
Self-Assembled Nanostructures: Ge on Si

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Outline

Limits of Device Scaling

Alternative Device Concepts

Self-Assembled Nanostructures

Forming small structures

Putting them where we want them

Zero-dimensional structures

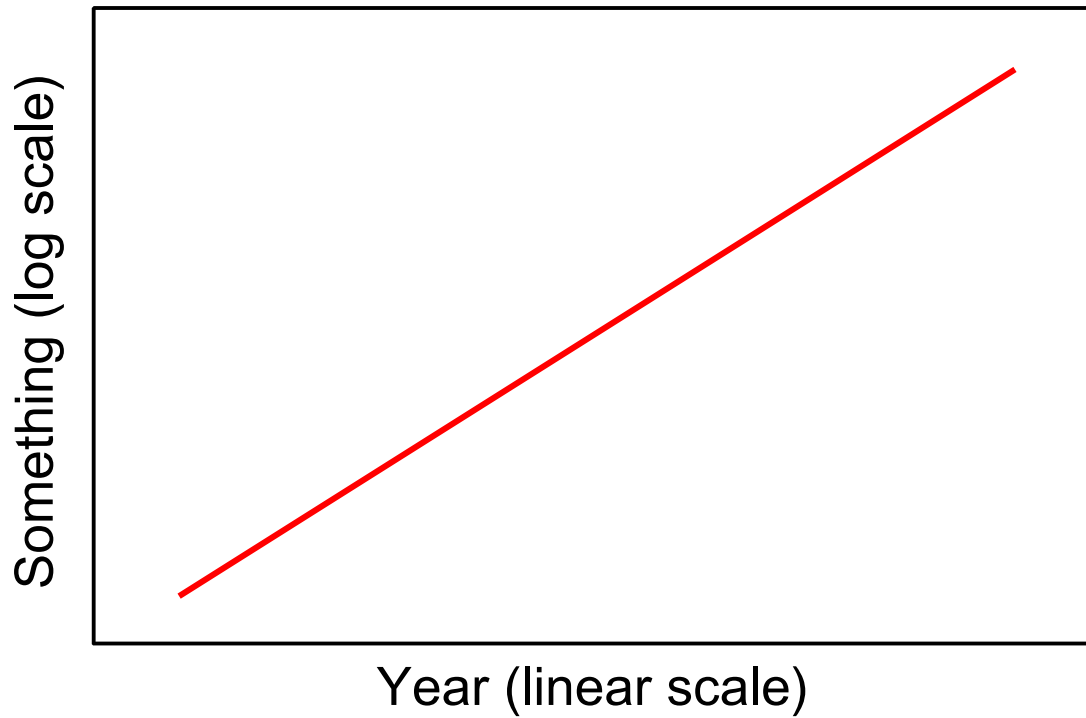
Strain from lattice mismatch

Enabling Concept

Defect Tolerance



Moore's Law (General Case)

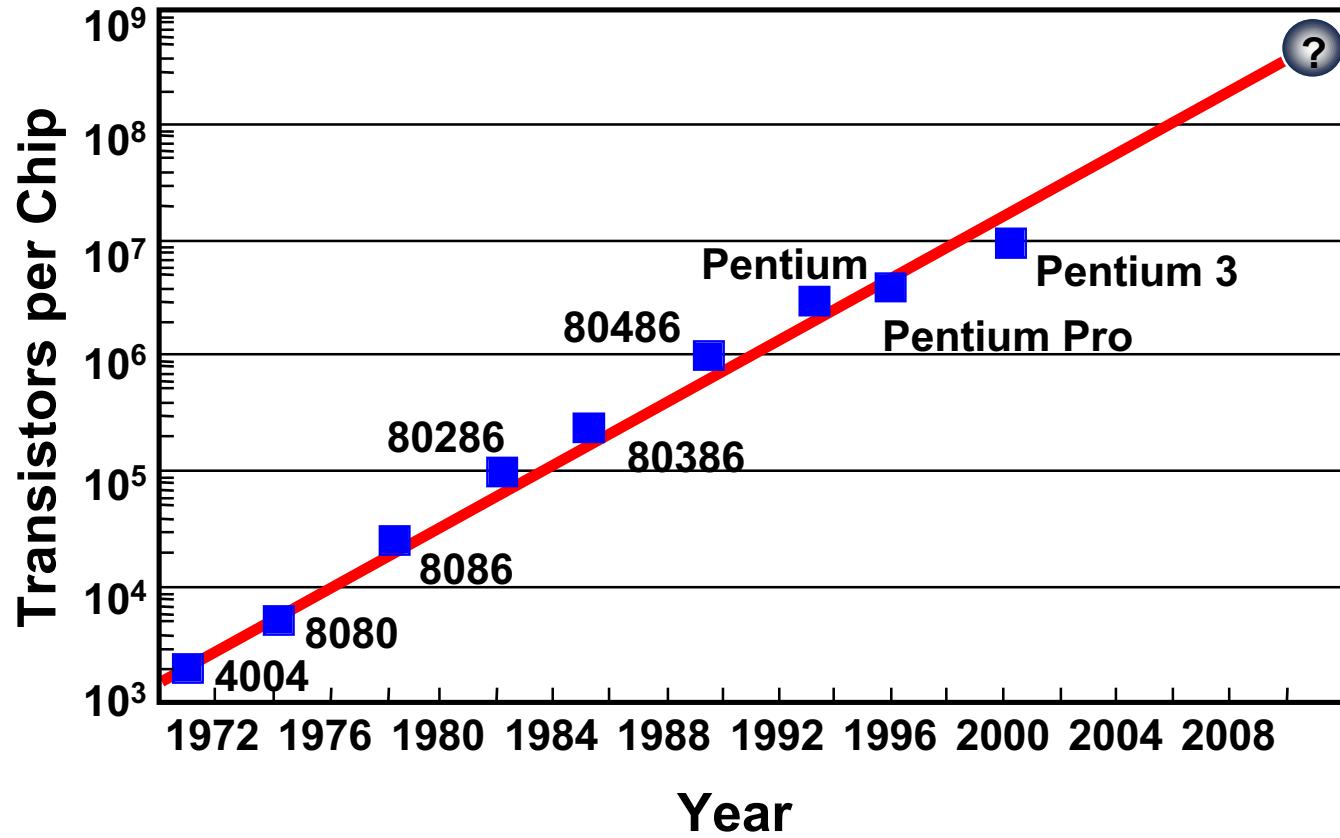


Even Dilbert uses Moore's Law

(Reference: Scott Adams "Dilbert," July 15, 1997)

Moore's Law

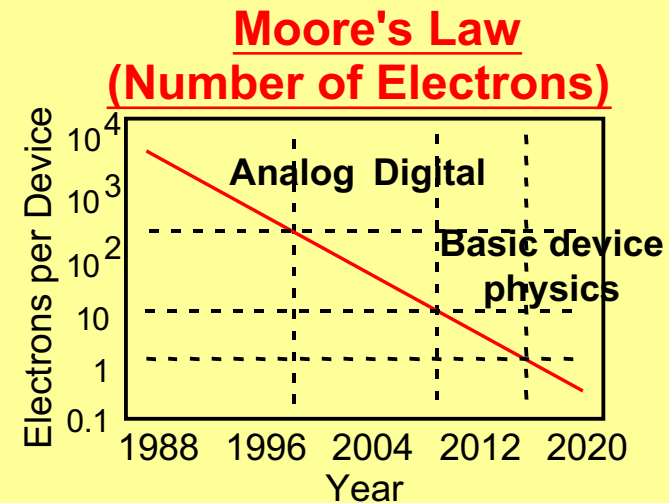
Number of Transistors



Critical Issues

Device size and density

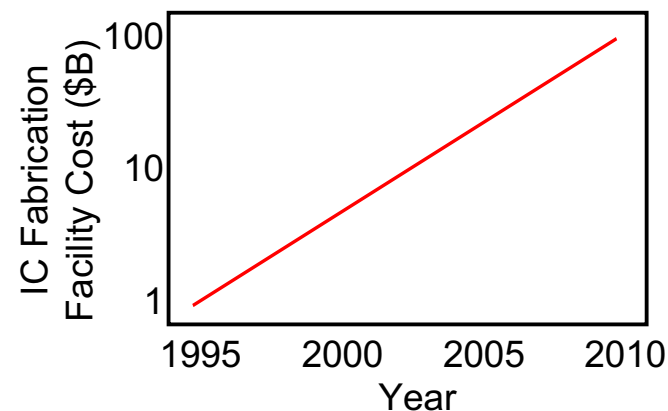
- Physically small features
- Operation with small features
- Limited number of electrons
- Interconnections



Cost

- Minimize expensive lithography
- Self (or directed) assembly
- Simpler architecture
- Defect-tolerant architecture

Moore's "Second Law" Cost of IC Fabrication Facility



Potential Devices

Single-electron devices
Quantum cellular automata
Molecular electronics
Quantum computing

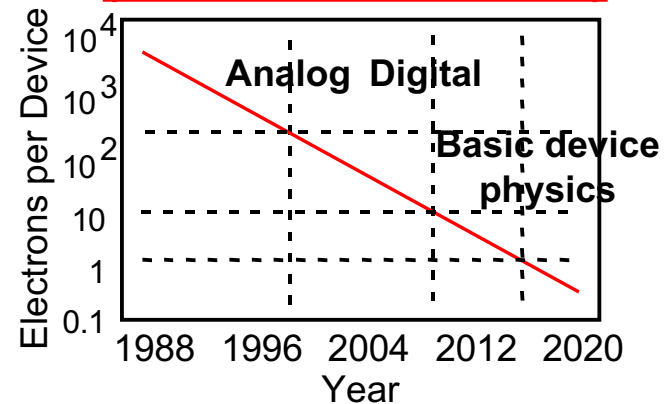


Critical Issues

Device size and density

- Physically small features
- Operation with small features
- Limited number of electrons
- Interconnections

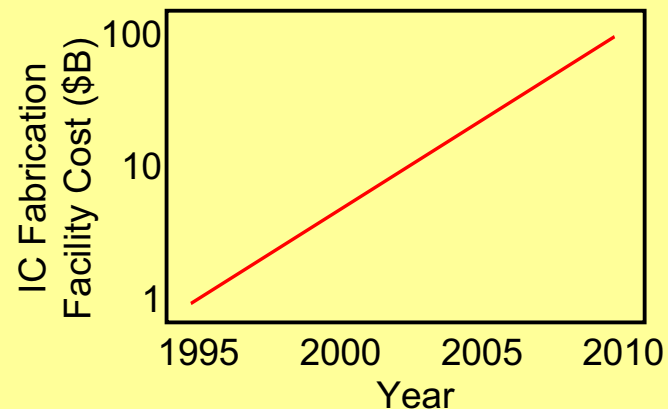
Moore's Law (Number of Electrons)



Cost

- Minimize expensive lithography
- Self (or directed) assembly
- Simpler architecture
- Defect-tolerant architecture

Moore's "Second Law" Cost of IC Fabrication Facility



Self-Assembled Nanostructures Zero Dimensional Islands on Si

Use directed-assembly to extend Moore's law

Determine critical dimensions by choice of materials and deposition kinetics ("self assembly"), not lithography
Use lithography to position devices or arrays of devices ("directed assembly")

Use small-size effects to perform logic, storage, and computation

Coulomb blockade or quantum confinement

Methods of self- or directed- assembly

Strain from lattice mismatch
Catalytic wire growth on nanoparticle

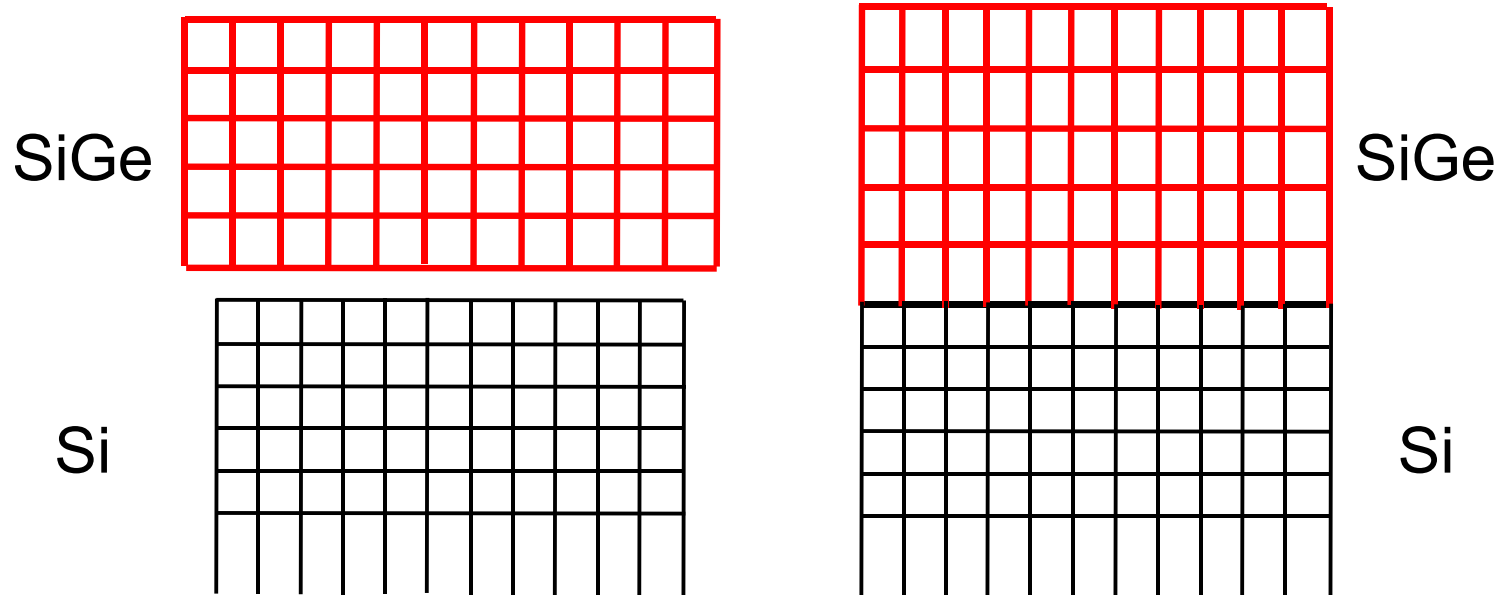
Thermodynamically assembled structures

Several percent defects
Need defect-tolerant architecture



Strained-Layer Epitaxy

Compress SiGe lattice to match silicon

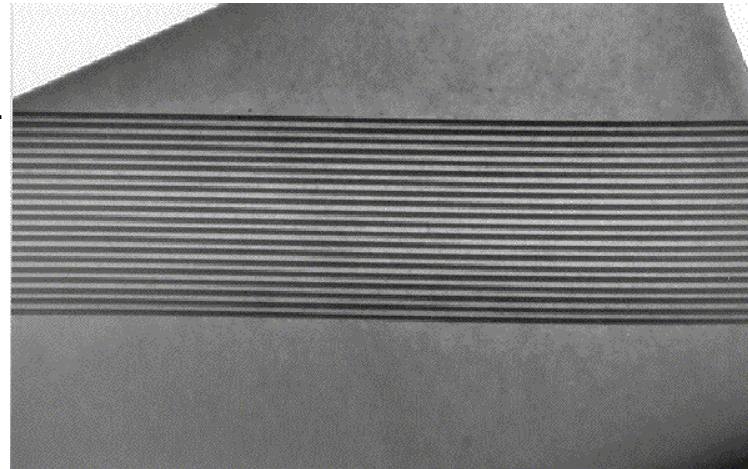


Can Accommodate Moderate Strain Multilayer Si/SiGe Structure

150 nm Si cap

20 x 3 nm SiGe
19 x 3.5 nm Si

Si substrate



- Average SiGe layer thickness: 3 nm + 0.2 nm
- Average Si layer thickness: 3.5 nm + 0.2 nm
- Si source: SiH_2Cl_2
- Temperatures: 625°C (SiGe), 690°C (Si)

Large Strain + Surface Diffusion Allows Surface Roughening

Deposit one material on another

Large strain → self-assembled islands (quantum dots)

Small islands → quantum or Coulomb-blockade effects

Focus on Ge on Si

Why Ge on Si?

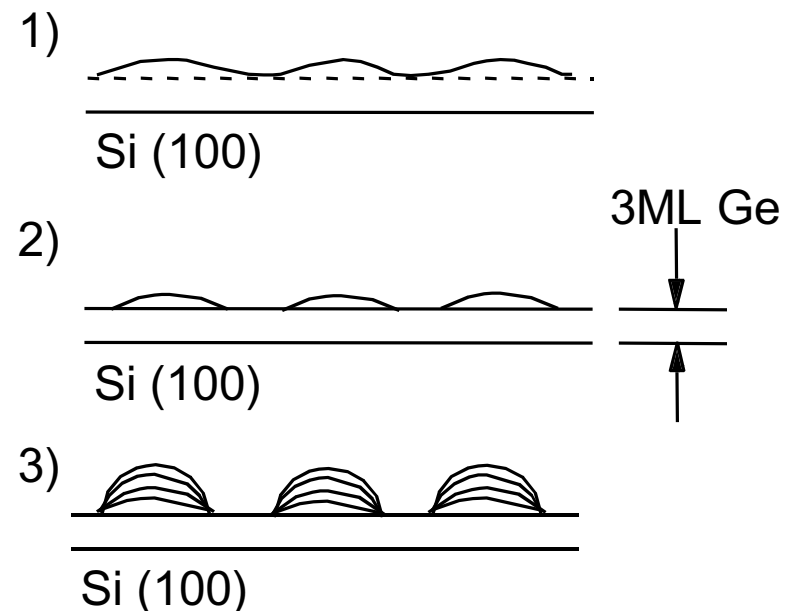
Compatible with Si IC technology

Deposition by

Chemical Vapor Deposition

(or Physical Vapor Deposition)

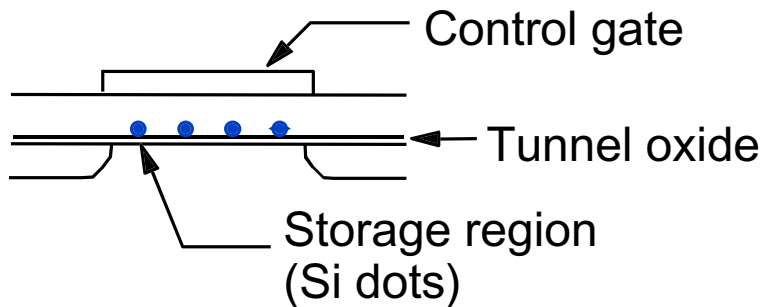
Energy and Kinetics Influence Island Formation



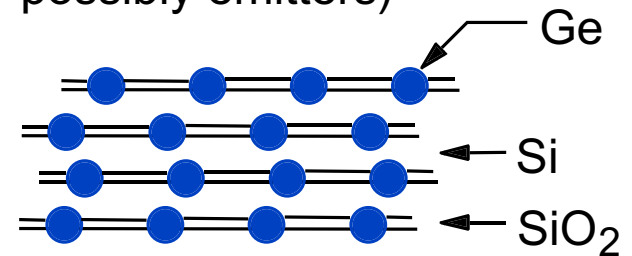
Possible Device Applications

Random Arrangement

Nonvolatile memory



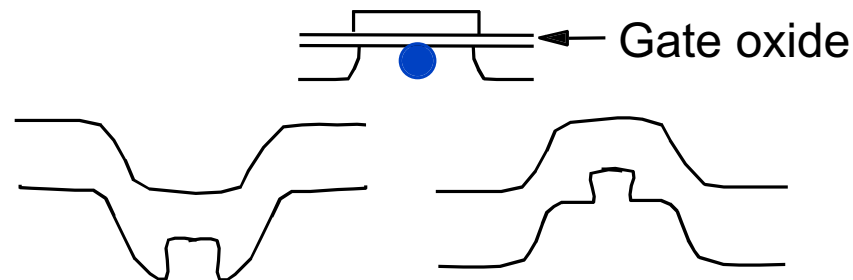
Long-wavelength photodetectors
(or possibly emitters)



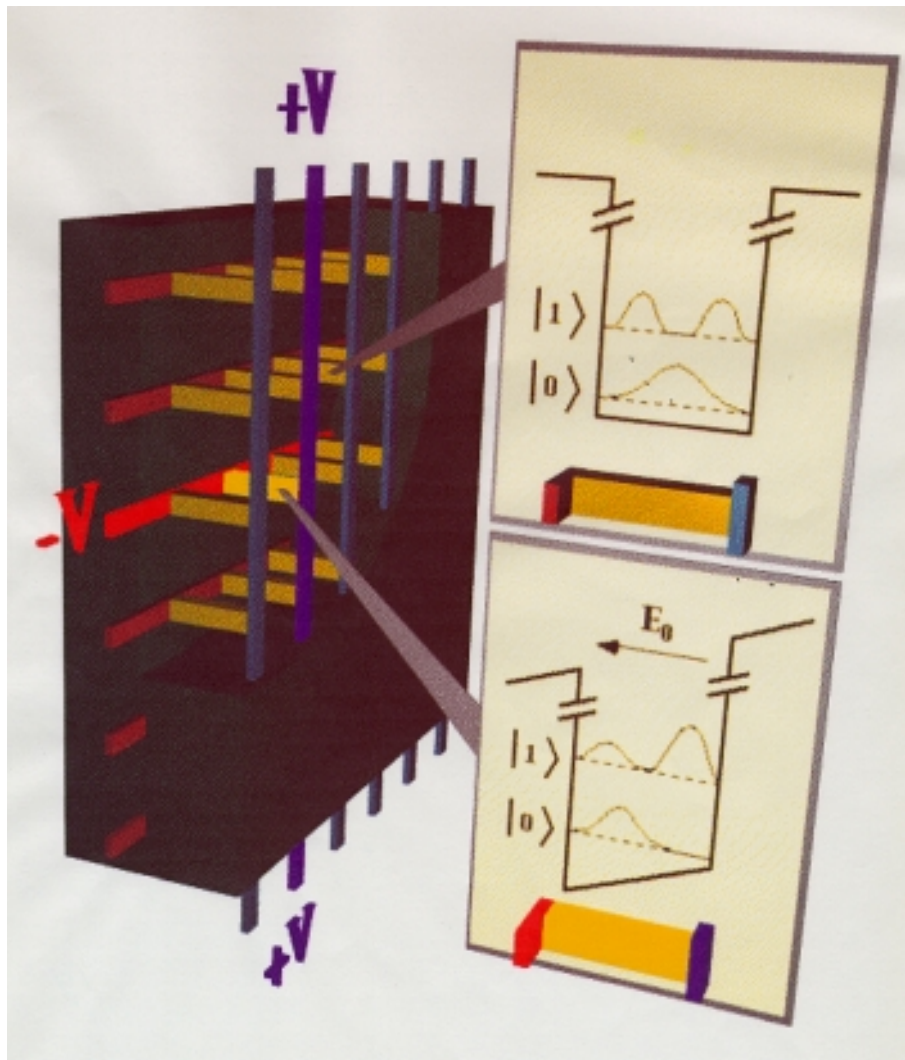
Aligned

MOS for logic

Possible barrier to short-channel (substrate) effects



Quantum Dot Computer



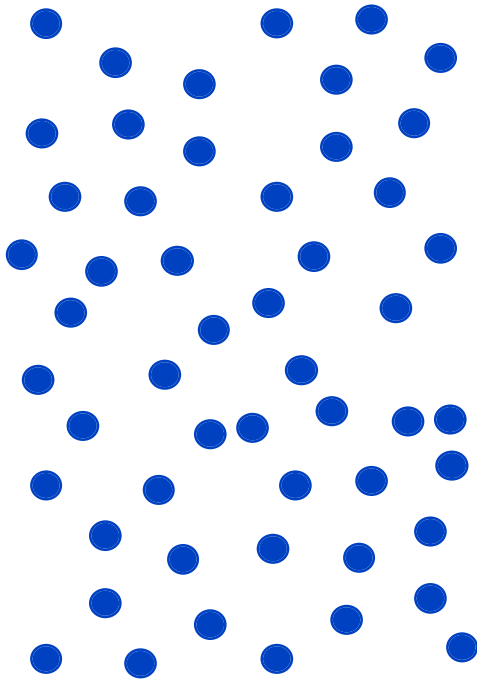
Oxford University

Artur Ekert

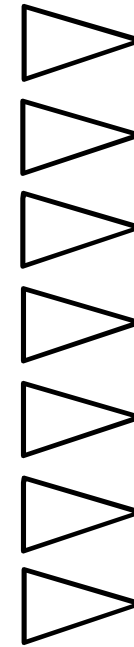
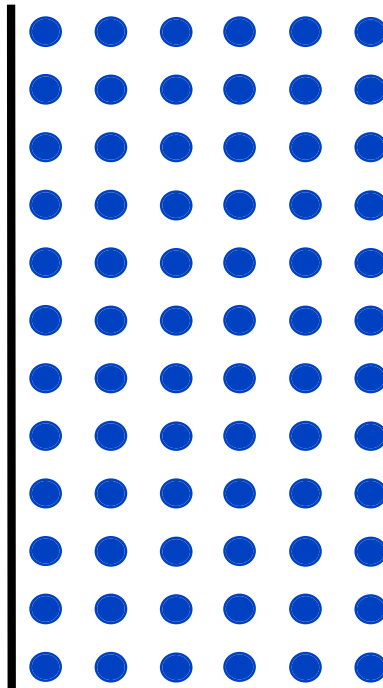
Key to Using Self-Assembled Islands

Forming and Positioning Islands

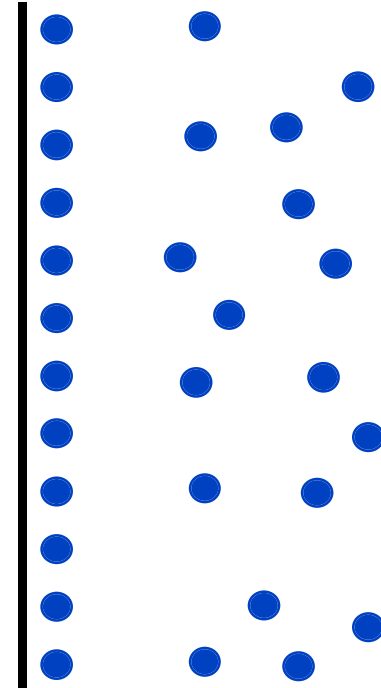
**Uniform Size
(Randomly Arranged)**



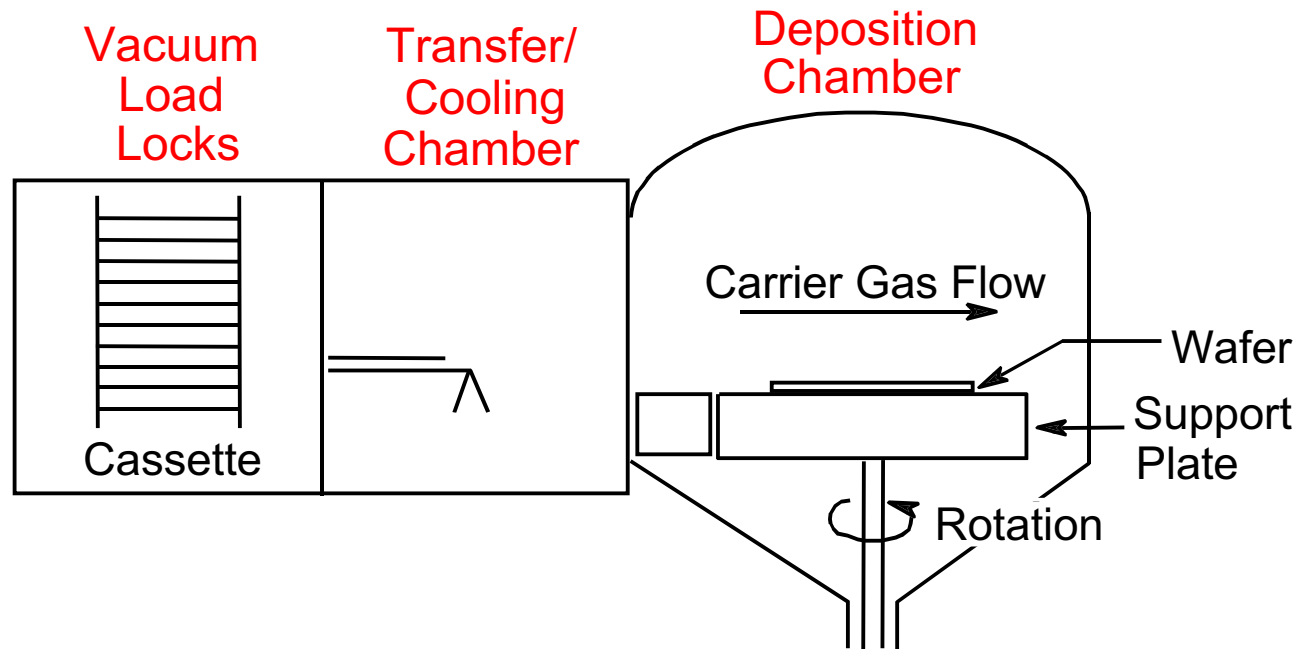
Ordered



Aligned



Applied Materials Centura



Cluster/multichamber system

RP wafer transfer

Cooldown chamber

Chamber volume: 11 liters

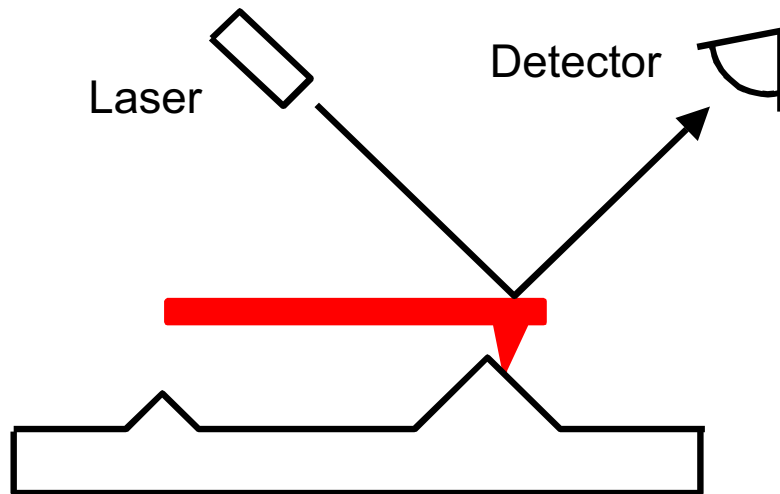
$P \sim 1 - 600$ Torr (10 Torr)

$T \sim 550 - 1200^{\circ}\text{C}$ (600°C)

Layers deposited in two different single-wafer CVD reactors
(and also by PVD)

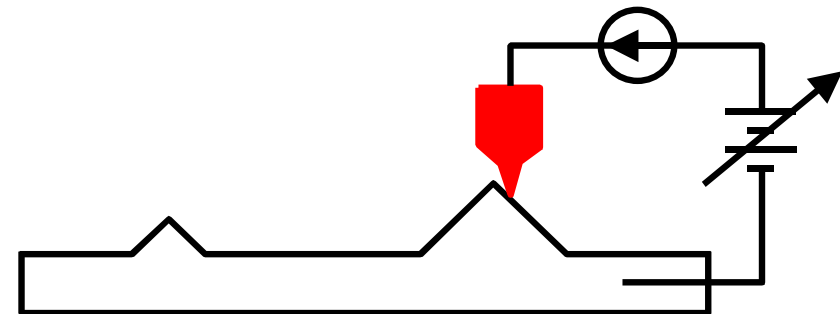
Scanning-Probe Microscopy

Atomic-Force Microscope (AFM)



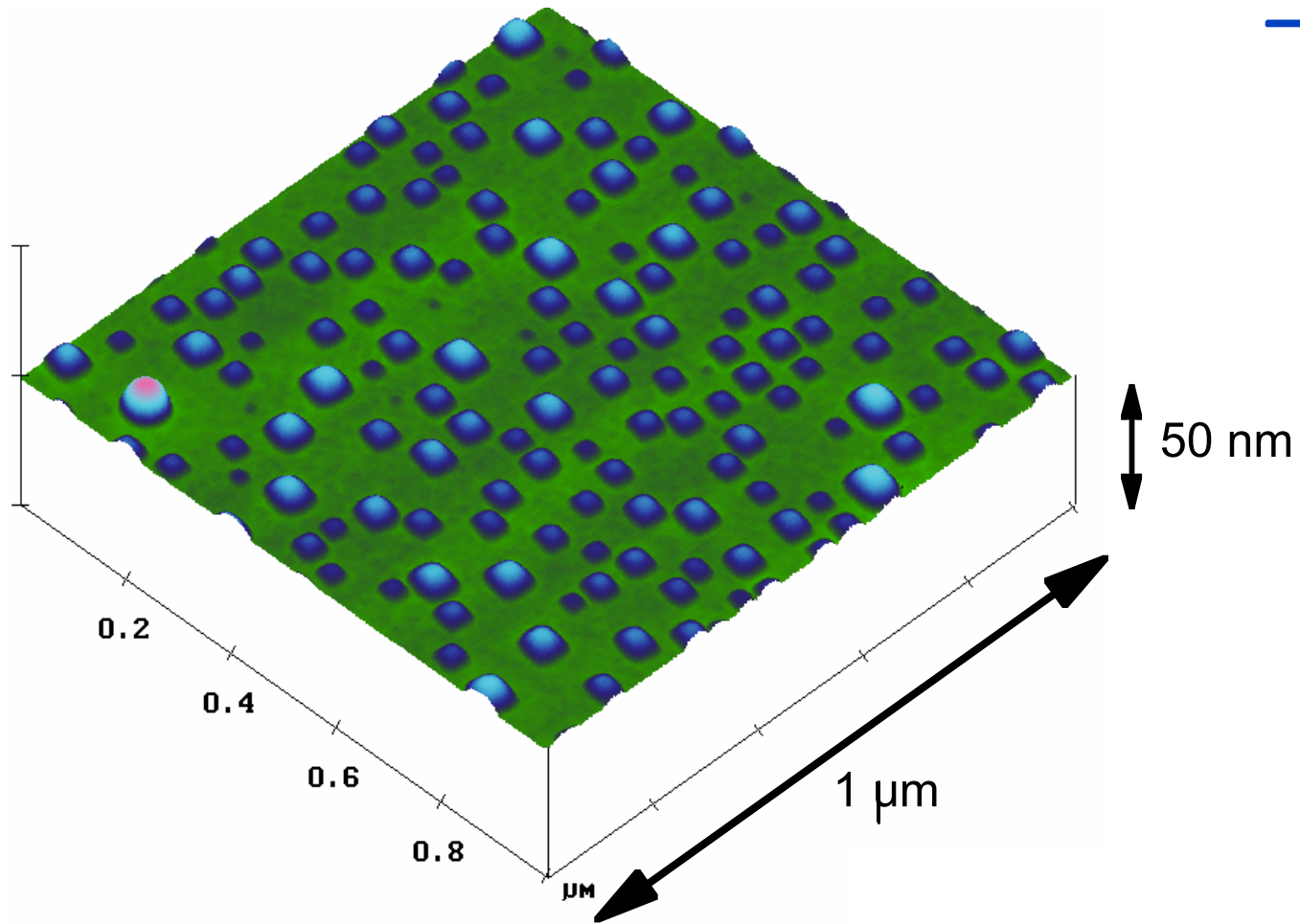
CVD and *ex situ* characterization

Scanning-Tunneling Microscope (STM)

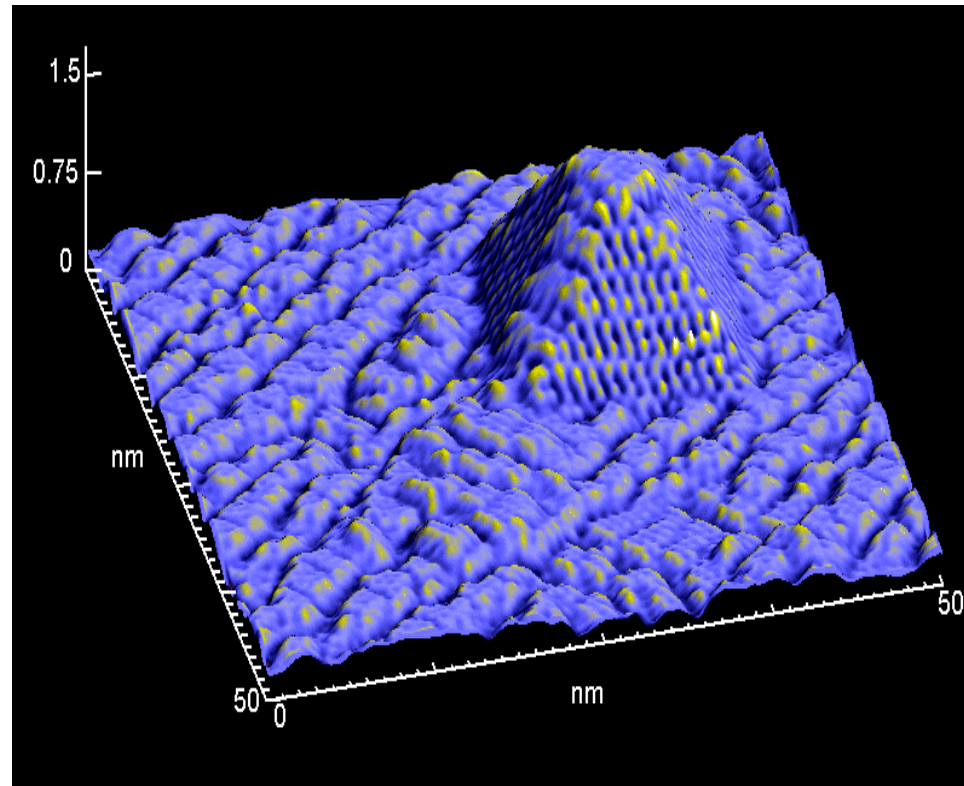


PVD and *in situ* characterization

Ge/Si(001): 6 eq-ML at 600°C

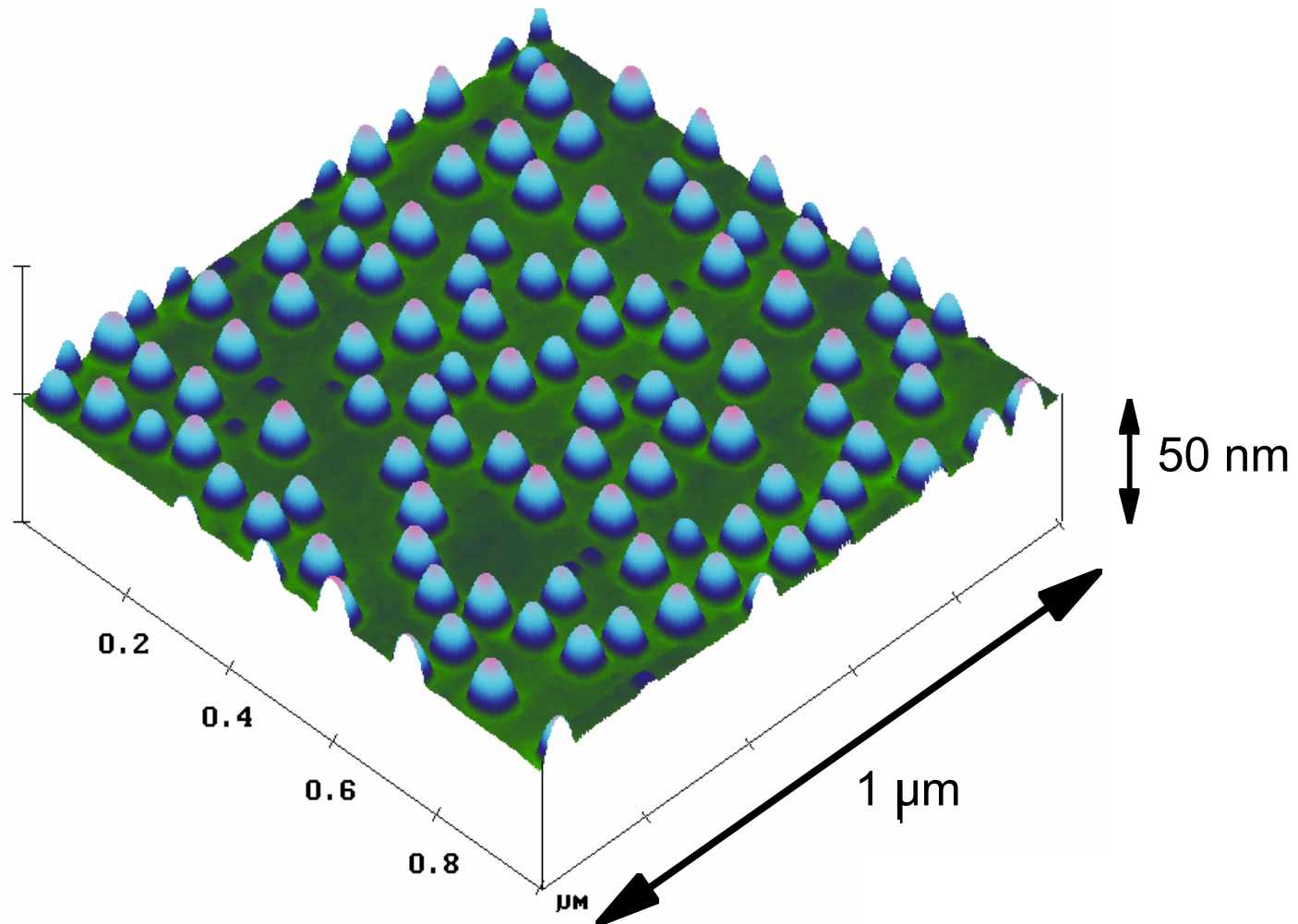


Very Small Ge Pyramid



Scanning Tunneling Micrograph by G. Medeiros-Ribeiro, HPL

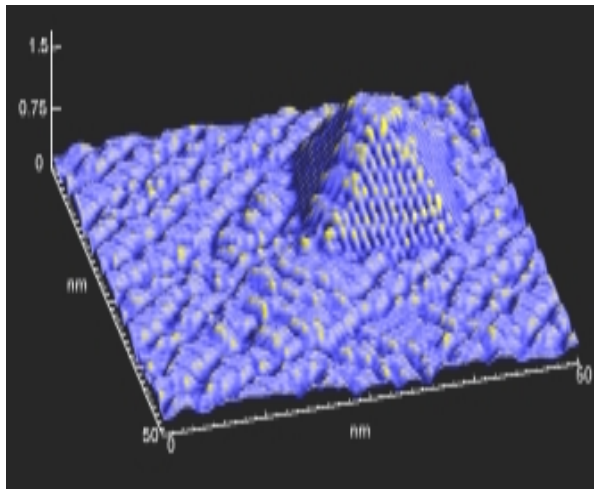
Ge/Si(001): 11 eq-ML at 600°C
Domes



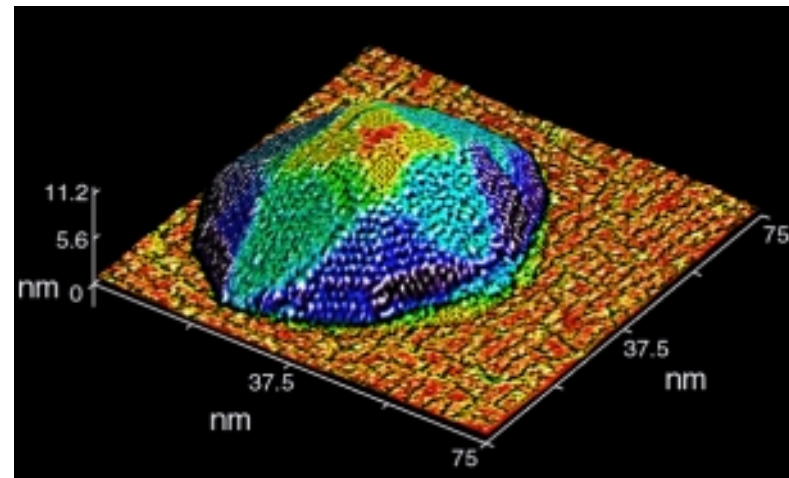
Self-Assembled Nanostructures

Strain from lattice mismatch forms 3D structure

Small Ge “pyramid”
on Si(001)



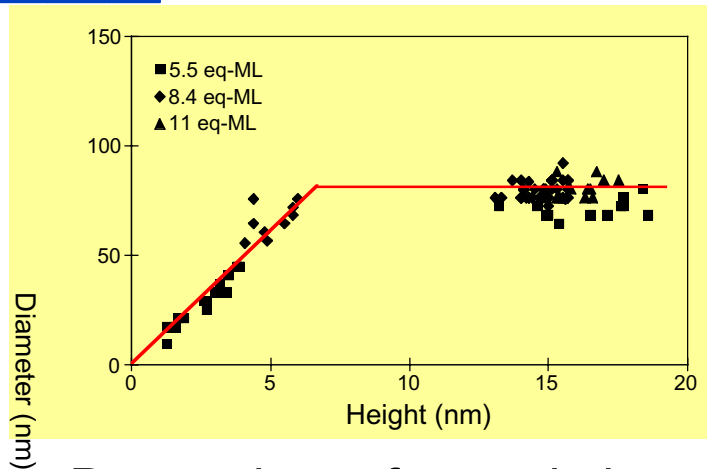
Larger Ge “dome”:
on Si(001)



Scanning-tunneling micrographs

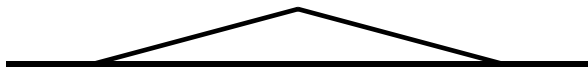
Gio Medeiros-Ribeiro, HPL

Island Distribution



Domes have favored size
Pyramids do not

Pyramids



Bounded by {105} facets only

Proportional:

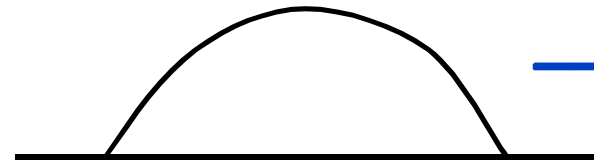
Surface area

Interface area

Edge length



Domes



Bounded by several facets

Area ratio can vary

Need not be proportional:

Surface area

Interface area

Edge length

Can vary to minimize energy

Harder to add atoms beyond

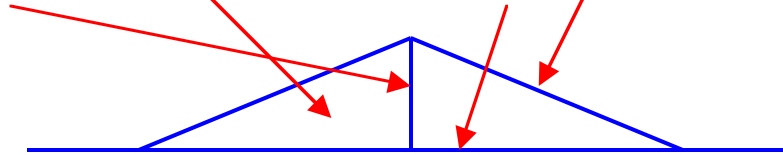
this energy minimum

Strain relaxation near top of island



Minimize Energy

Volume strain energy, facet surface energy,
edge energy, (interface energy - surface energy)



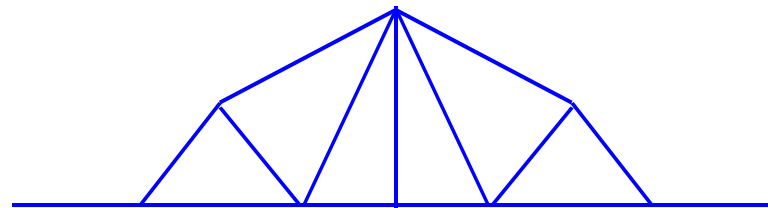
$$\Delta E(n) = C n + B n^{2/3} + A n^{1/3} \ln(a_c/n^{1/3})$$

C (C < 0): volume strain energy

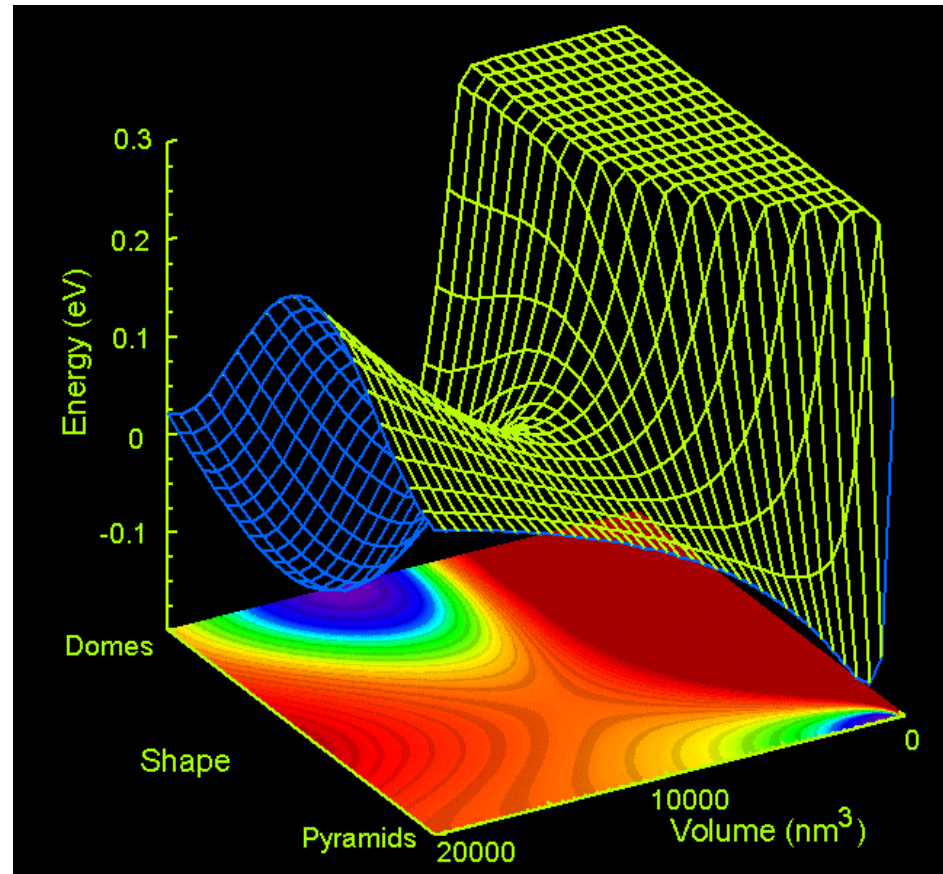
B (B < > 0): facet and interface energies

A (A > 0): edge energies

$$\Delta E(n)/n = C + B n^{-1/3} + A n^{-2/3} \ln(a_c/n^{1/3})$$



Shape Determined by Energy Minimization



Manipulating Islands

How to get

- Uniform size distribution?
- Smaller islands?

Domes have narrower distribution
Potentially more useful

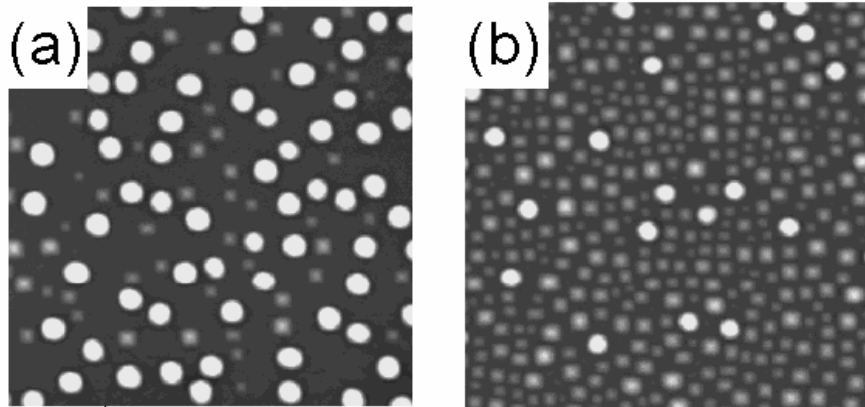
How to get smaller domes?

Change kinetics or thermodynamics

- Add HCl during deposition:
Primarily changes kinetics
- Etch with HCl after deposition
Reduces island height, not base
- Use Ti (TiSi_x)
Larger lattice mismatch

Using HCl to Control Islands

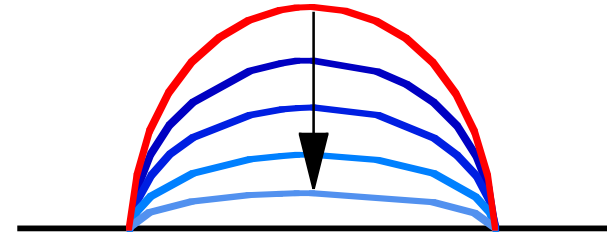
Adding HCl during Deposition



0
1.5
HCl Partial Pressure (Pa)

Adsorbed Cl impedes Ge surface diffusion

Etching with Gaseous HCl
after Deposition



Shorter, but not narrower

Manipulating Islands

How to get smaller domes?
Change thermodynamics

Island shape determined by

- Volume energy
- Surface energy
- Interface energy
- Edge and corner energies

Add something that binds well
to surface, changes surface
energy (and perhaps ratio of
energies of different surfaces)

Phosphorus or arsenic
n-type dopants

Initiation of arsenic
incorporation slow
Little in thin layer

Phosphorus more useful as
dopant

Doped Ge islands



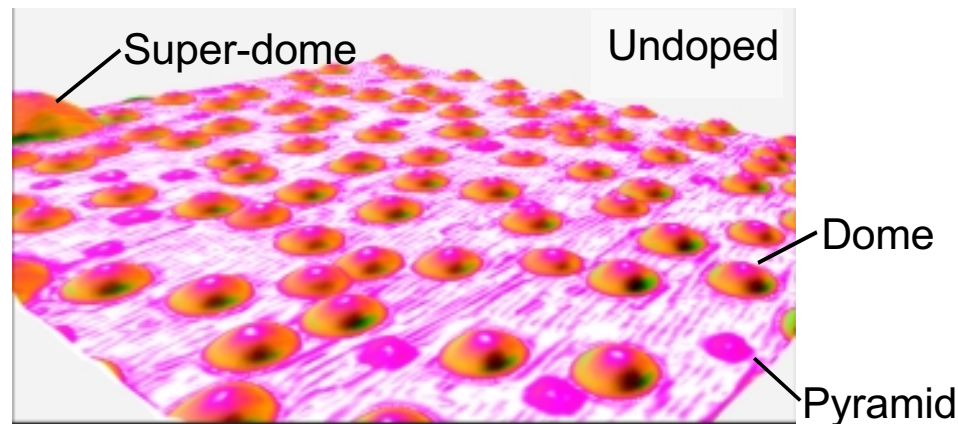
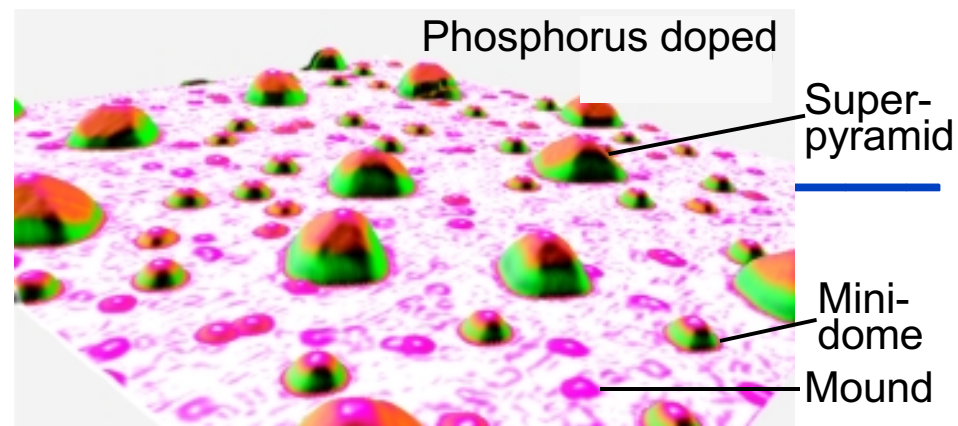
Temperature: 600°C

Partial pressures:

GeH_4 : $3\text{-}6 \times 10^{-2}$ Pa ($2.5\text{-}5 \times 10^{-4}$ Torr)

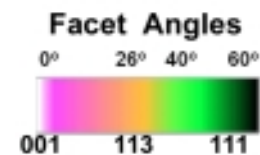
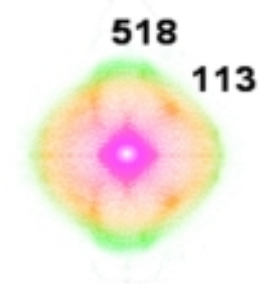
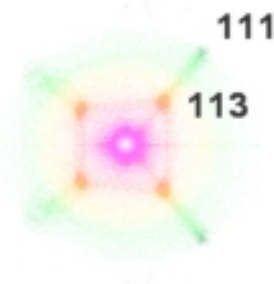
PH_3 : 1.7×10^{-3} Pa (1.4×10^{-5} Torr)

H_2 : 1.3 kPa (10 Torr)



Doped

Undoped



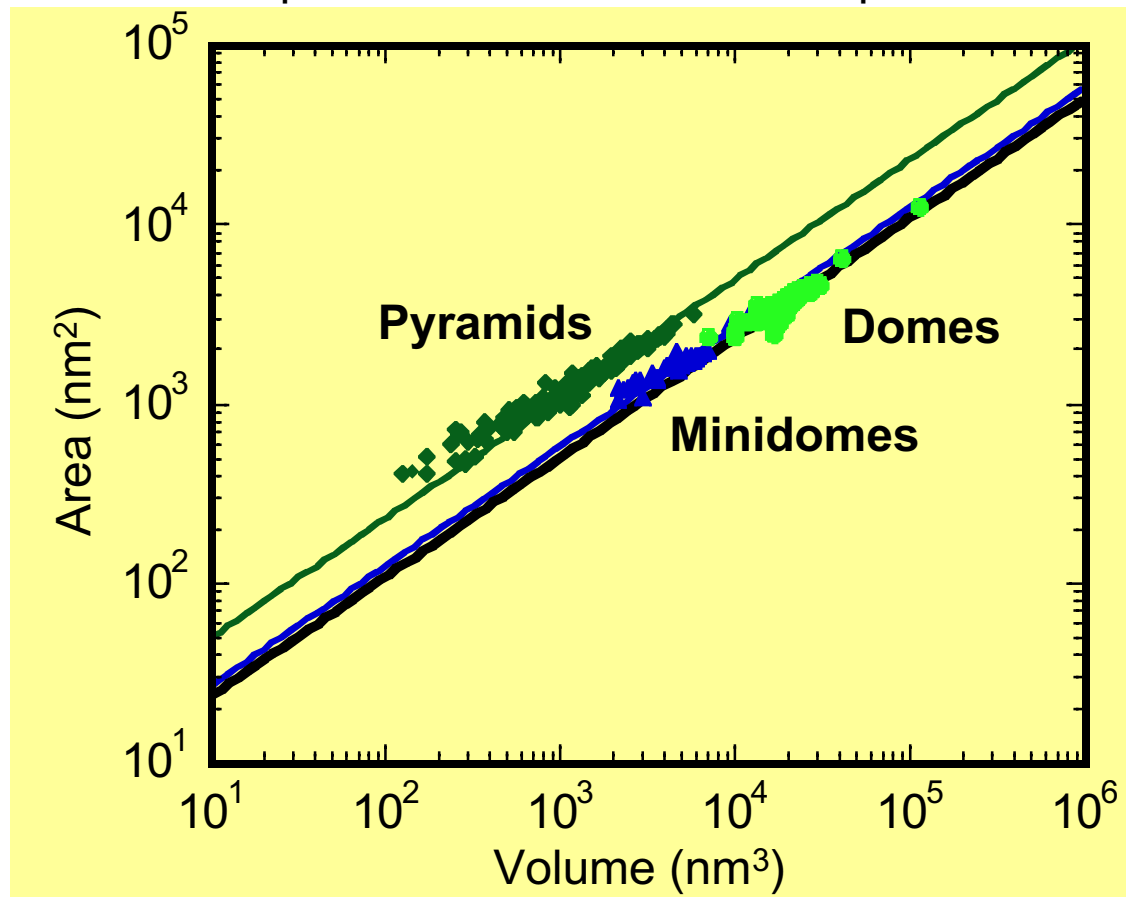
Island Shape Analysis

Undoped: Pyramids and Domes

Doped: Mini-domes

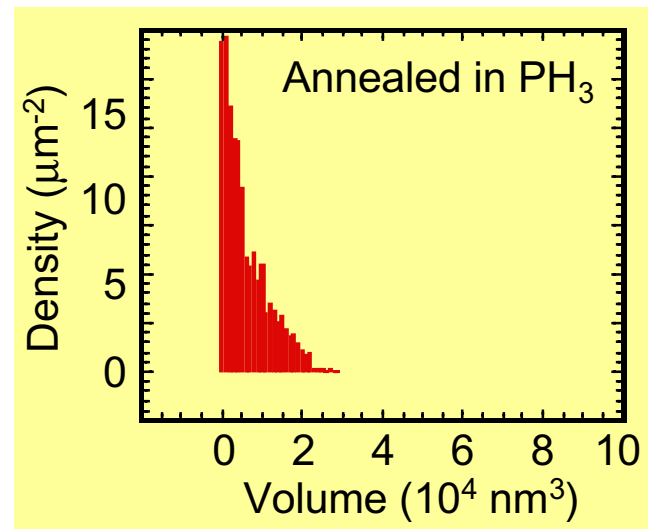
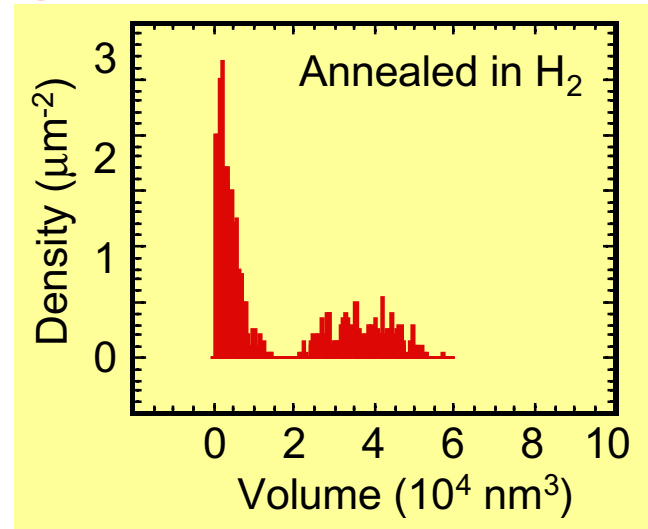
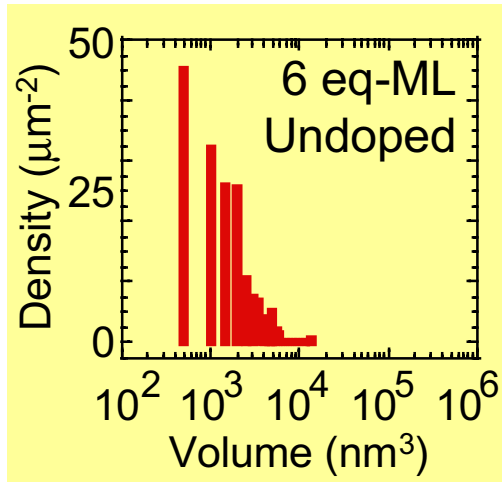
Points of one shape lie on line with slope = 2/3

Intercept different for different shapes



Phosphorus Also Changes Annealing Kinetics

6 eq-ML undoped Ge
Mainly pyramids



Effect of annealing

H_2 : Islands coarsen -
many convert to domes

PH_3 : Coarsening retarded

Phosphorus-Doped Ge Islands

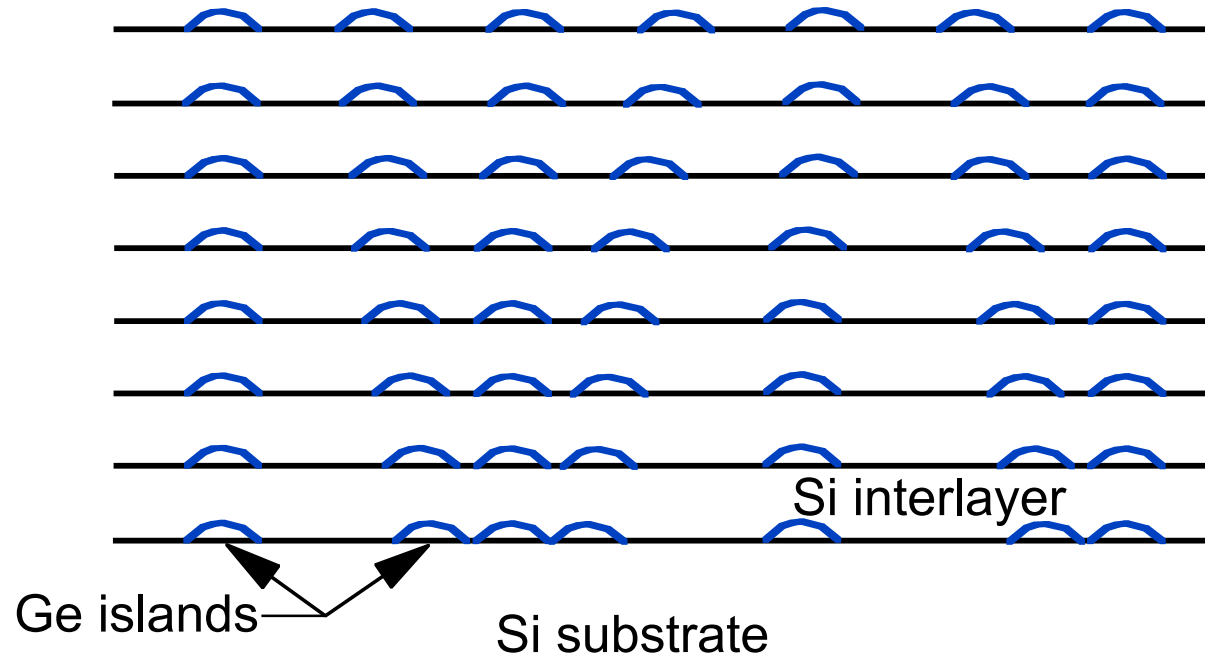
- Island shape influenced by surface energy
- Phosphorus...
 - Modifies energies and relative energies of different surface planes
 - Changes favored island shape
 - Retards coarsening
- Additional method for controlling island size, shape, and uniformity
- Slow buildup of high surface phosphorus concentration over 10s of monolayers

Manipulating Islands

Ordering and aligning

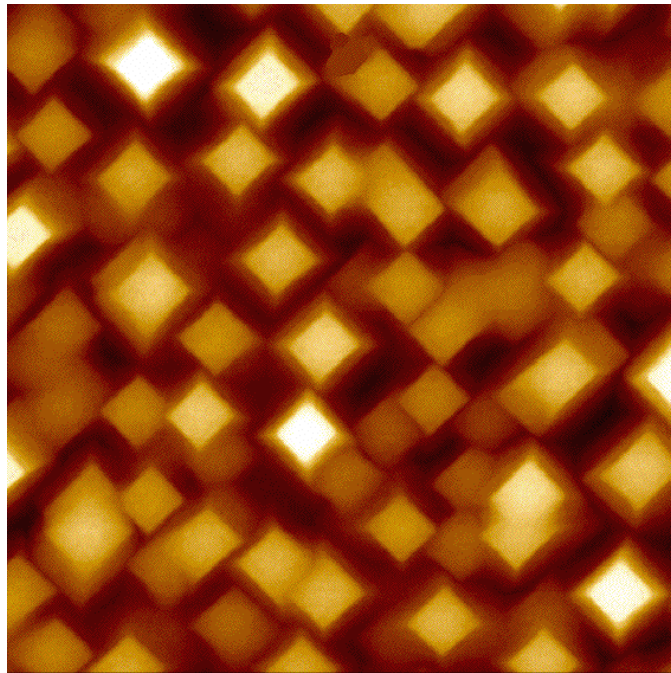
Ordering in Successive Layers

Cross Section

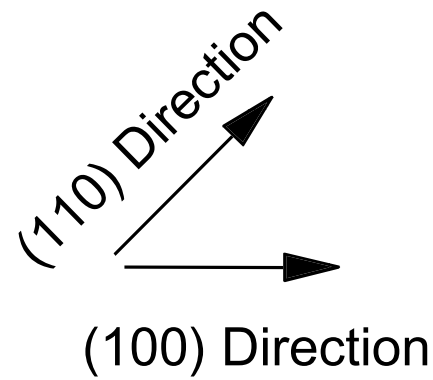


10 Layers of Si/Ge (Pyramids) Nano Picasso

Top View

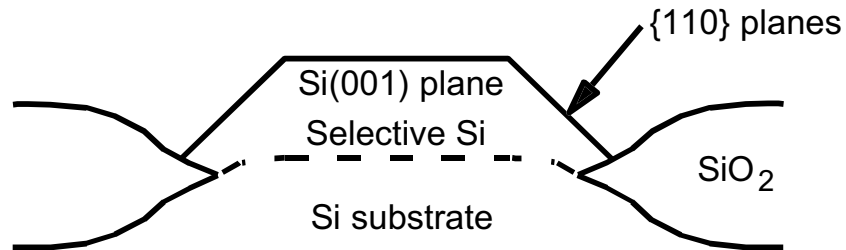


← 1 μm →

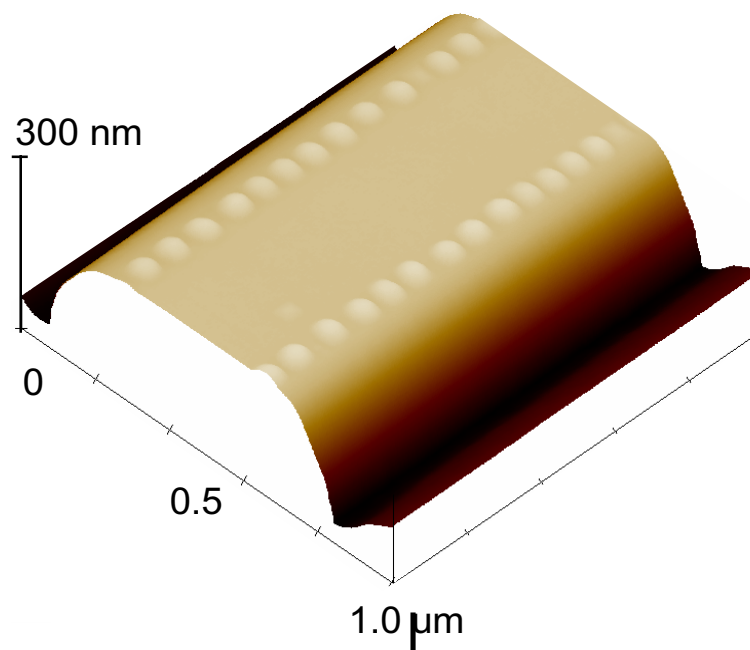
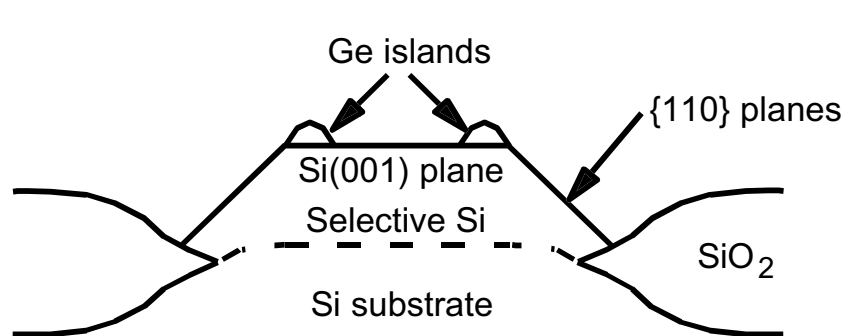


Height scale: 20 nm

Positioning Islands: Self-Assembled Ge Islands on Patterned Si substrate



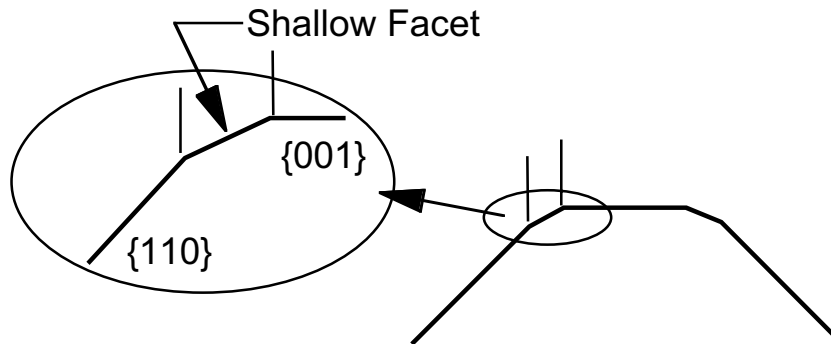
Positioning Islands: Self-Assembled Ge Islands on Patterned Si substrate



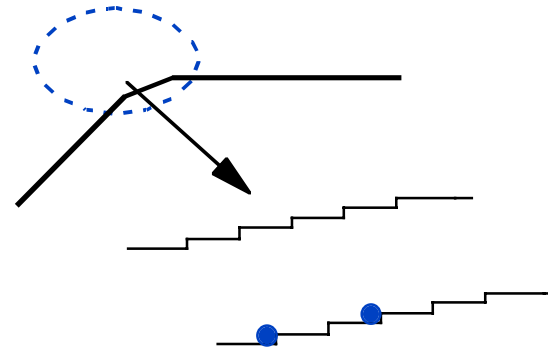
T.I. Kamins and R. Stanley Williams,
Appl. Phys. Lett. **71**, 1201 (1997)

What Causes Alignment?

Shallow facet

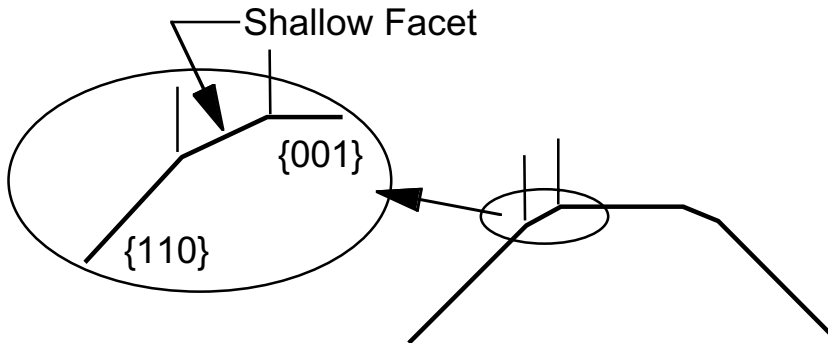


Facet provides steps for Ge nucleation

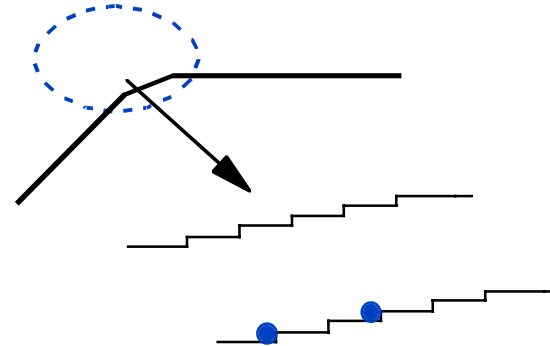


What Causes Alignment?

Shallow facet

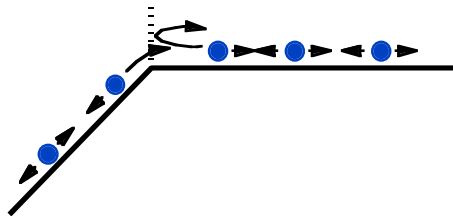


Facet provides steps for Ge nucleation



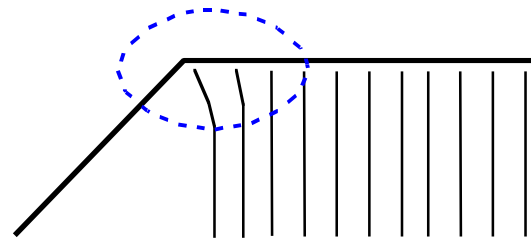
Surface Diffusion?

Anisotropic diffusion causes Ge accumulation near edge

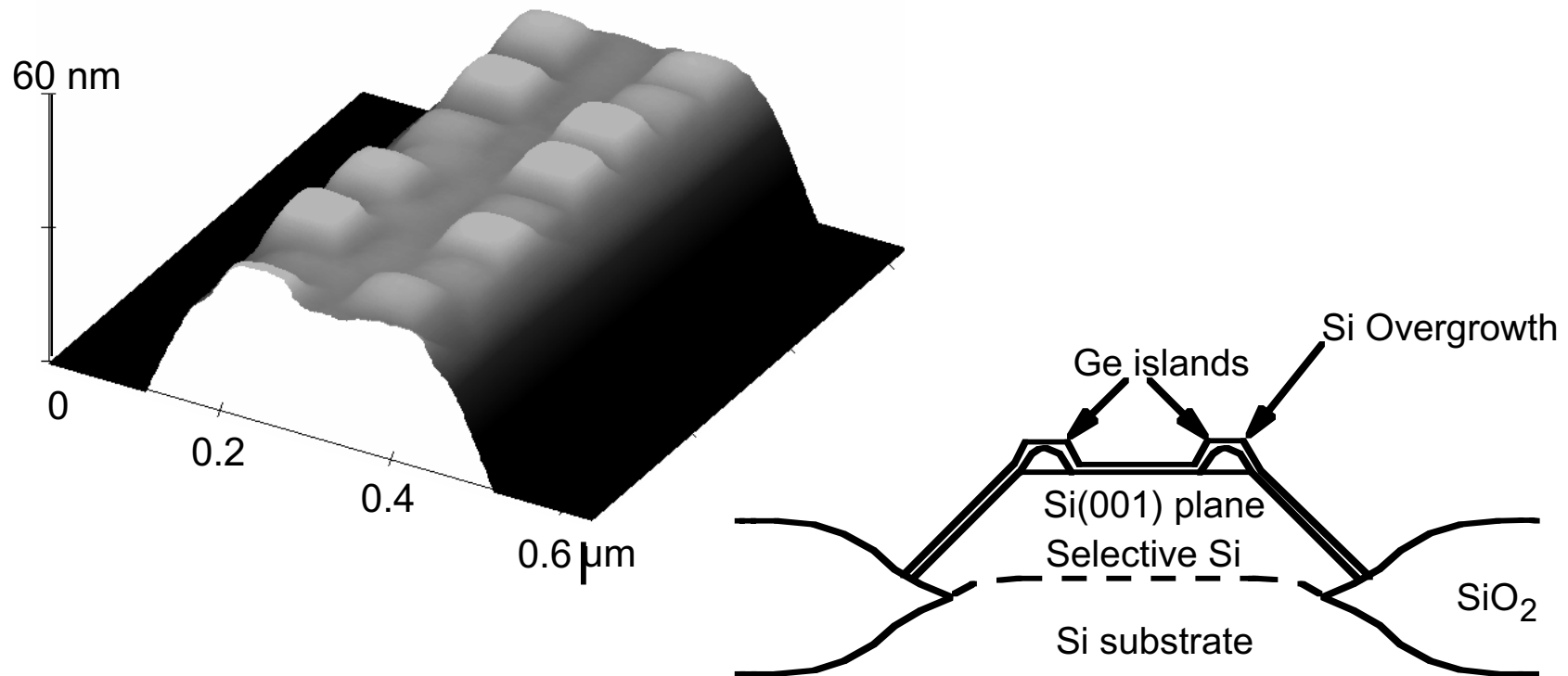


Strain?

Ge stretches Si lattice near edges
Relieves stress
Lowers energy barrier for nucleation



Si-Capped Ge Islands on Patterned Si Substrate



In-plane orientation of Ge islands and Si cap are different: Ge || [100], Si || [110] directions

Anisotropic Stress

Ge on Si:

Lattice mismatch same in x and y directions

⇒ equi-axed islands

Different lattice mismatch in different directions

⇒ anisotropic islands (ie, “wires”)

Anisotropic lattice mismatch:

ErSi₂ [0001] || Si<110>: +6.5%

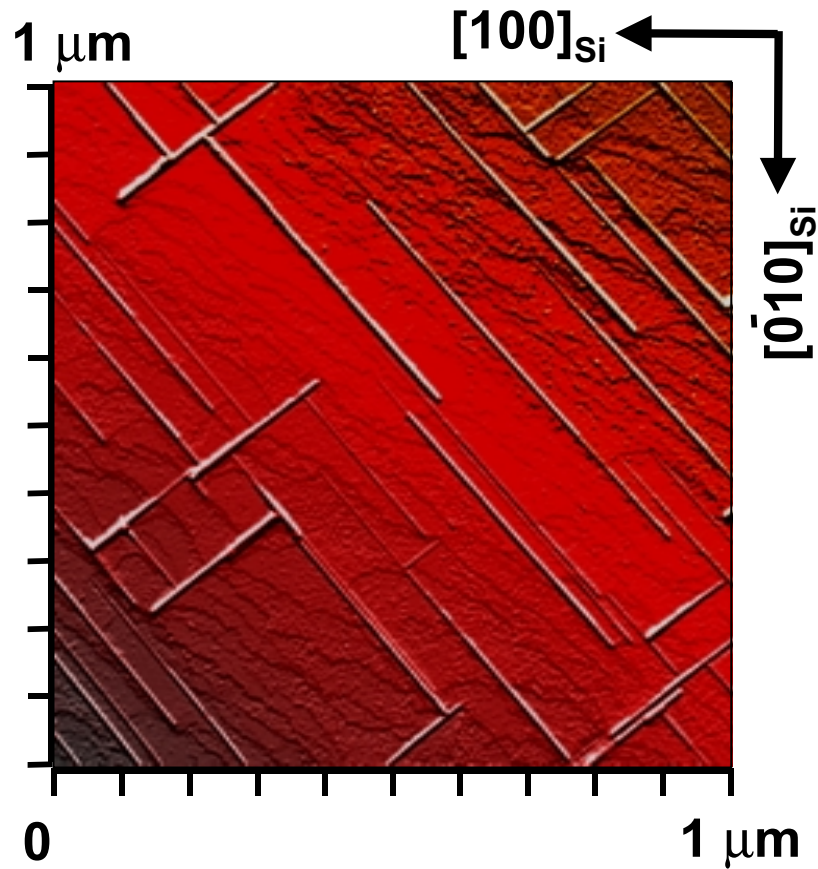
ErSi₂ [11 $\bar{2}$ 0] || Si<110>: -1.3%

Constraint on growth in one direction

Elongated (wire) growth in perpendicular direction

Y. Chen, D. A. A. Ohlberg, G. Medeiros-Ribero,
Y. A. Chang, and R. Stanley Williams,
Applied Physics Letters **76**, 4004 (26 June 2000)

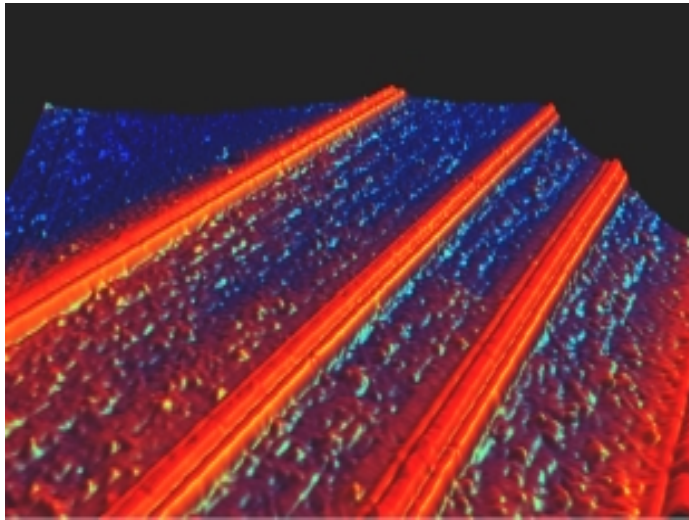
ErSi₂ on Si



Yong Chen and Doug Ohlberg, HPL

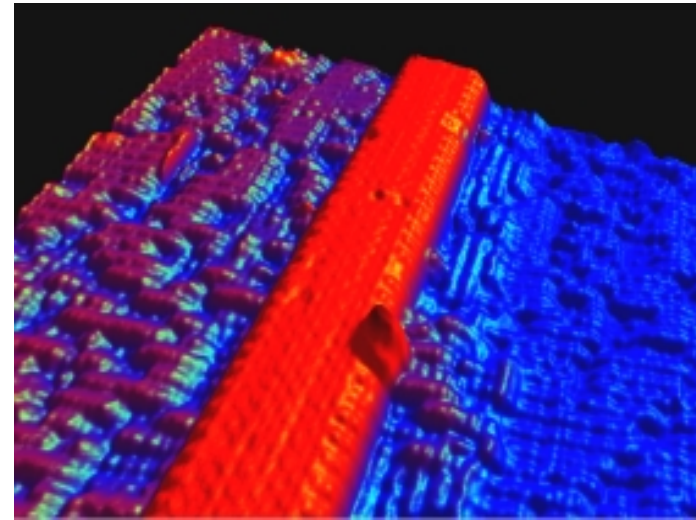
Self-Assembled Nanostructures

**Anisotropic lattice strain
forms 1D structure**



Scanning tunneling
micrographs

ErSi₂ “wires” on Si(001)



Yong Chen and Doug Ohlberg, HPL

Defect Tolerance

Self-assembled, self-ordered system will not be perfect

Several percent defects

How to live with less-than-perfect parts in a system?

Structurally simple architecture (eg, crossbar array)

Parallel straight wires

Map defects

Configure around defects

(Can also be applied to conventional fabrication
to reduce costs)

Normal computer:

Design (configure), build, test

Defect-tolerant computer:

Build, test (to locate defects), configure around defects



Summary

Limits of scaling

Alternative devices

Self-assembled nanostructures

Forming small structures

Putting them where we want them

Strain from lattice mismatch

Zero-dimensional islands: Ge, Ti

One-dimensional wires: ErSi₂

Catalytic wire growth

Ti-catalyzed Si nanowire growth

Patterned substrate to position features

Defect-tolerant architecture