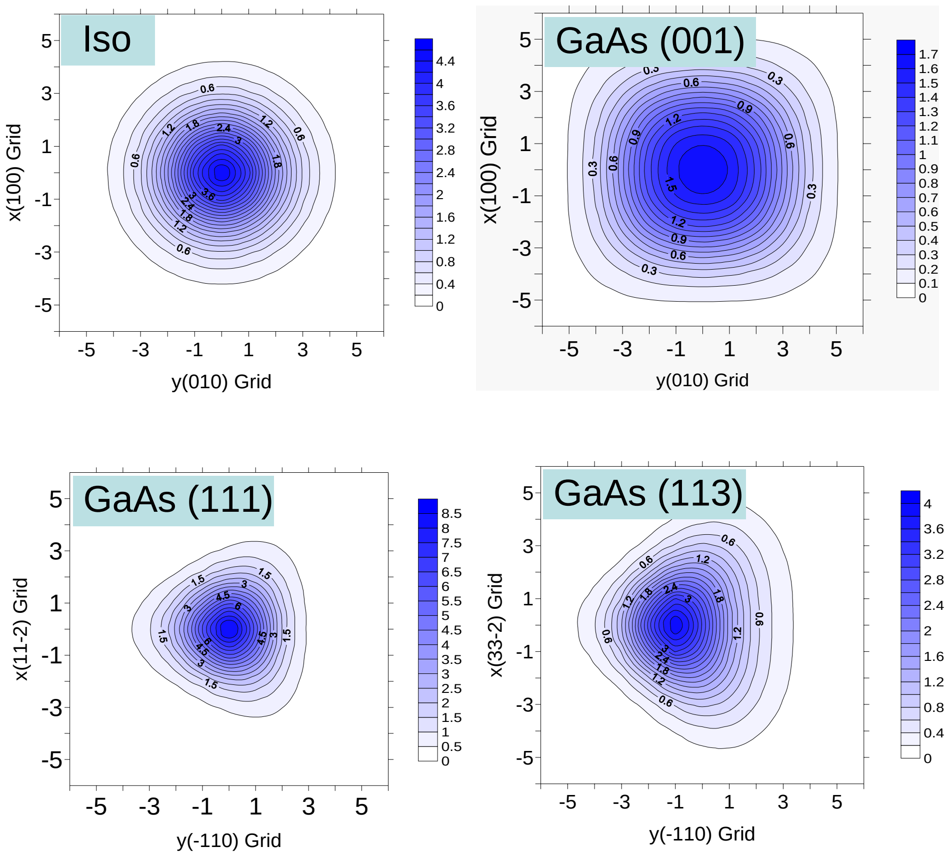
$$C = \begin{bmatrix} 172.6 & 53.8 & 53.8 & 0 & 0 & 0 \\ 53.8 & 172.6 & 53.8 & 0 & 0 & 0 \\ 53.8 & 53.8 & 172.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 59.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 59.4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 59.4 \end{bmatrix} \text{GPa}$$

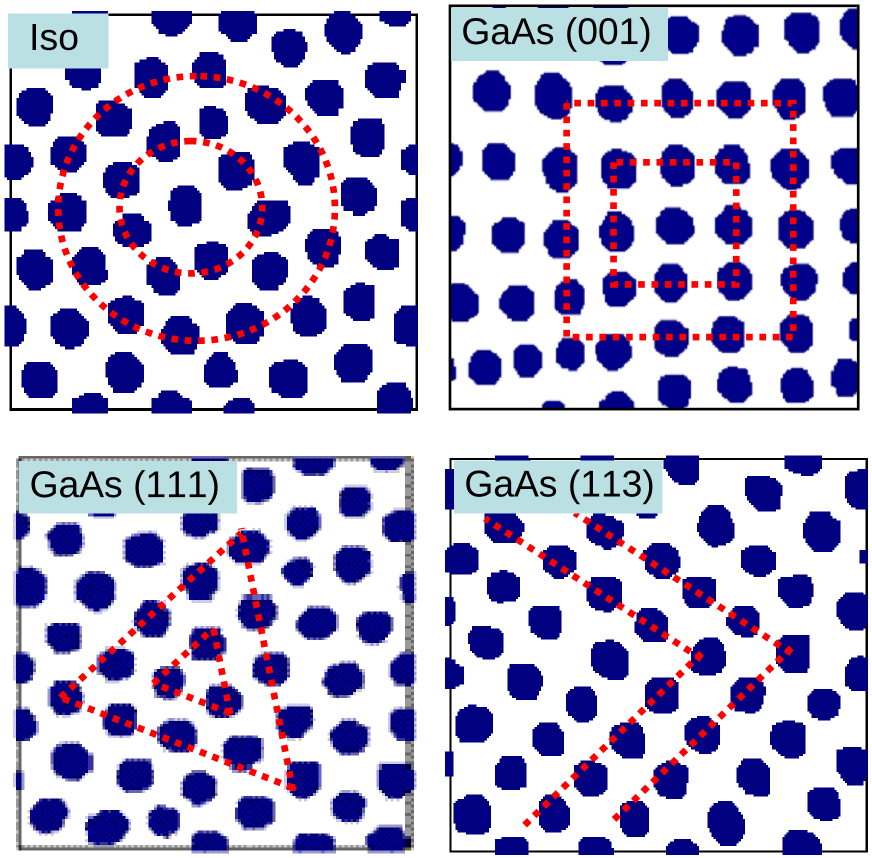
Strain Energy Distribution



(Pan, Zhu, and Chung, JAP, 2006)

QDs Patterns with Different Substrate Directions





<u>QDs patterns</u>

T=750K, *F*=1.0Ml/s, *c*=20%, and t_i=200s, on a 200×200 grid.

(Pan, Zhu, and Chung, JAP, 2006)

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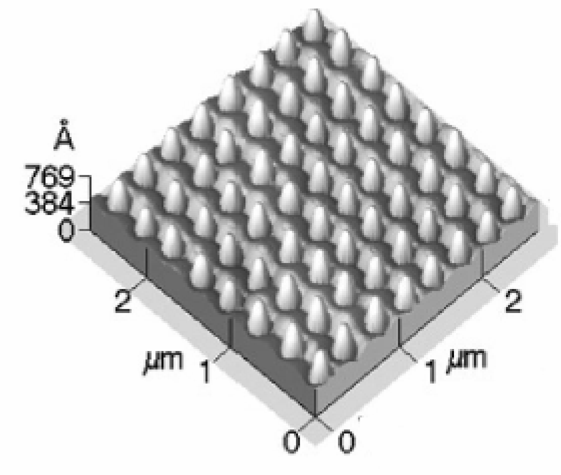
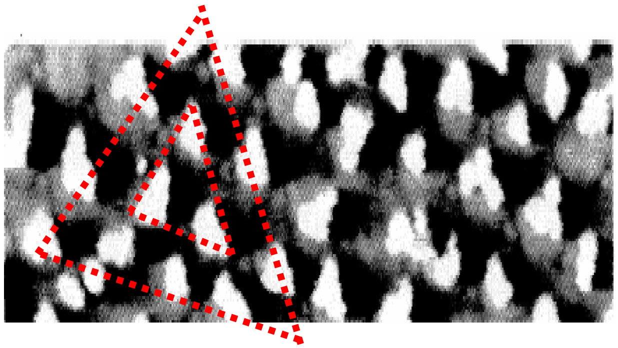
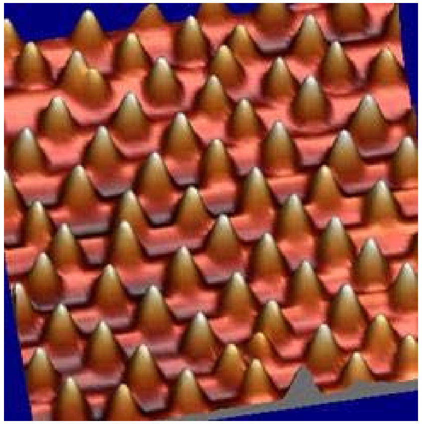
Compare of Experimental and Simulated QDs Patterns



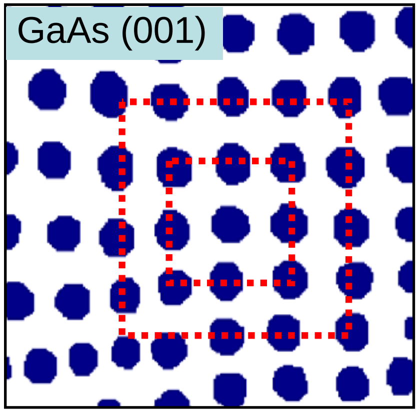
(Zhong and Bauer, APL 2004)



(Brune et al., Phys. Rev. B 1995)



(Seyedmohammadi website)



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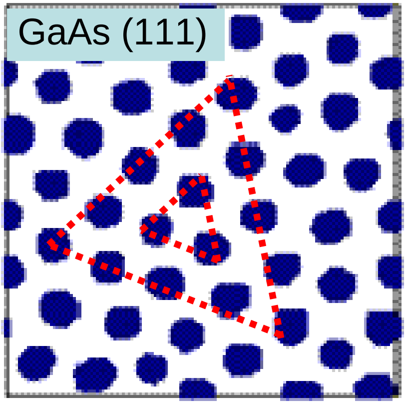

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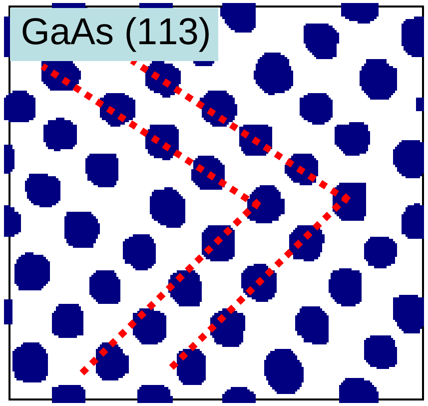

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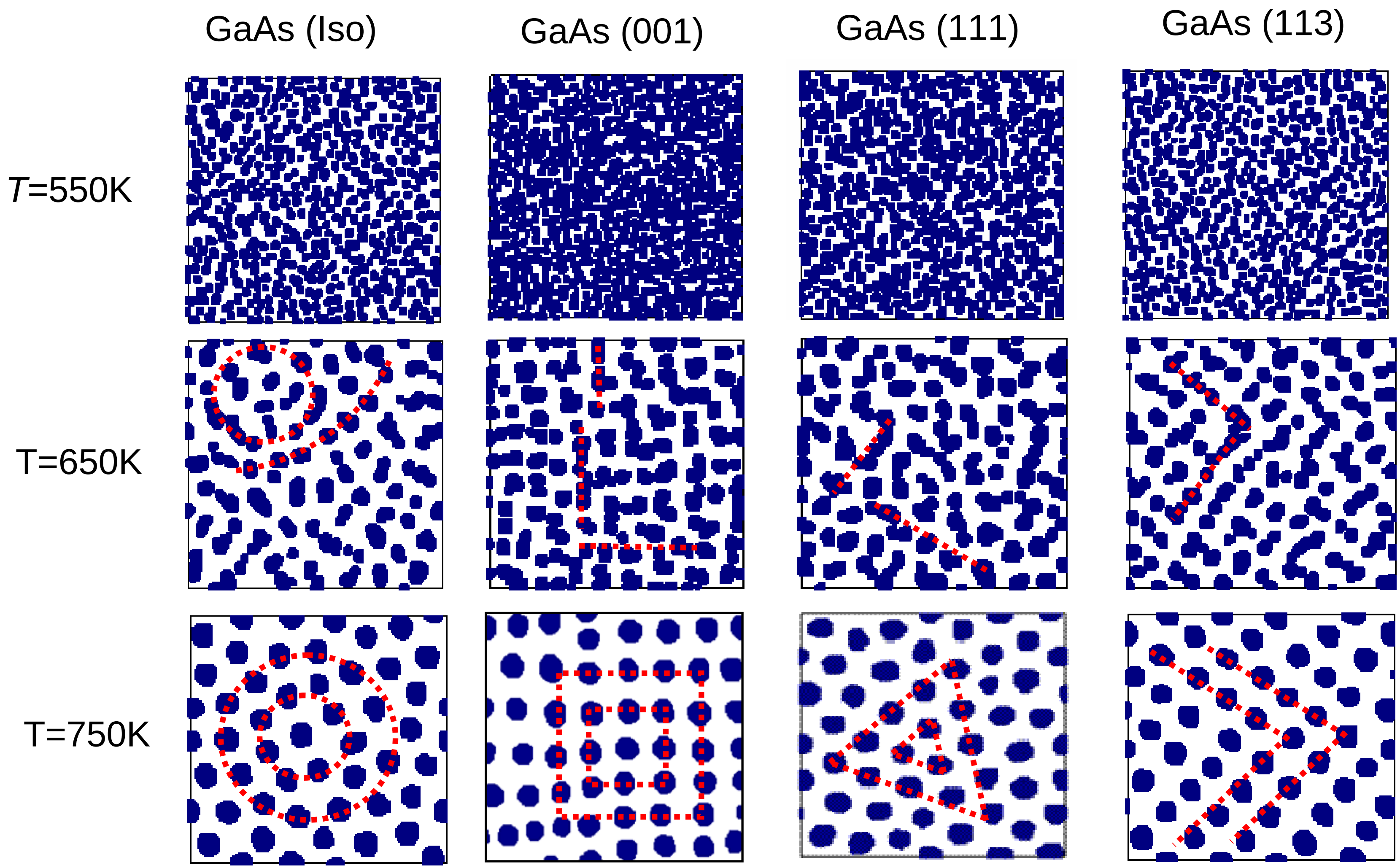
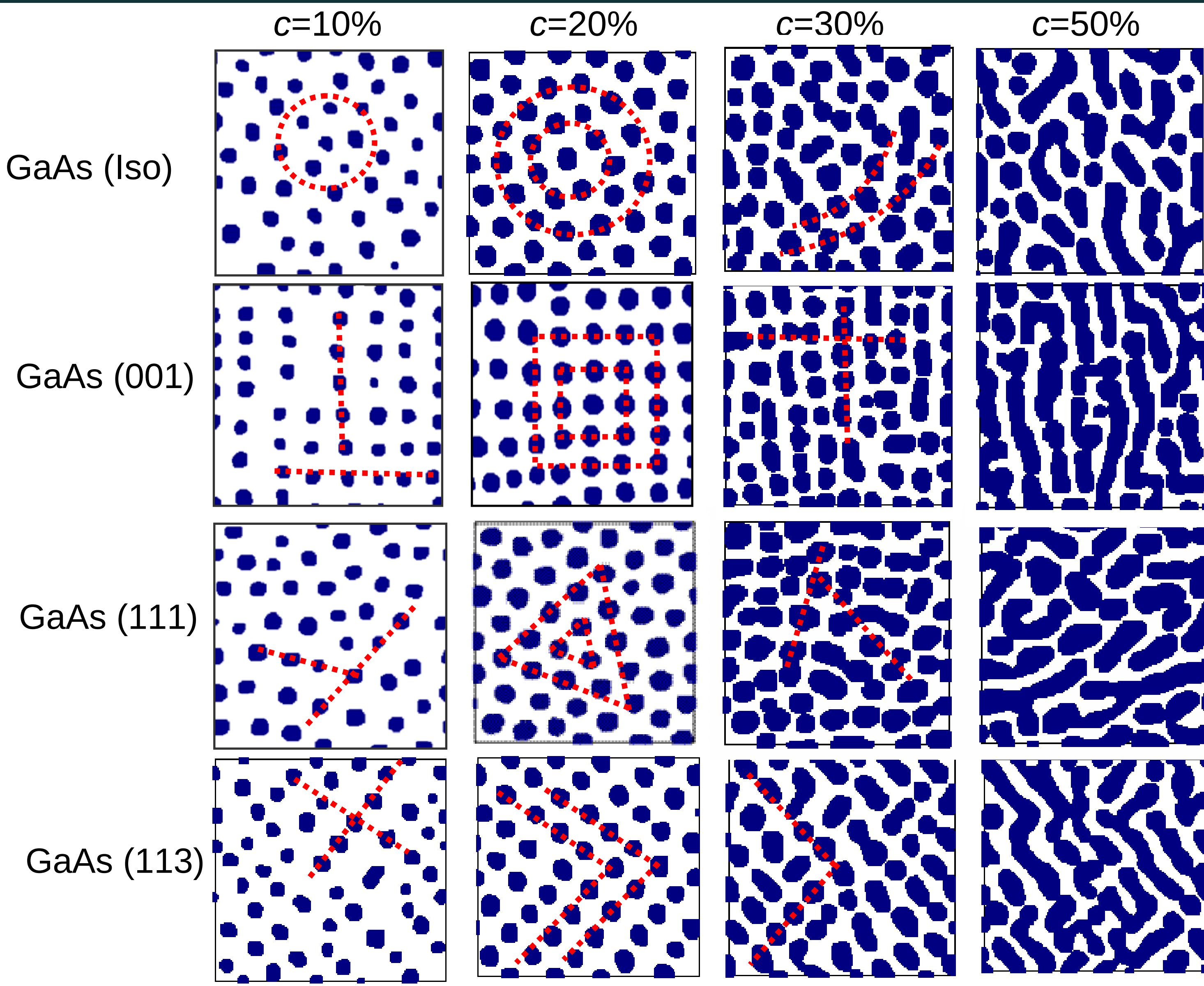
QDs Patterns vs. Temperatures



Flux rate F=1.0Ml/s, coverage c=20% and interruption time t_i=200s on a 200×200 grid

(Pan, Zhu, and Chung, JAP, 2006)

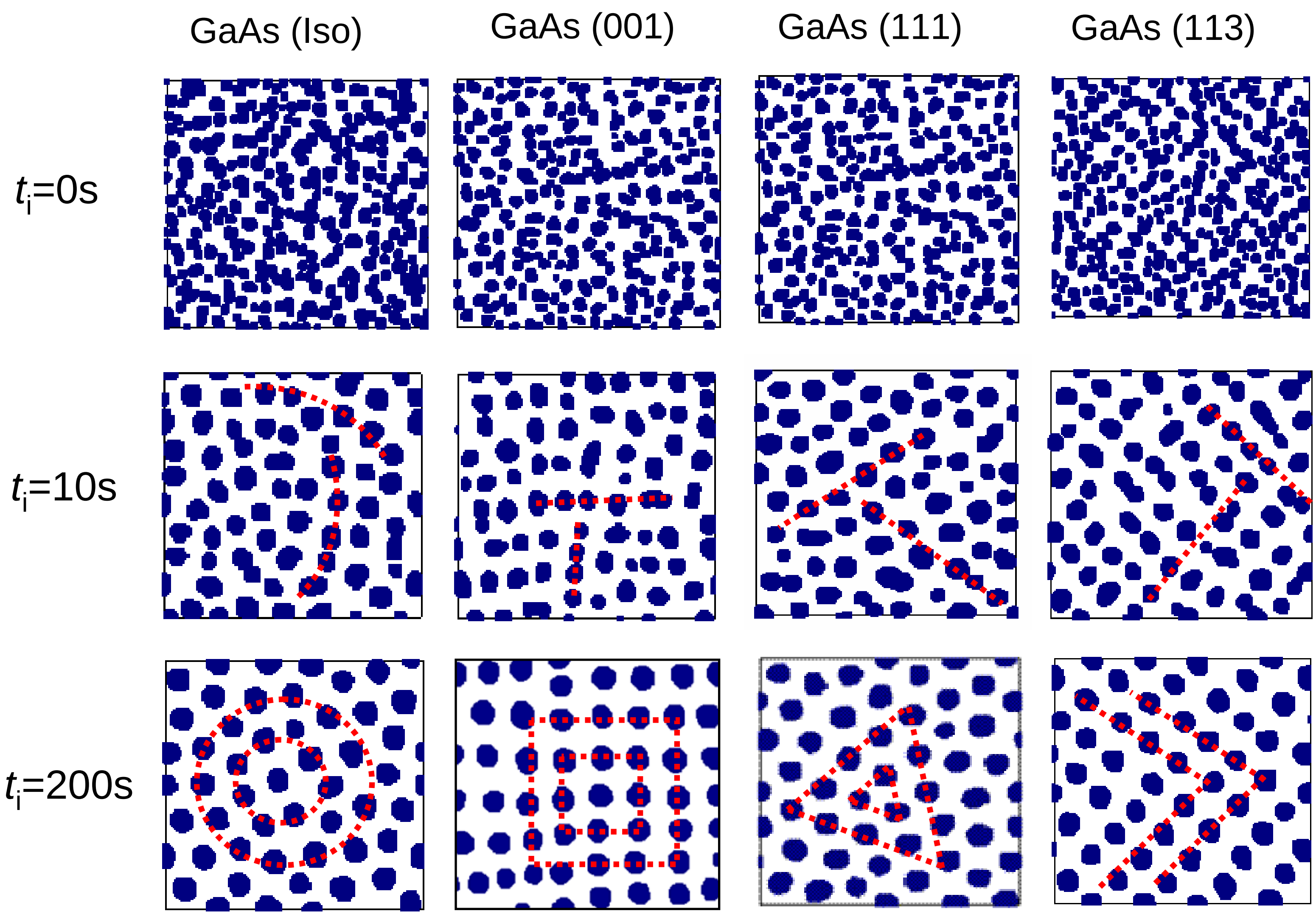
QDs Patterns vs. Coverage *c*



Temperature T=750K, flux rate F=1.0Ml/s, interruption time t_i=200s on a 200×200 grid

(Pan, Zhu, and Chung, JAP, 2006)

QDs Patterns vs. Interruption Time t_i



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The End