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# Lecture 2
# Strain and structure of thin films

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Sapporo 2010

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# Outline

- Strain in epitaxial systems
  – Leads to structure
  – Quantum dots and their arrays
- Atomistic strain model
  – Lattice statics model
  – Lattice mismatch
- Numerical methods
  – Algebraic multigrid (AMG)
  – Artificial boundary conditions (ABC)
- Application to nanowires
  – Step bunching instability
- Summary

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# Strain in Epitaxial Systems

- Lattice mismatch leads to strain
  - Heteroepitaxy
  - Ge/Si has 4% lattice mismatch
  - 1.3% lattice mismatch for AlSb on InAs
  - 7% for GaAs on InAs
- Device performance affected by strain
  - band-gap properties
- Relief of strain energy can lead to geometric structures
  - Quantum dots and q dot arrays

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# Band Gap Shift due to Strain Induced by Alloy Composition in $In_xGa_{1-x}As/GaAs$

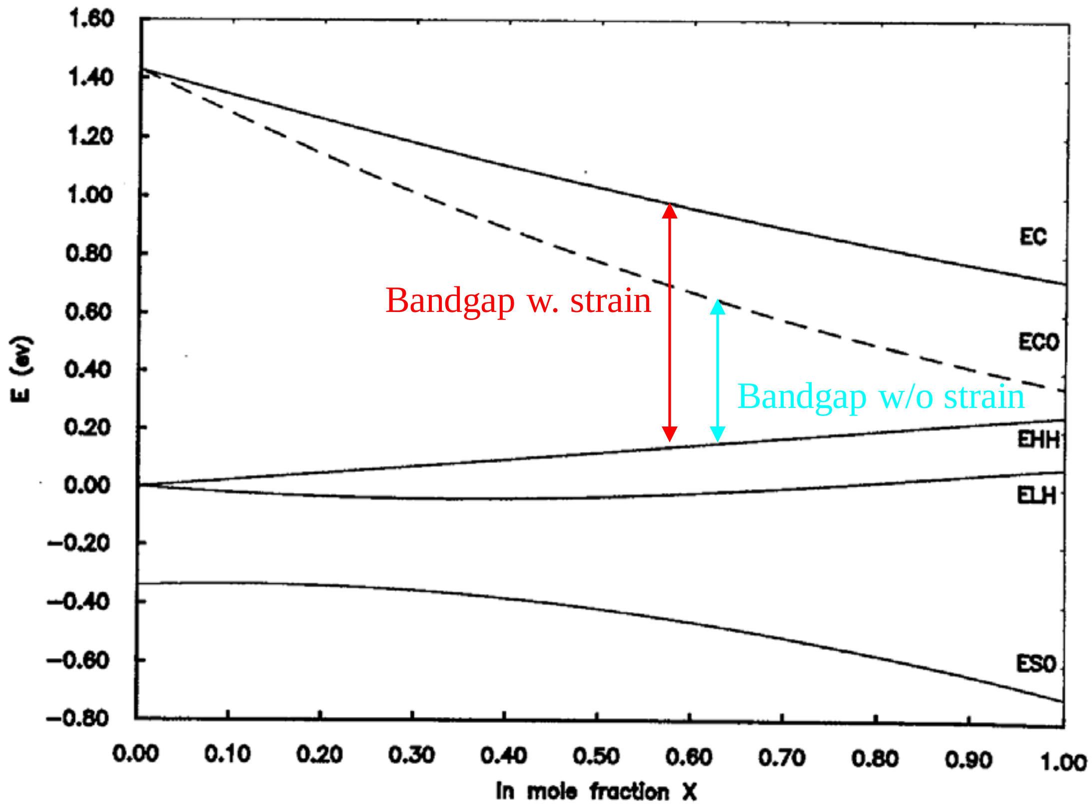
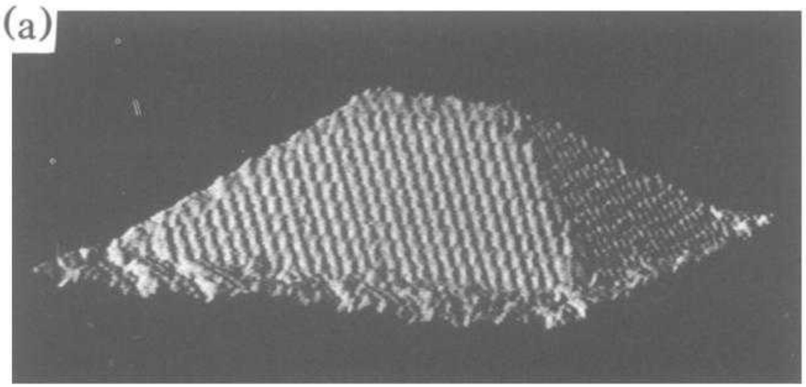
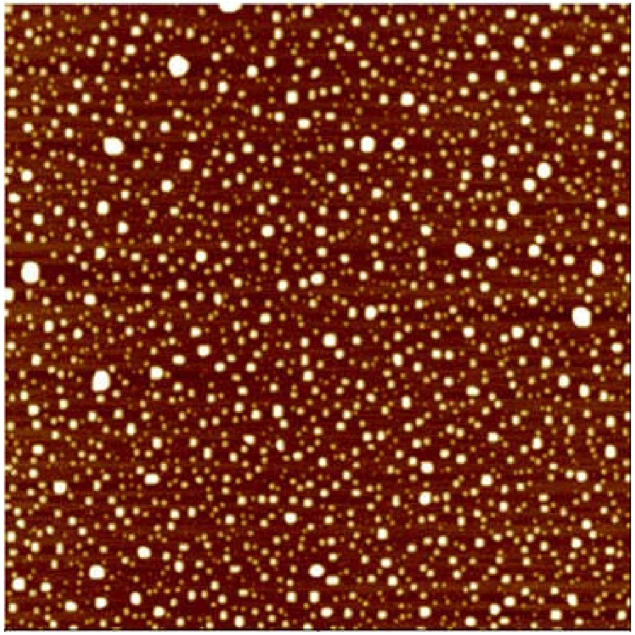



FIG. 12. Relative shifts of the band-edge extrema as a function of the InAs mole fraction x in GaInAs as 300 K. ECO is the variation of the unstrained conduction band with the valence band depth at 0 eV. EC is the variation of the conduction band due to the hydrostatic strain component. HH, LH, and SO are the variation of the heavy-hole, light-hole, and splitt-off band due to the shear-strain component (for convenience, the hydrostatic shift is attributed entirely to the conduction band).

Mandeville, in Schaff et al. 1991

# Quantum dots and Q Dot Arrays



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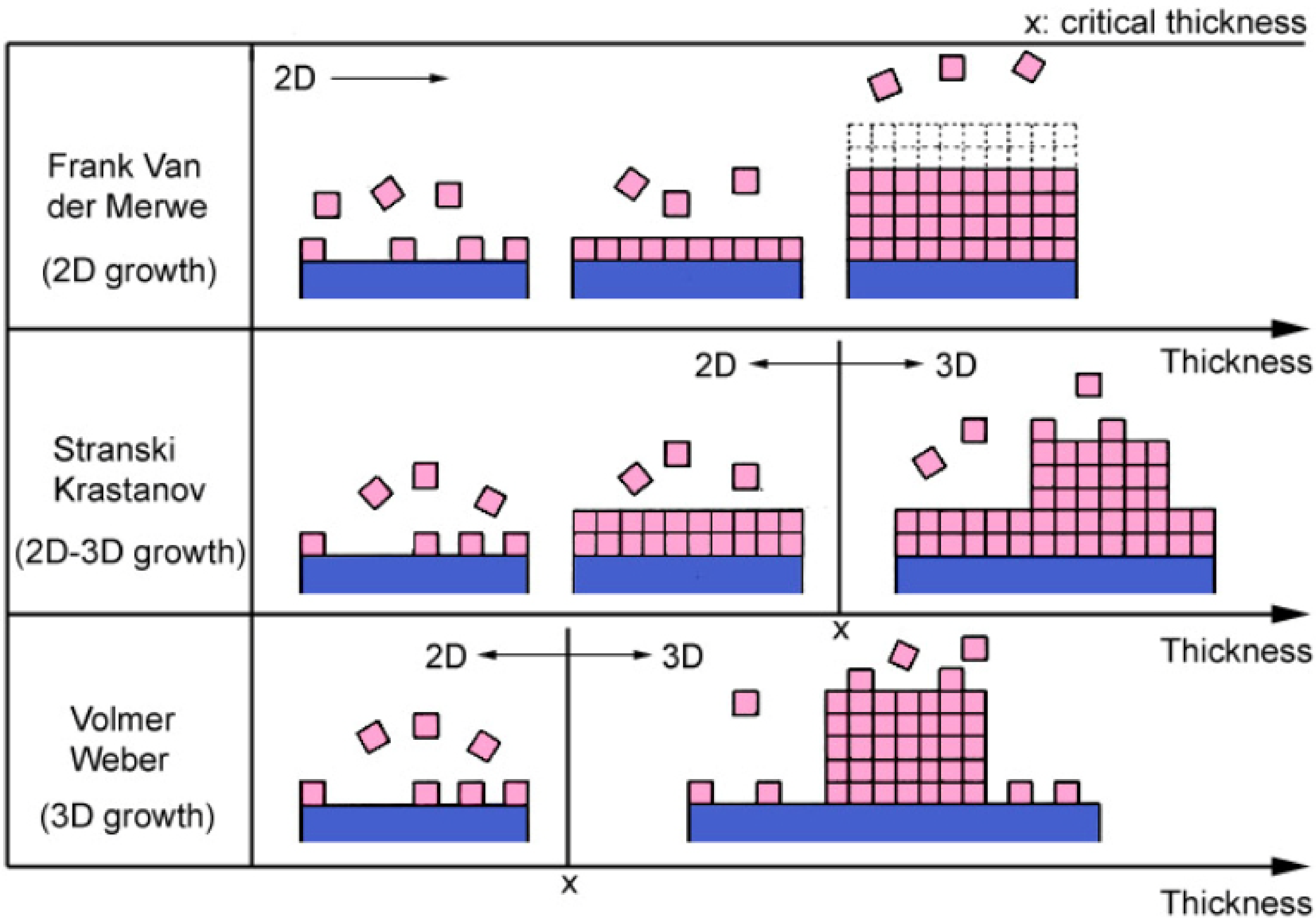
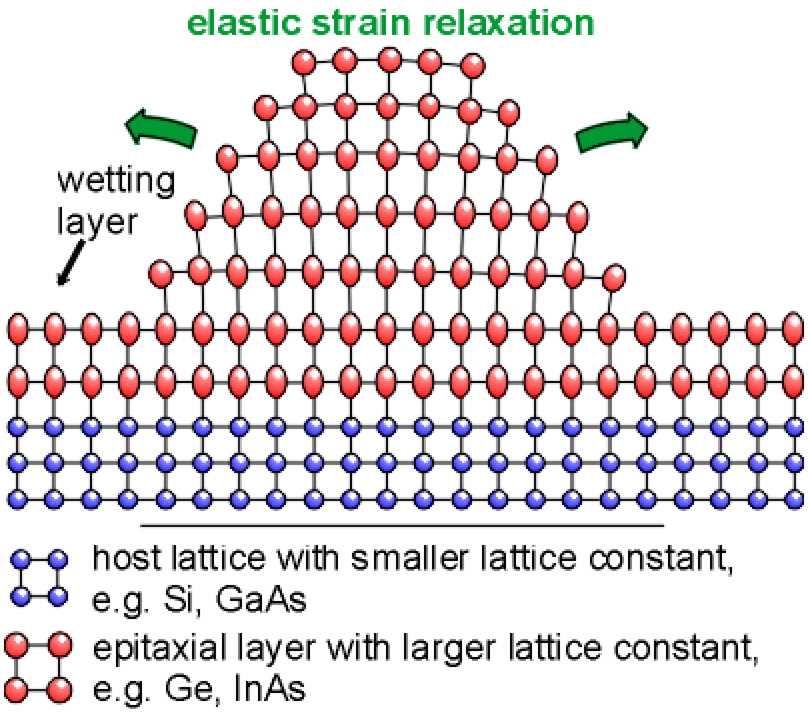
# Epitaxial Growth Modes



# Stranski-Krastanow Growth

- Formation of 3D structures (q-dots) preceded by wetting layer
  - Most frequently seen growth mode



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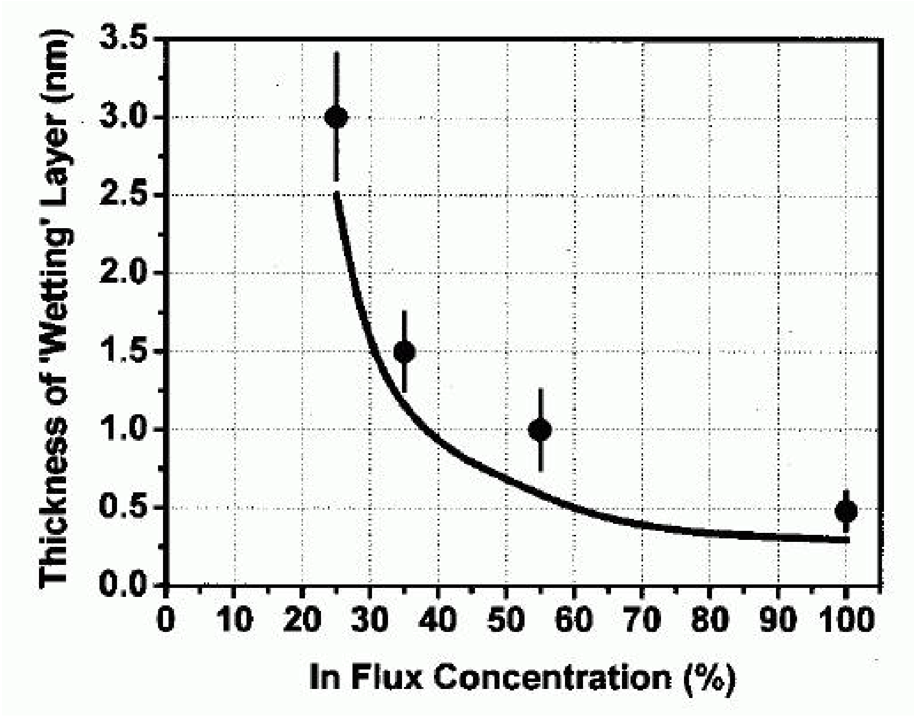
# Wetting Layer Thickness in SK Growth

- Wetting layer thickness can vary from 1 to many atomic layers.
- Recent results suggest that alloy segregation (vertical) determines thickness.
  - Cullis et al PRB 2002
  - Tu & Tersoff PRB 2004
- Not successfully simulated.



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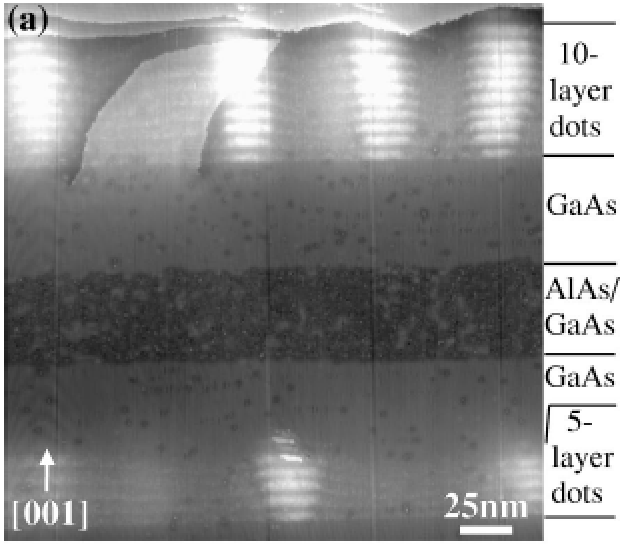
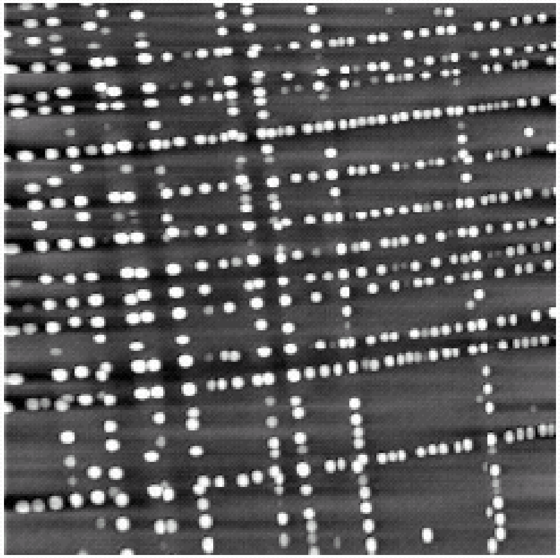
- Vertical allignment of q dots in epitaxial overgrowth (left)
- Control of q dot growth over mesh of buried dislocation lines (right)

$Al_xGa_{1-x}As$ system




B. Lita et al. (Goldman group), APL **74**, (1999)

GeSi system



H. J. Kim, Z. M. Zhao, Y. H. Xie, PRB **68**, (2003).

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# Continuum Models of Strained Growth

- Continuum elasticity
  - Marchenko & Parshin Sov. Phys. JETP 1980
  - Spencer, Voorhees, Davis (1991,…); Freund & Shenoy (2002)
  - apply continuum elasticity equations in thin film
  - prediction of strain induced instabilities,
  - fully developed q dots
- Green's function on step edges
  - Tersoff et al. (1995,…)
  - Kukta & Bhattacharya (1999)
  - describe influence of step edge via monopole and dipole forces, using Green's function
  - Singularity requires cutoff of Green's function for curved step edge
    - Similar to singularity of vortex line
  - prediction of step edge dynamics
  - inapplicable (or difficult to use) for inhomogeneous materials

# Step Bunching

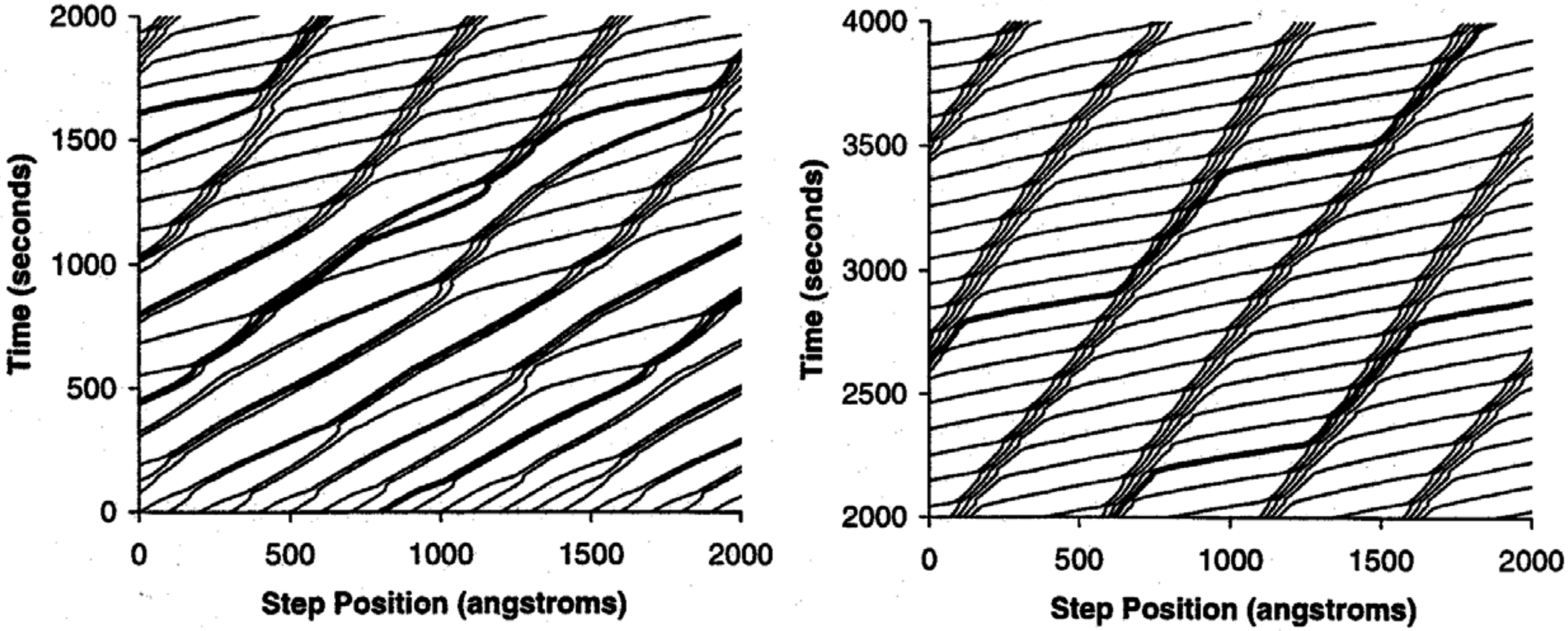


Figure 4. Plots of step position versus time calculated for a step train subjected to stress. Periodic boundary conditions were imposed with 15 steps per period. Bold traces demarcate a period. Initially equidistant steps become unstable, dynamically bunching and unbunching in an irregular manner (left). At later times (right), bunching and unbunching continues, yet the step traces form a regular pattern with four step per bunch on average.

Kukta & Bhattacharya (1999)
(similar work by Tersoff et al.1995,…)

# Atomistic Modeling of Strain in Thin Films

- Lattice statics for discrete atomistic system,
  - minimize discrete strain energy (Born & Huang, 1954)
  - Application to epitaxial films,
    - E.g., Stewart, Pohland & Gibson (1994), Orr, Kessler, Snyder & Sander (1992),
- Idealizations
  - Harmonic potentials, Simple cubic lattice
  - General, qualitative properties
    - Independent of system parameters
  - Computational speed enable additional physics & geometry
    - 3D, alloying, surface stress
- Atomistic vs. continuum
  - atomistic scale required for thin layer morphology
    - strain at steps
  - continuum scale required for efficiency
    - KMC requires small time steps, frequent updates of strain field

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# Microscopic Model of Elasticity with Harmonic Potentials

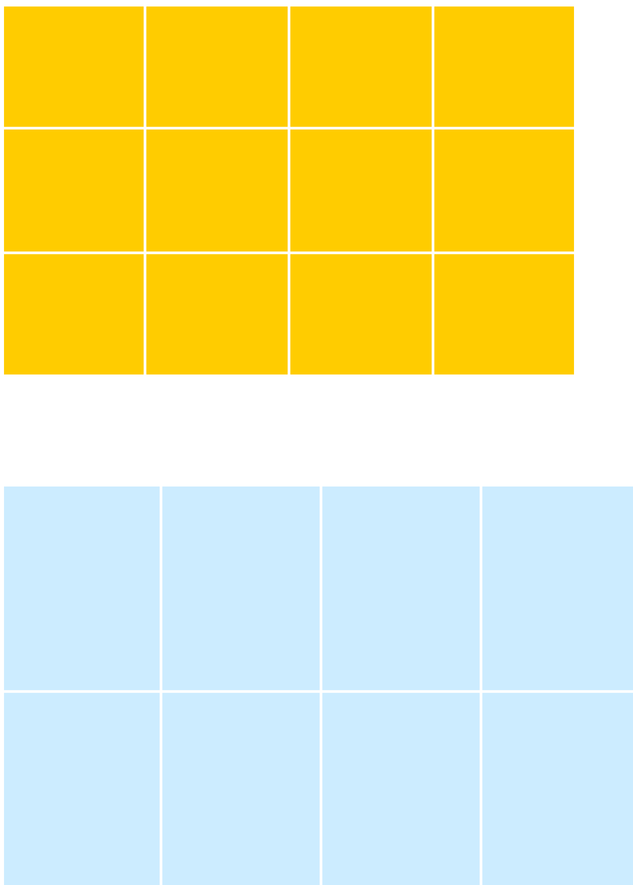
- Continuum Energy density
  - isotropic $$E = \lambda(S_{xx} + S_{yy})^2 + \mu(S_{xx}{}^2 + S_{yy}{}^2 + 2S_{xy}{}^2)$$
  - cubic symmetry $$E = \alpha(S_{xx}{}^2 + S_{yy}{}^2) + \beta S_{xy}{}^2 + \gamma S_{xx} S_{yy}$$
- Atomistic Energy density
  - Nearest neighbor springs
    $$E = k(S_{xx}{}^2 + S_{yy}{}^2)$$
  - Diagonal springs
    $$E = \ell(S_{xx} + 2S_{xy} + S_{yy})^2 + \ell(S_{xx} - 2S_{xy} + S_{yy})^2$$
  - Bond bending terms
    $$E = mS_{xy}{}^2$$
- Elastic equations $\partial_u \mathcal{E}[u] = 0$

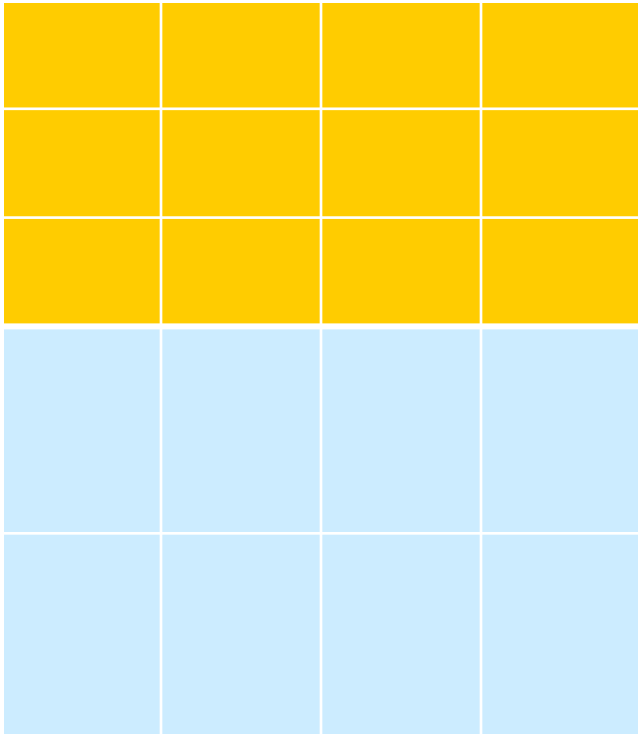
# Cauchy Relations

- Elasticity based on two-particle potentials
  - → $\mu = 4\,\lambda$ (Lame coefficients) for cubic symmetry
  - – Cauchy relations
- Access to full range of elasticity requires 3-body terms in energy
  - – E.g. bond bending terms: $(\cos\theta)^2$
  - – Keating model for Si consists of nearest neighbor springs and bond bending terms

$\theta$

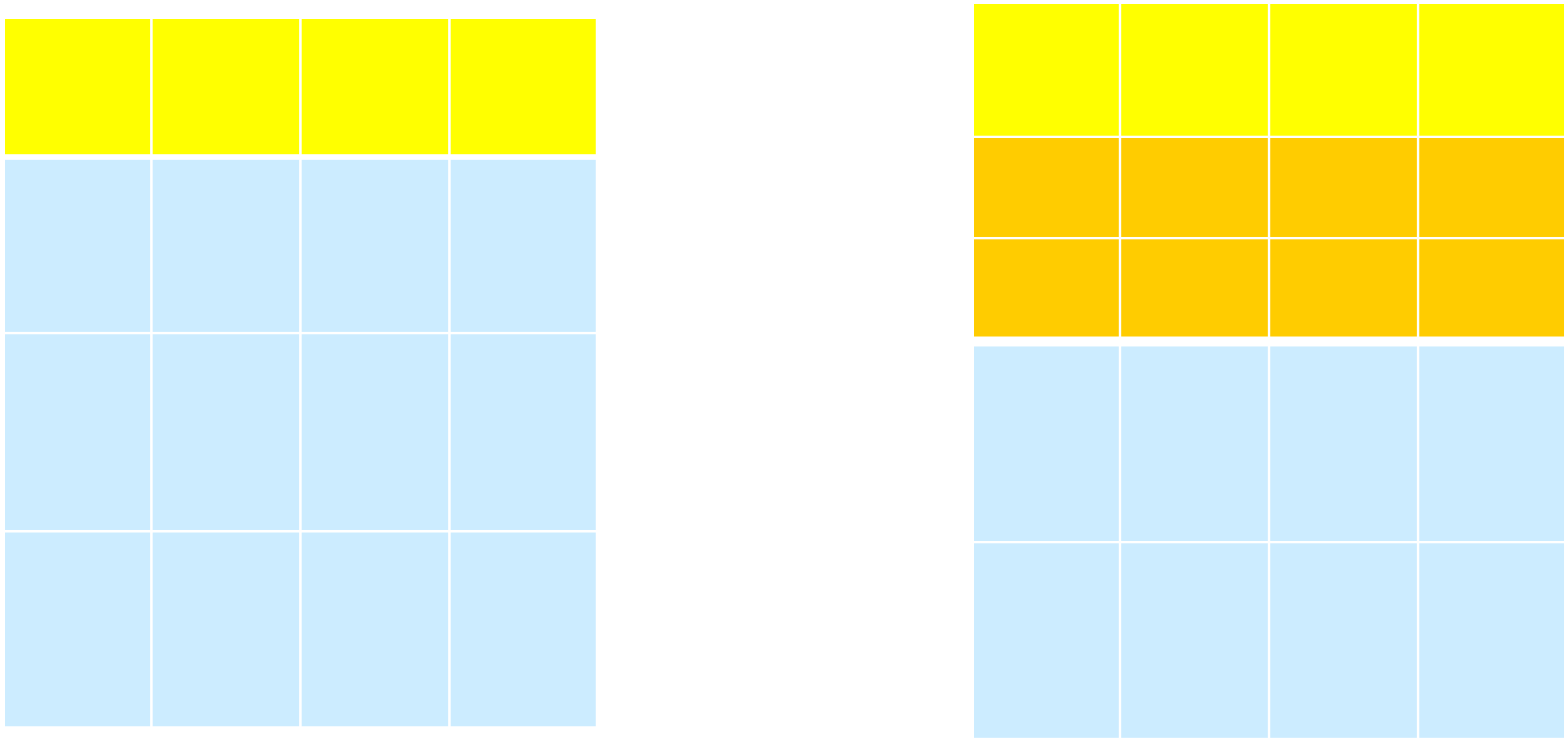
# Strain in an Epitaxial Film Due to Lattice Mismatch



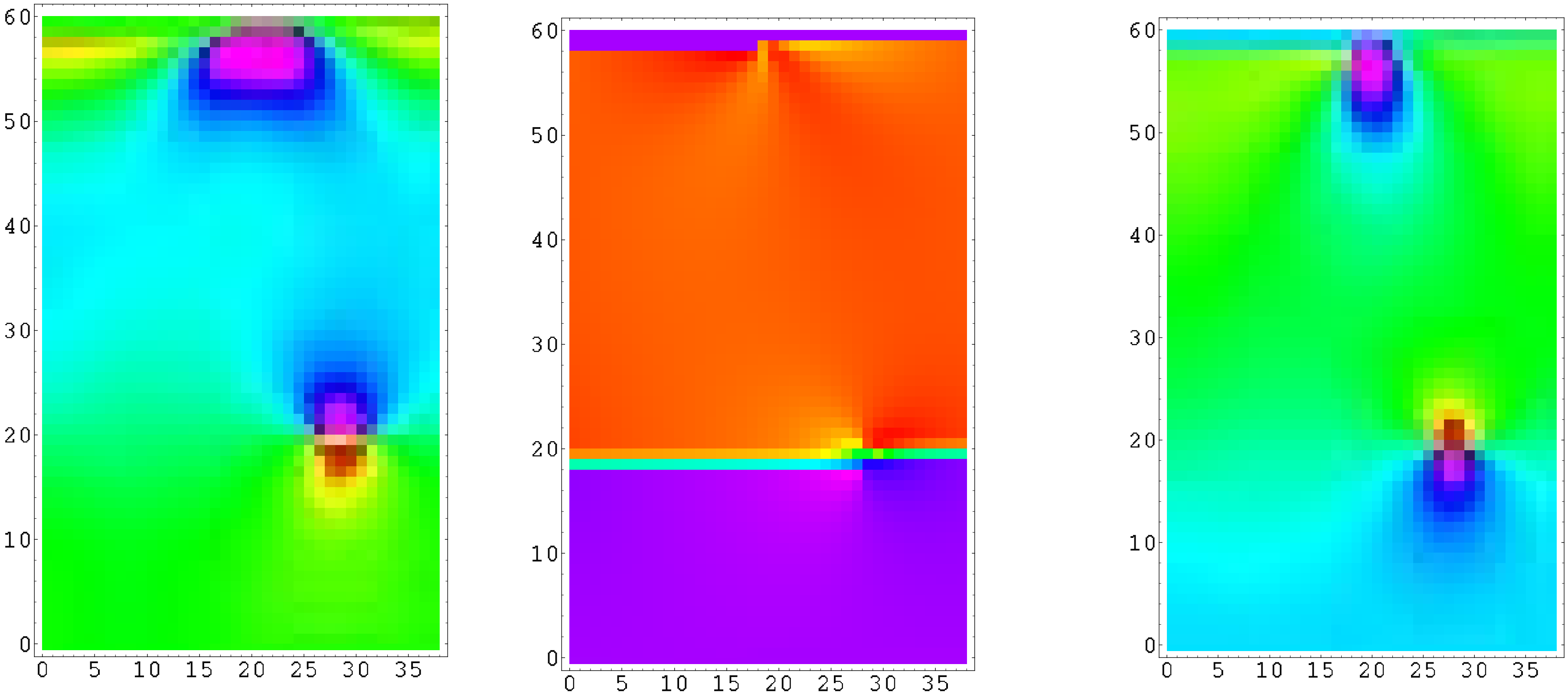


- lattice mismatch
  - lattice constant in film a
  - lattice constant in substrate h
  - relative lattice mismatch $\varepsilon=(a-h)/h$

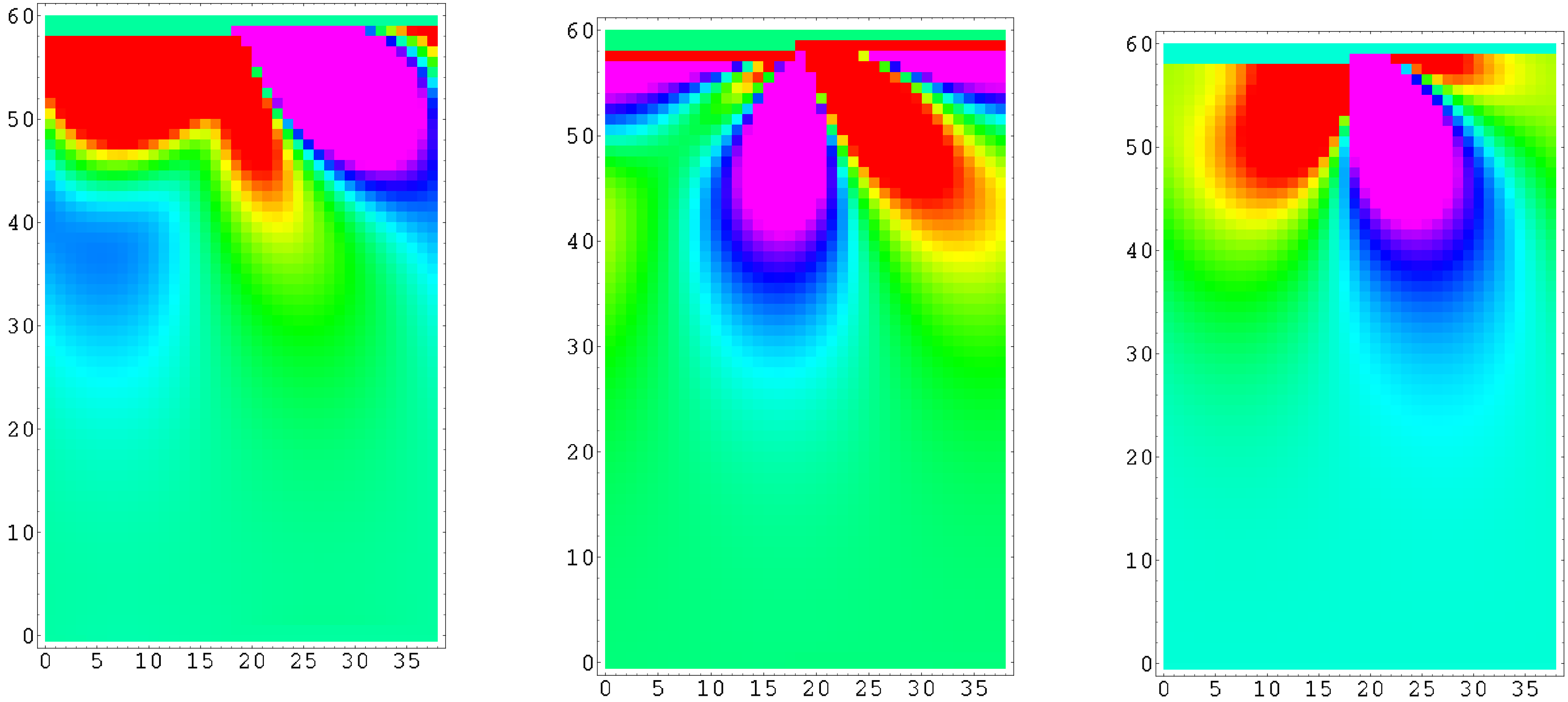
# Deformation of Surface due to Intrinsic Surface Stress



# Strain Tensor
# Step with No Intrinsic Surface Stress



# Strain Tensor
# Step with Intrinsic Surface Stress
# No lattice mismatch

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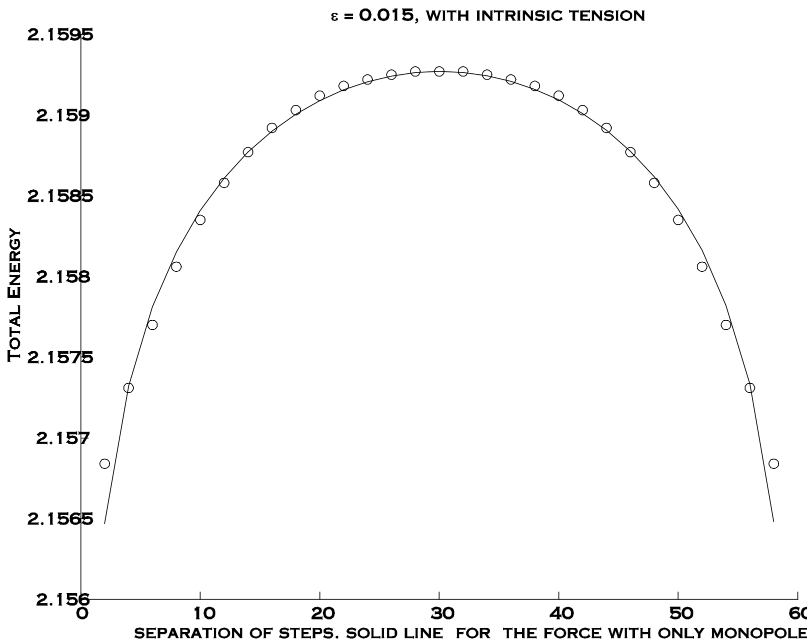
# Interaction of Surface Steps

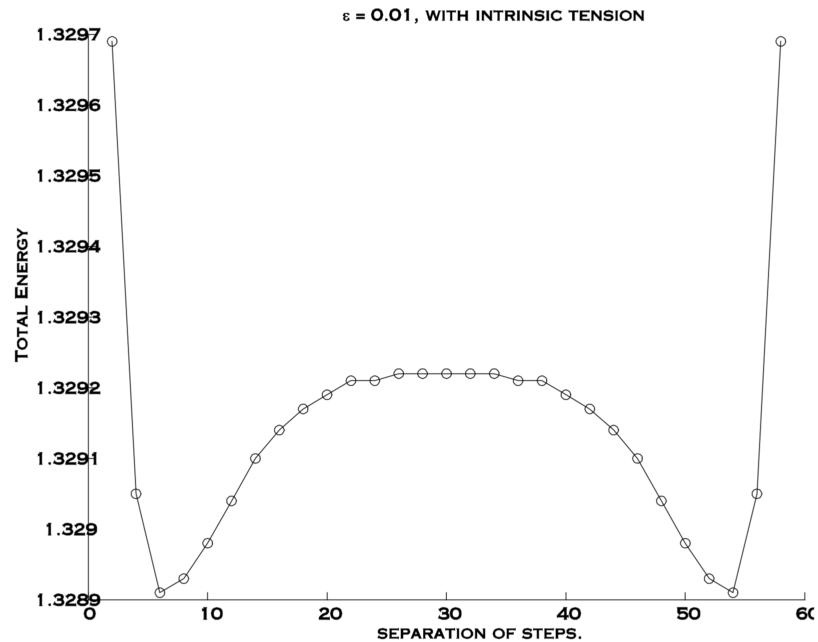
- Steps of like "sign"
  - Lattice mismatch → step attraction
    - Step aggregation allows increased relaxation
  - Surface stress → step repulsion
    - Step separation reduces interfacial curvature

# Energy vs. Step Separation

Step attraction due to lattice mismatch




Repulsion of nearby steps due to intrinsic surface stress



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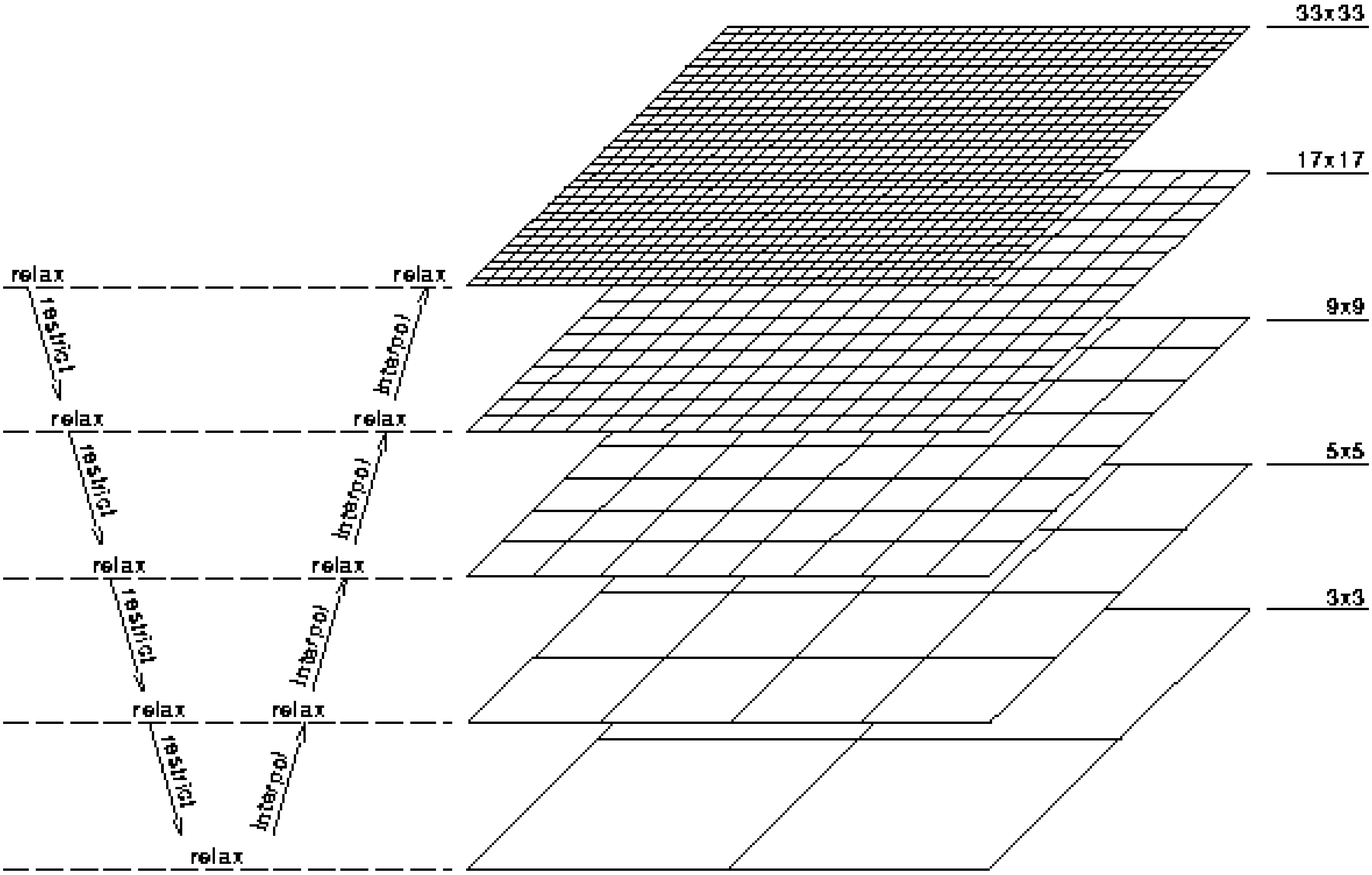
# Numerical method for Discrete Strain Equations

- Algebraic multigrid with PCG
- Artificial boundary conditions at top of substrate
  - Exact for discrete equations
- 2D and 3D, MG and ABC combined
  - Russo & Smereka (JCP 2006),
  - Lee, REC & Lee (SIAP 2006)
  - REC, Lee, Shu Xiao, Xu (JCP 2006)

# Multigrid

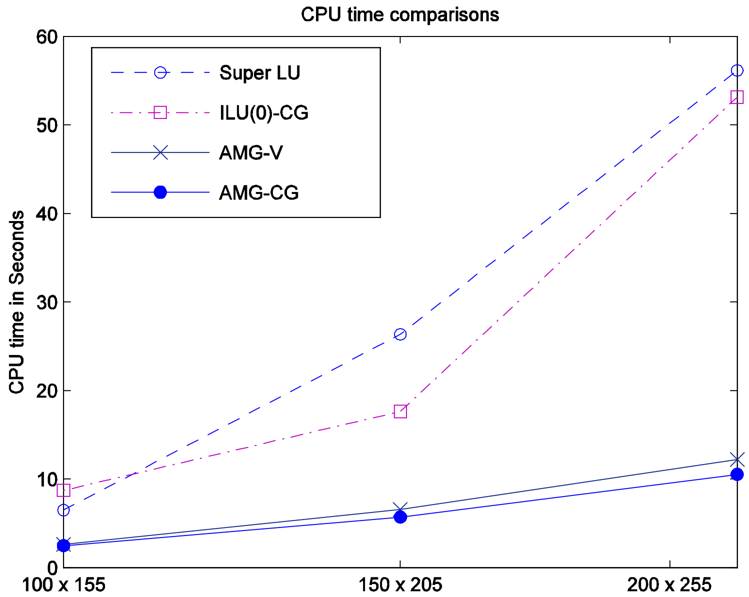
- Solution performed on grids of different resolution
  - Average (fine grid) → coarse grid
  - Interpolate(coarse grid) → fine grid
  - Interaction between grids  accelerates communication across the grid and convergence
- (Geometric) multigrid (MG)
  - Averaging is performed over geometric neighbors
- Algebraic multigrid (AMG)
  - Sparse matrix elements define a graph
  - Average is performed over adjacent points on graph

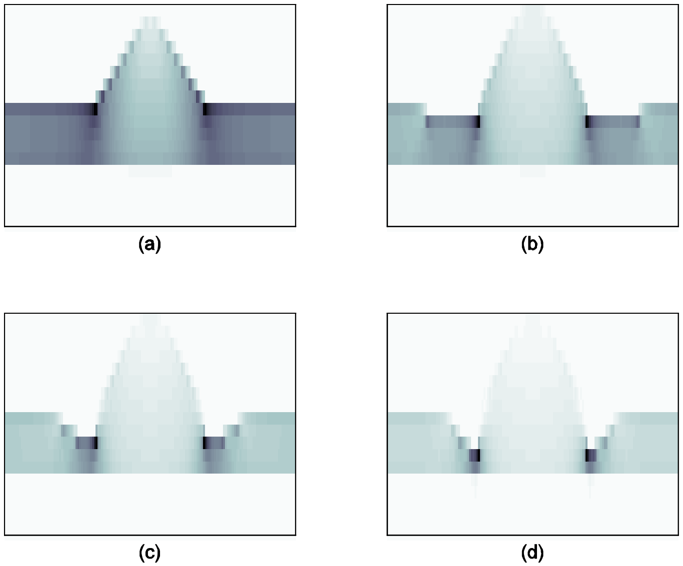
# Multigrid



relax
restrict
relax
interpol
relax
restrict
relax
interpol
relax
restrict
relax
interpol
relax
restrict
relax
interpol
relax
33x33
17x17
9x9
5x5
3x3

# AMG for Atomistic Strain




CPU speed (sec) vs. lattice size for strain computation in a 2D quantum dot system

Similar results in 3D and with ABC

Strain energy density for 160 atom wide pyramid in 2D with trenches, for various trench depths

# Artificial Boundary Conditions

- For heteroepitaxial system, forces occur only at substrate/film interface
  - Below the interface, homogeneous elasticity
  - Exact solution in terms of Fourier transform
- Reduction of solution domain
  - $\Gamma$ = plane below interface
  - $\Omega_1$ = region above $\Gamma$, $\Omega_2$ = region above $\Gamma$
  - Exact artificial bdry condition (ABC) on $\Gamma$
  - Solution only required on $\Omega_1$, using ABC on $\Gamma$
  - Formula for energy of entire system ( $\Omega_1 + \Omega_2$ )
- Exact ABCs developed for continuous and discrete systems

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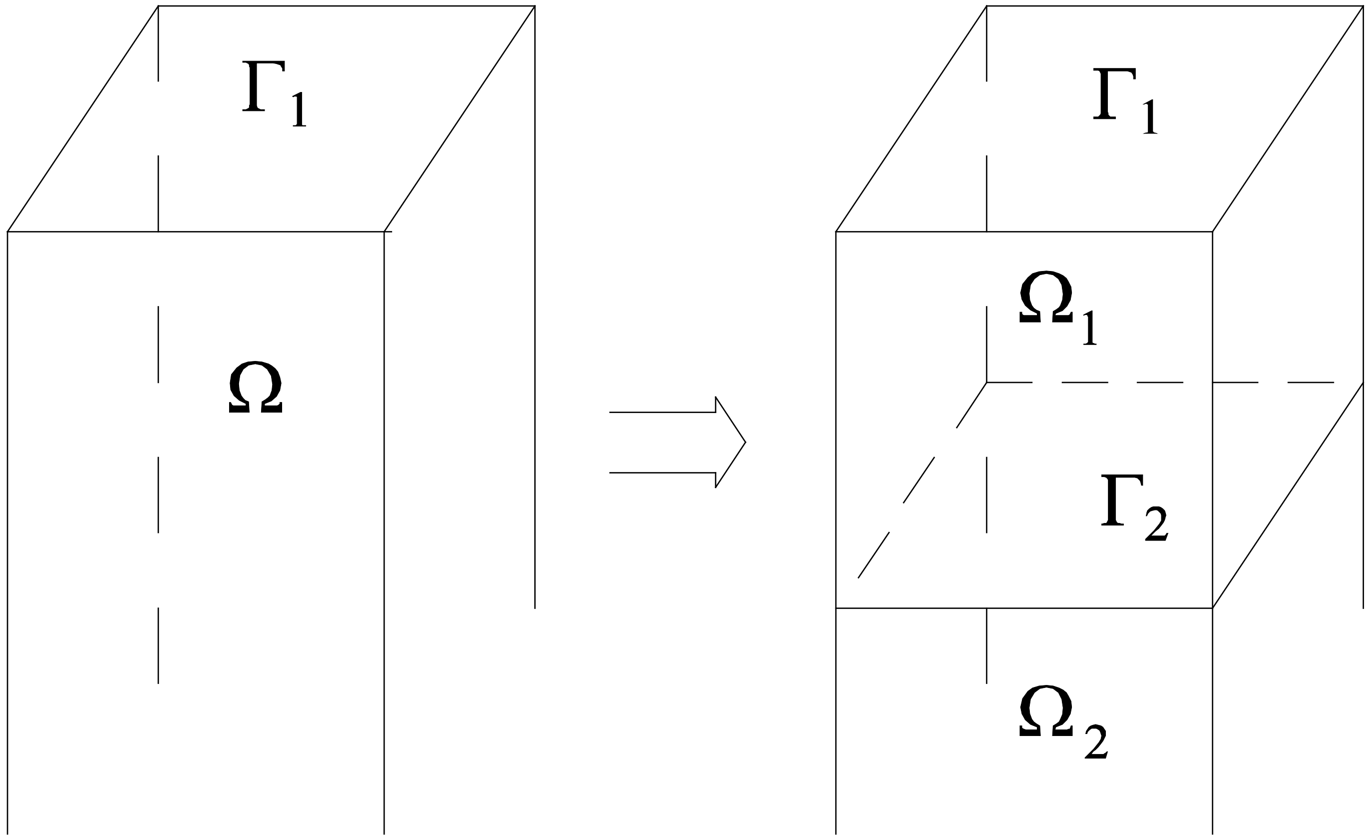
# Artificial Boundary Conditions



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# Example of ABCs

- Laplace eqtn in $R^2$

  $\Delta u = f$ in $\Omega_1 = \{y>0\}$

  $\Delta u = 0$ in $\Omega_2 = \{y<0\}$

- Solution: k-th mode $u_k$,
  - BC $u_k \to 0$ as $y \to \infty$

$$u_k(x, y) = e^{ikx} e^{|k| y}$$

- ABC on $\Gamma=\{y=0\}$
  - Eqtn satisfied by $u_k$

$$\partial u / \partial y = \partial H u / \partial x$$

$$\hat{H u}(k) = \operatorname{sgn}(k)\, \hat{u}(k)$$

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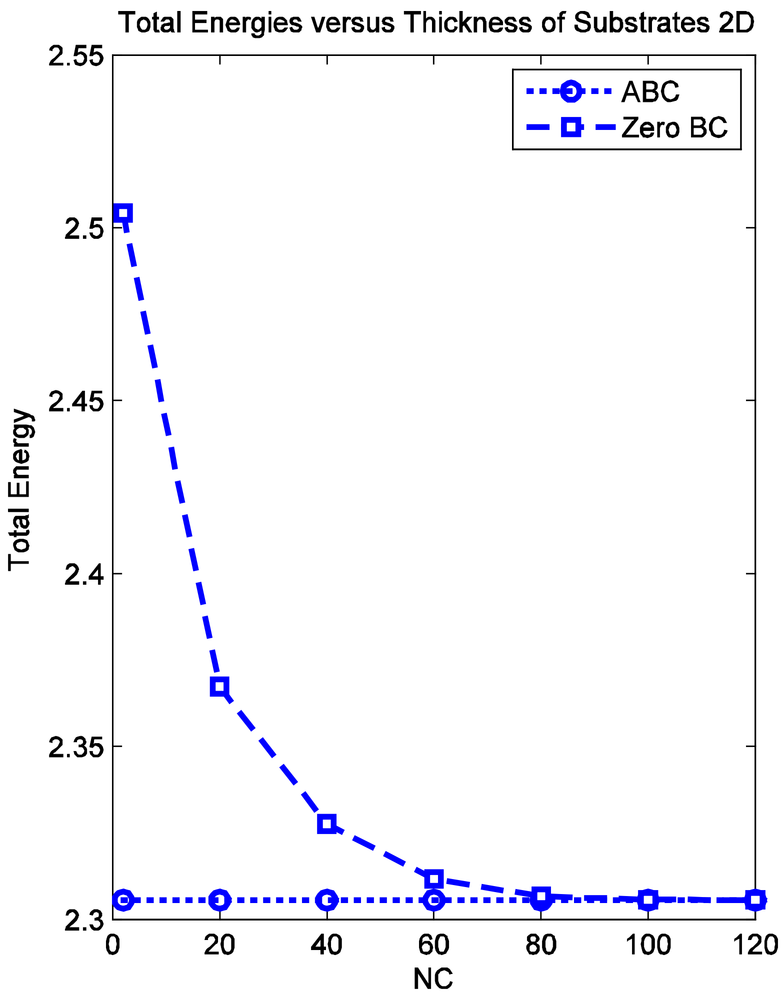
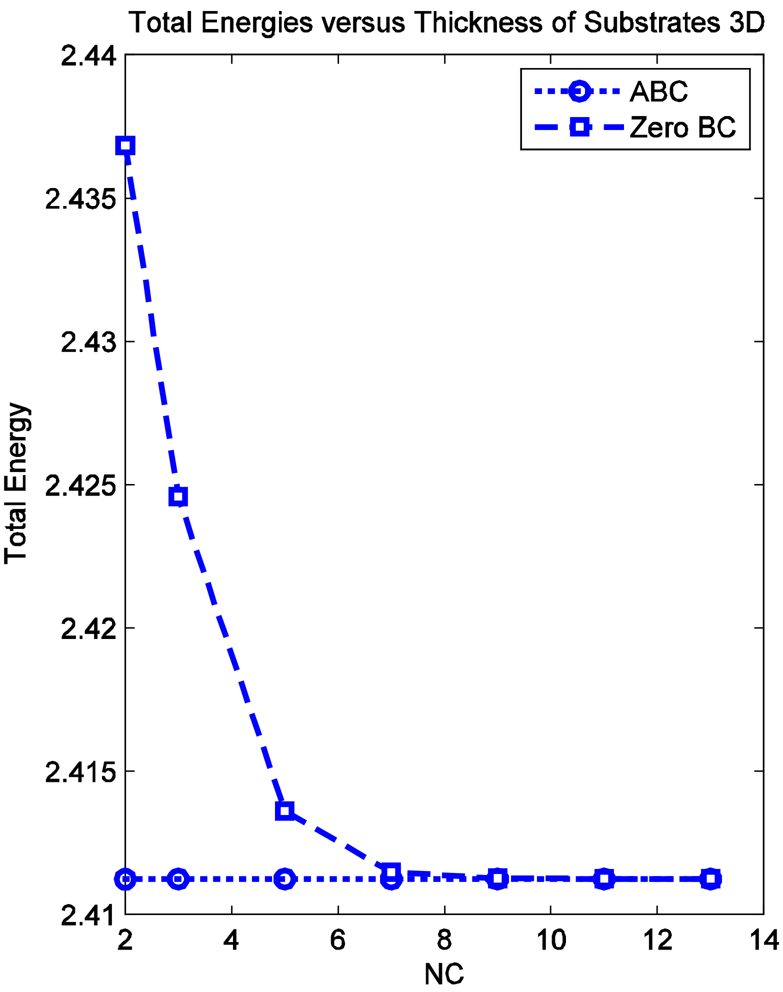
# Artificial Boundary Conditions



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# Nanowires

- Growth catalyzed by metal cluster (Au, Ti, …)
- Epitaxial
- Application to nano-electronics
- Stability difficulties

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# Ti-Nucleated Si Nanowires

Kamins, Li & Williams, APL 2003

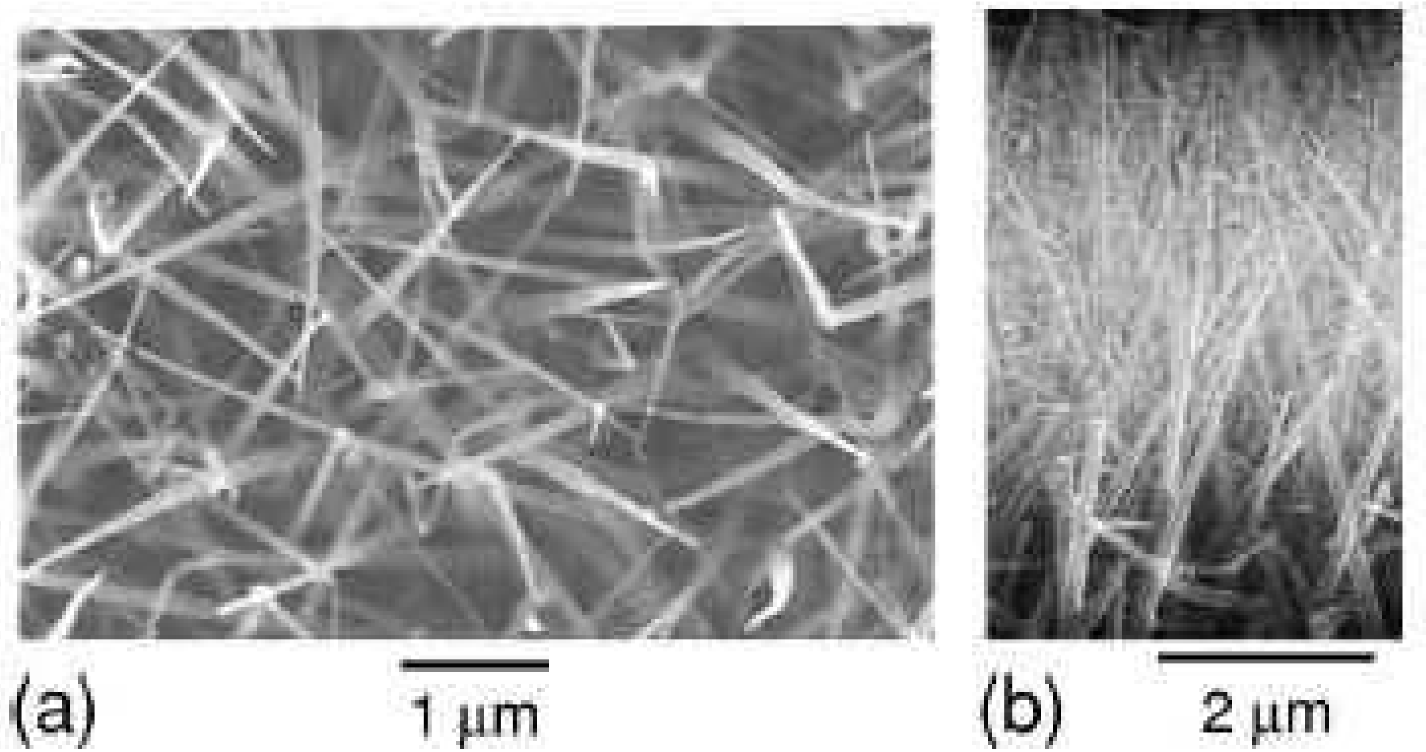


FIG. 1. (a) Plan-view and (b) cross-sectional scanning-electron micrographs of Ti-nucleated Si nanowires (60 min growth) after annealing in $H_2$ at 850 °C for 1 h.

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# Nanowire Geometry Changes at Higher Temperatures

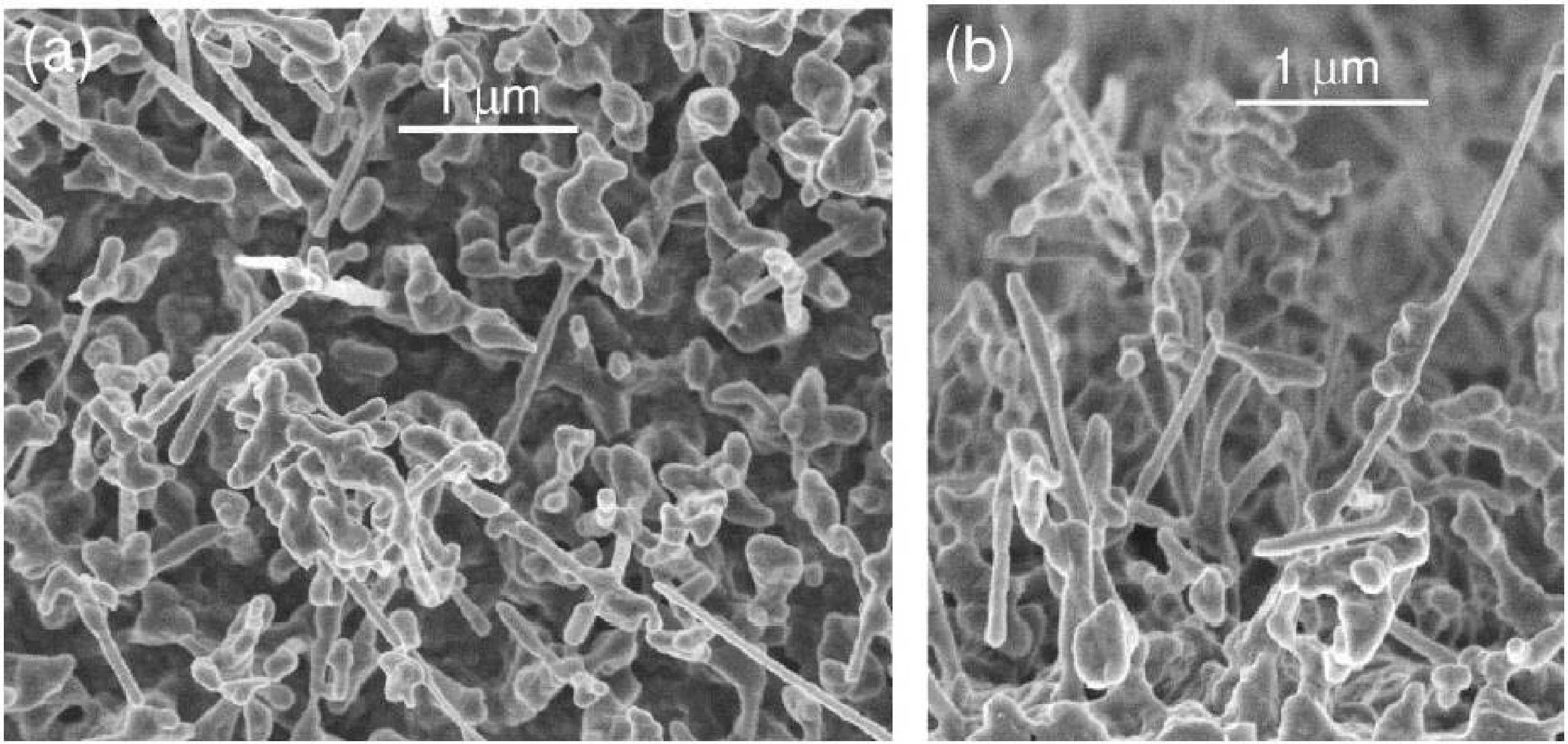


FIG. 2. (a) Plan-view and (b) cross-sectional scanning-electron micrographs of Ti-nucleated Si nanowires (60 min growth) after annealing in $H_2$ at 900 °C for 1 h.

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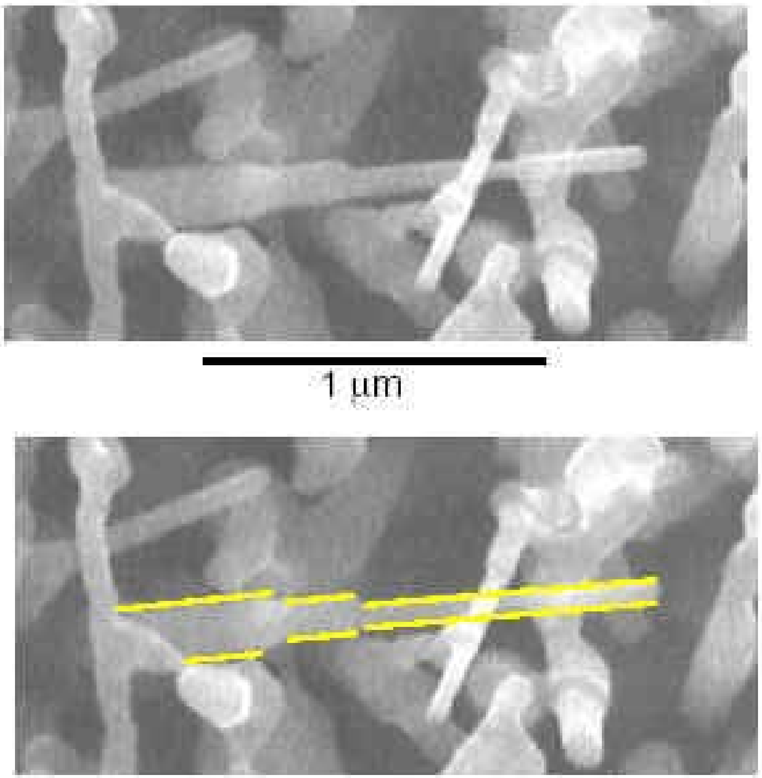
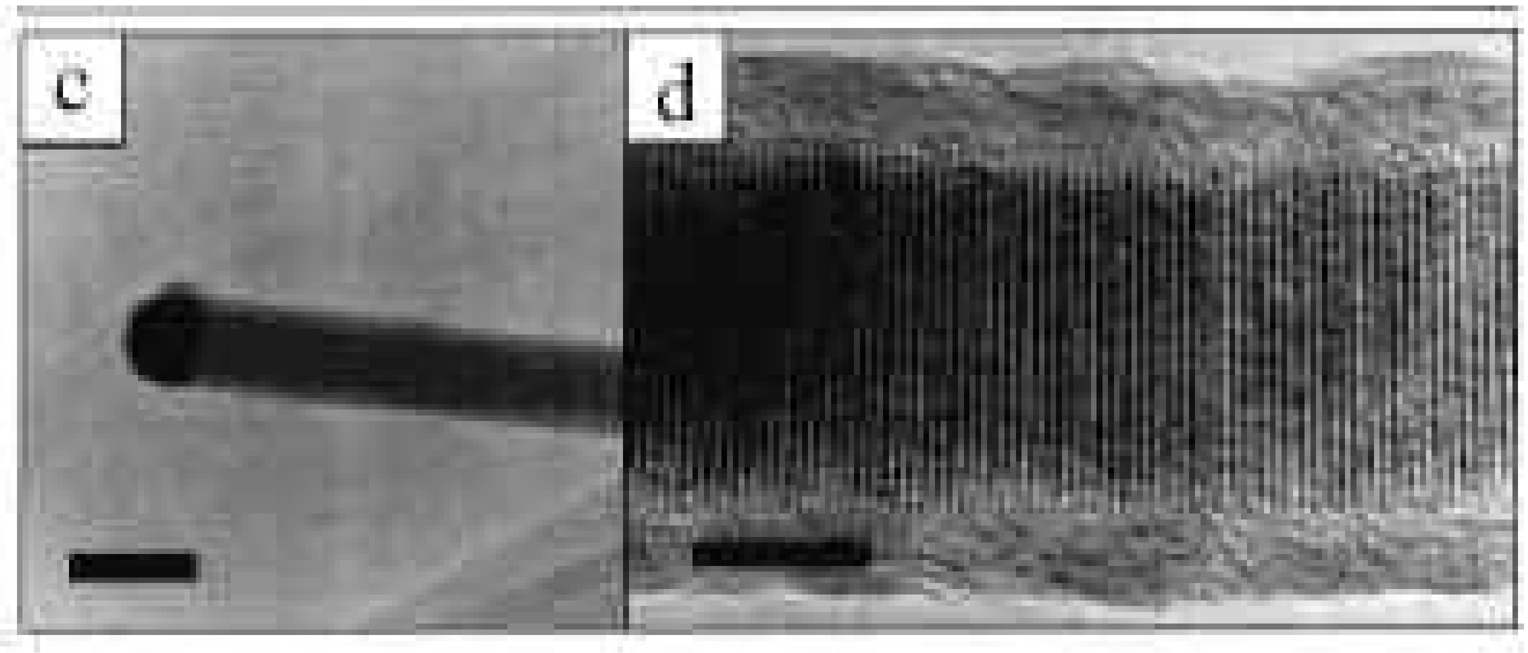
# Instability in Metal Catalyzed Growth of Nanowires

- Epitaxial structure
  - Tapered shape due to side attachment
- Instability at high temperature
  - Tapered shape → terraced shape
  - Step bunching



# Nanowire is Epitaxial



# Simulation of Nanowires

2D

3D

- Simulate system with two steps
  - Find step separation L that minimizes energy minimizer
  - Fixed mass
  - Harmonic potential, intrinsic surface stress, no lattice mismatch
- Extend to be antisymmetric and periodic
  - $L \ll \mathbf{L_1}$ & $L \ll \mathbf{L_2}$
  - Remove translation and rotation degeneracies

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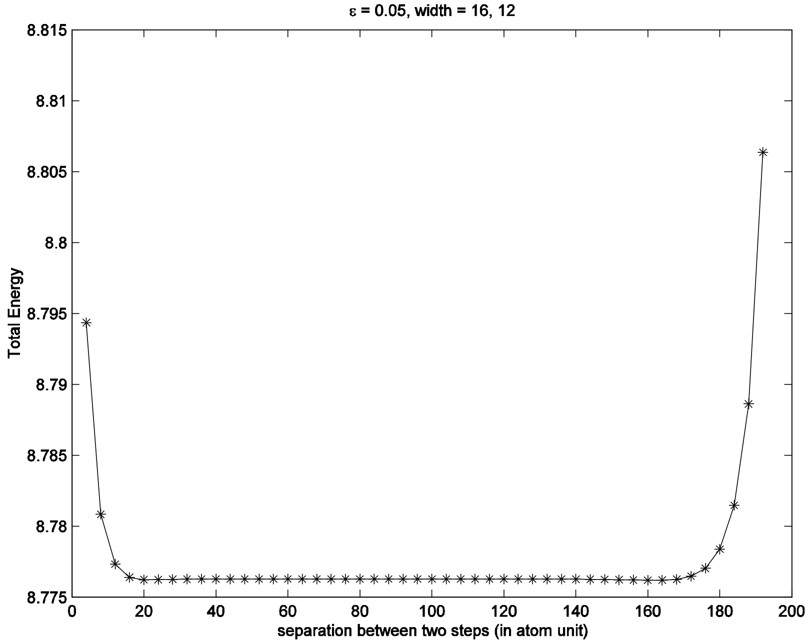
# 2D Simulation of Nanowires

- Step repulsion in 2D
  - As in planar steps
- No step bunching in 2D



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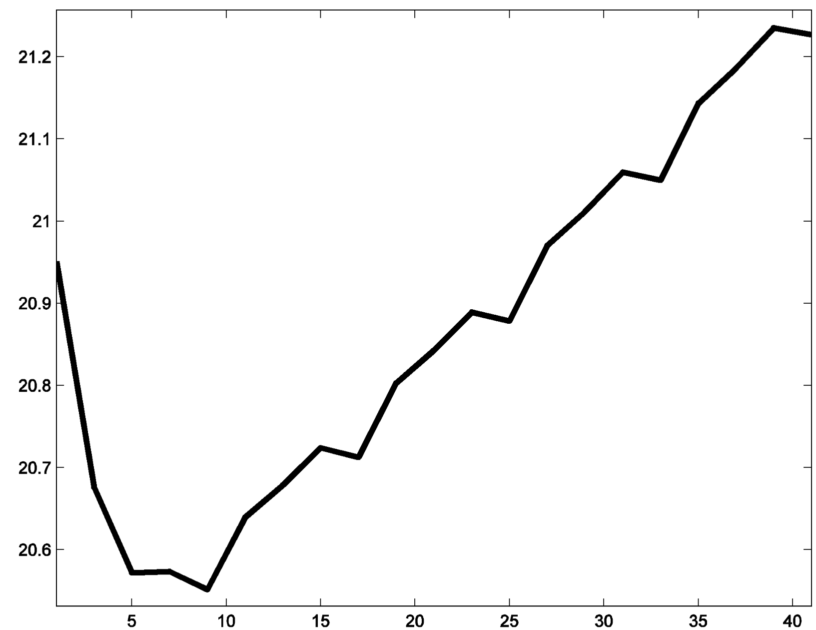
# 3D Simulation of Interaction between Steps on Nanowires

- Interactions of two steps
  - $r = R_1$ for $z<z_1$
  - $r = R_2$ for $z_1 < z < z_2$
  - $r = R_3$ for $z_2 < z$
  - $L= z_2-z_1$ = inter-step distance
  - z = axial distance, r = wire radius
- Energy minimum occurs for small L
  - Step bunching
- Results are insensitive to parameters
  - Step size ($R_1 – R_2$ or $R_2 – R_3$)
  - Surface stress
  - Wire radius, shape
- Lowest value of energy E occurs for small value of separation L
  - System prefers bunched steps
- System size, up to 100 x 15 x 15

$(R_1 , R_2 , R_3) = (3,4,5)$



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- Strain model
  - Harmonic potential
  - Minimal stencil
  - Surface stress represented by variation in lattice constant
- Numerical methods
  - AMG
  - ABC
- Nanowires
  - Surface stress
  - No step bunching in 2D
  - Step bunching in 3D