UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

SMR.998d - 17

Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM WELLS, DOTS, WIRES
AND SELF-ORGANIZING NANOSTRUCTURES
11 - 22 AUGUST 1997

"Self-organized Nanostructures in Strained Multilayer Films"

FENG LIU
Materials Science Center
University of Wisconsin
Madison, WI 53706
U.S.A.

These are preliminary lecture notes, intended only for distribution to participants.

Self-organized Nanostructures in Strained Multilayer Films

I. Background

II. Recent development and understanding

Feng Liu

University of Wisconsin-Madison

Introduction:

strained films $\longrightarrow$ devices

---- using strain as a key ingredient to engineer the electronic band structure

---- strain-induced self-assembly and self-organization of nanostructures

Nanofabrication

"man-made" vs. "nature-made"

Self-organization

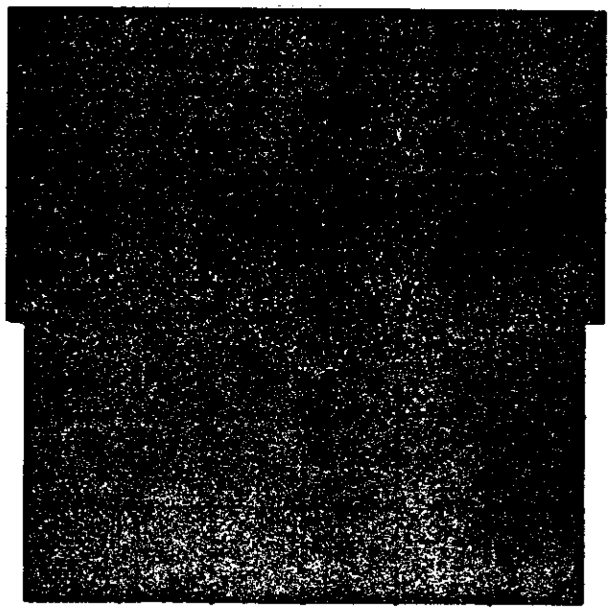
Atomic scale → minimizing chemical free energy

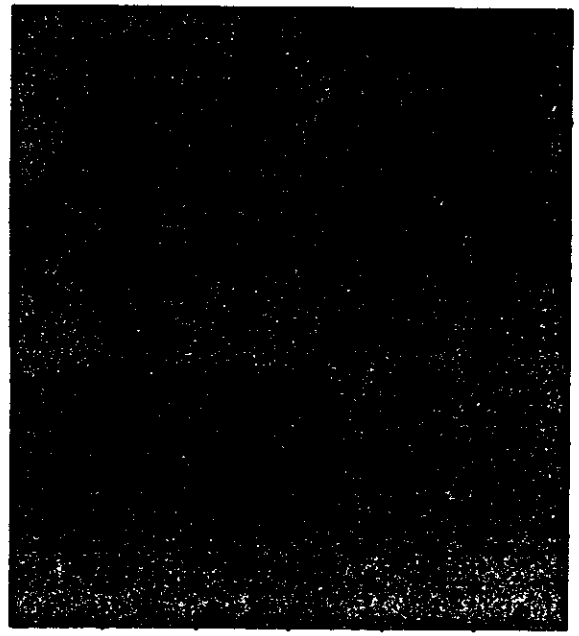
crystal growth: selforganization of atoms

Nano scale → minimizing strain free energy

Self-organization of quantum dots (islands) and quantum wires (step bunches)

Modes of strain relaxation:





--- dislocation formation
--- surface roughening

Modes of strain relaxation:

--- formation of dislocation

--- surface roughening

University of Wisconsin - Madison

Dislocation formation:

$$\Delta E = E_{creation} - E_{relaxation}$$

$$\mathbf{R} = Ae^{-\Delta Ec/kt}, \ \Delta E_c \sim \varepsilon^{-1}$$

S.V. Kamat and J.P. Hirth, JAP **67**, 6844 (1990).
F.K. LeGoues, P.M. Mooney, and J. Tersoff, PRL **71**, 396 (1993)

Surface roughening:

---- surface reconstruction
(steps and vacancies)
---- formation of 3D islands
(faceting)
---- step bunching
---- formation of undulations

Surface stress $\longrightarrow$ Surface roughening

$$E_{surf} = E_{formation} + E_{deformation}$$

$$\sigma_{ij} = \frac{1}{A}\frac{dE_{surf}}{d\varepsilon_{ij}} = \gamma\delta_{ij} + \frac{d\gamma}{d\varepsilon_{ij}}$$

strained films: misfit $\longrightarrow \sigma_{ij}$

Surface elastic relaxation energy:

$$f_i(\mathbf{r}) = \partial_j \sigma_{ij}(\mathbf{r}), \quad \mathbf{r} = (x,y)$$

$$u_i(\mathbf{r}) = \int d^2r' \, \chi_{ij}(\mathbf{r}-\mathbf{r}') \, f_j(\mathbf{r}')$$

$$E_r = -\frac{1}{2} \int d^2r \, f_i(\mathbf{r}) \, u_i(\mathbf{r})$$

$$= -\frac{1}{2} \iint d^2r \, d^2r' \, \chi_{ij}(\mathbf{r}-\mathbf{r}') f_i(\mathbf{r}) f_j(\mathbf{r}')$$

Surface reconstruction:

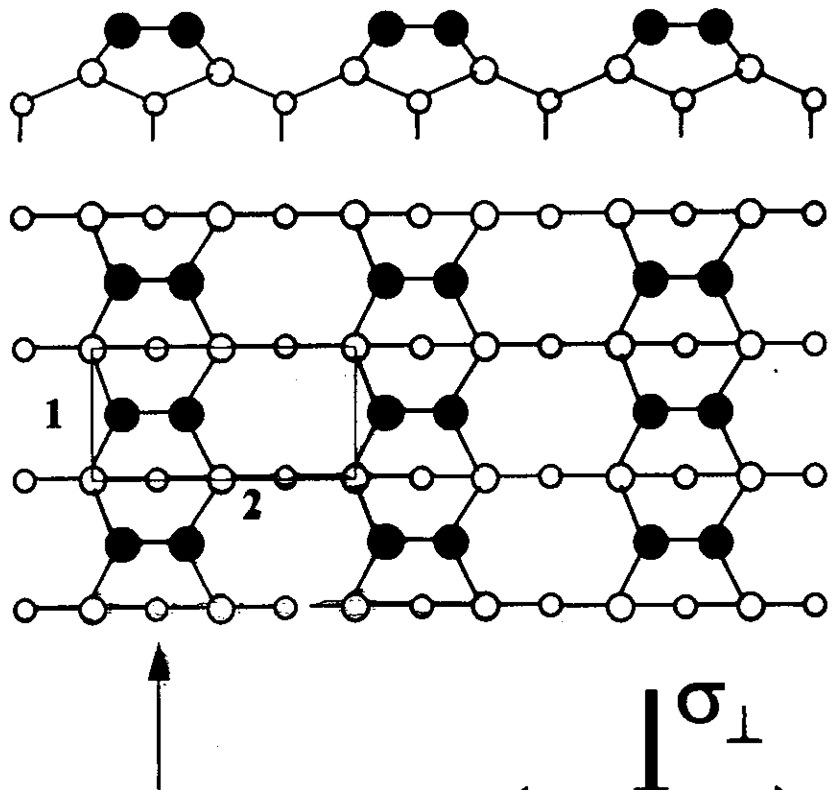
---- Si(001): stress-domain structure

---- Ge-covered Si(001):

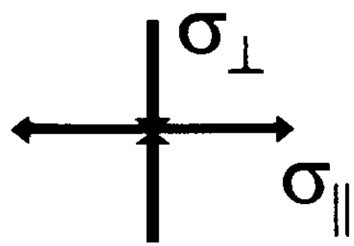
1.) reversal of surface stress anisotropy

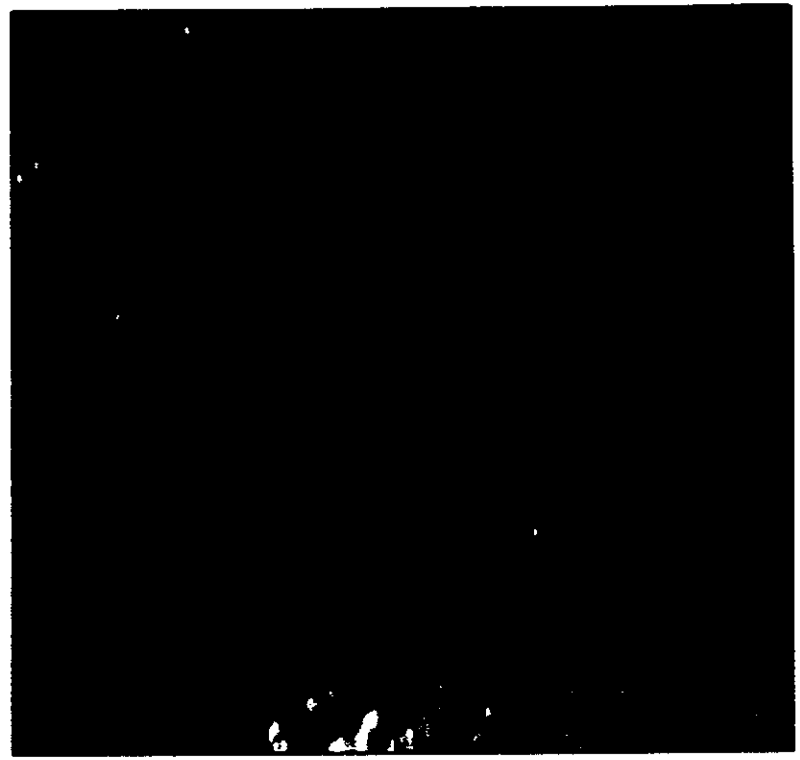
2.) $2 \times n$ reconstruction

Si(001) - 2x1



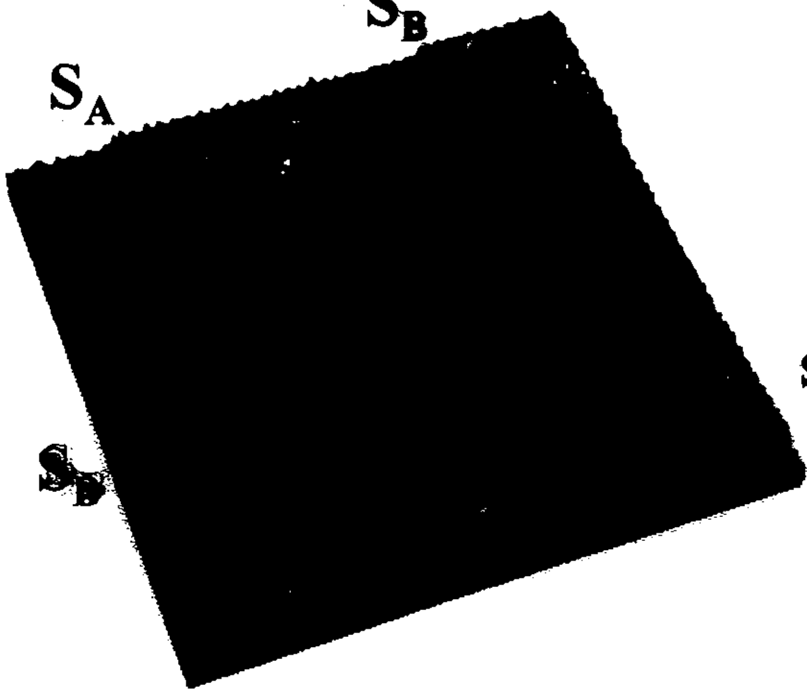
dimer row

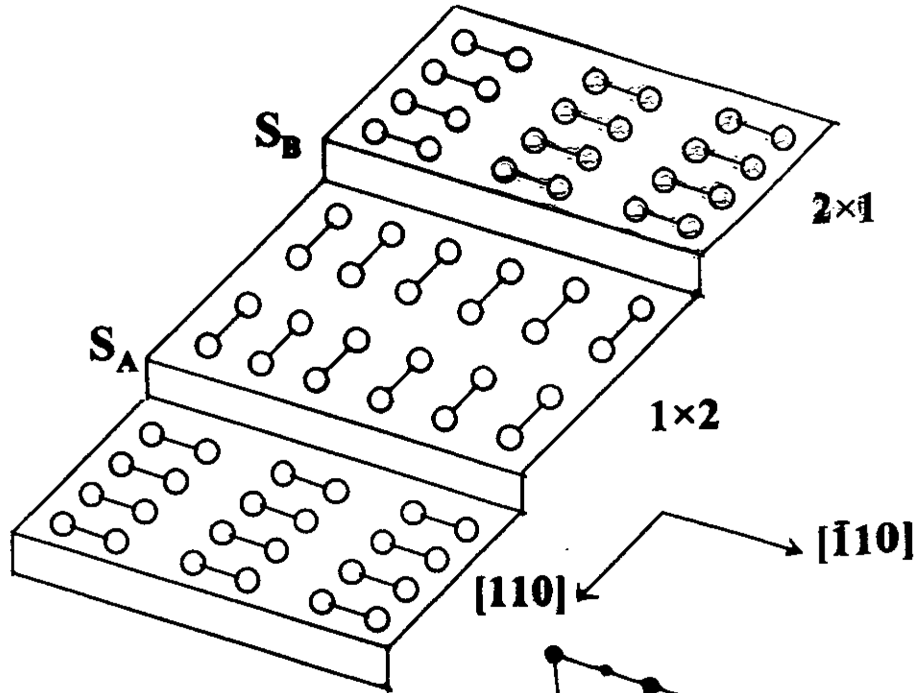


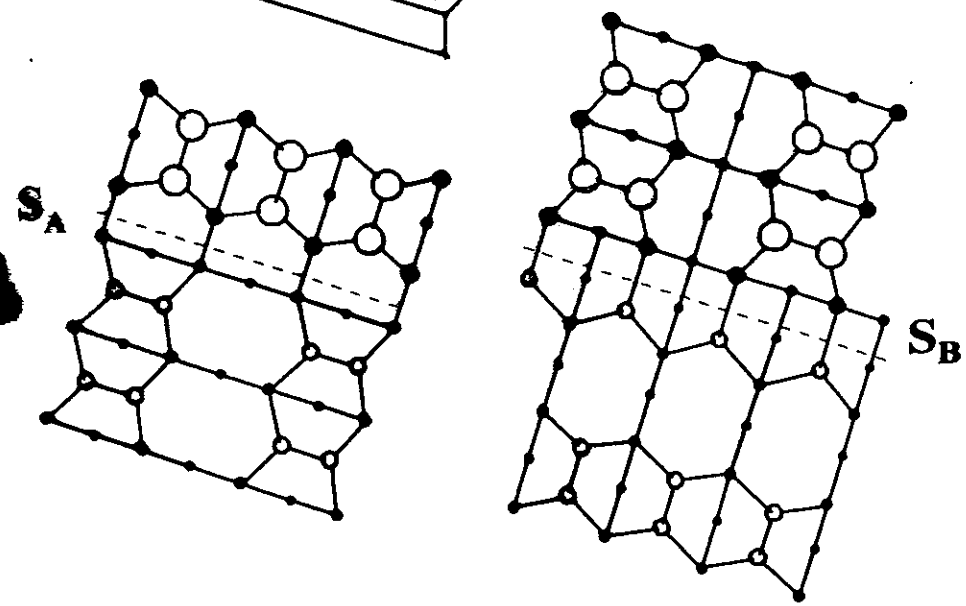


dimer row

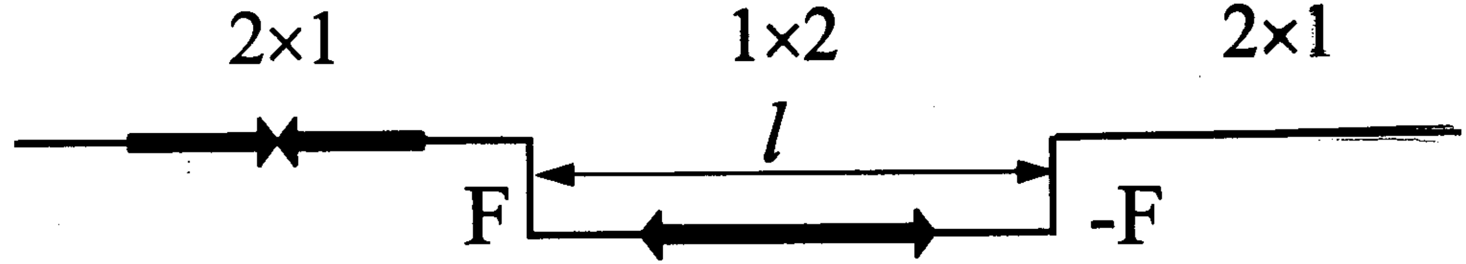
Vicinal Si(001)







University of Wisconsin - Madison



$$\sigma^{2x1} = \begin{pmatrix} \sigma_\perp & 0 \\ 0 & \sigma_\parallel \end{pmatrix} \quad \sigma^{1x2} = \begin{pmatrix} \sigma_\parallel & 0 \\ 0 & \sigma_\perp \end{pmatrix}$$

Surface stress anisotropy: $F = \sigma_\parallel - \sigma_\perp$

$$f_i(\mathbf{r}) = \pm F\, \delta_{ix}\, \delta(x - x_0)$$

$$E_r = -c \ln(l/a), \quad c = F^2 \frac{1-\nu}{2\pi\mu}$$

V.I. Marchenko, JETP Lett. **33**, 381 (1981).

F ➡ step-step interaction

$$E_r = -c \ln(l/\pi a), \quad l = l_{2\times 1} = l_{1\times 2}$$

ε (external uniaxial strain) ➡

$$E_r = -c \ln[(l/\pi a)\cos(\pi p/2)] + 0.5\varepsilon p F$$

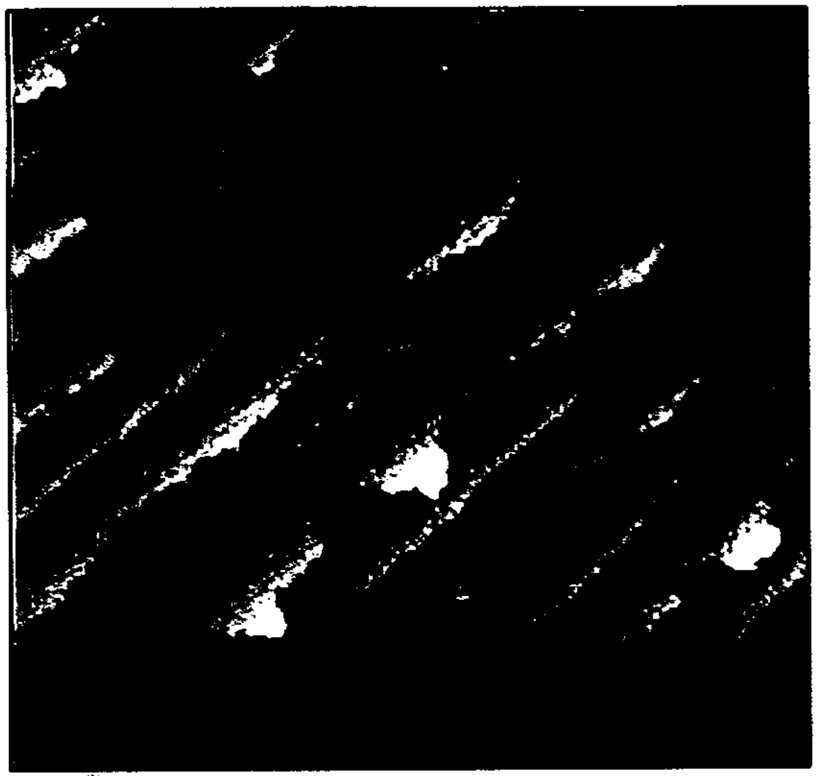
$$l_{2\times 1}/\, l_{1\times 2} = (1+p)/(1-p)$$

O.L. Alerhand *et al.*, PRL **61, 1973 (1988)**

University of Wisconsin - Madison

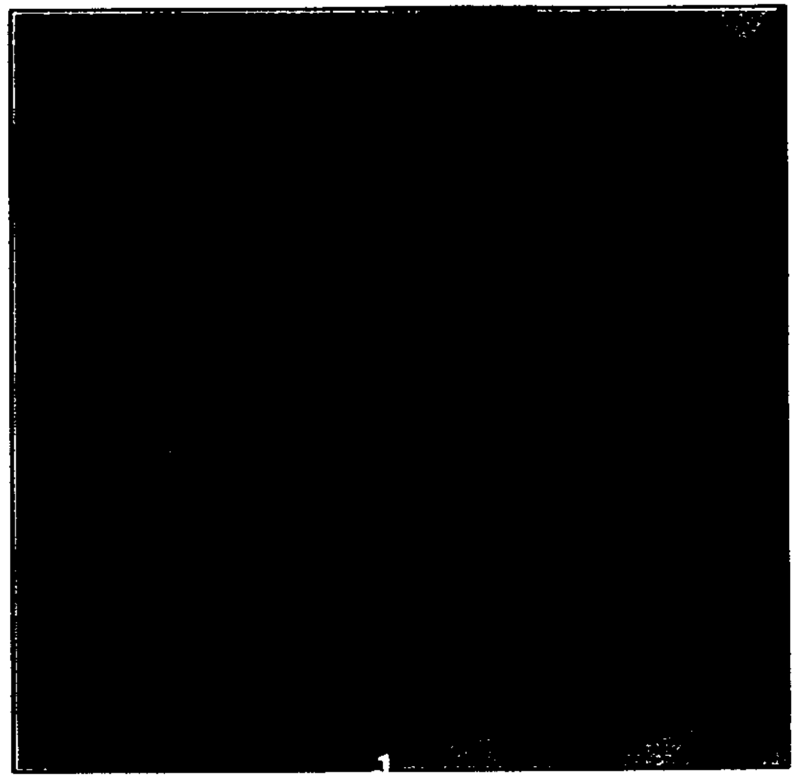
Effect of External Stress on Si(001)

3000 Å



Before

3000 Å



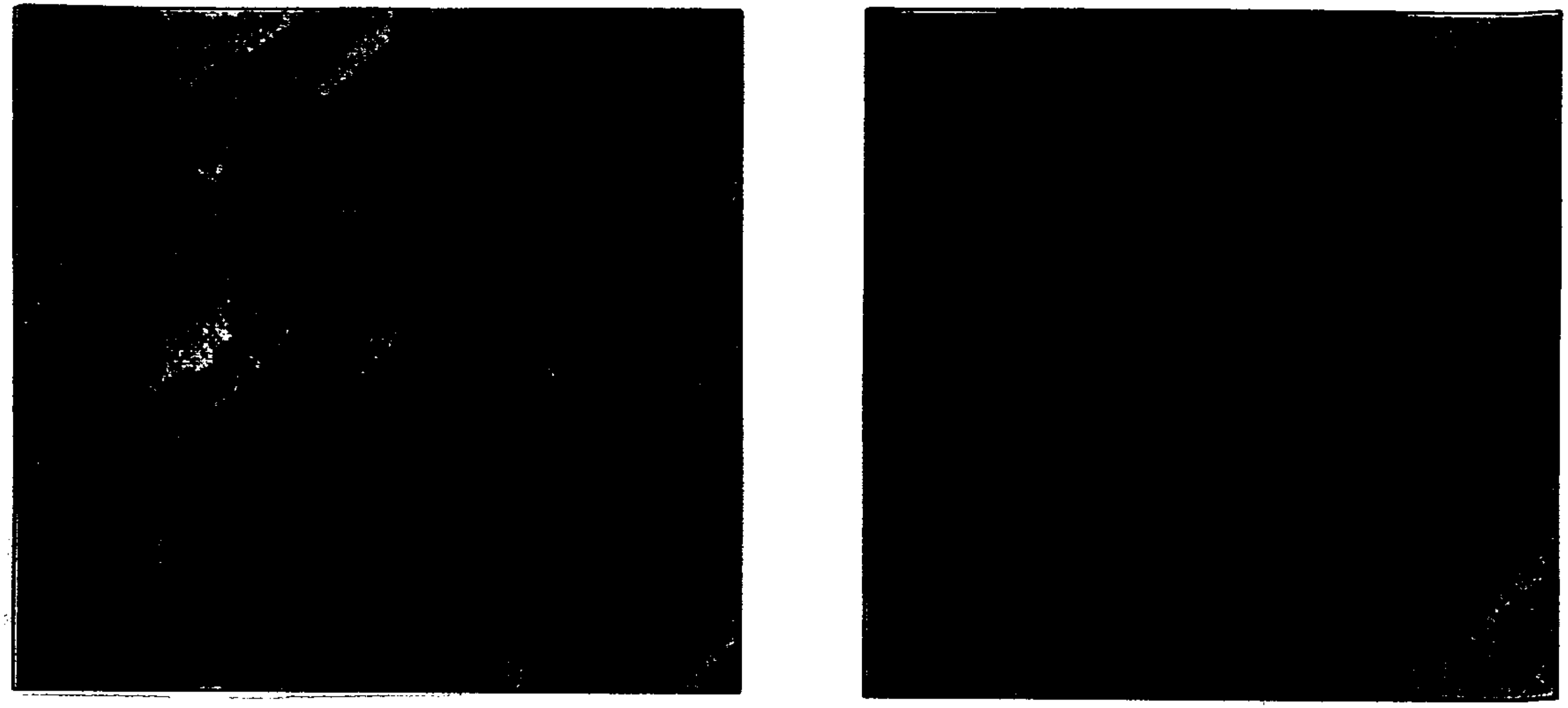
After

ε

University of Wisconsin - Madison

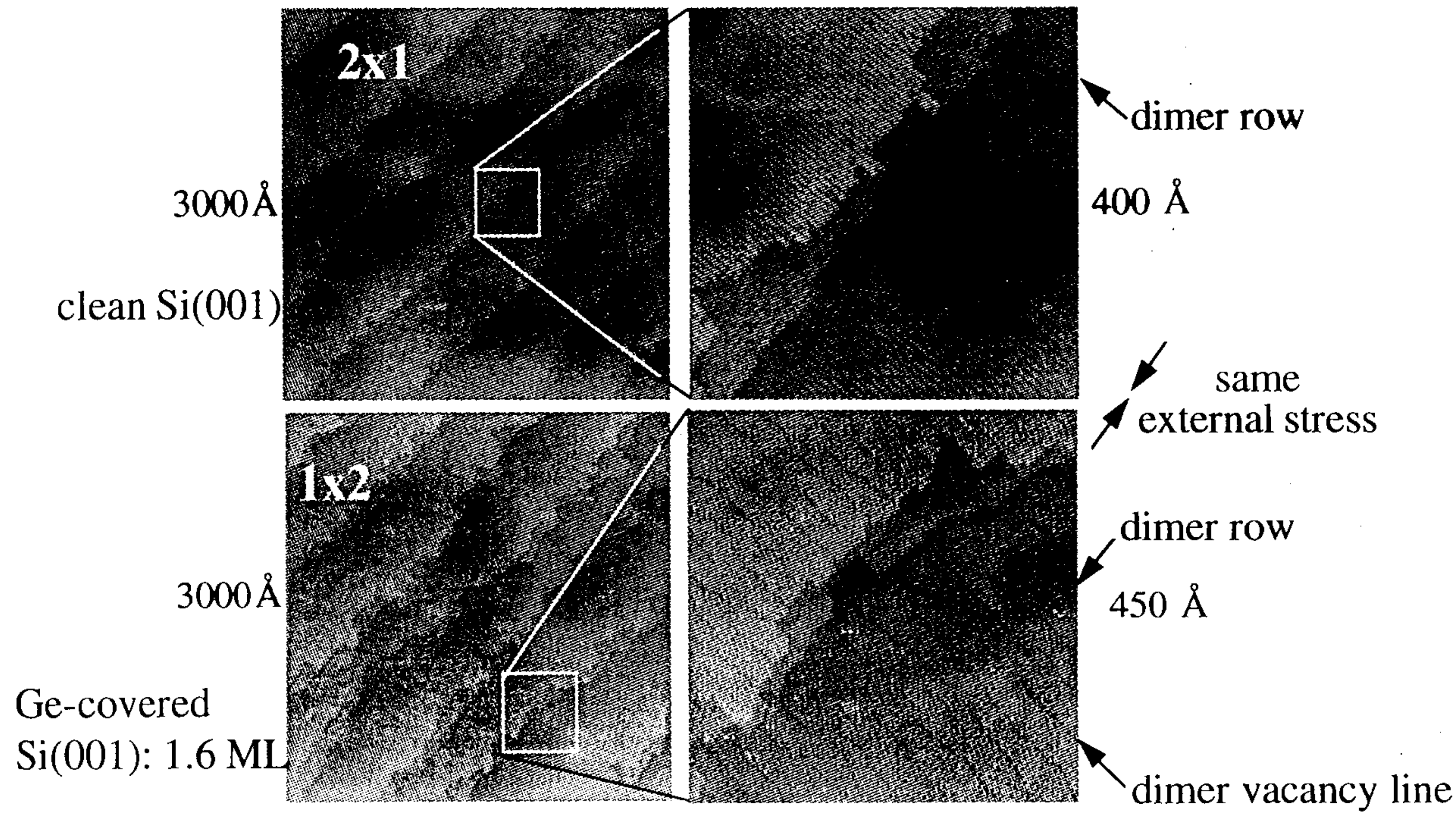
Effect of External Stress on Ge/Si(001)

$\theta_{Ge} \sim 1.6$ ML

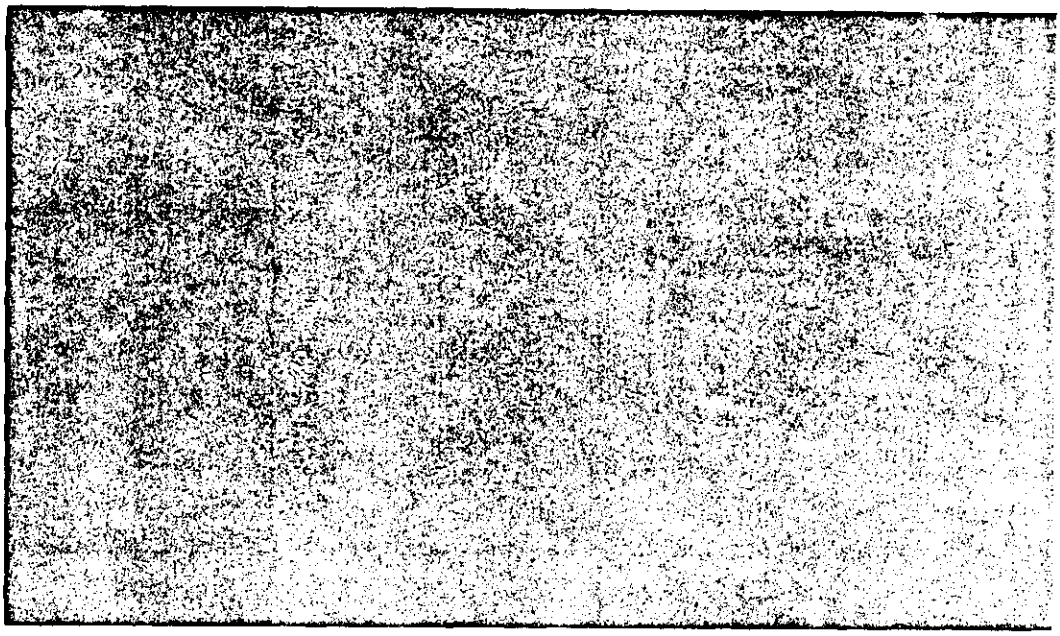


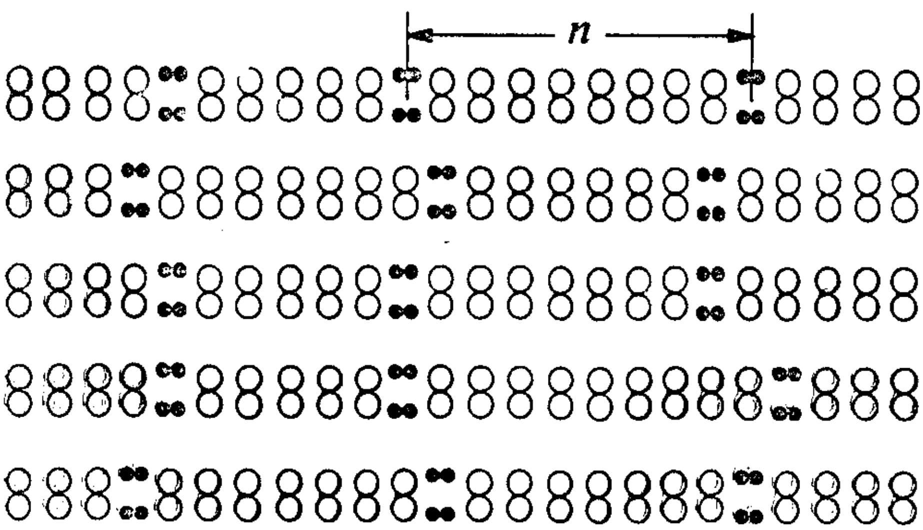
University of Wisconsin - Madison

Opposite Response of Steps to the Same External Stress: Reversal of Surface Stress Anisotropy

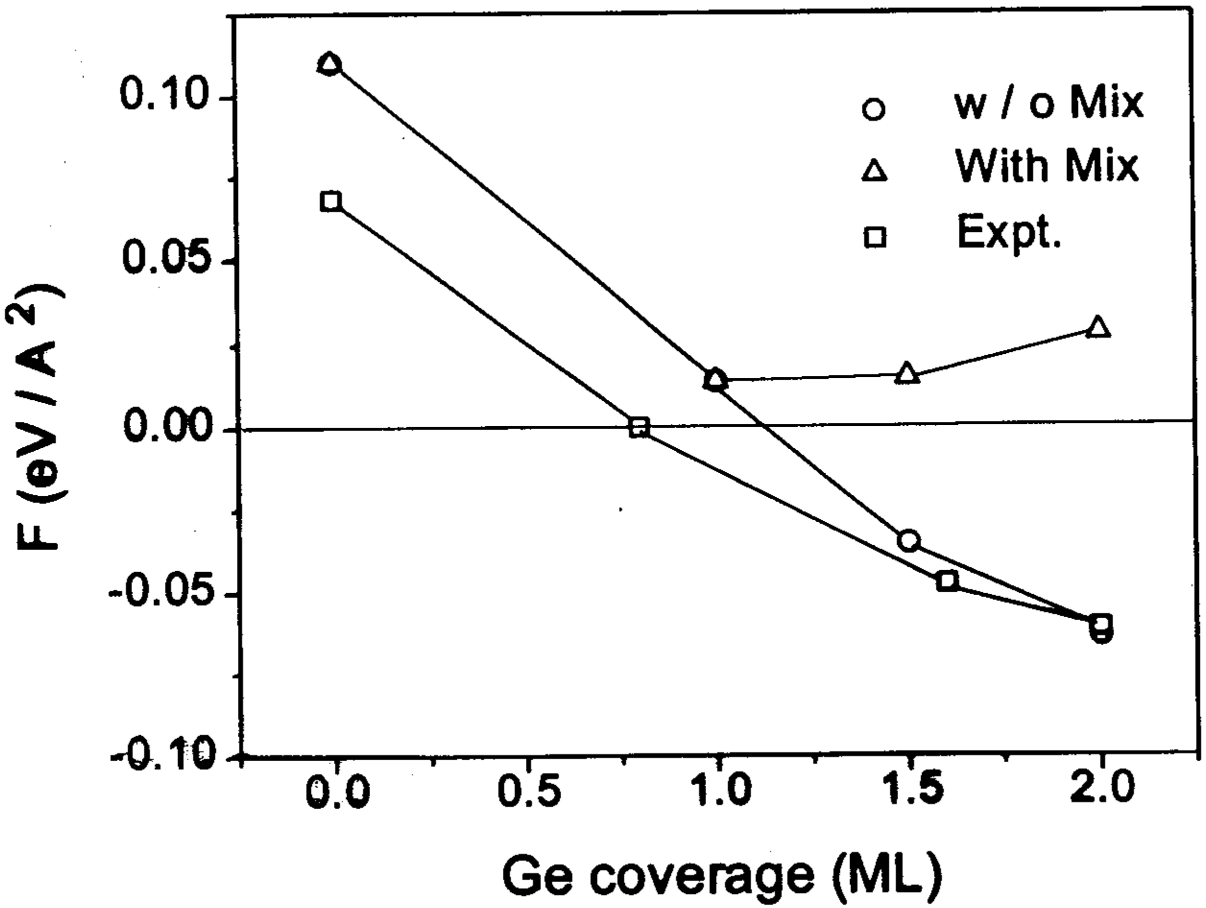


$2 \times n$ reconstruction:



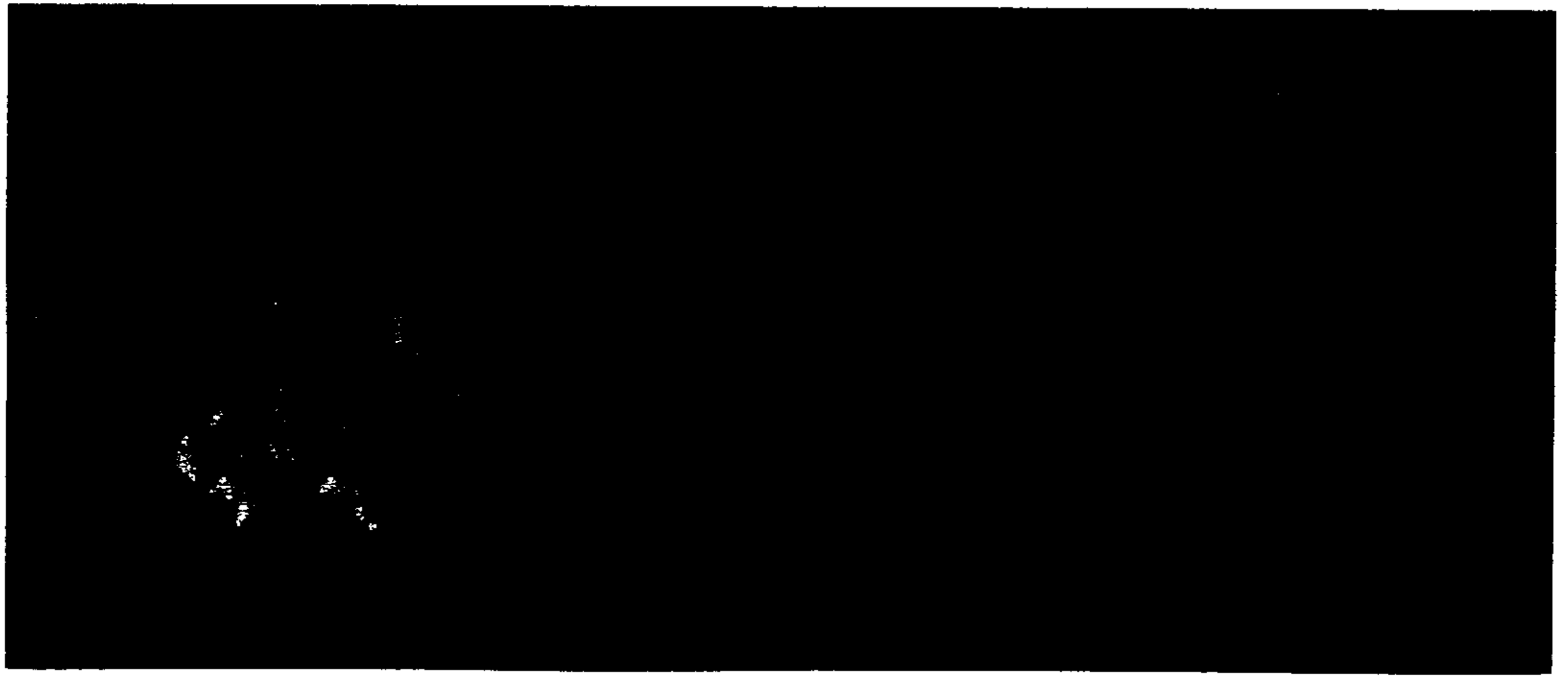


Surface stress anisotropy ~ Ge coverage



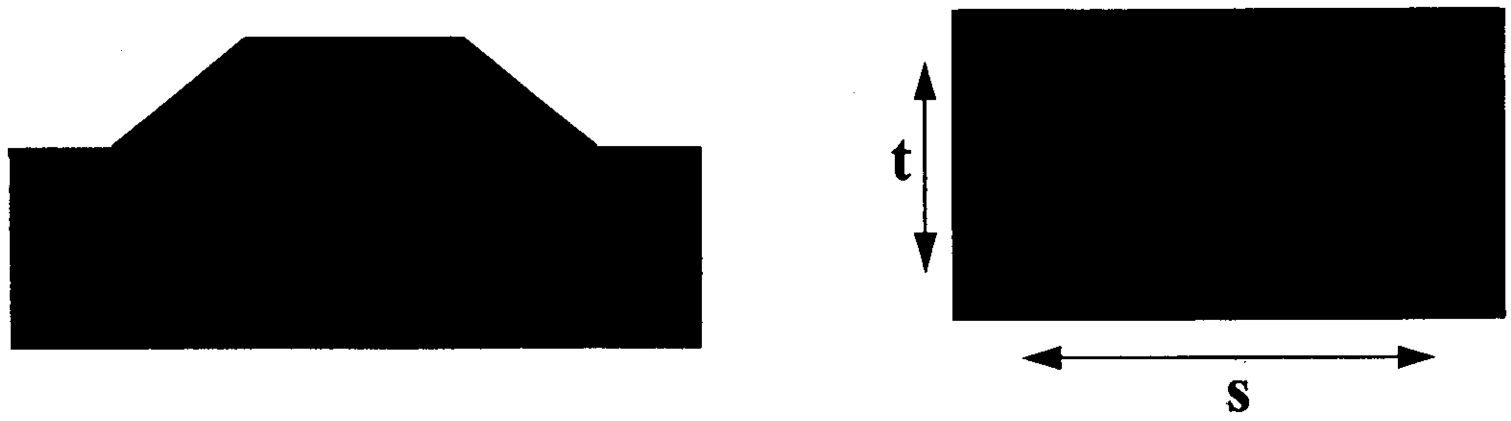
Fang Wu and M.G. Lagally, PRL **75**, 2534 (1995).
Feng Liu and M.G. Lagally, PRL **76**, 3156 (1996).

Formation of 3D islands:



Y.W. Mo, *et al.*, PRL **65**, 1020 (1990).

Elastic relaxation in strained islands:



$E_s = 2(s+t)h\Gamma, \quad \Gamma = \gamma_e \csc\theta - \gamma_s \cot\theta$

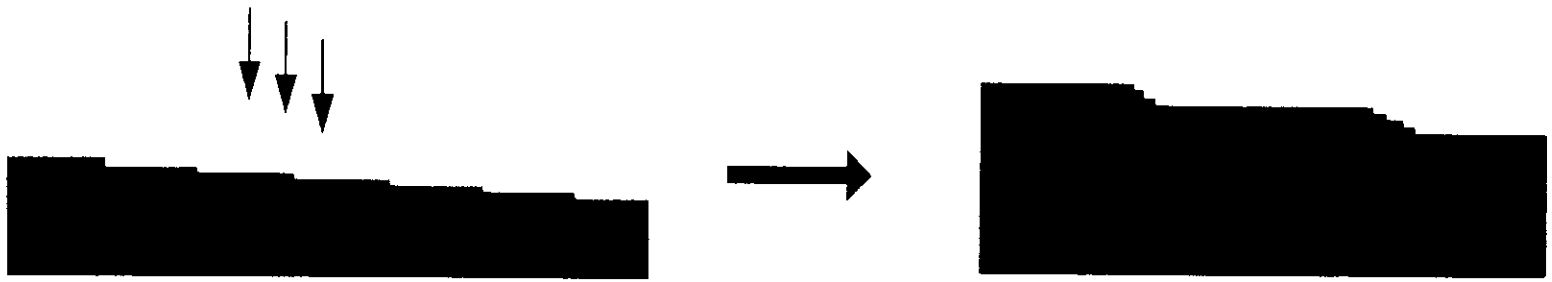
$E_r = -2ch^2[s\ln(te^{3/2}/h\cot\theta) + t\ln(se^{3/2}/h\cot\theta)]$

$\Delta E = E_s + E_r = 4\Gamma V^{2/3} \tan^{1/3}\theta - 6cV\tan\theta$

$\Delta E_0 \sim c^{-2} \sim \varepsilon^{-4}$

J. Tersoff and F.K. LeGoues, PRL **72**, 3570 (1994).

Step Bunching:

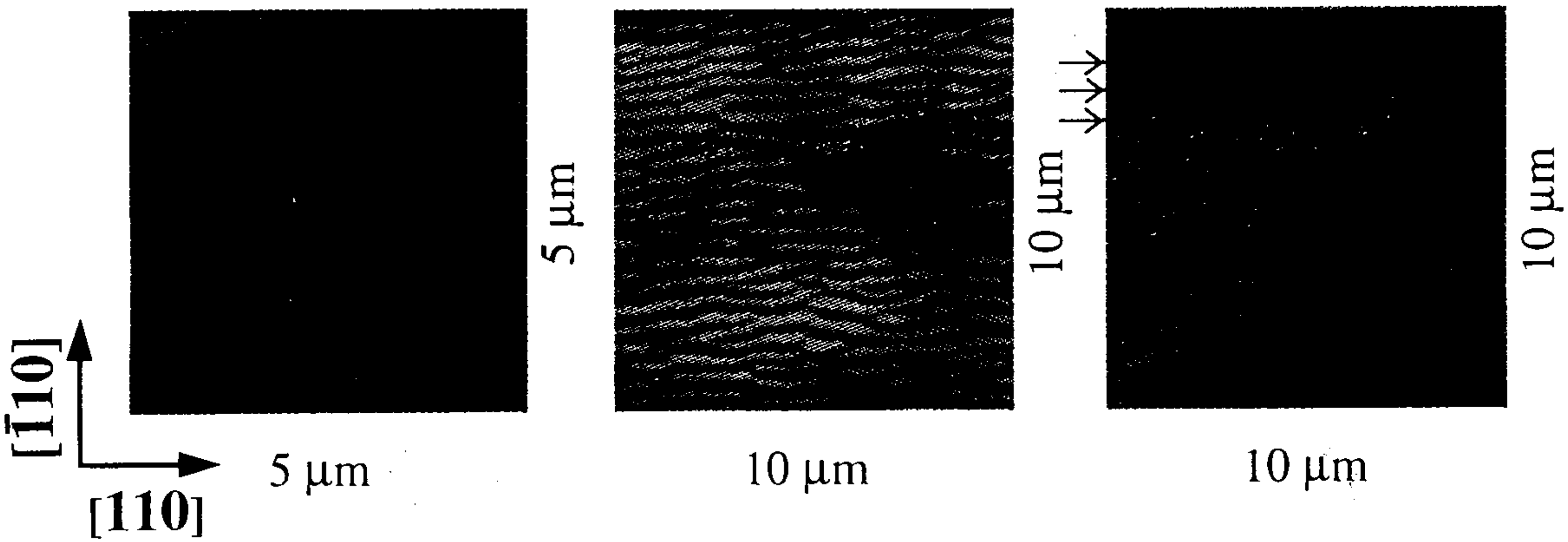


$\Delta E < 0$

bunching rate $\sim B\alpha_1^2$

J. Tersoff *et al.*, PRL **75**, 2730 (1995).

Effect of alloy composition

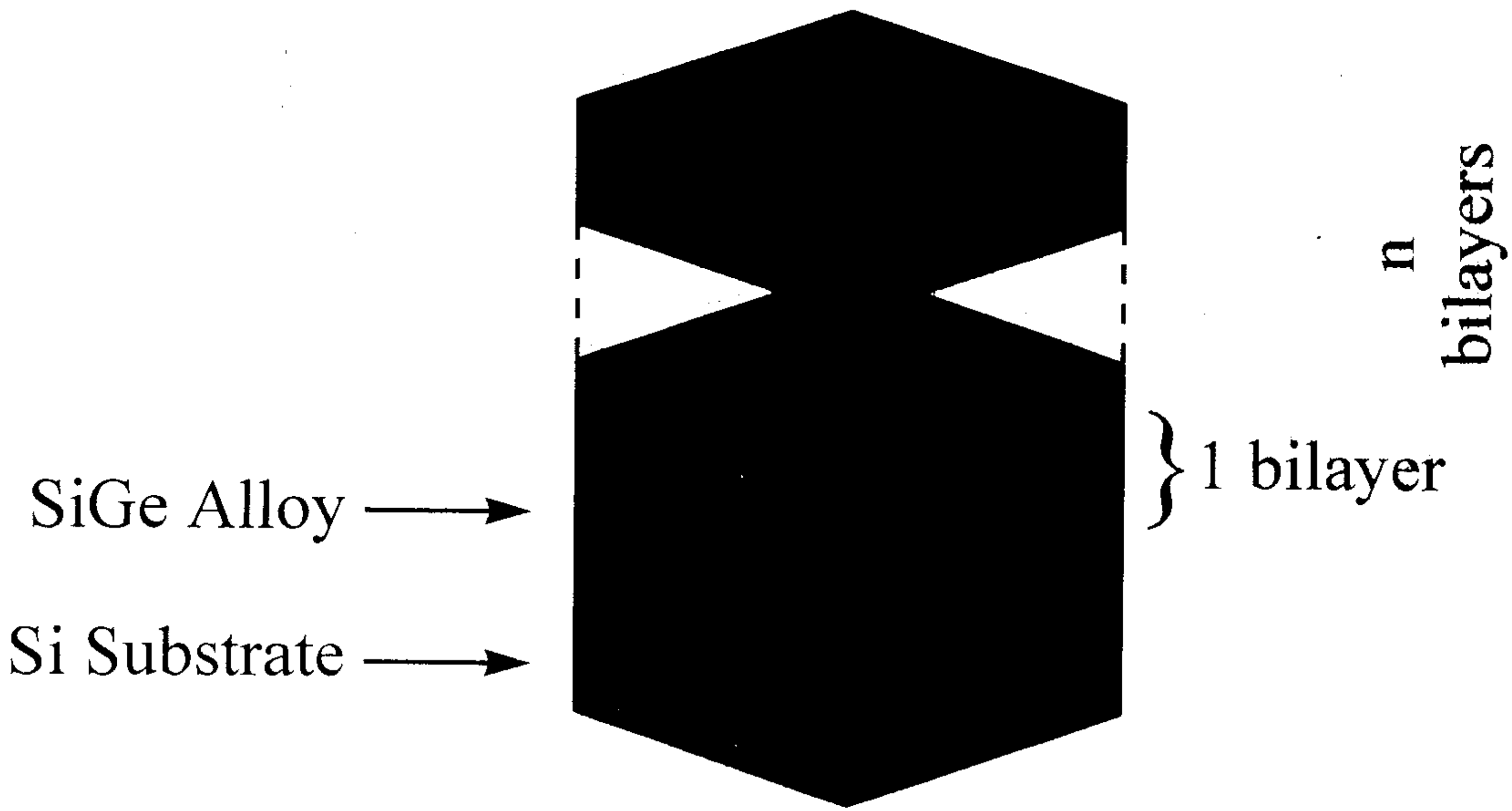


$x_{Ge} = 0.20$ $\sigma = 0.15$ nm

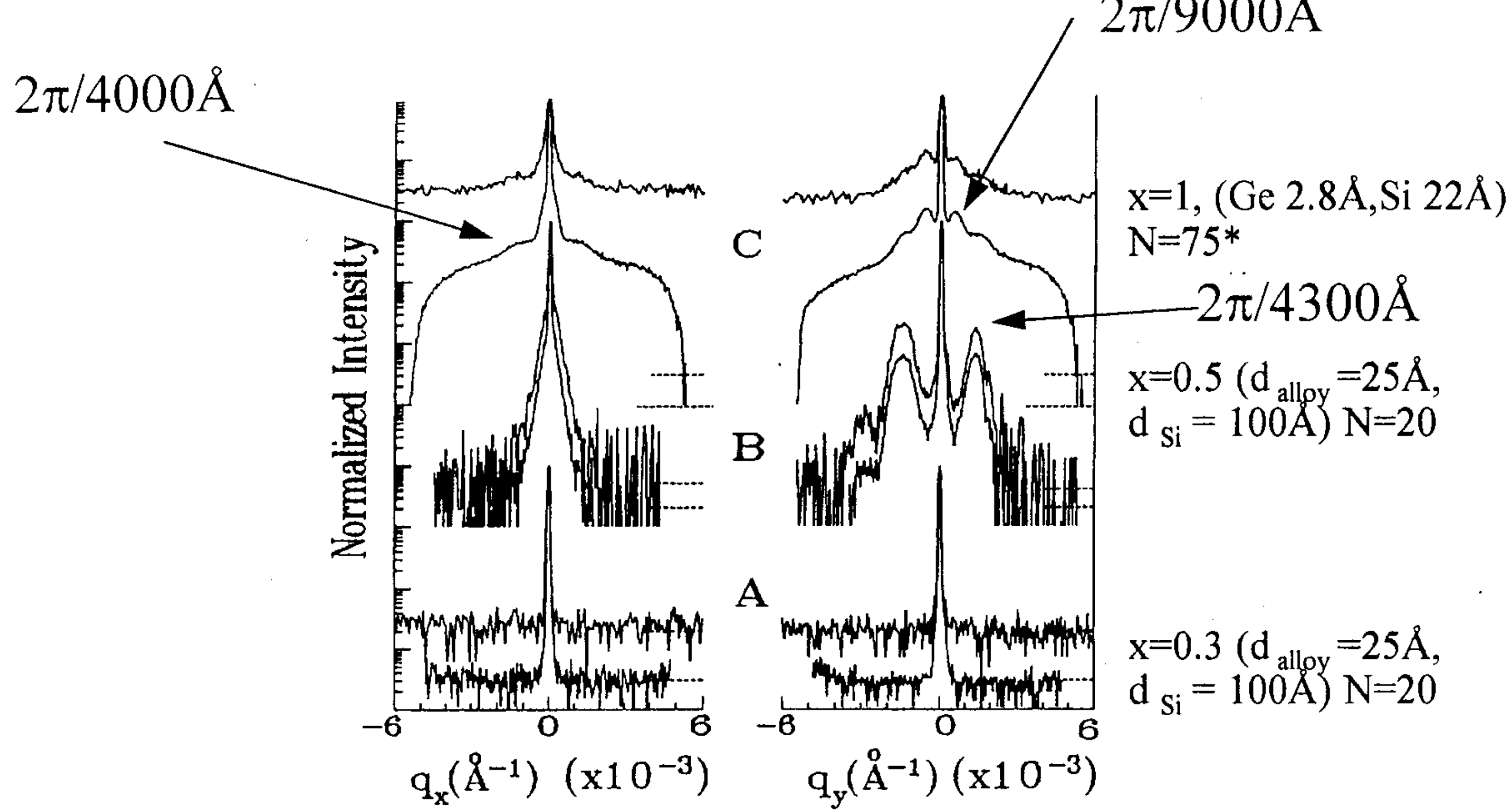
$x_{Ge} = 0.45$ $\sigma = 0.35$ nm

$x_{Ge} = 0.75$ $\sigma = 2.2$ nm

Multilayer Film Growth



Transverse scans for different Ge Concentrations:

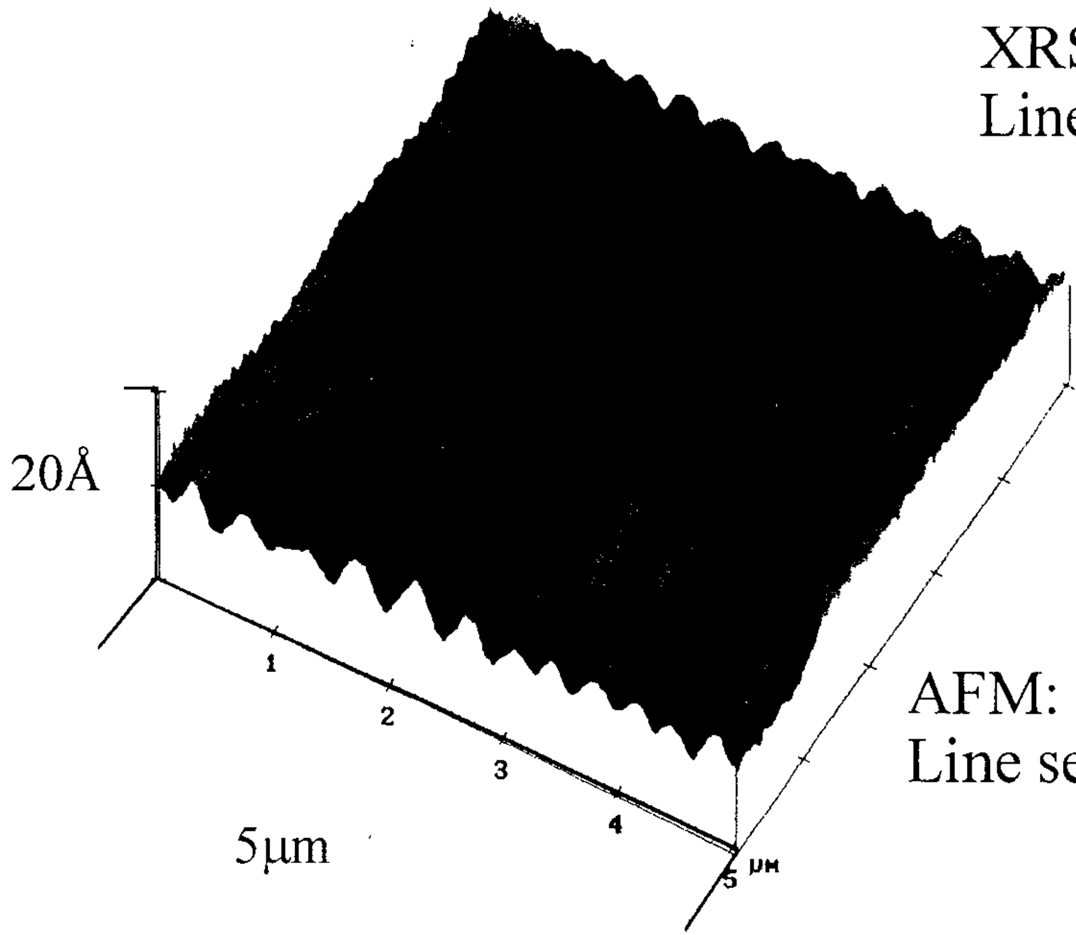


* Supplied by E. Kasper

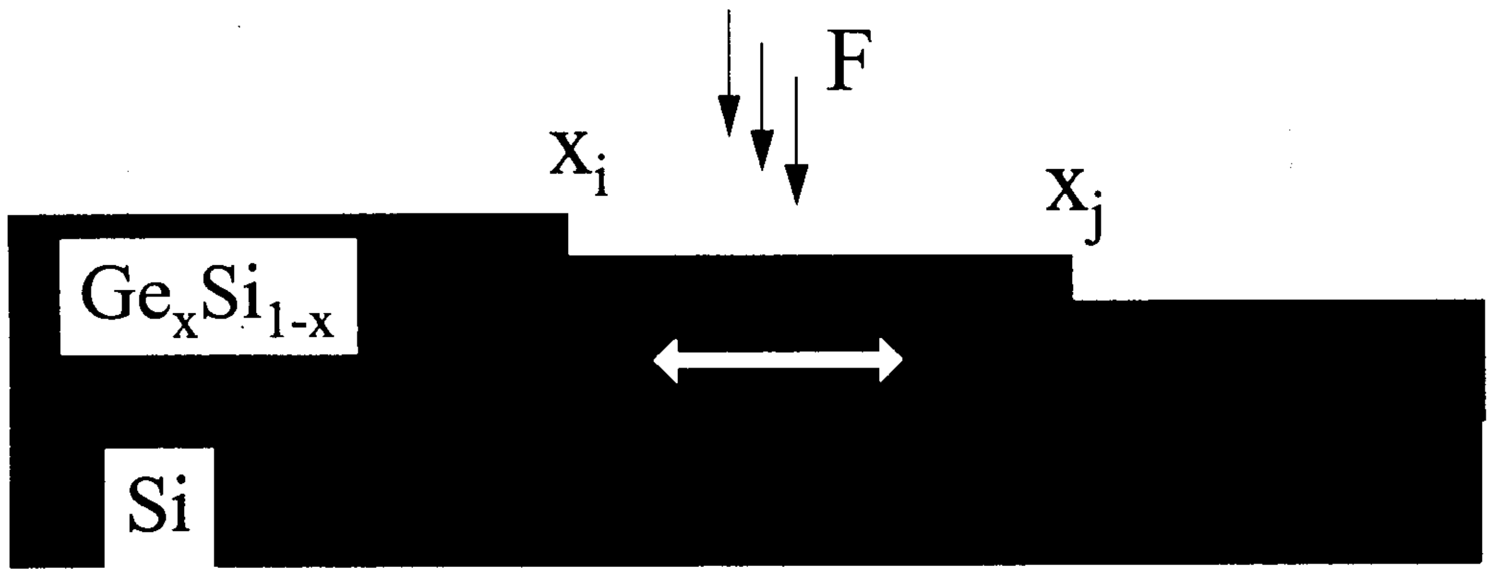
University of Wisconsin-Madison

Comparison of XRS with AFM:
Sample B x=0.5, N=20

XRS: $\sigma = 4.5$Å,
Line separation = 4300Å ±300Å



AFM: $\sigma = 3.5$Å,
Line separation = 4450Å ± 200Å



$$f_i = \sum_{i \neq j} \left(\frac{\alpha_1}{(x_j - x_i)} - \frac{\alpha_2}{(x_j - x_i)^3} \right)$$

$$v_i = F\left(\frac{x_{i+1} - x_{i-1}}{2}\right) - B\left(\frac{f_{i+1} - f_i}{x_{i+1} - x_i} - \frac{f_{i-1} - f_i}{x_{i-1} - x_i}\right)$$

$$B = \frac{DA}{2kT} e^{-Ed/kT}$$

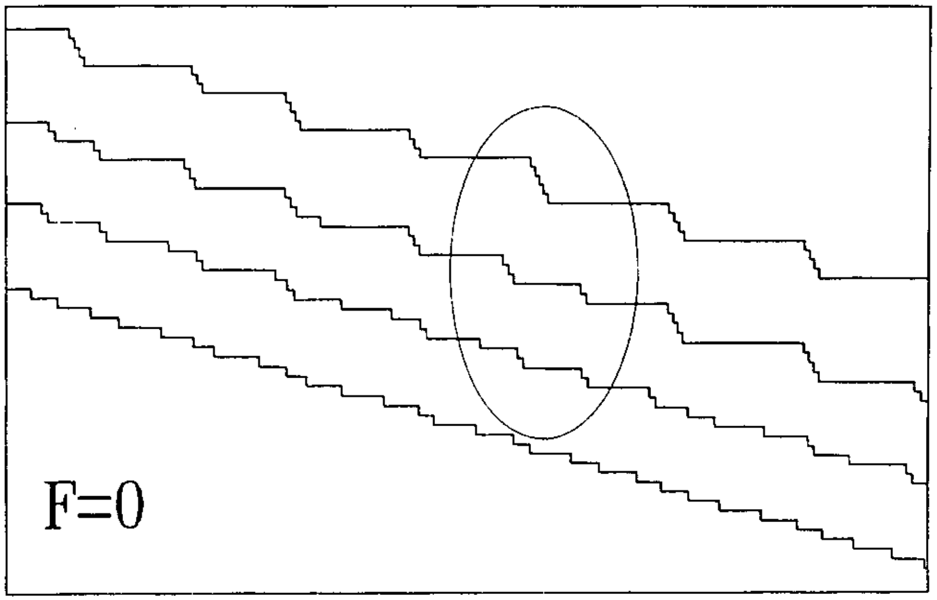
Step-Bunching Instability of Strained Vicinal Surface

attraction due to a net "force monopole" at each step

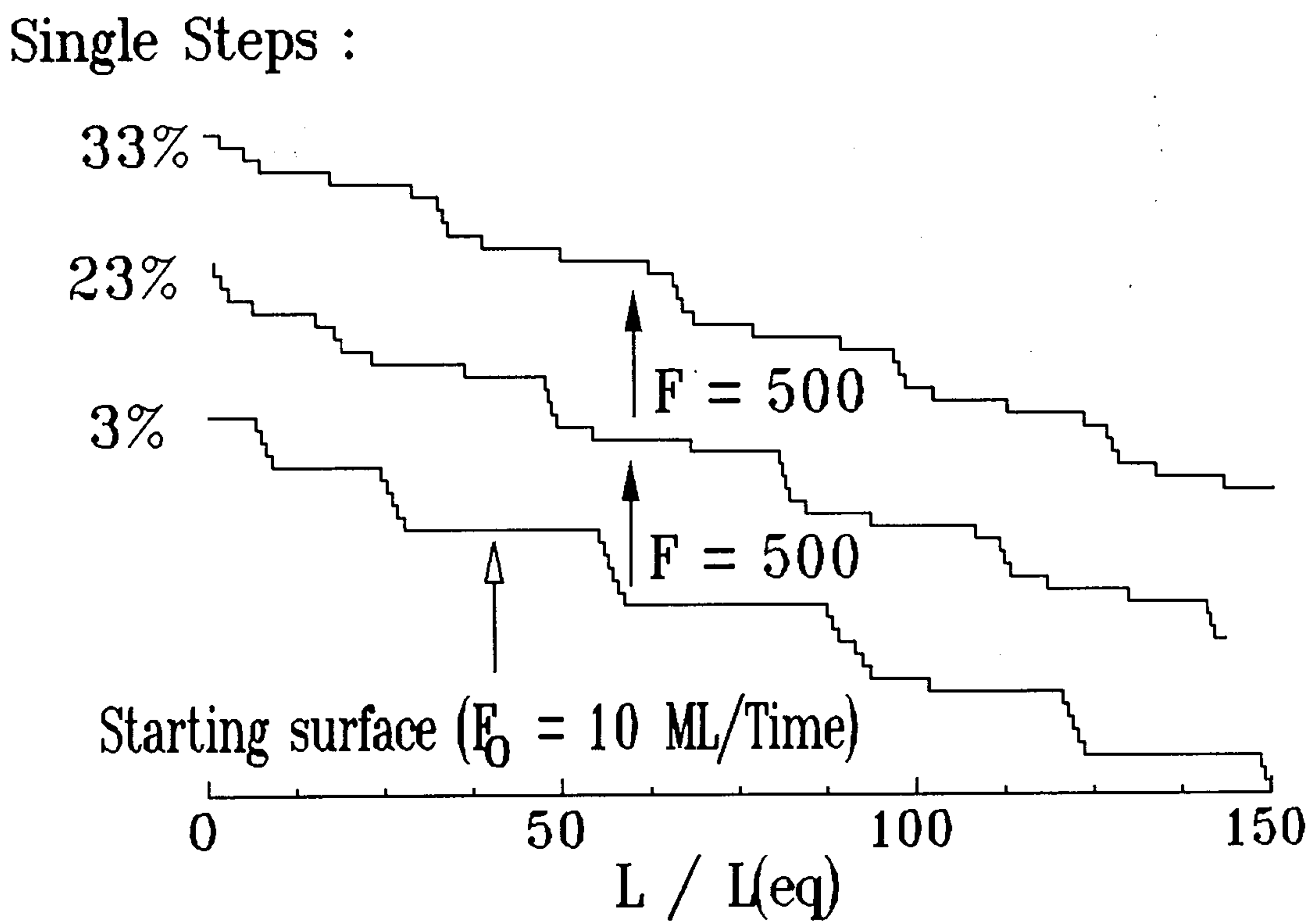
force dipole repulsion

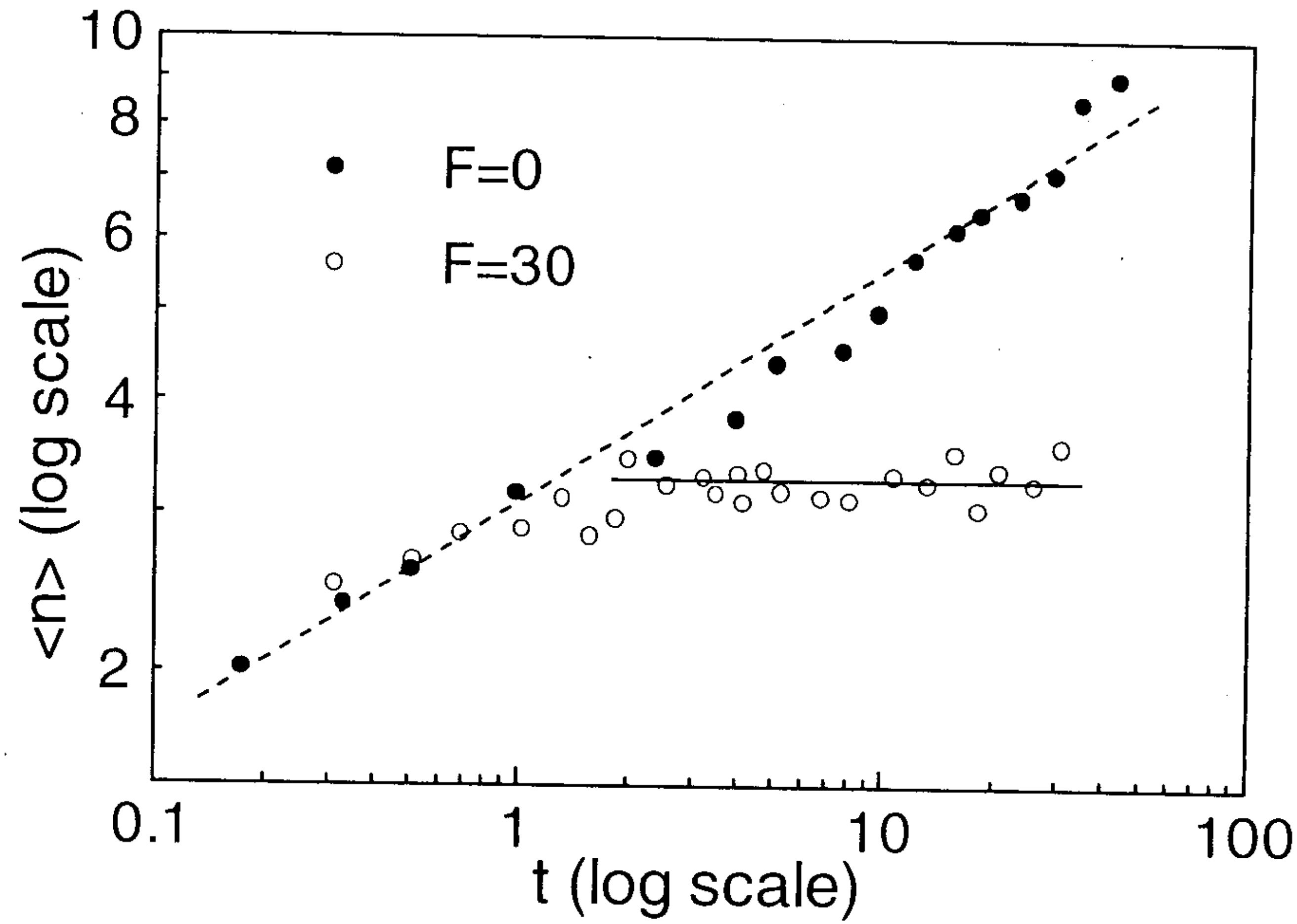
total force per unit length on step

$$f_m = \sum_{n \neq m} \left(\frac{\alpha_1}{(x_n - x_m)} - \frac{\alpha_2}{(x_n - x_m)^3} \right)$$

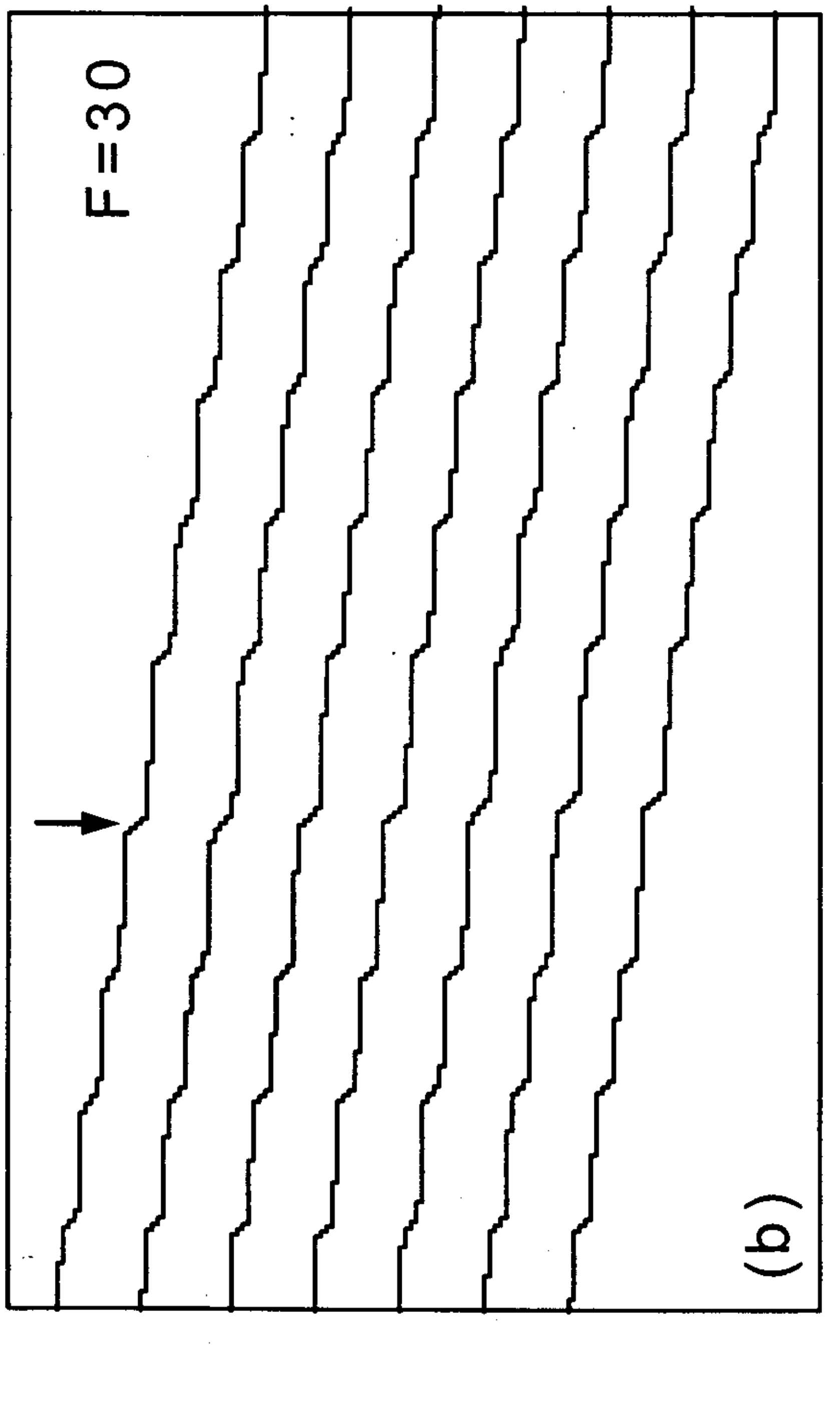


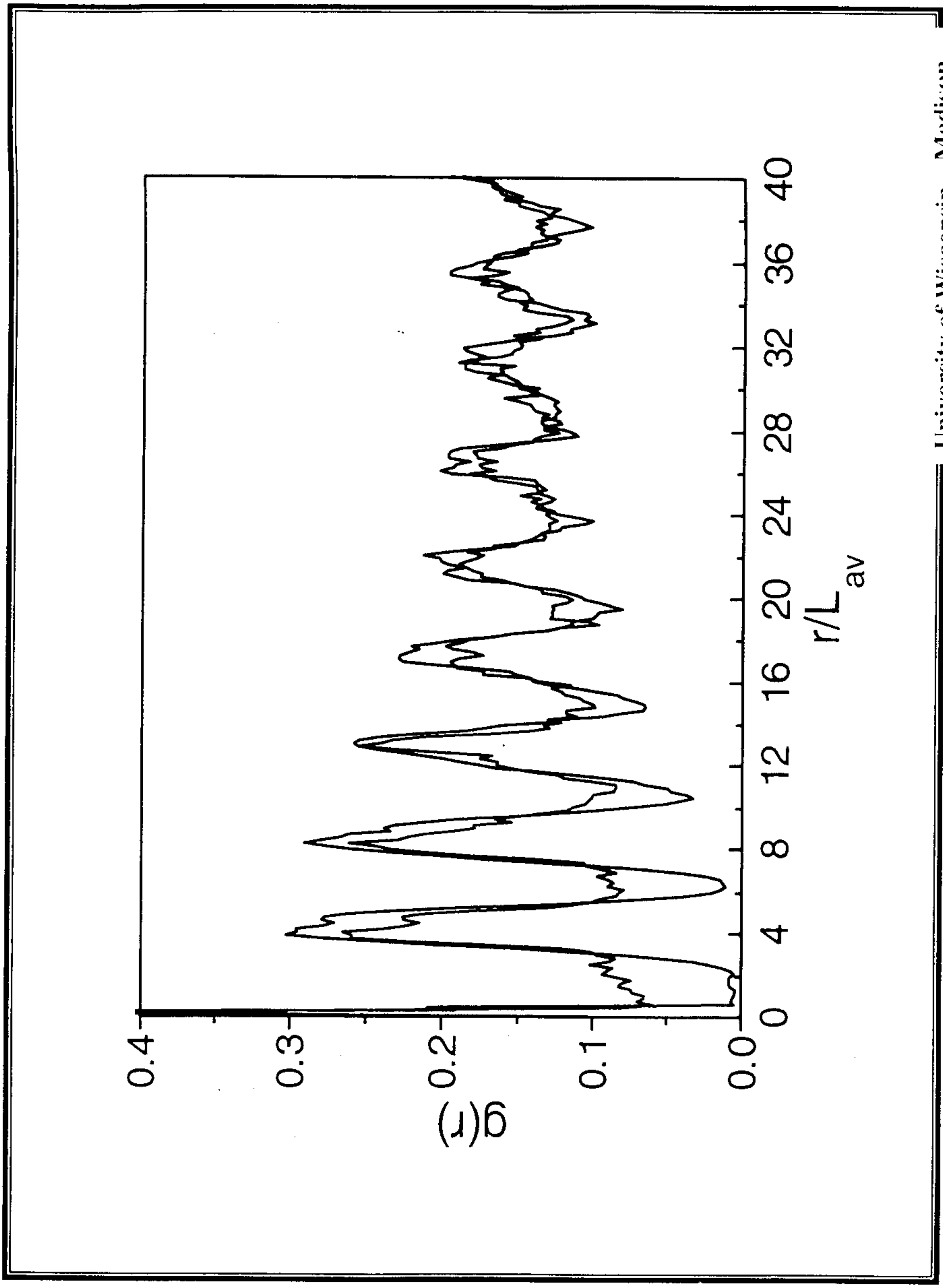
Debunching By Faster Deposition

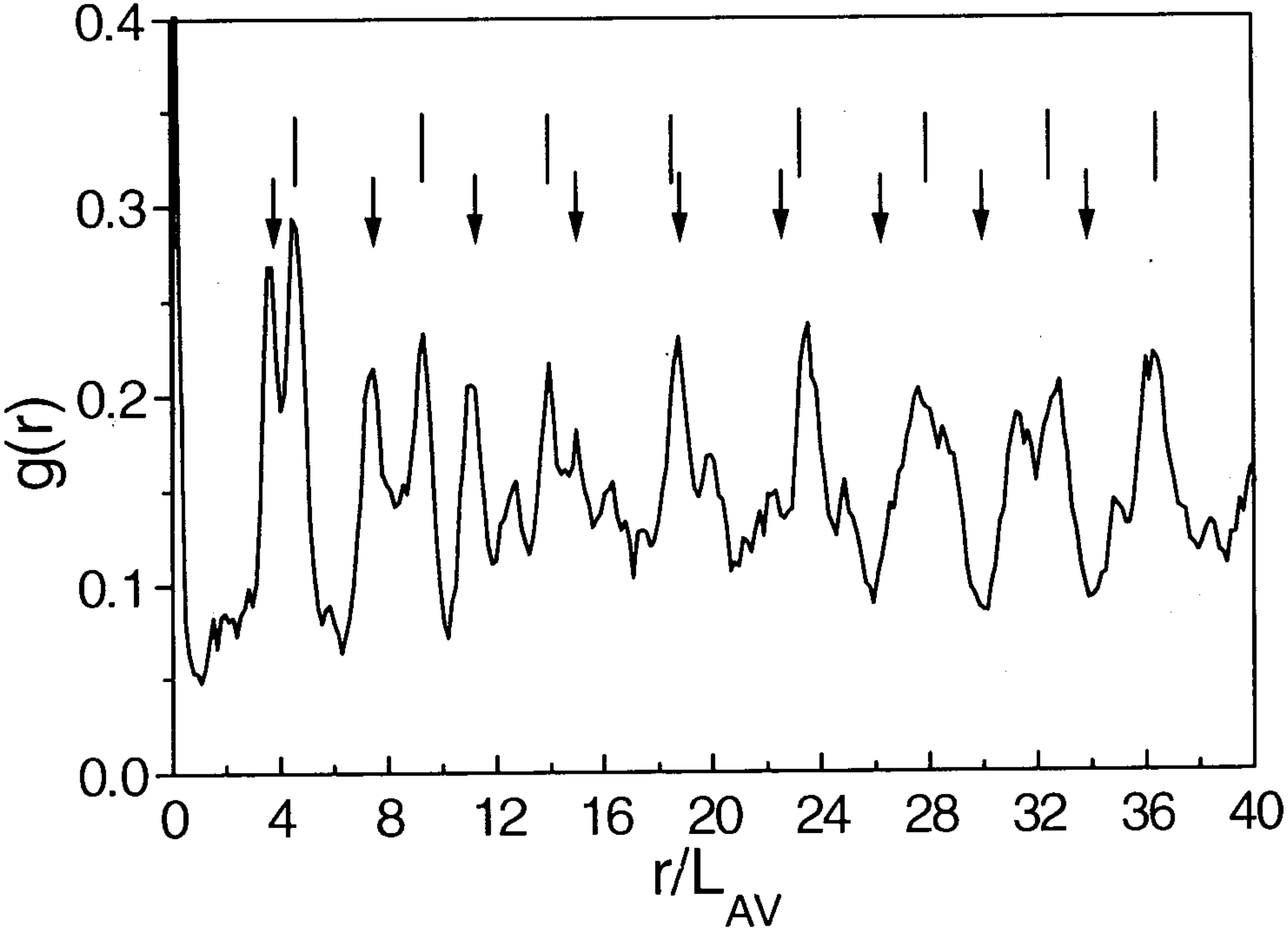


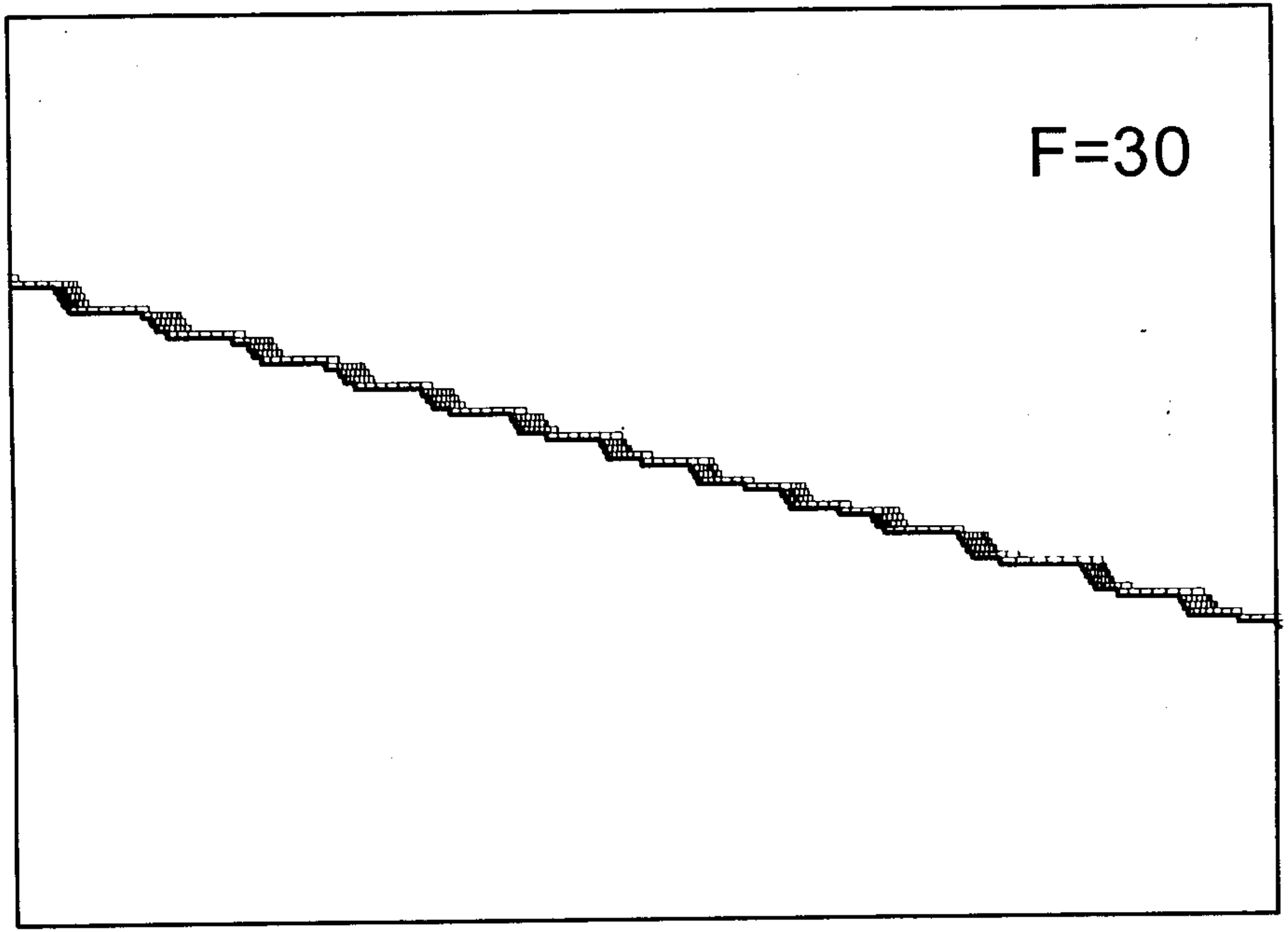


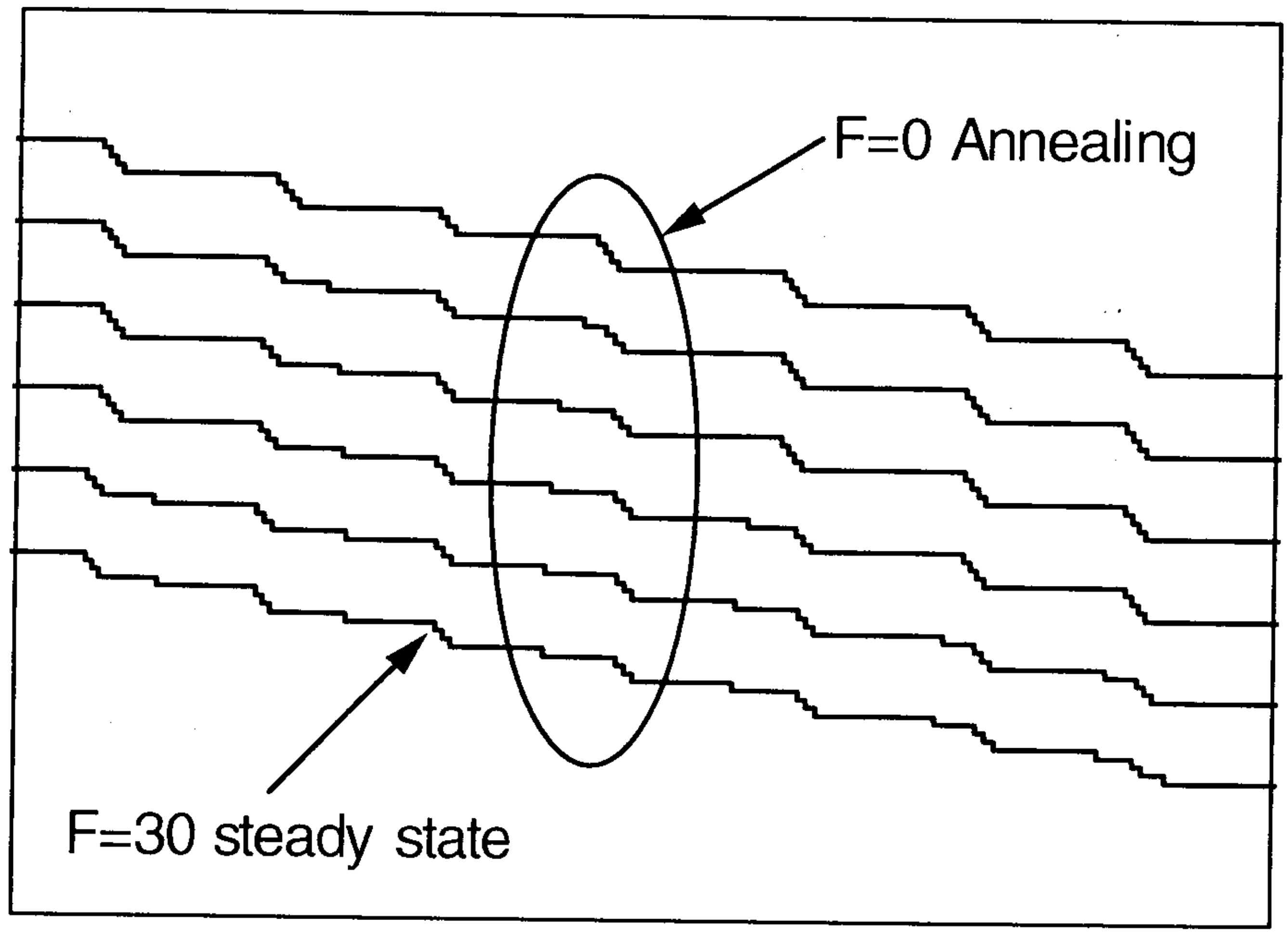
F=0
F=30
<n> (log scale)
t (log scale)
10
8
6
4
2
0.1
1
10
100

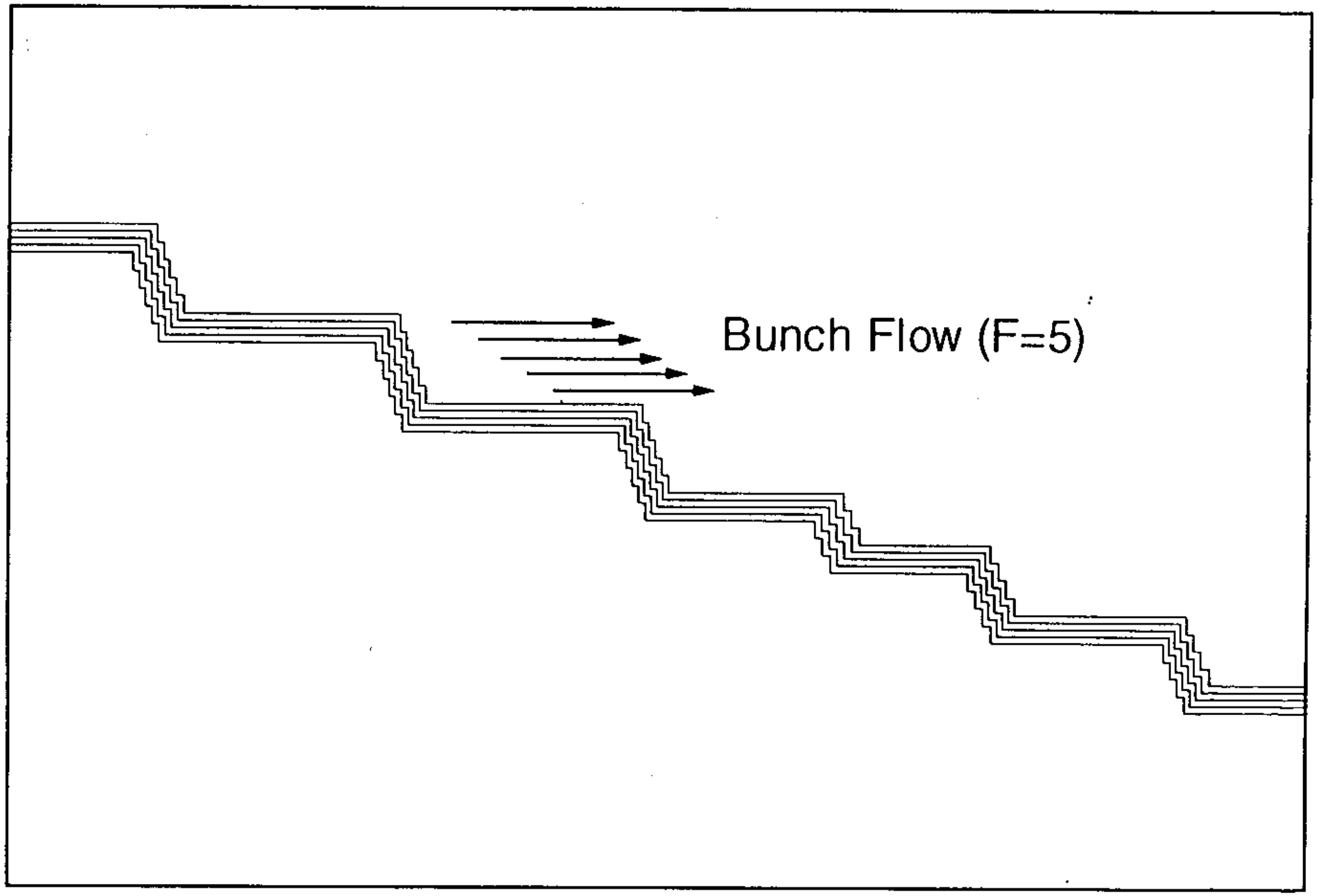

F=30
(b)

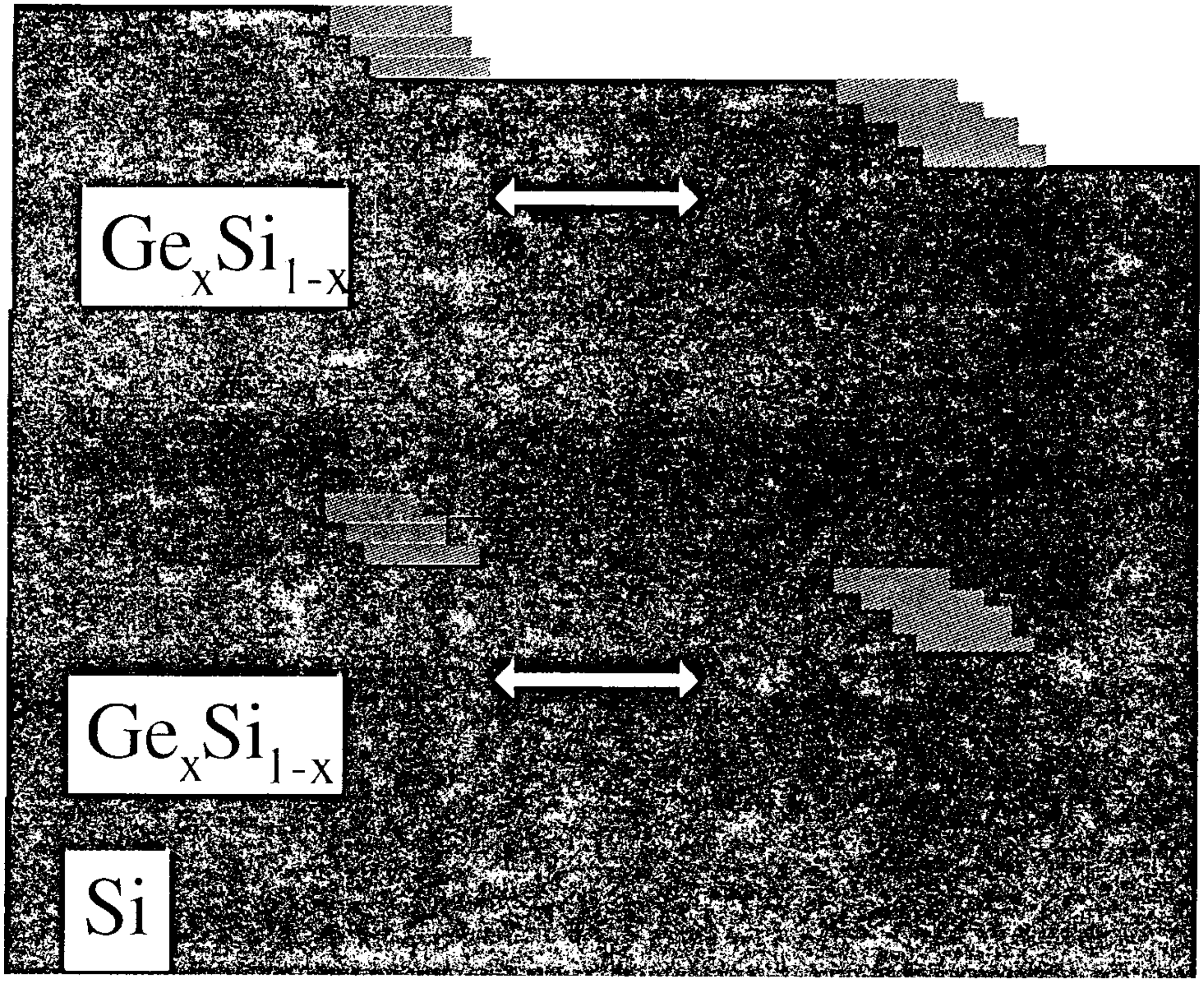

g(r)
r/L_av
0.0
0.1
0.2
0.3
0.4
0
4
8
12
16
20
24
28
32
36
40
University of Wisconsin - Madison


0.4
0.3
0.2
0.1
0.0
g(r)
0
4
8
12
16
20
24
28
32
36
40
r/L_AV


F=30


F=0 Annealing
F=30 steady state


Bunch Flow (F=5)


GexSi1-x
GexSi1-x
Si

Quantum-wire Fabrication:

---- surface patterning

---- 3D islands with a long thin shape

---- preferential growth at steps

*** **step-bunch arrays**

Conclusions:

self-organized step bunches → quantum wires

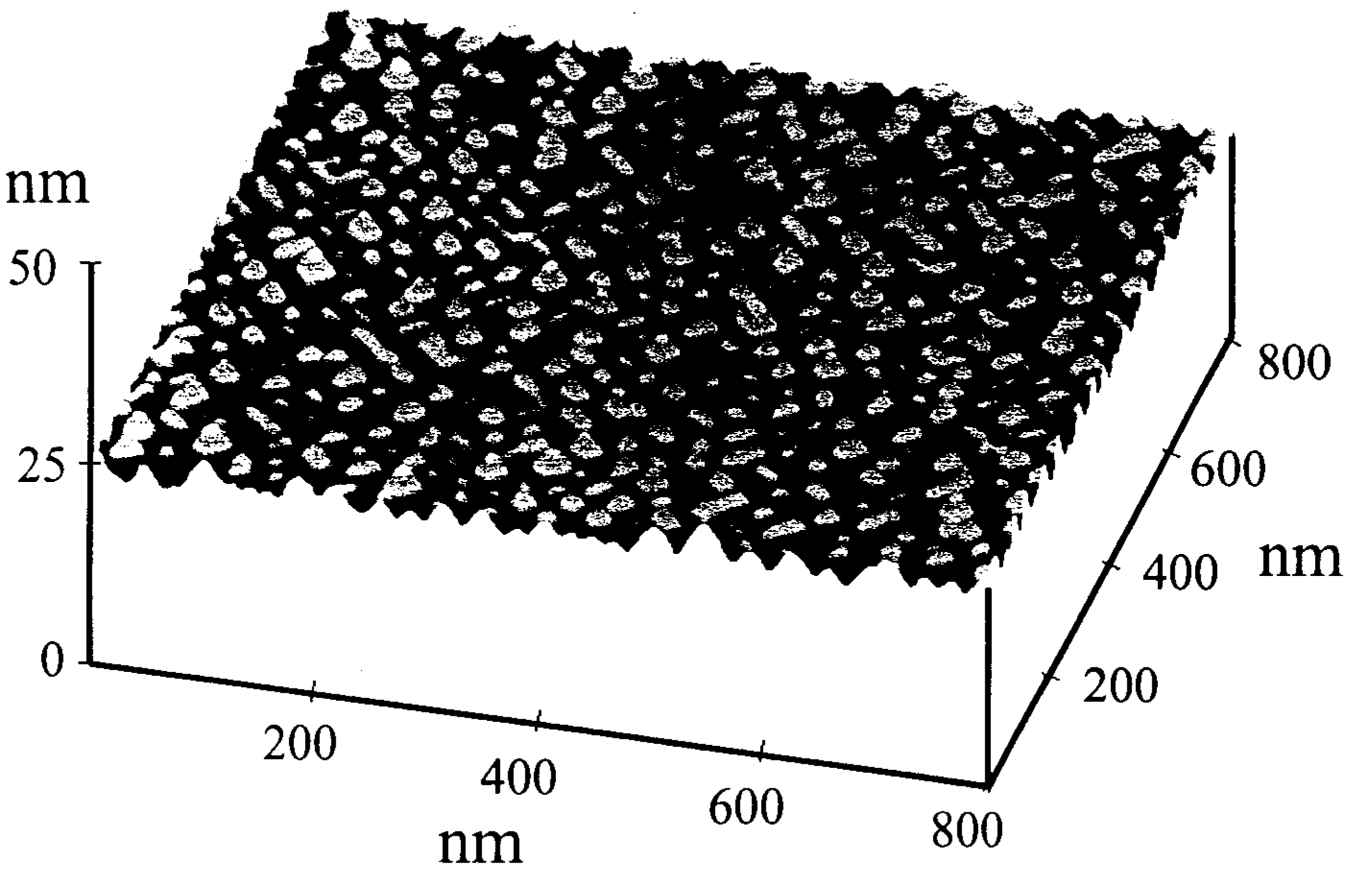
--- bunches are straighter than steps

--- high degree of uniformity and order

--- controlled structural features

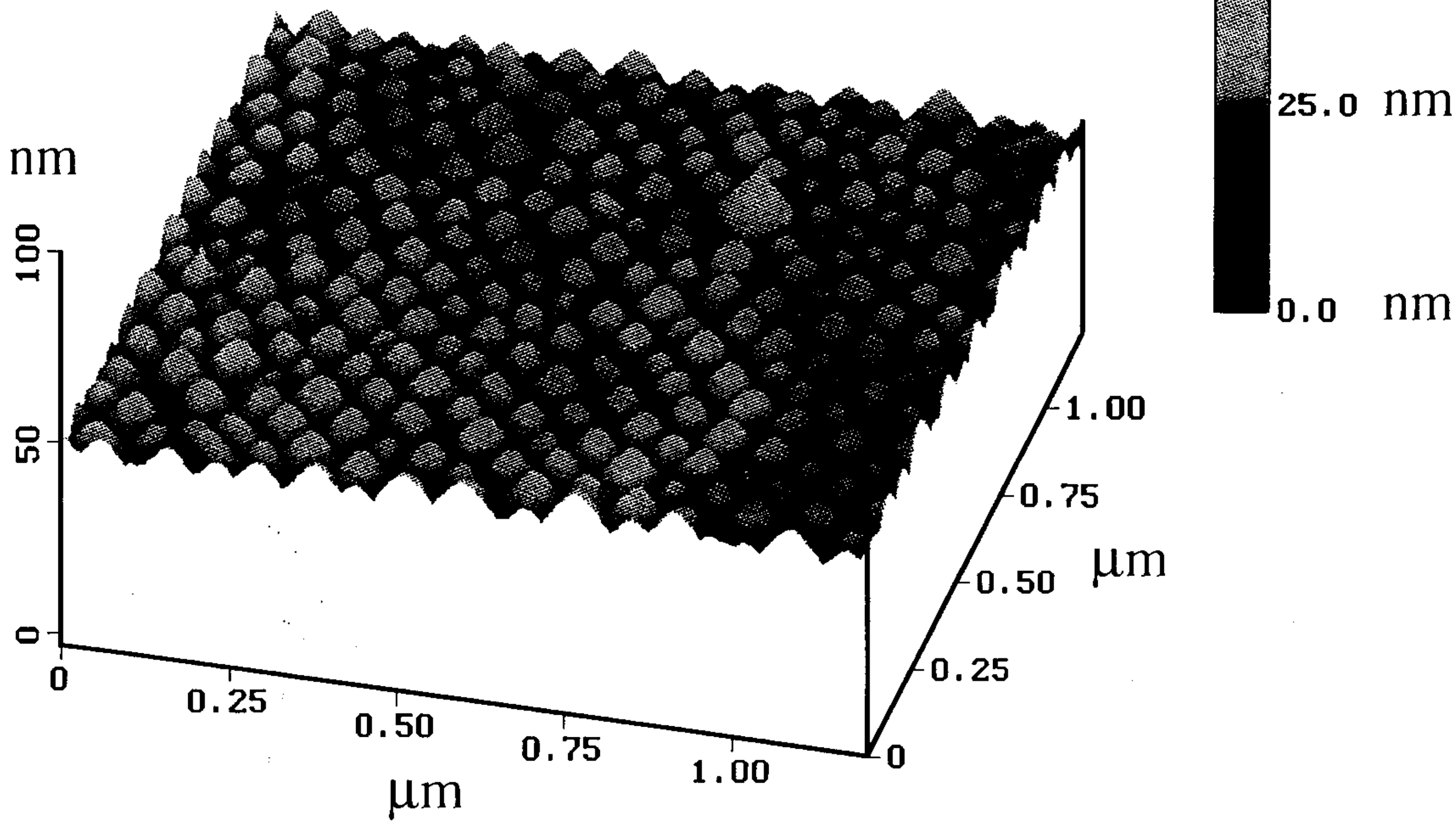
(bunch size, spacing, and long-range order)

2.5 nm $Si_{0.25}Ge_{0.75}/Si(001)$

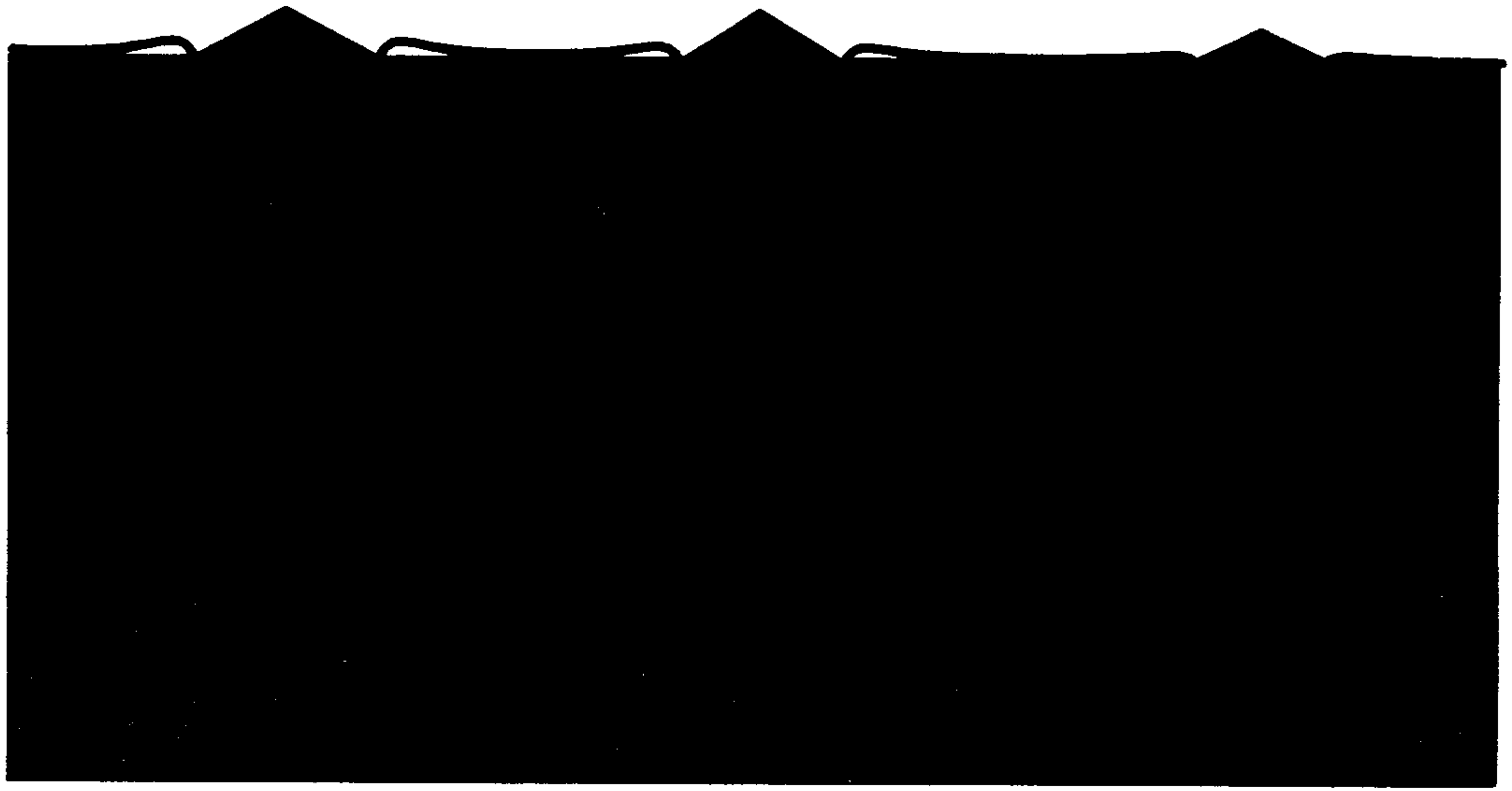


University of Wisconsin-Madison

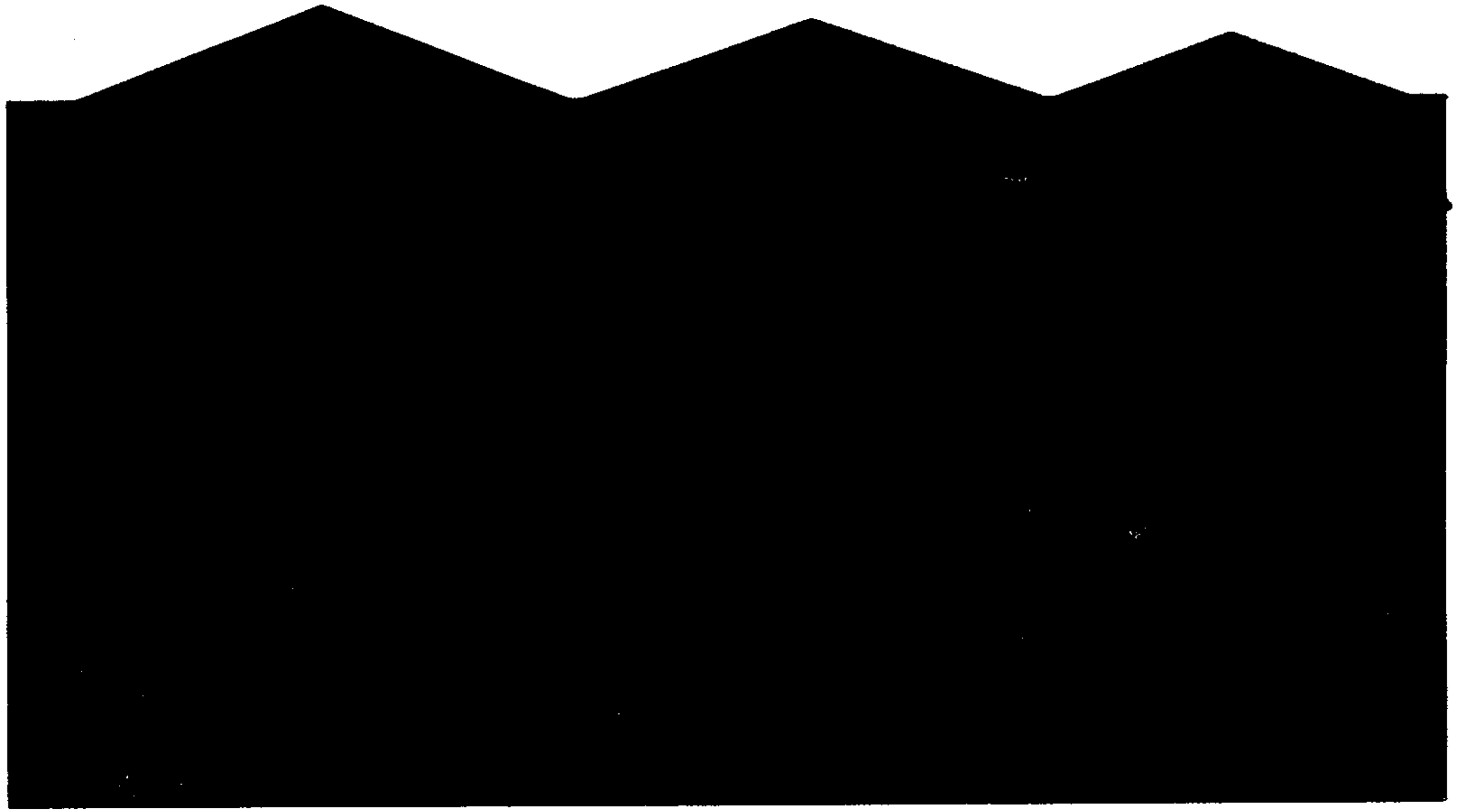
20 x (2.5 nm $Si_{0.25}Ge_{0.75}$ / 10 nm Si) on Si(001)



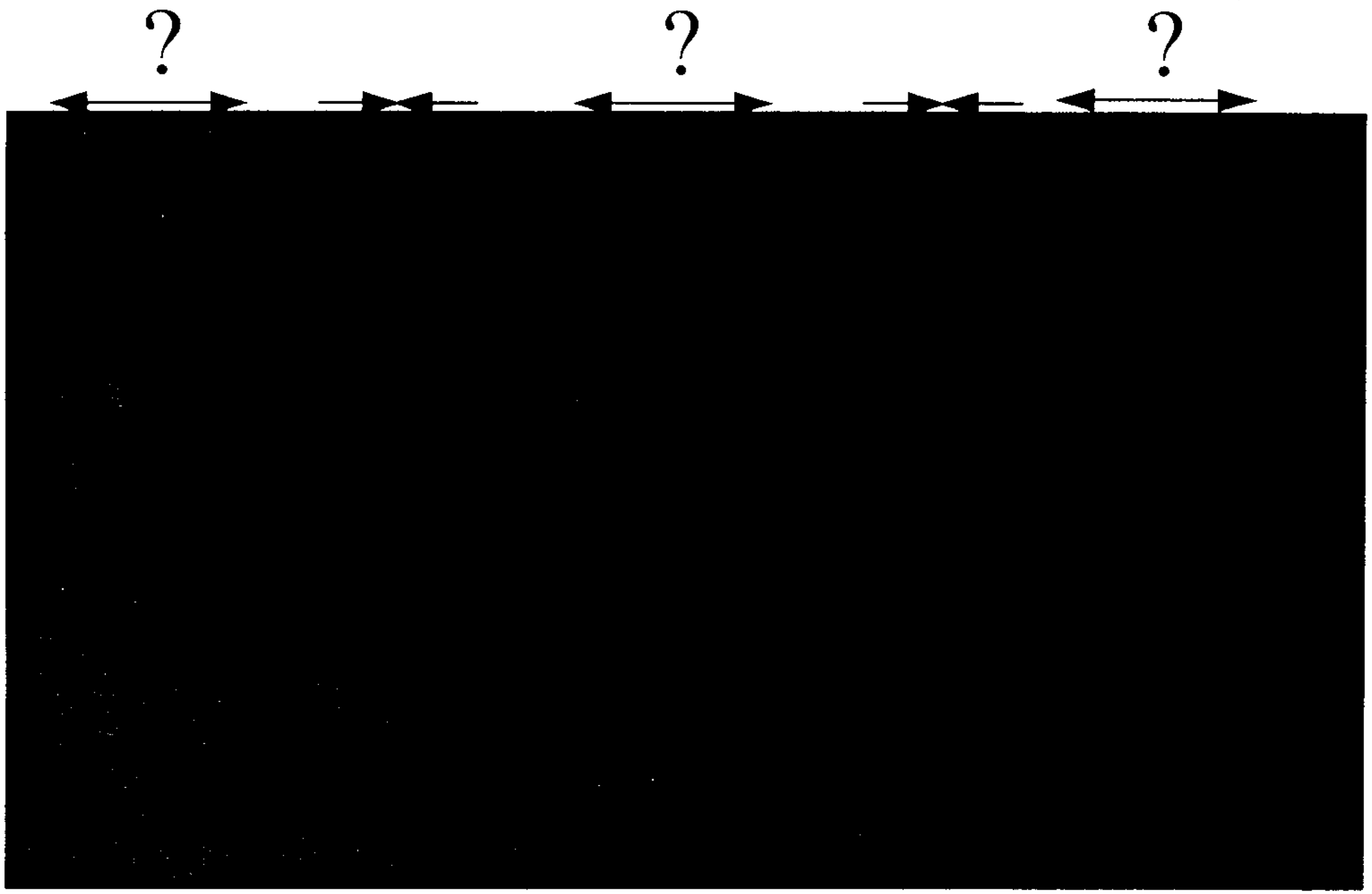
Determine island location and size:



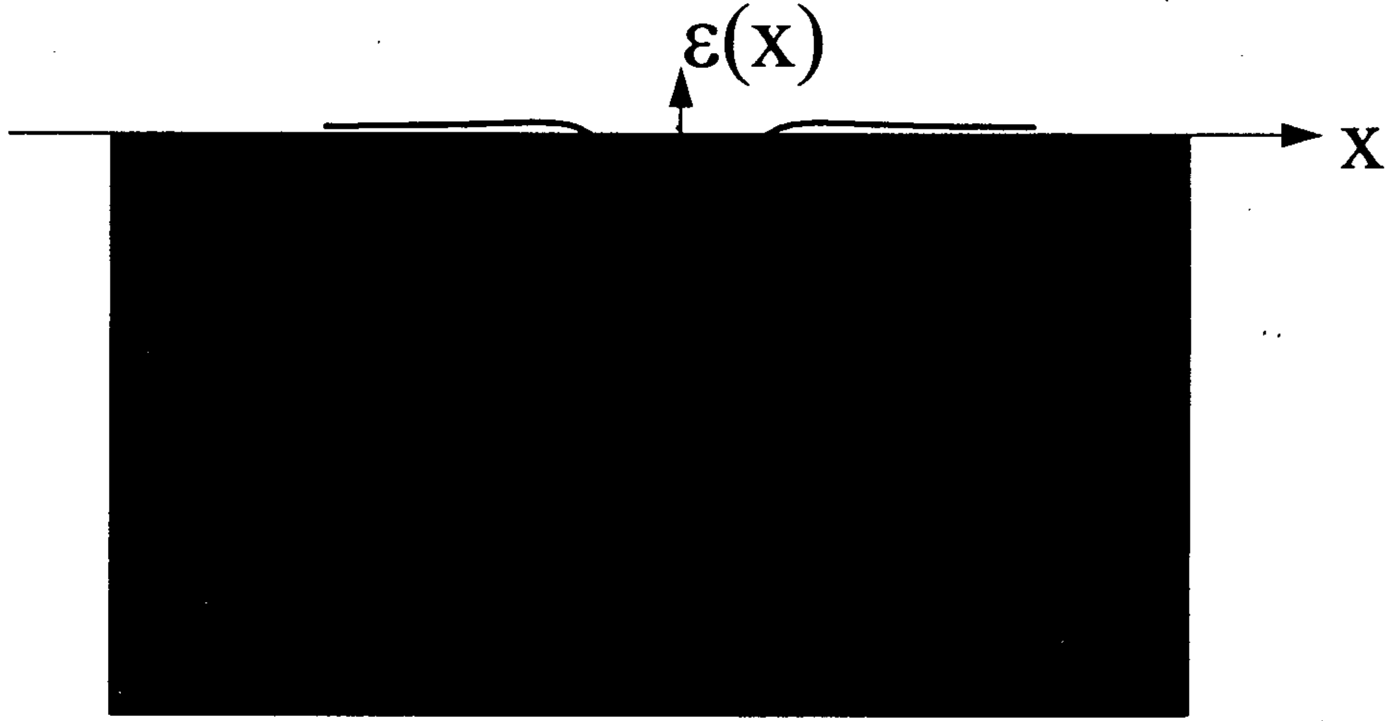
Determine island location and size:



Island formation in multilayer film:



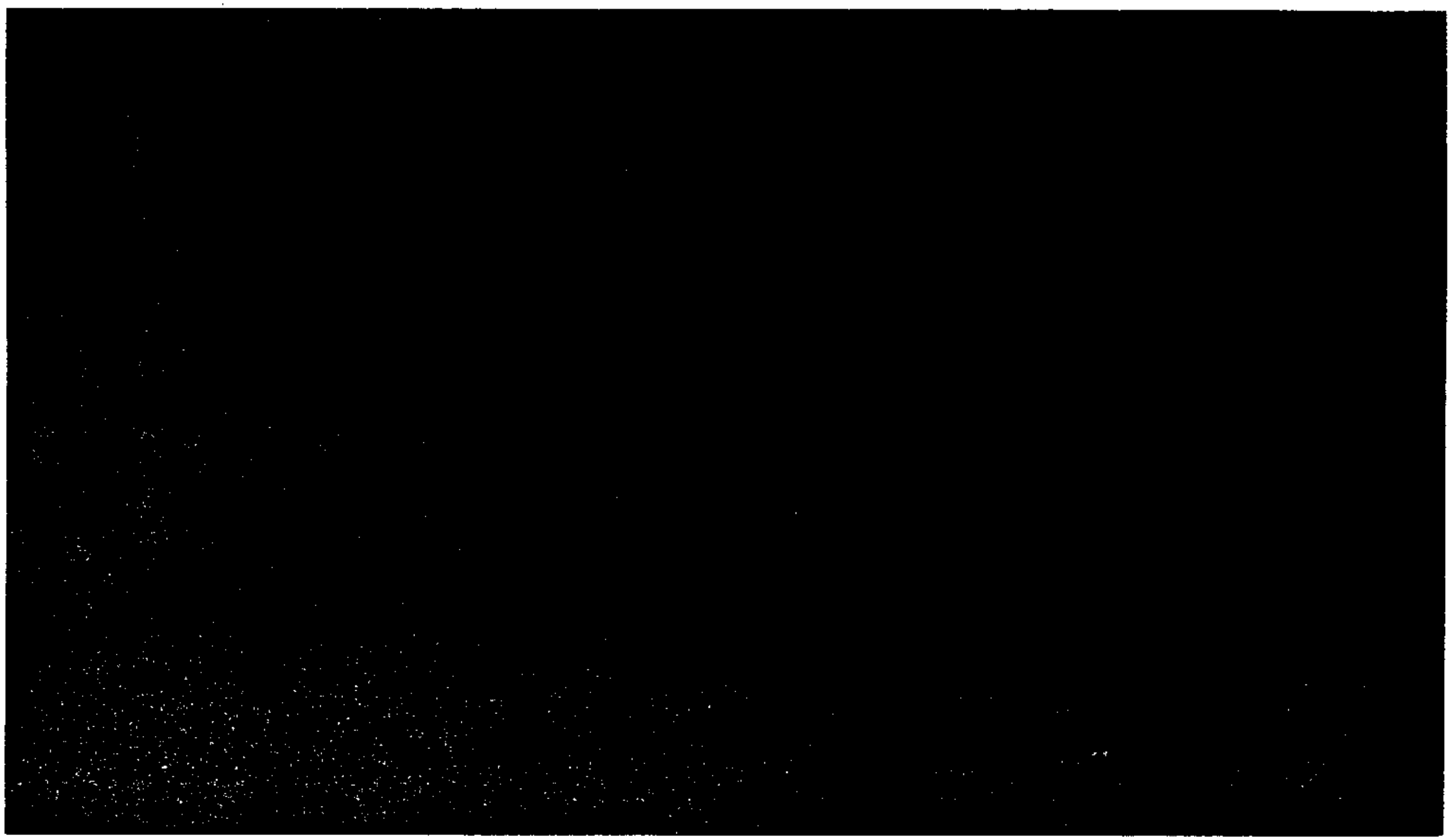
Surface strain due to a point island:



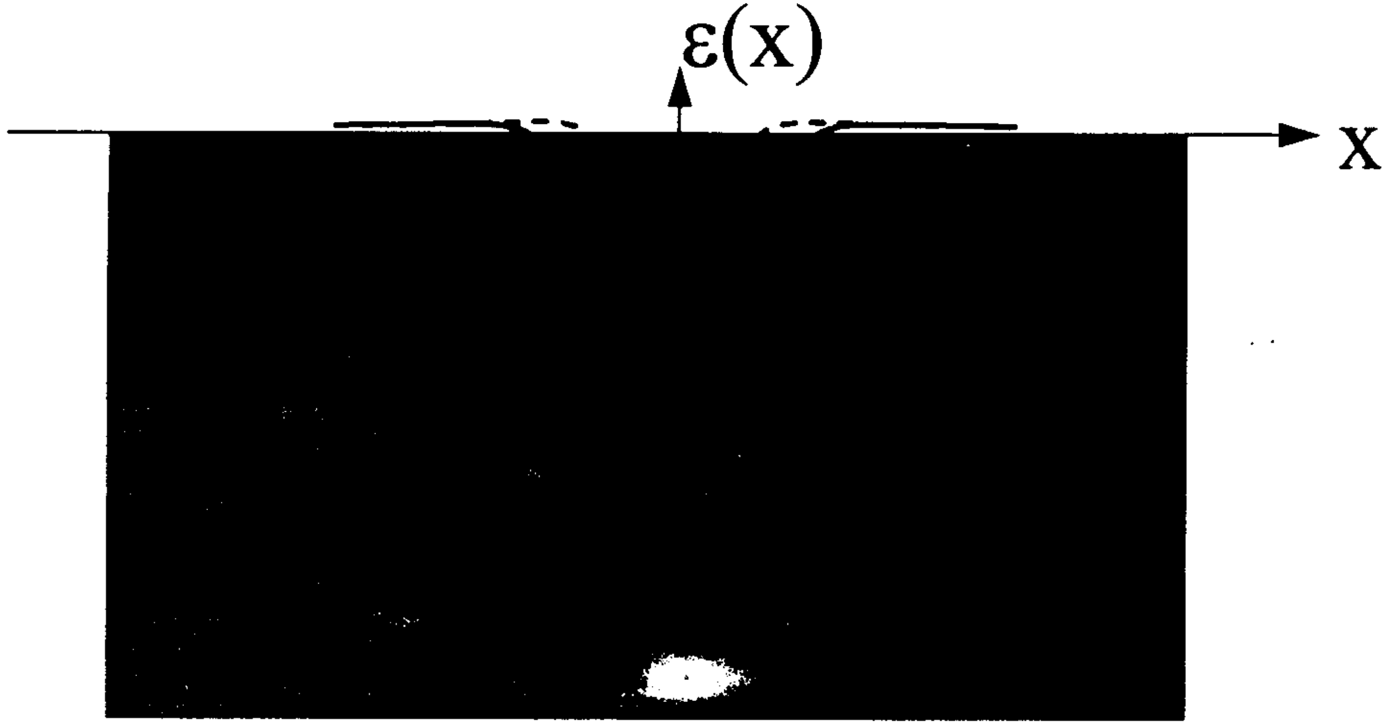
$$\varepsilon(x) = c(x^2+L^2)^{-3/2}[1-3L^2/(x^2+L^2)].$$

A.A. Maradudin and R.F. Wallis, Surf. Sci. **91**, 423 (1980).
J. Tersoff, C. Teichert, and M.G. Lagally, PRL **76**, 1675 (1996).

Island shape after overgrowth:



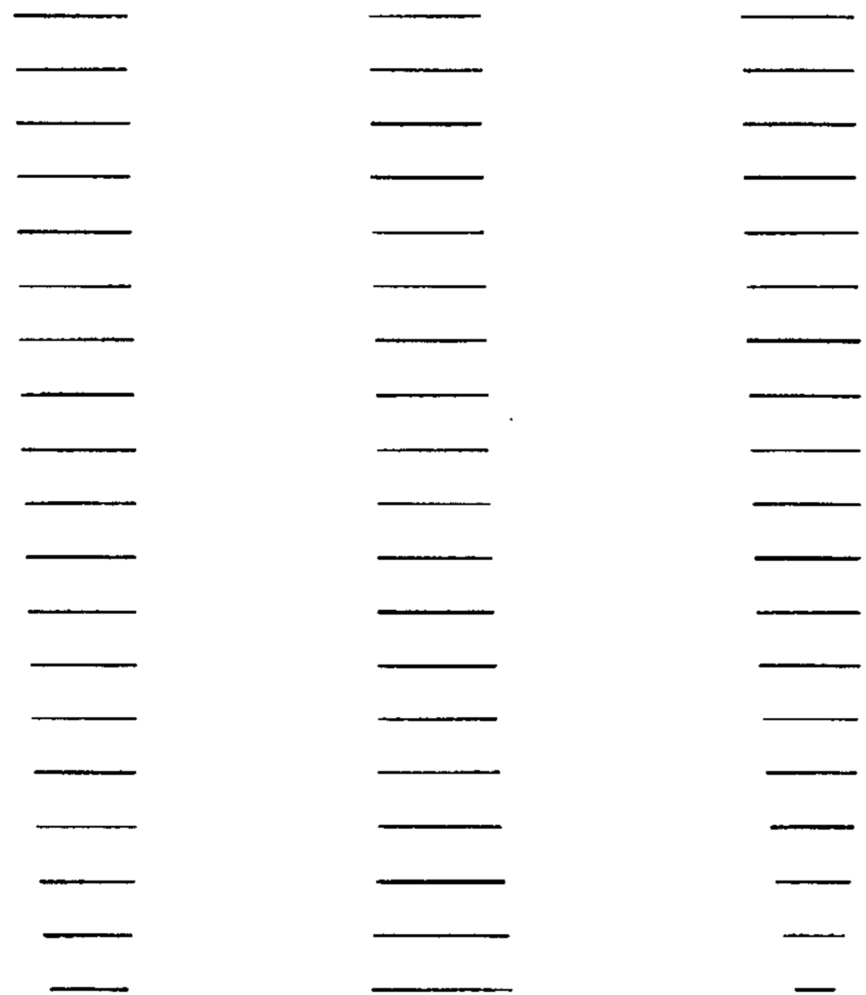
Surface strain due to a rectangle island:



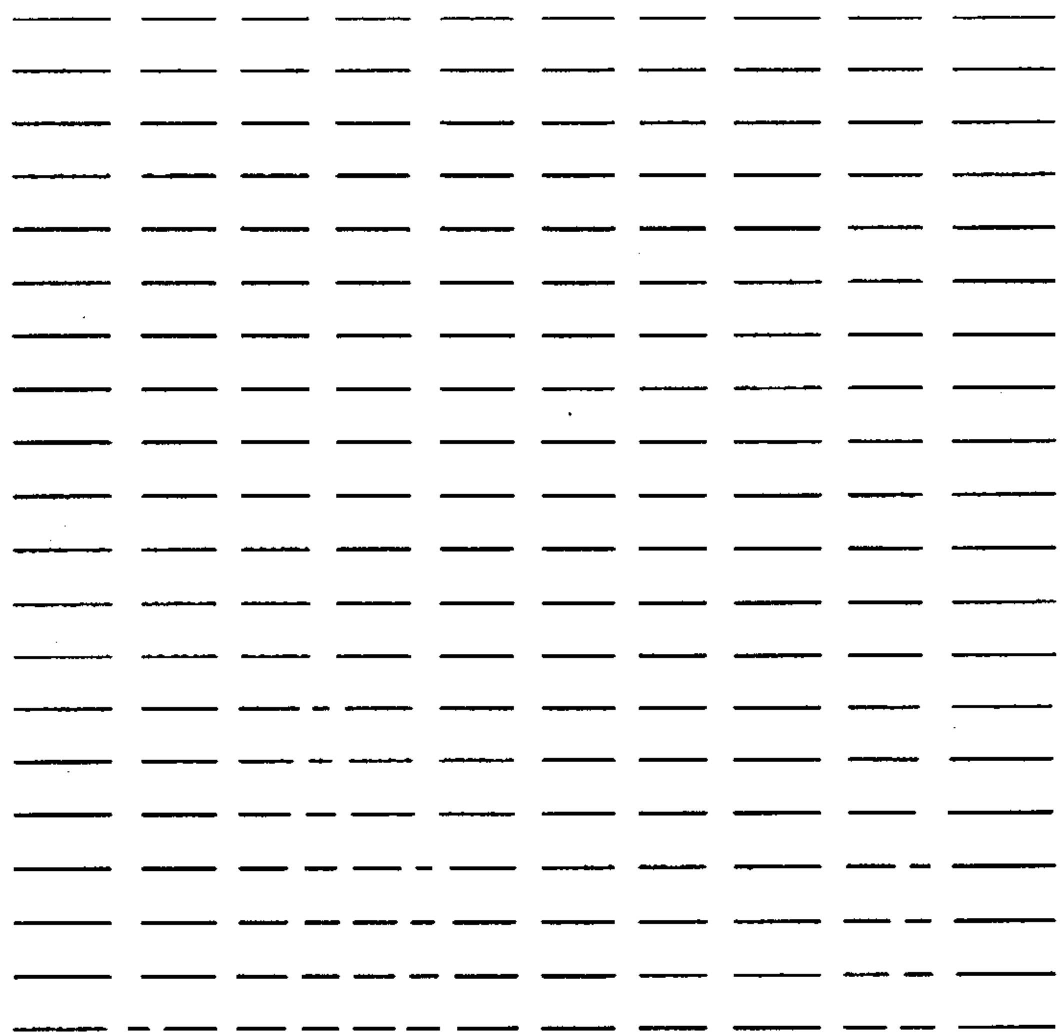
$$\varepsilon(x) = -ch(x+d)[2+(x+d)^2/L^2][(x+d)^2+L^2]^{-3/2}$$
$$+ch(x-d)[2+(x-d)^2/L^2][(x-d)^2+L^2]^{-3/2};\ h \ll d.$$

Feng Liu, Sarah Davenport, and M.G. Lagally, to be published.

Growth of single islands in multilayer films



Growth of close-lying islands in multilayer films



University of Wisconsin - Madison

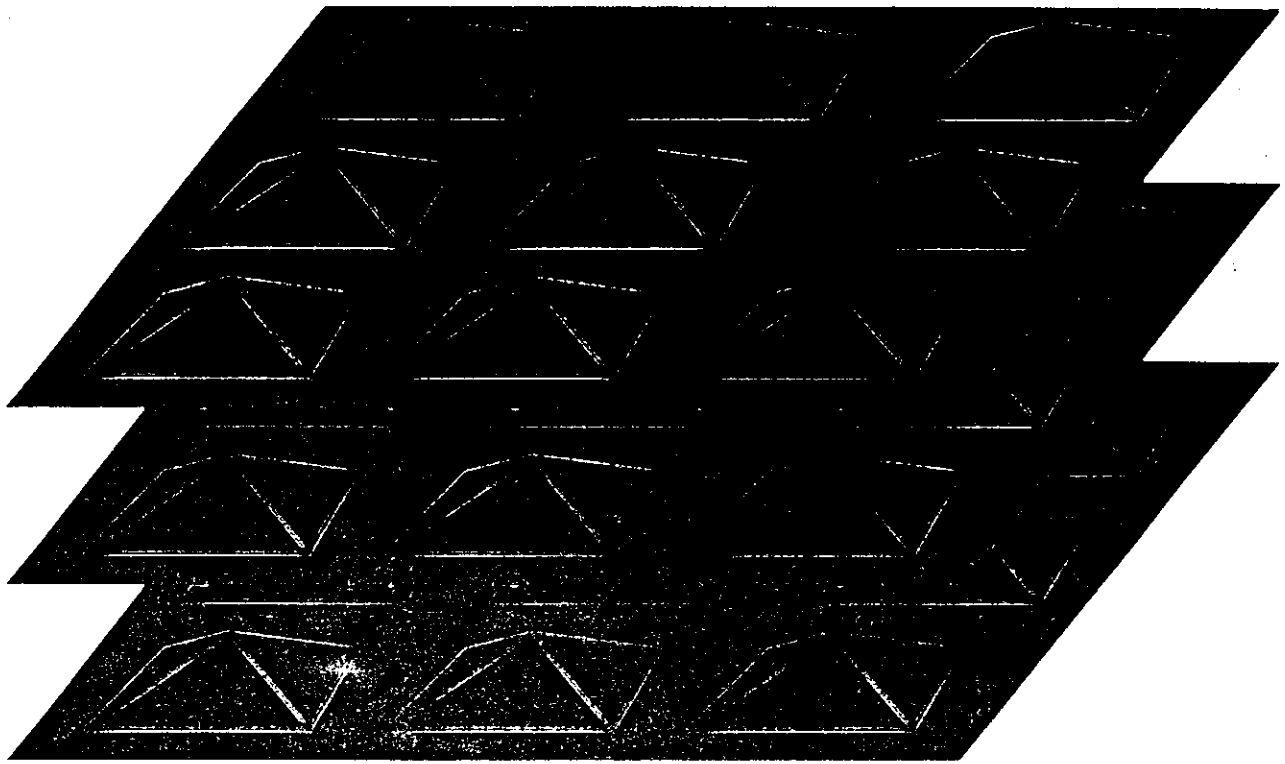
Table 1: Comparison of the Standard Deviations of Island Size of Closely Spaced Islands where L = 12nm

Layer Number	Average Island Size (nm)	Standard Deviation of Island Size (nm)
1	26.75	12.86
5	36.06	10.14
10	39.06	6.59
15	39.06	6.59
20	39.06	6.59

Table 2: Increase in Average Island Size after 20 Layers for Initially Closely Spaced Islands

Layer Thickness (nm)	Average Island Size after 20 layers (nm)	Standard Deviation of Island Size after 20 layers (nm)
12	39.06	6.59
14	38.56	7.52
16	42.48	11.19
18	51.92	9.04
20	58.50	8.15

Self-Organization in Three Dimensions



3-D "superlattice" of group IV clusters

University of Wisconsin

Conclusions:

Stress (strain) management and multilayer thin-film growth provide an attractive route to nanofabrication of quantum wires and quantum dots.