Morphological evolution of SiGe nanostructures

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OUTLINE

Introduction

Morphological evolution of SiGe layers on :

*** Si(111)**

*** Si(001)**

Conclusion

CONFIGURATIONAL FORCE

= Gradient in μ

Isothermal ($T_{sub} = T_{res}$), Isobaric ($P_{sub} = P_{res}$) subsystem

➡ $G_{subsystem}$ minimized in equilibrium

$$dG = -SdT + VdP + \mu dN$$

$$\mu \equiv \left(\frac{\partial G}{\partial N}\right)_{T,P}$$

Solid phase "β", single component, surrounded by phase "α":

$$\mu^{\beta} = \underbrace{\mu^{\beta}_{\substack{\text{stress-free}\\ \text{bulk}}}(T)}_{\text{Term 1}} + \underbrace{\frac{1}{2}\mathbf{C}^{\beta}\boldsymbol{\varepsilon}^{2}}_{\text{Term 2}} - \underbrace{\sigma_{\text{normal}}\Omega^{\beta}}_{\text{Term 3}} + \underbrace{\left[\left(\gamma^{\alpha\beta} + \frac{d^{2}\gamma^{\alpha\beta}}{d\theta_{1}^{2}}\right)\frac{1}{R_{1}} + \left(\gamma^{\alpha\beta} + \frac{d^{2}\gamma^{\alpha\beta}}{d\theta_{2}^{2}}\right)\frac{1}{R_{2}}\right]\Omega^{\beta}}_{\text{Term 4}}$$

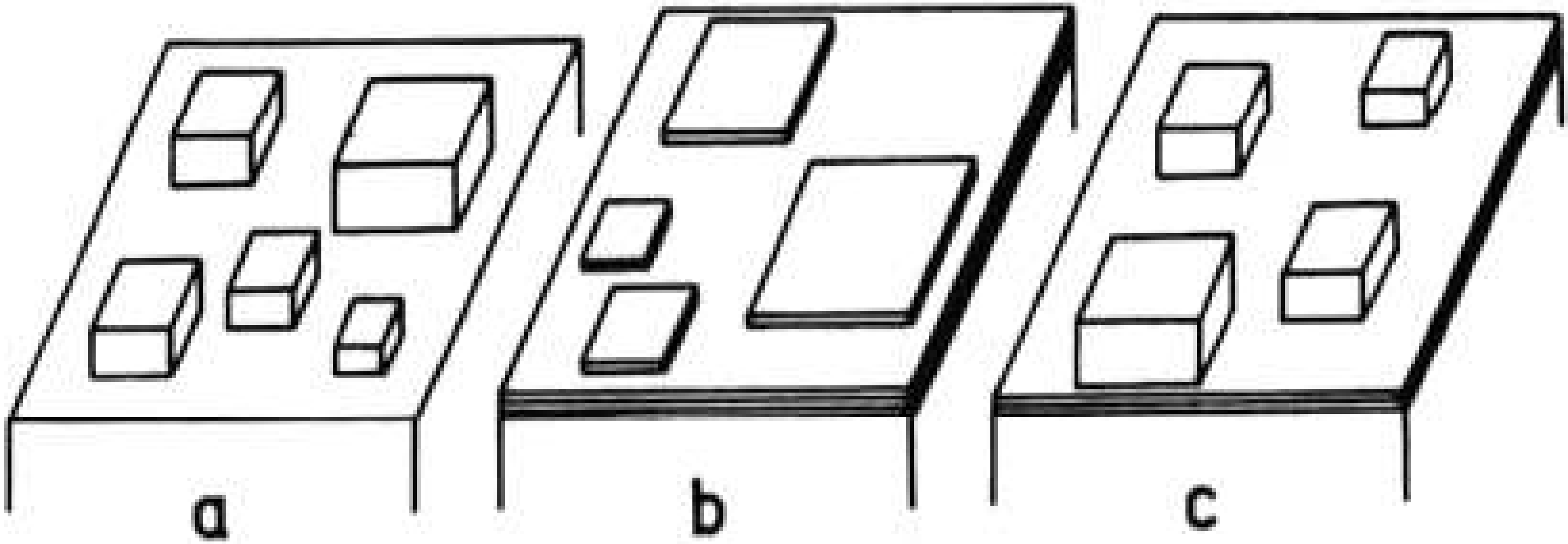
Term 1: depends on phase: bonding, etc.

Term 2: elastic strain energy density

Term 3: PV work to push surroundings out of the way

Term 4: total surface energy (including anisotropy)
Ω = atomic (or molecular) volume
R = principal radius of curvature
θ = surface orientation

GROWTH MODES



Volmer Veber	Frank van der Merwe	Stranski Krastanov
or island growth	or layer by layer growth	or layer by layer growth followed by 3D islands
$d\mu / dn < 0$	$d\mu / dn > 0$	$d\mu / dn >/< 0$

During epitaxy

Strain energy

Surface energy

$$\mu^{\beta} = \underbrace{\mu^{\beta}_{\substack{\text{stress-free}\\ \text{bulk}}}(T)}_{\text{Term 1}} + \underbrace{\frac{1}{2}\mathbf{C}^{\beta}\boldsymbol{\varepsilon}^{2}}_{\text{Term 2}} - \underbrace{\sigma_{\text{normal}}\Omega^{\beta}}_{\text{Term 3}} + \underbrace{\left[\left(\gamma^{\alpha\beta} + \frac{d^{2}\gamma^{\alpha\beta}}{d\theta_{1}^{2}}\right)\frac{1}{R_{1}} + \left(\gamma^{\alpha\beta} + \frac{d^{2}\gamma^{\alpha\beta}}{d\theta_{2}^{2}}\right)\frac{1}{R_{2}}\right]\Omega^{\beta}}_{\text{Term 4}}$$

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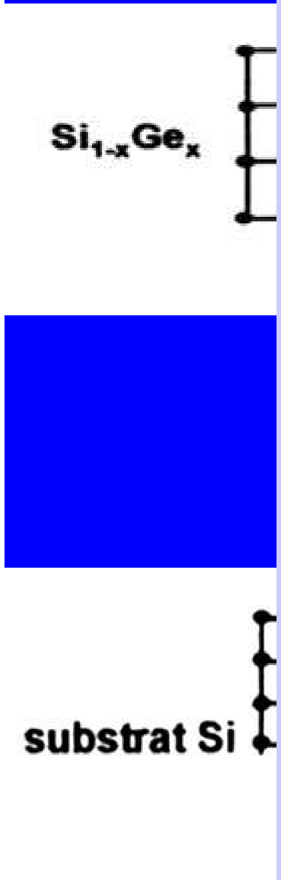
Stranski-Krastanov growth mode : 2 critical thickness

Misfit $\varepsilon = \Delta a / a = 4.2\ \%$

$a_{Si} = 5.4311$ Å

$a_{Ge} = 5.6579$ Å

h_{cr} / H_{cr}



h_{cr}

Strain energy

H_{cr}

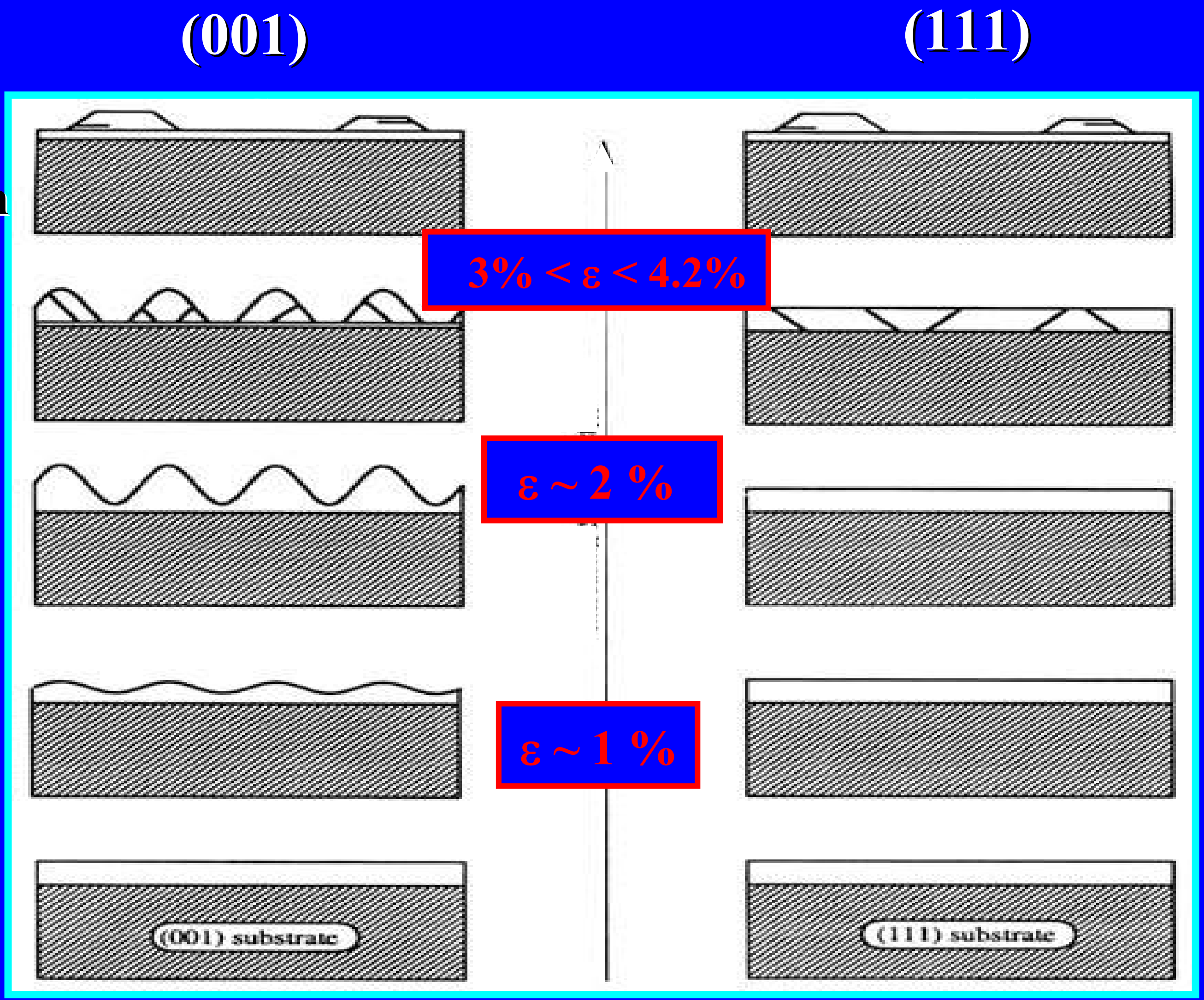
Chemical potential

Comparaison (111) and (001)

S-K growth mode
with Plastic relaxation

Kinetic
growth instability
only on (001)

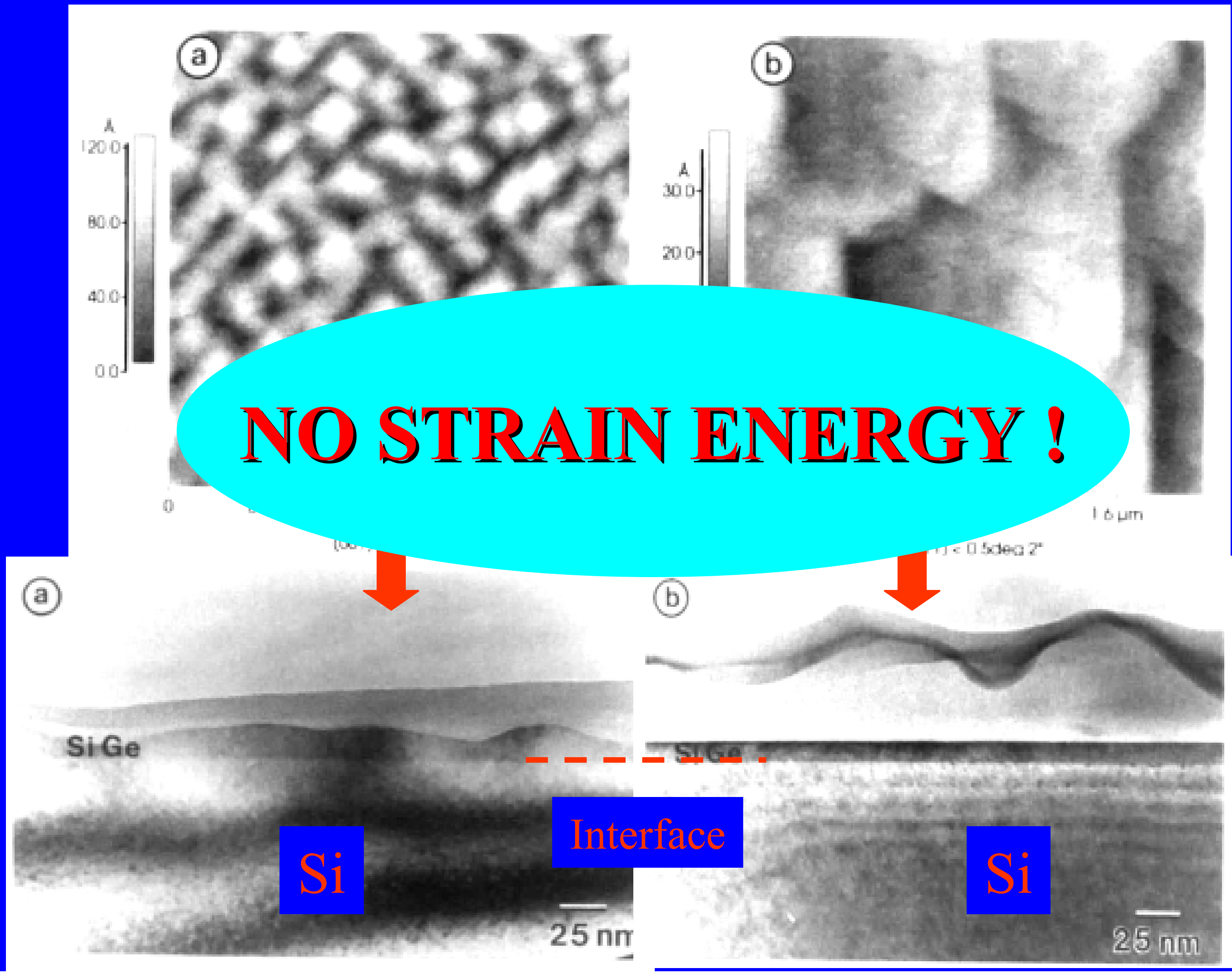
2D nucleation
layer by layer



WHY ?

(001)
Growth instability

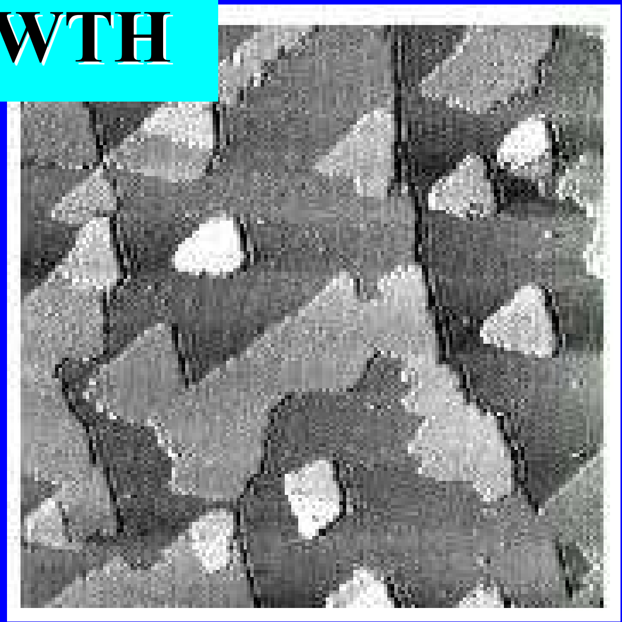
(111)
Layer by layer growth

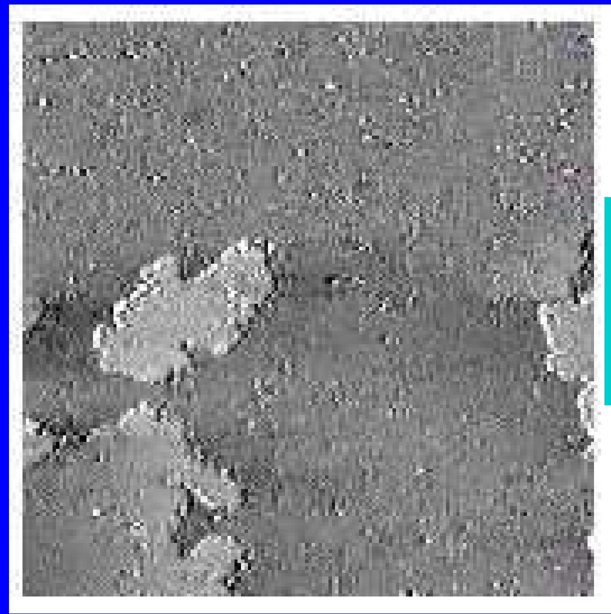


GROWTH OF SiGe ON Si(111)

REGIME I: 2D GROWTH

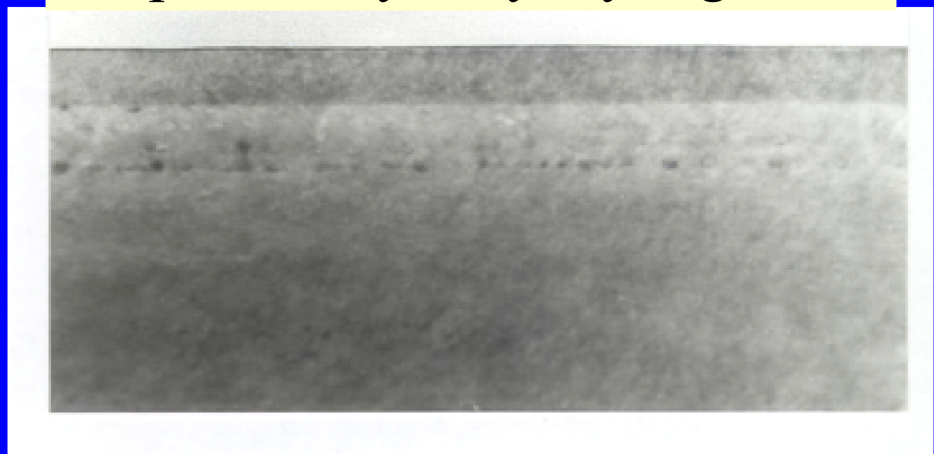
2D nucleation





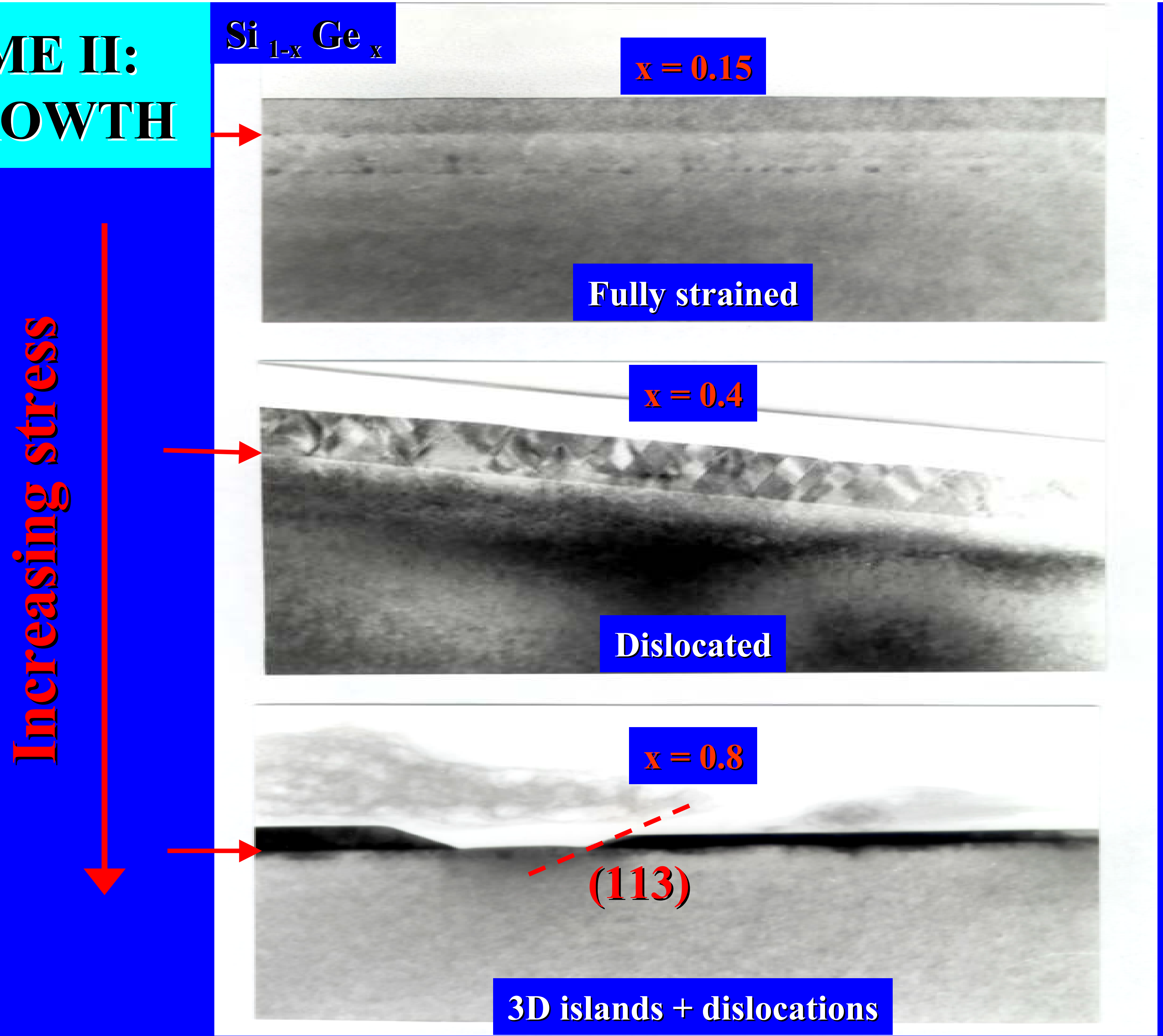
B. Voigtländer et al., Review of Scientific Instruments 67 (1996) 2568.

Step flow layer by layer growth



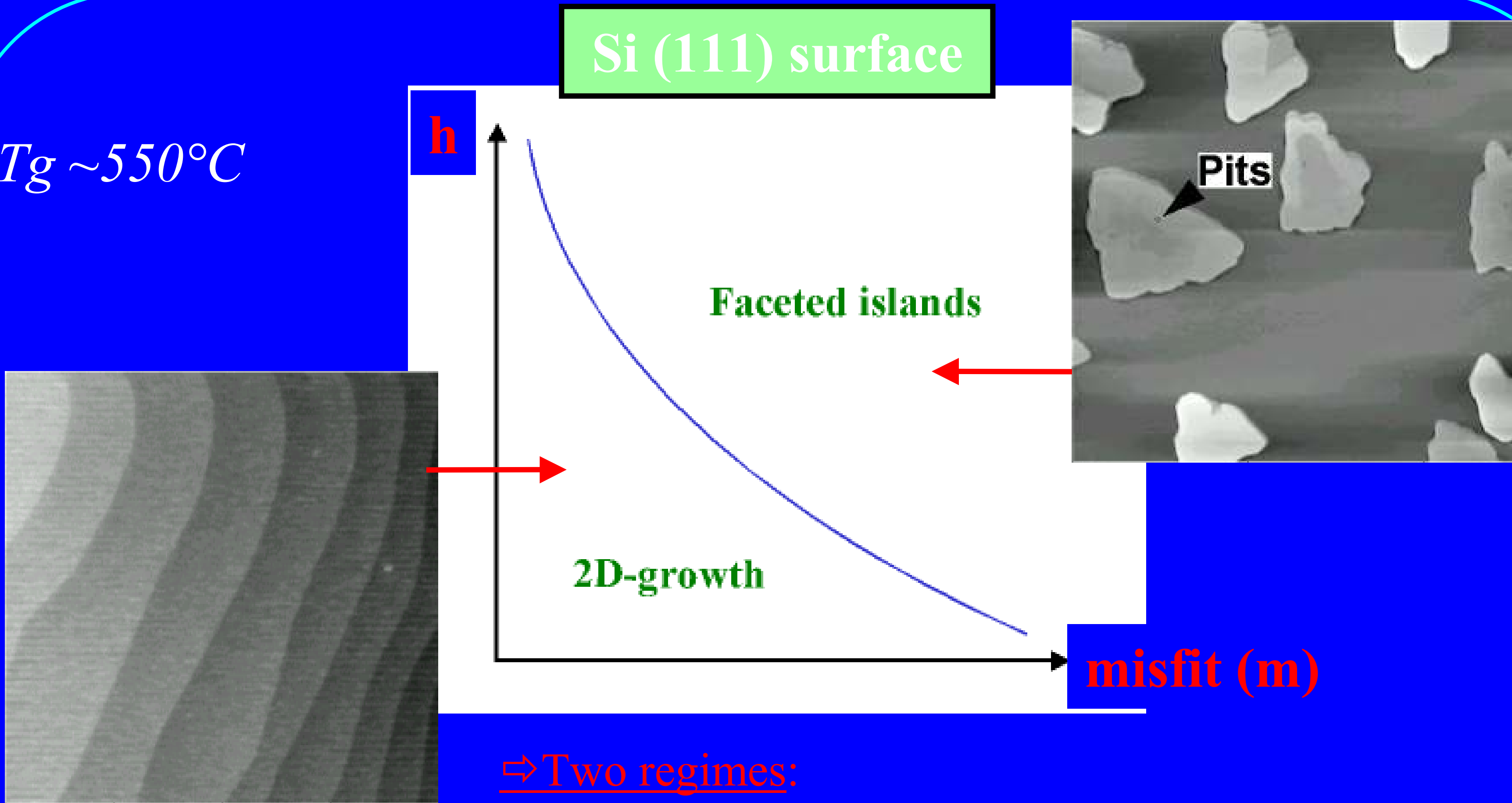
I. Berbezier et al., Surf. Sci. 412/413 (1998) 415

REGIME II: 3D GROWTH



Morphological Evolution of SiGe Layers:
Experimental « kinetic » phase diagrams, Si(111)

Tg ~550°C



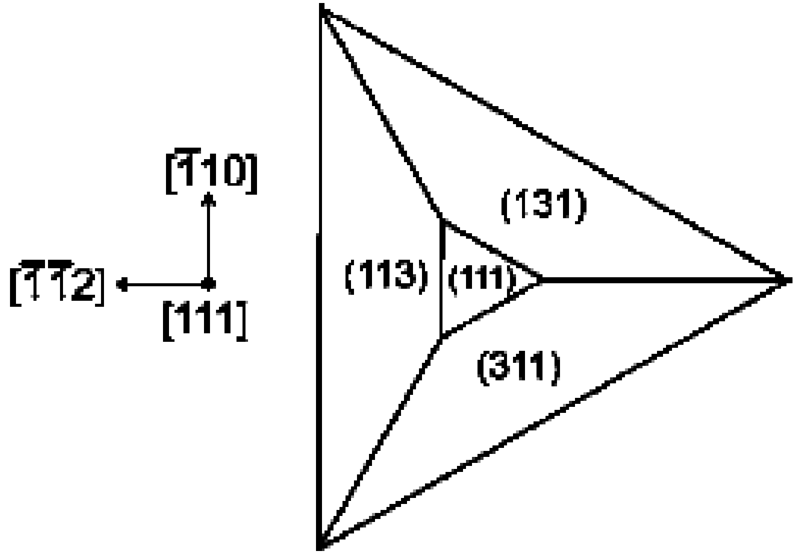
⇨Two regimes:

- 2D layer by layer at low (h,m)
- Classical SK growth (dislocated islands) at high (h,m)

Equilibrium shape of Ge / Si

$$E_{\text{total}} = E_{\text{elastic}} + E_{\text{surface}} + E_{\text{edge}}.$$

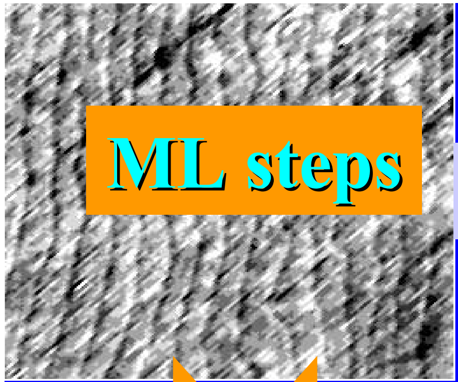
$$F_s = \frac{s\gamma_{\text{side}}}{\cos\theta}\left(\frac{3}{sm\tan\theta}V\right)^{2/3}(1-\varepsilon^3)^{1/3}$$



Corresponds to the experimental results

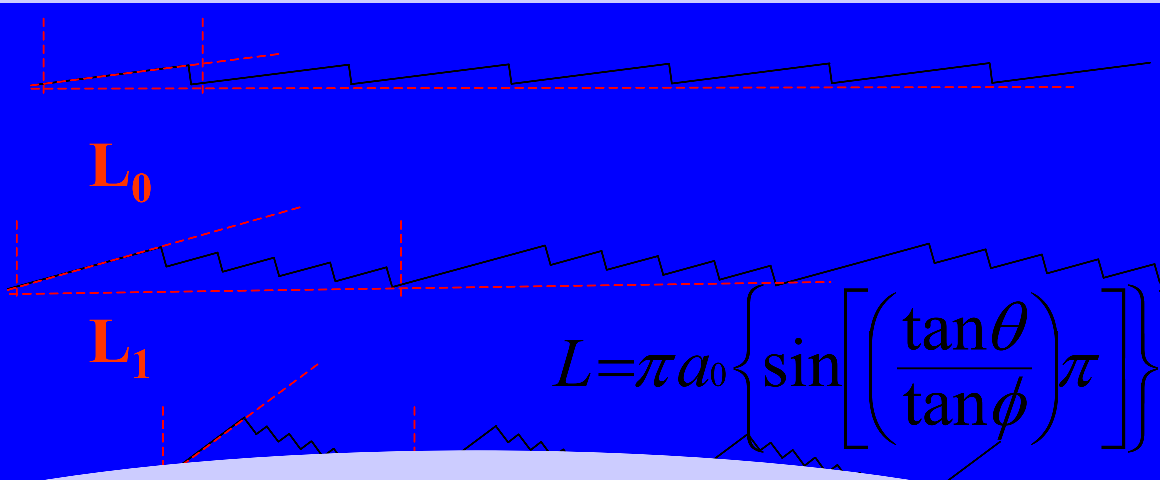
A. A. Stekolnikov and F. Bechstedt, PHYS. REV. B 72, 2005

INFLUENCE OF VICINAL SUBSTRATE

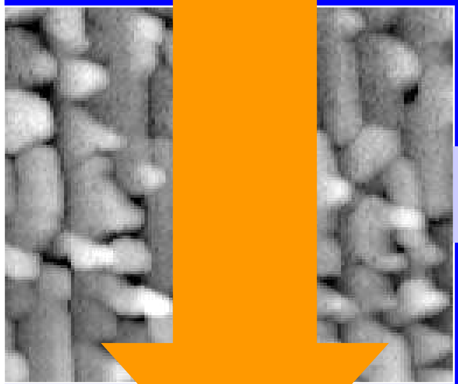


Scan size : 2 µn

0°off



$$L=\pi a_0\left\{\sin\left[\left(\frac{\tan\theta}{\tan\phi}\right)\pi\right]\right\}^{-1}$$



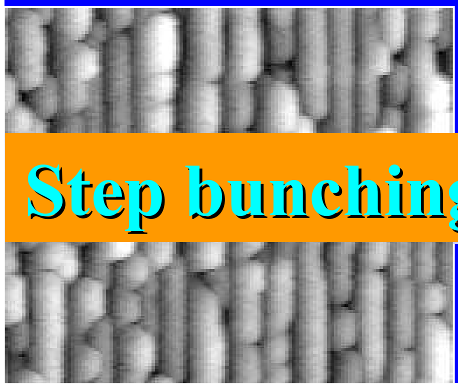
2

= Equilibrium shape of Ge / Si

P stable ... $(\theta_1)\,\Sigma_1 + \sigma_2\,(\theta_2)\Sigma_2$

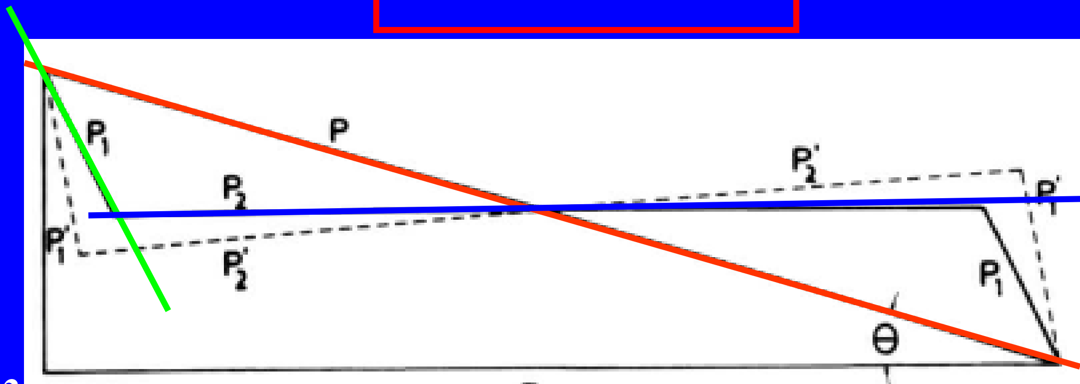
Condition of stability : **surface stiffness of p > 0**

$$\sigma^* = \sigma + \frac{d^2\sigma}{d\theta^2} > 0$$



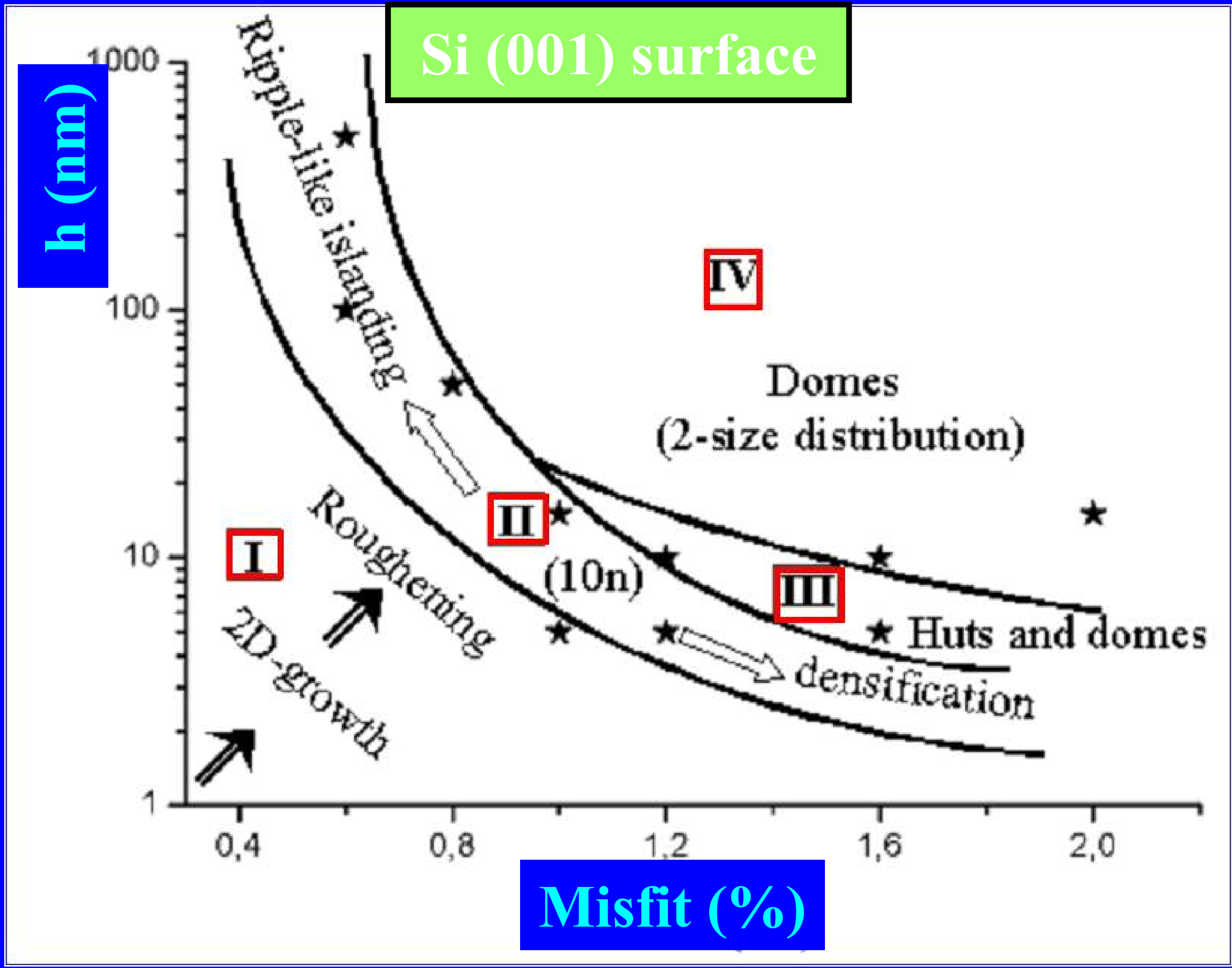
°off

h = 10 nm x = 0.3



GROWTH OF SiGe ON Si(001)

Morphological Evolution of SiGe Layers:
Experimental kinetic phase diagrams, Si(001)

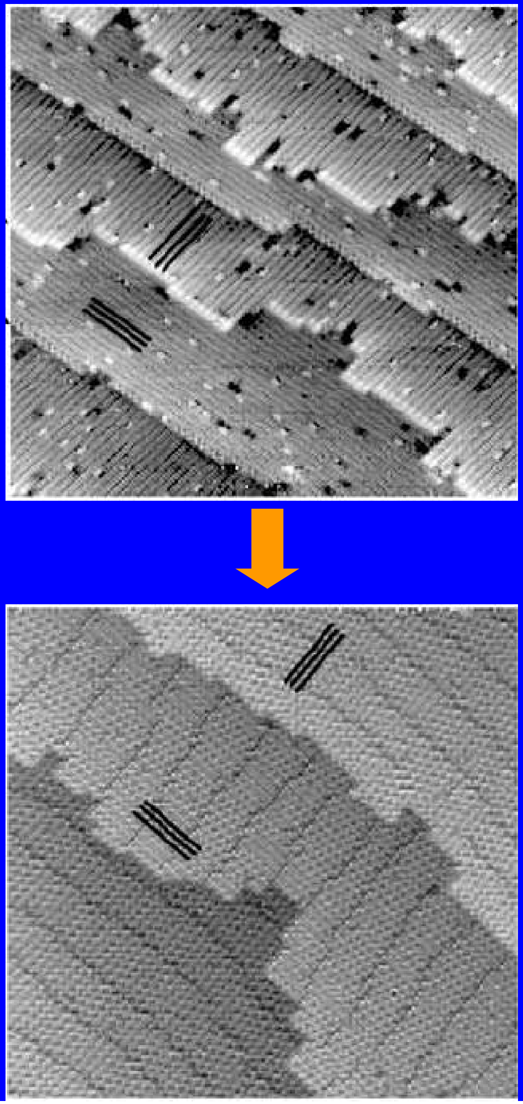


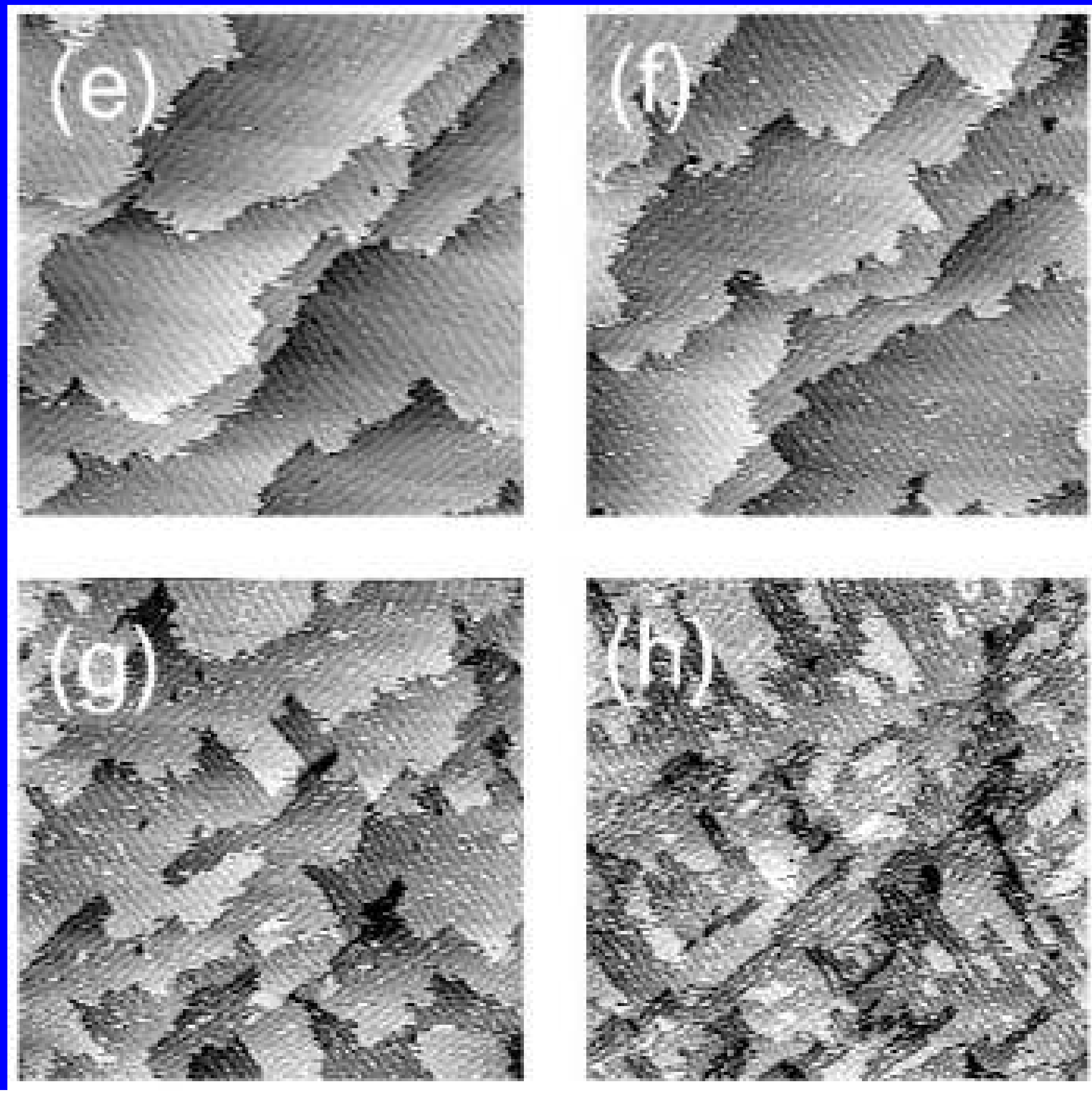
Tg ~550°C

➡ **4 growth regimes**

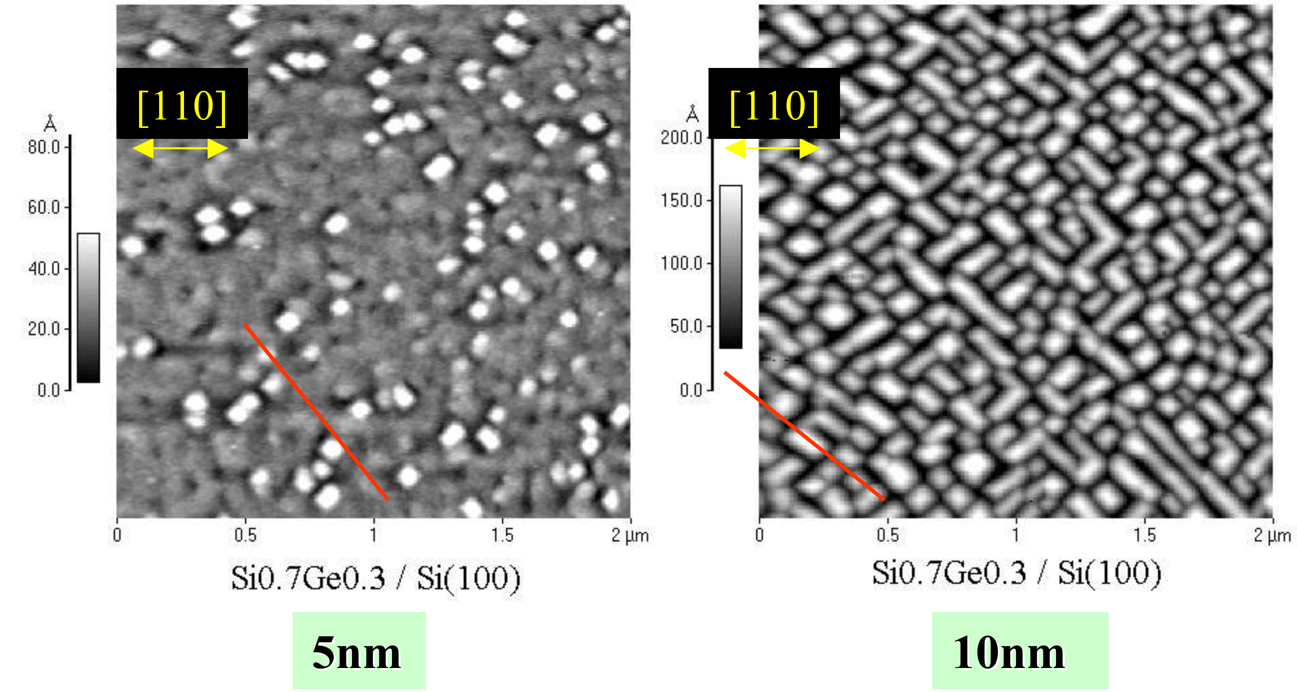
REGIME I: ROUGHENING

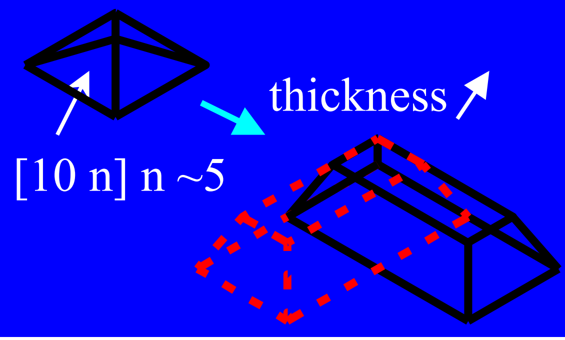
Remains flat during annealing



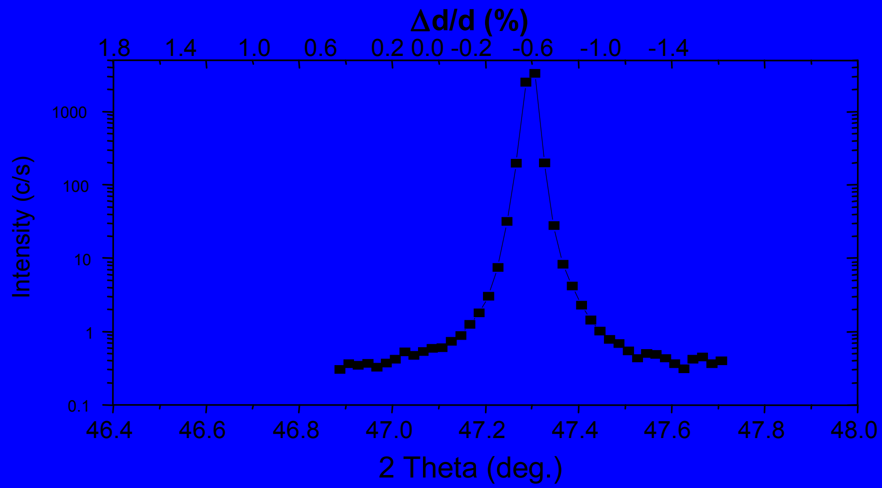


REGIME II : HUTS ISLANDS



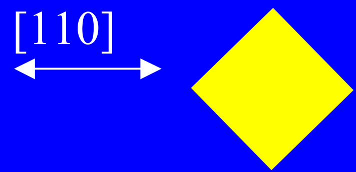


Stress Relaxation : *XRD analysis*

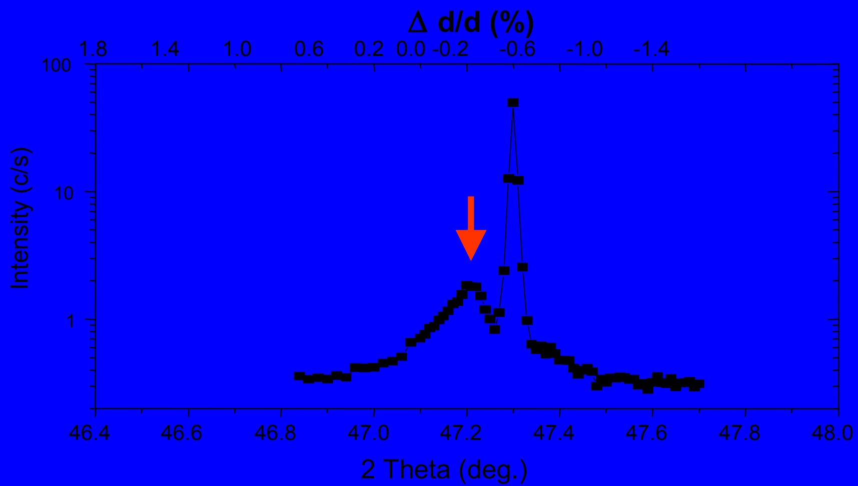


Si0.7Ge0.3/Si(100)

5nm

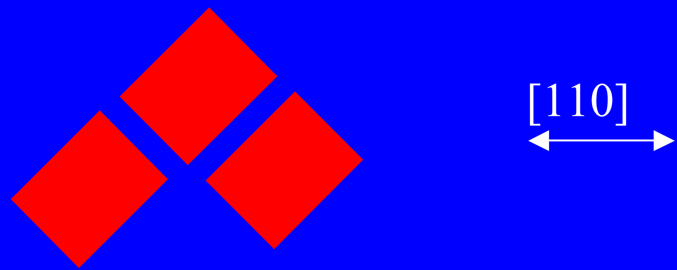


No relaxation



Si0.7Ge0.3/Si(100)

10nm

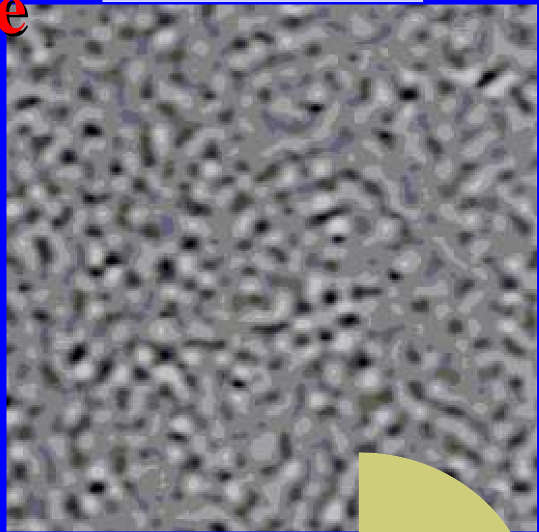


Small relaxation (0.2%)

(Δd/d~1.2% if total relaxation)

Rough / Ripple-like

As grown



Scan : 5 µm

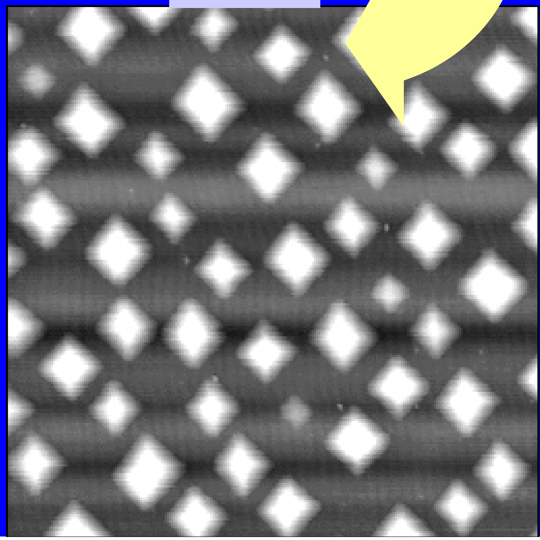
x=0.25

m=1%

h = 50Å

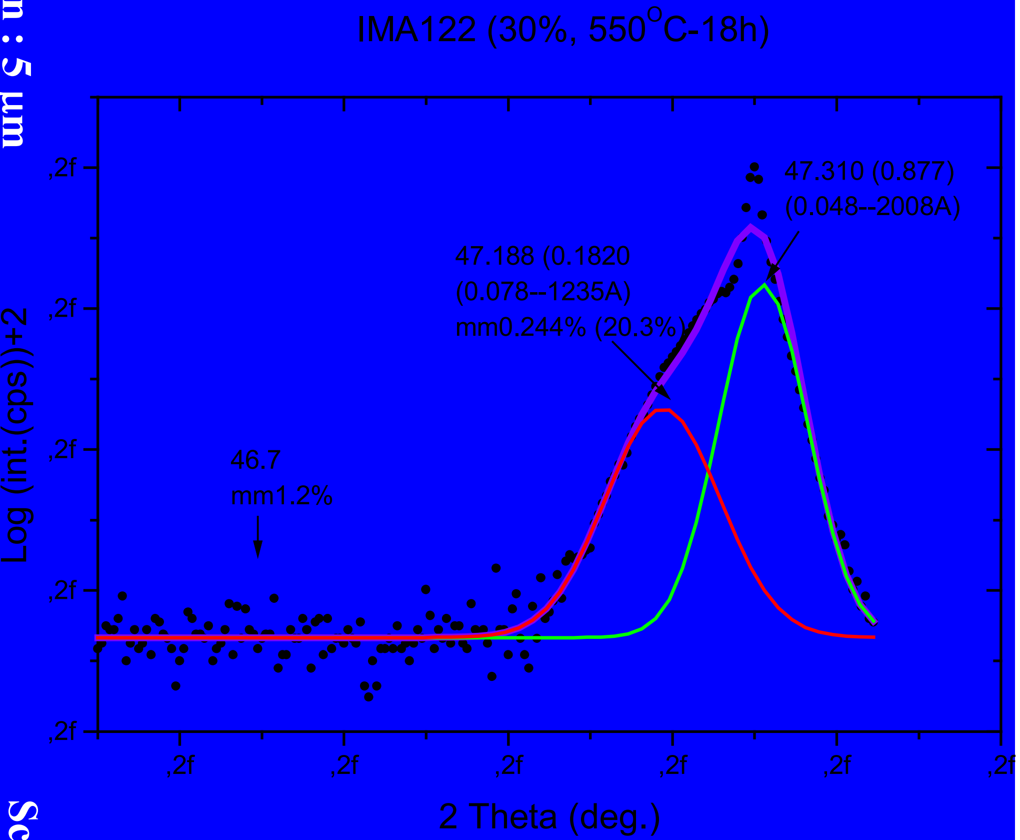
Annealing 550°C (1h30 - 18 h)

64 h

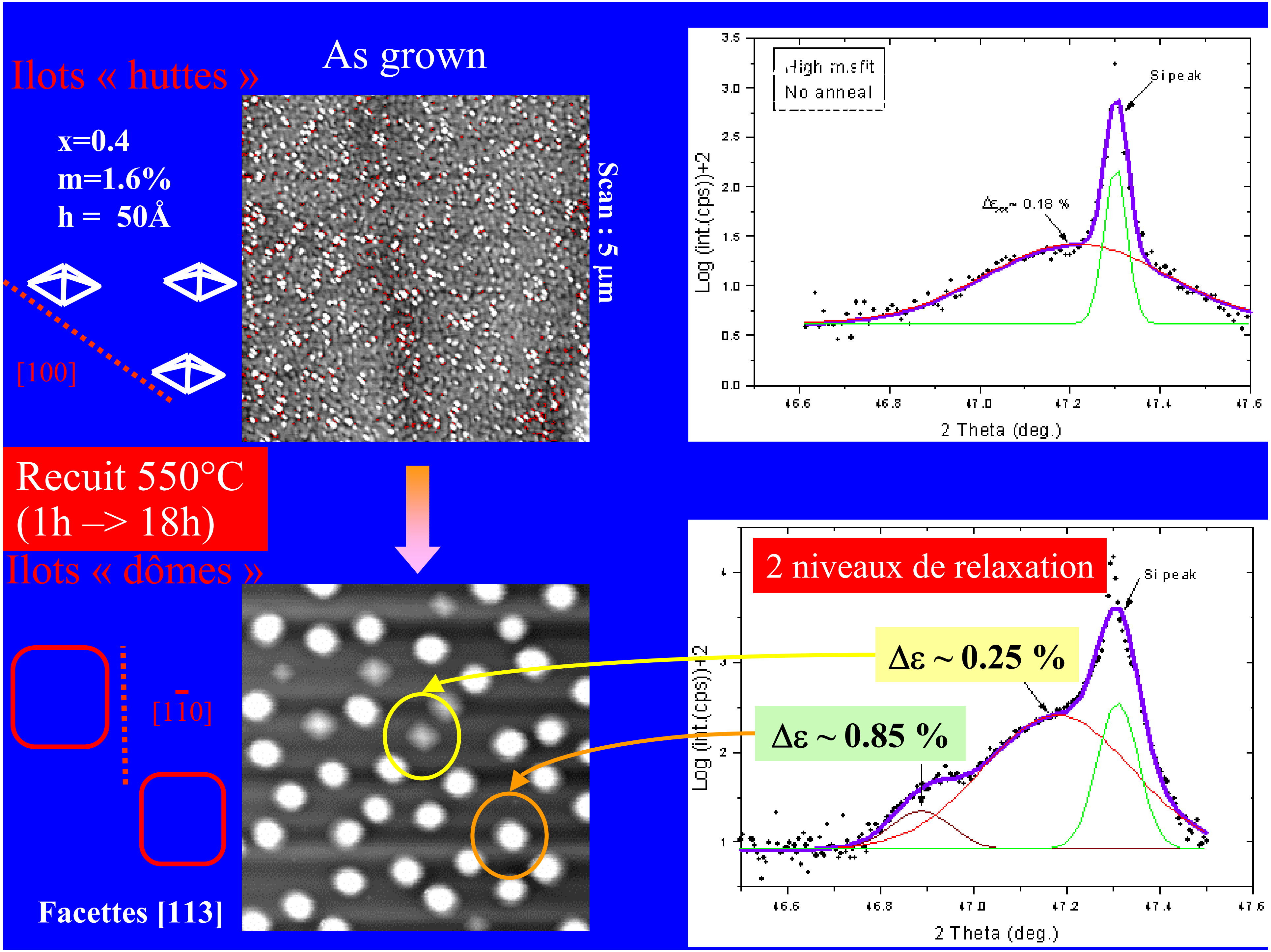


Scan : 2 µm

Huts



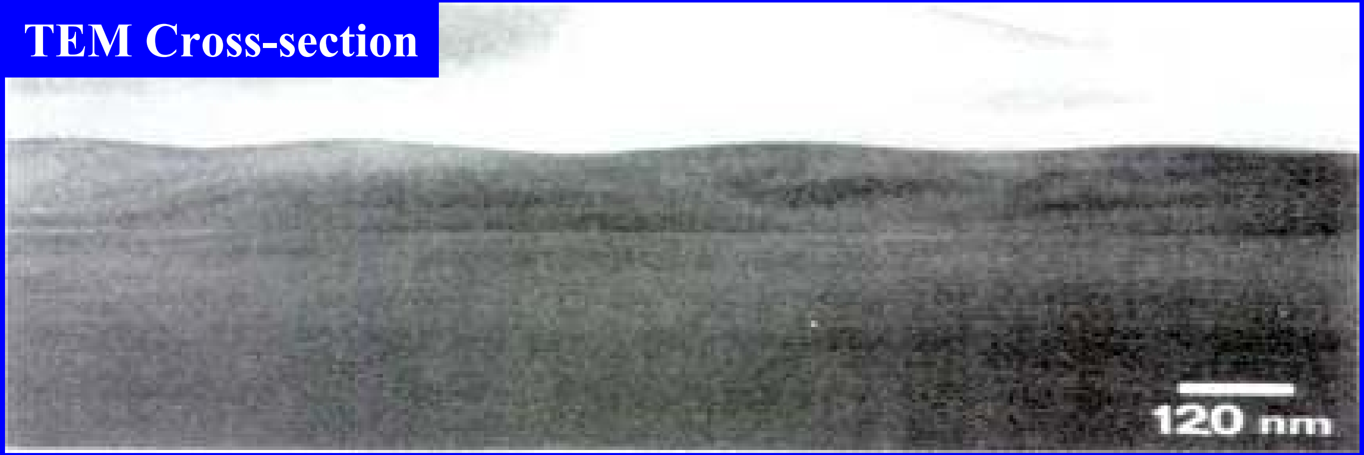
Δε = 0.25% relaxation

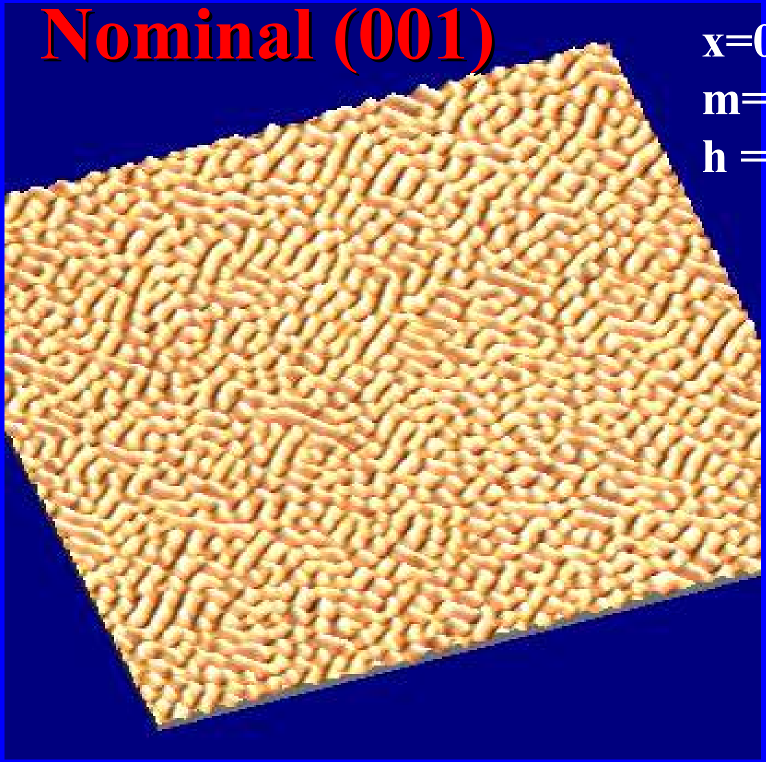


Ilots « huttes »
As grown
x=0.4
m=1.6%
h = 50Å
[100]
Scan : 5 µm
High misfit
No anneal
Si peak
Δε ~ 0.18 %
Log (int.(cps))+2
2 Theta (deg.)
Recuit 550°C
(1h –> 18h)
Ilots « dômes »
[1-10]
Facettes [113]
2 niveaux de relaxation
Si peak
Δε ~ 0.25 %
Δε ~ 0.85 %
Log (int.(cps))+2
2 Theta (deg.)

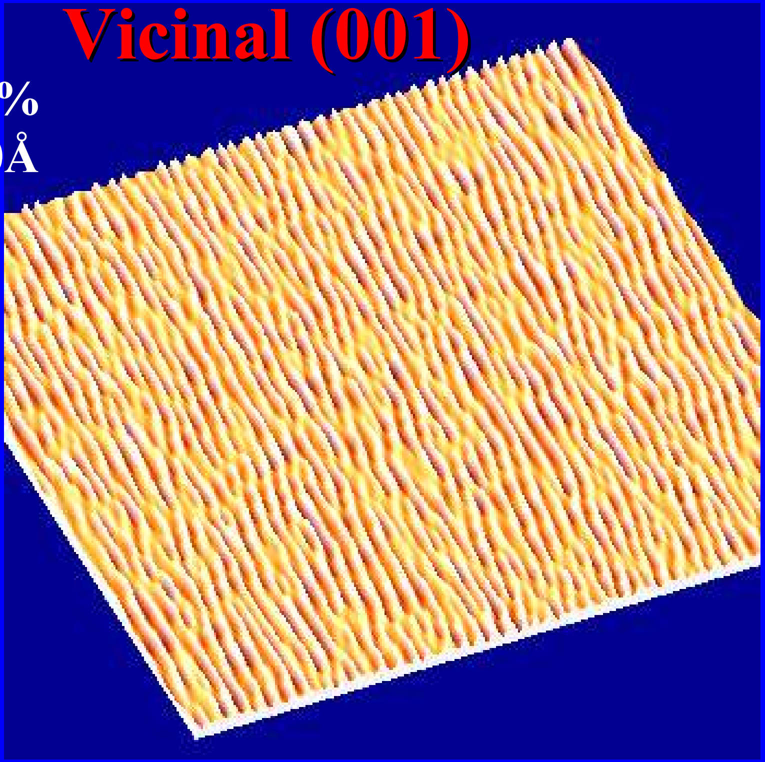
Influence of vicinal substrate

TEM Cross-section





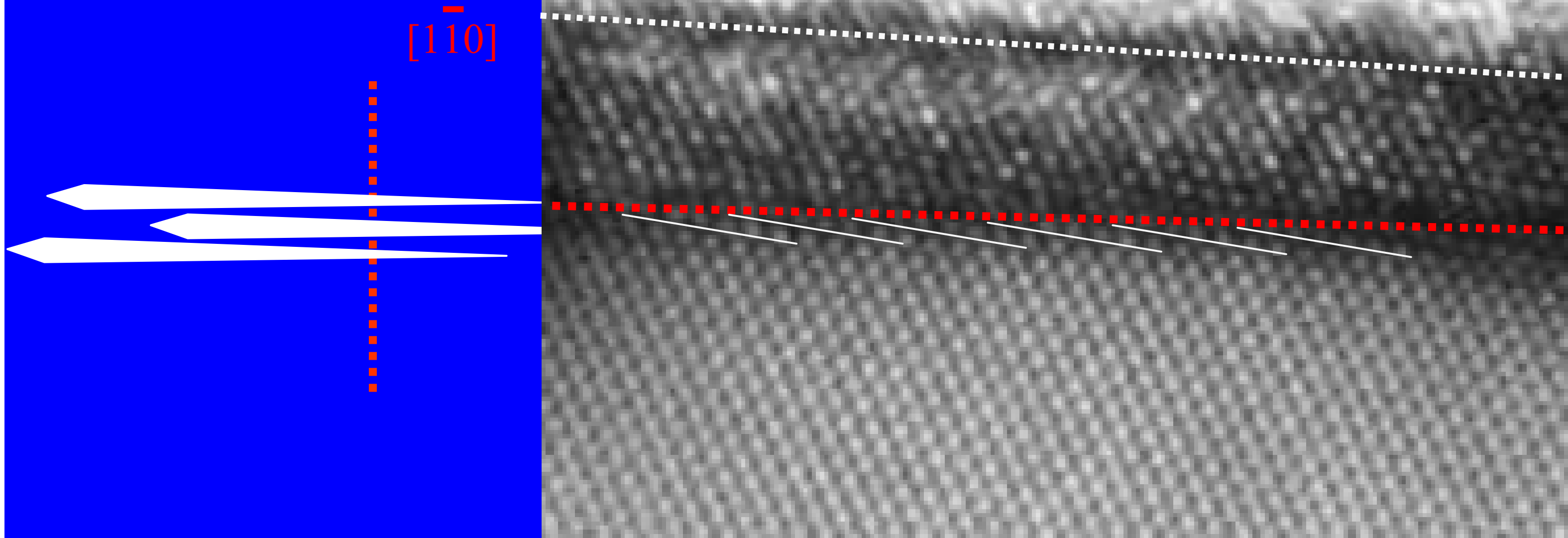
x=0.4
m=1.6%
h = 50Å



Scan : 5 µm

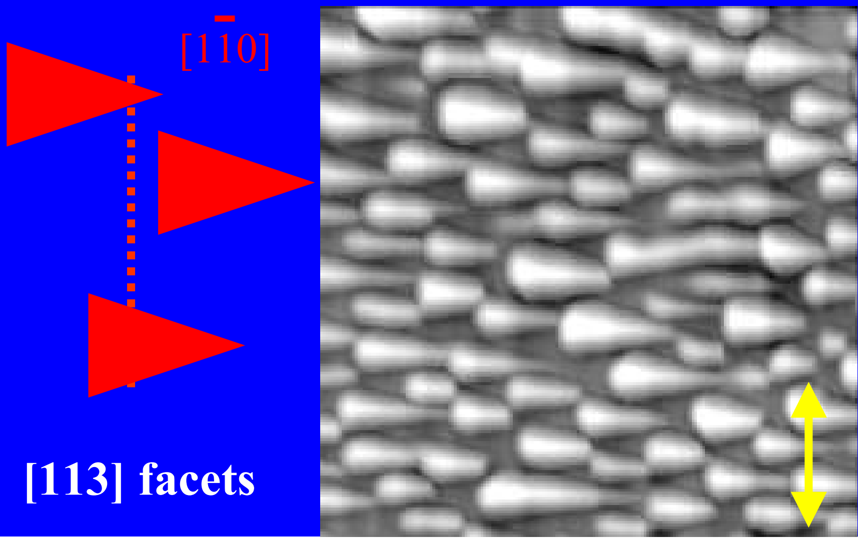
(118) Si = (001) 10° off

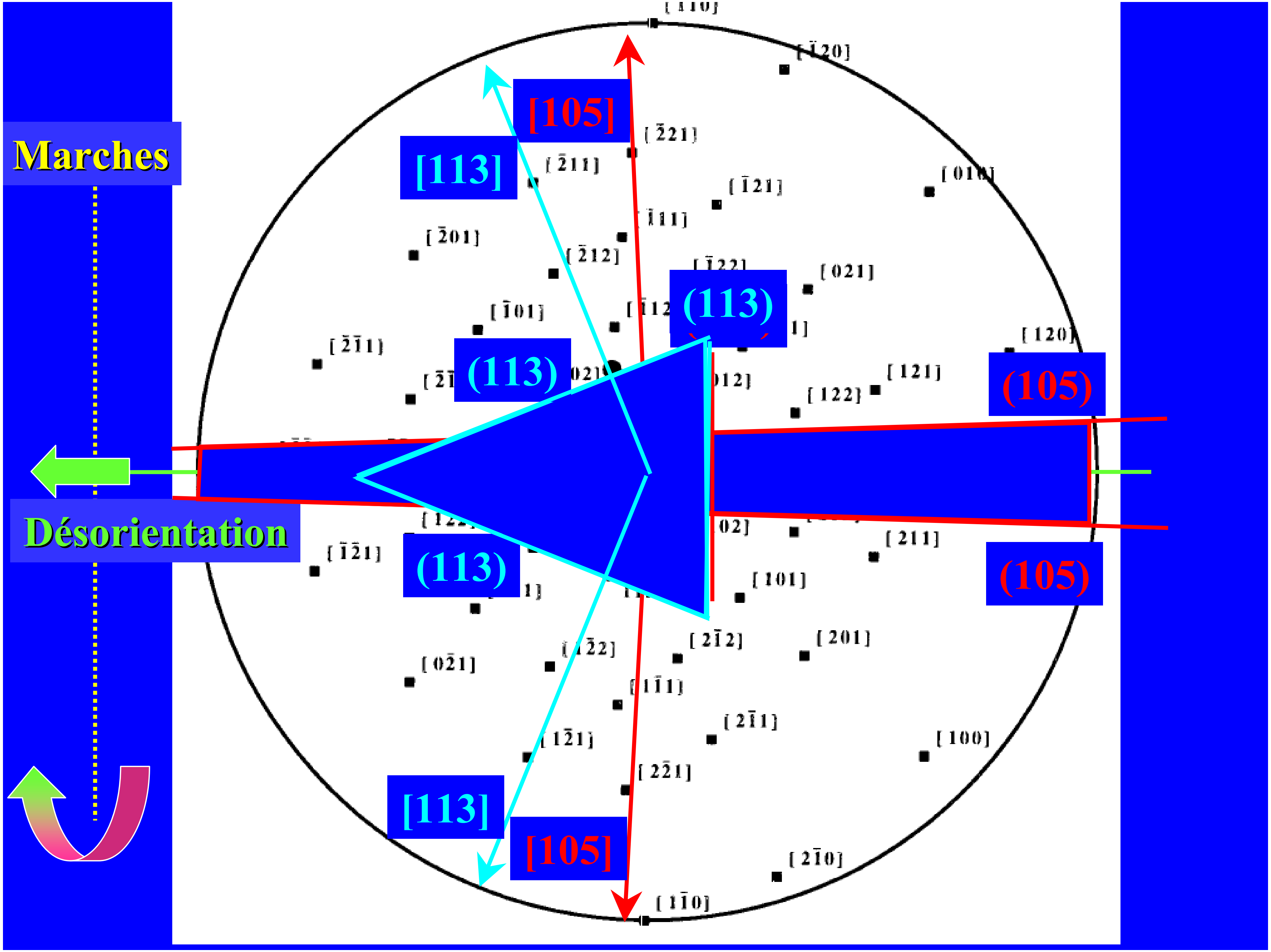
As grown



Annealed 550°C
(1h –> 18h)

« Domes » islands

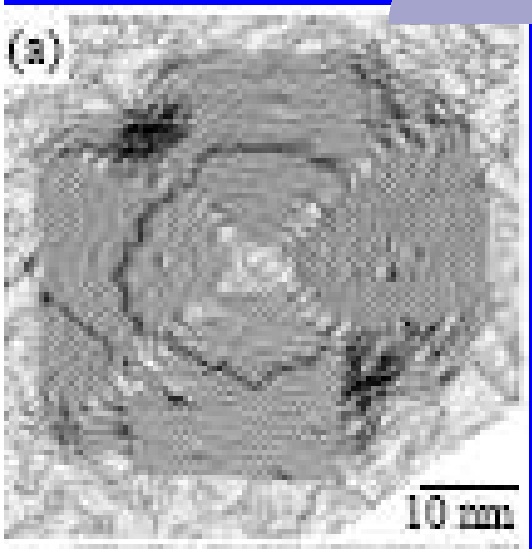


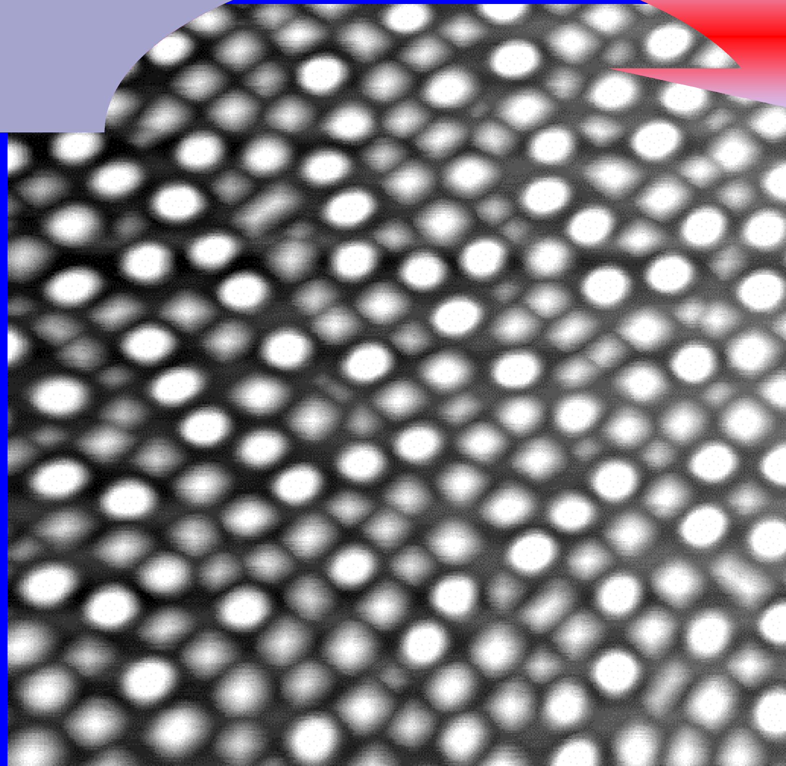


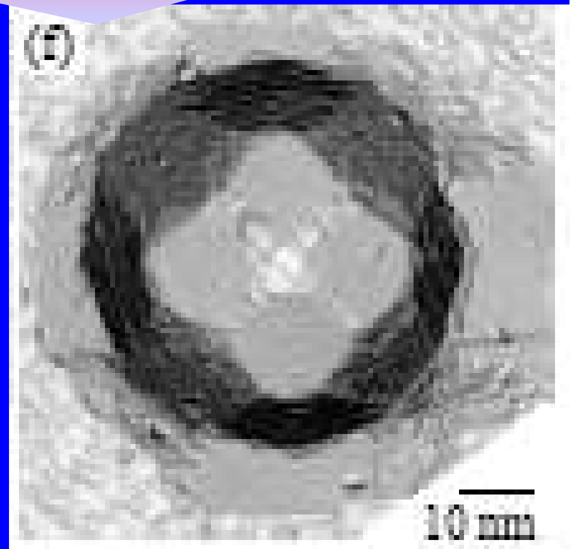
Marches
Désorientation
[105]
[113]
(113)
(113)
(105)
(113)
(105)
[113]
[105]

REGIME III: BIMODAL ISLANDS

Morphological shape transition







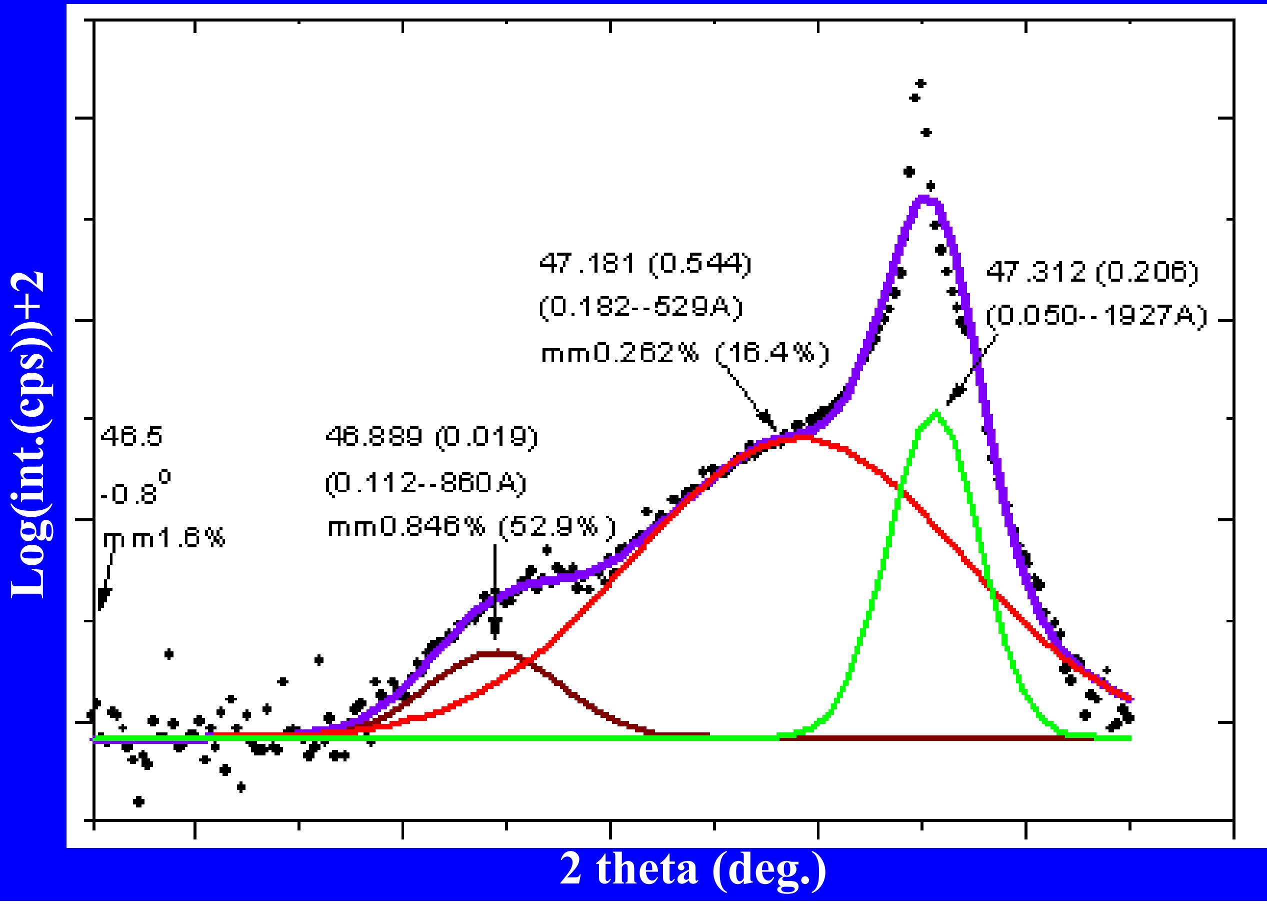
SiGe 35% 100 Å

Transition : Huts ⇨ Domes

Bimodal relaxation

Huts and Domes

0.25% and 0.85% relaxation



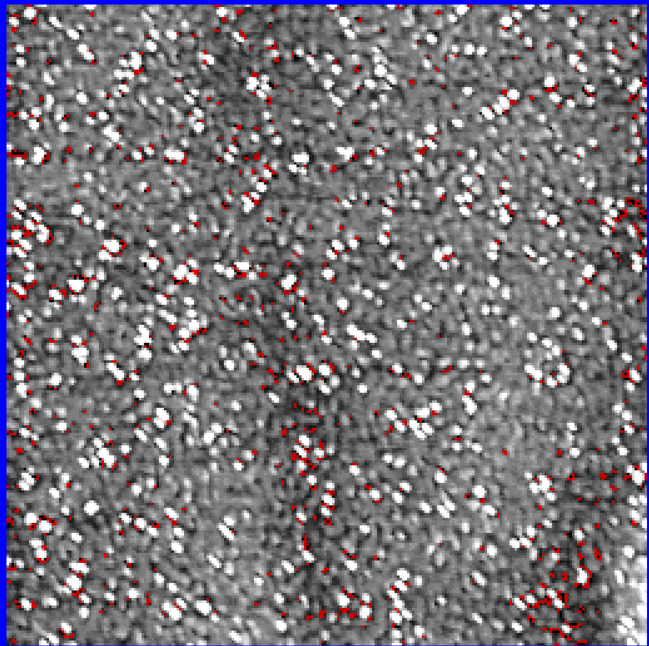
As grown | **Annealing 550°C 18 h**

Huts → Huts + Domes

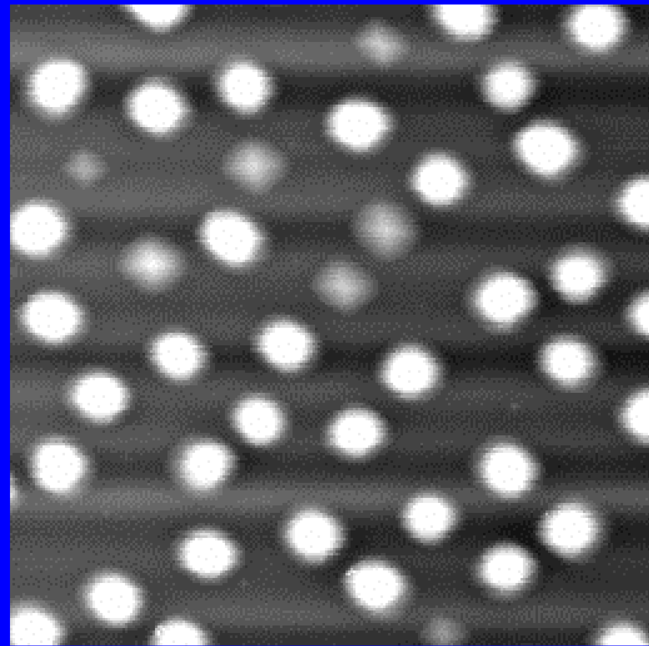
x=0.4

m=1.6%

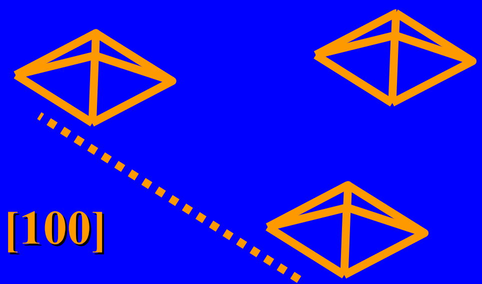
h = 50Å



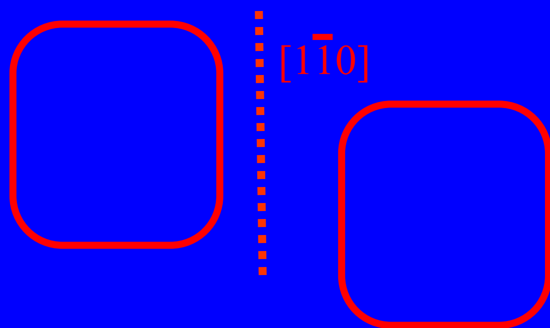
Scan : 5 µm



Scan : 2 µm

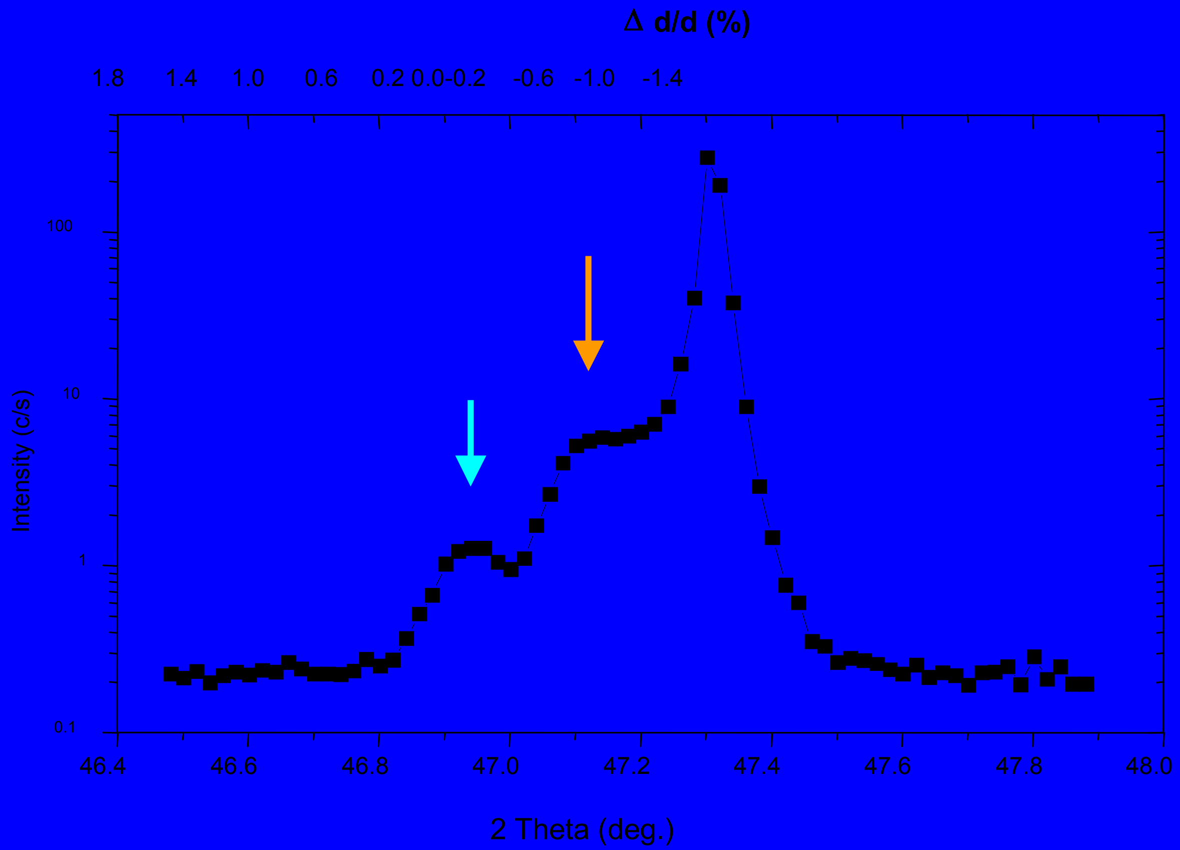


[105]* facets



[113]* facets

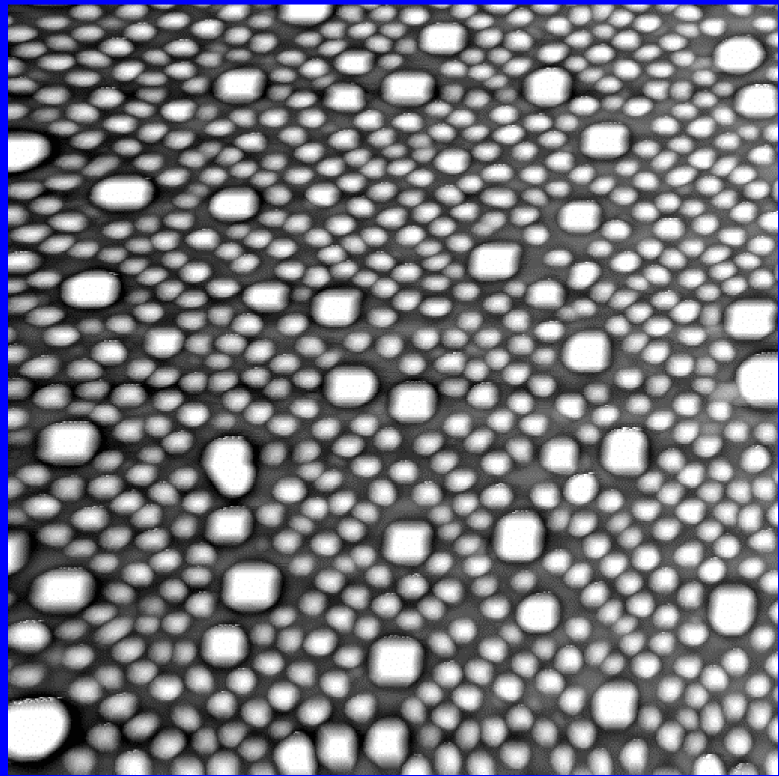
Stress Relaxation



Aspect ratio / Relaxation

REGIME IV: BIMODAL DOMES

Bimodal size distribution of Domes



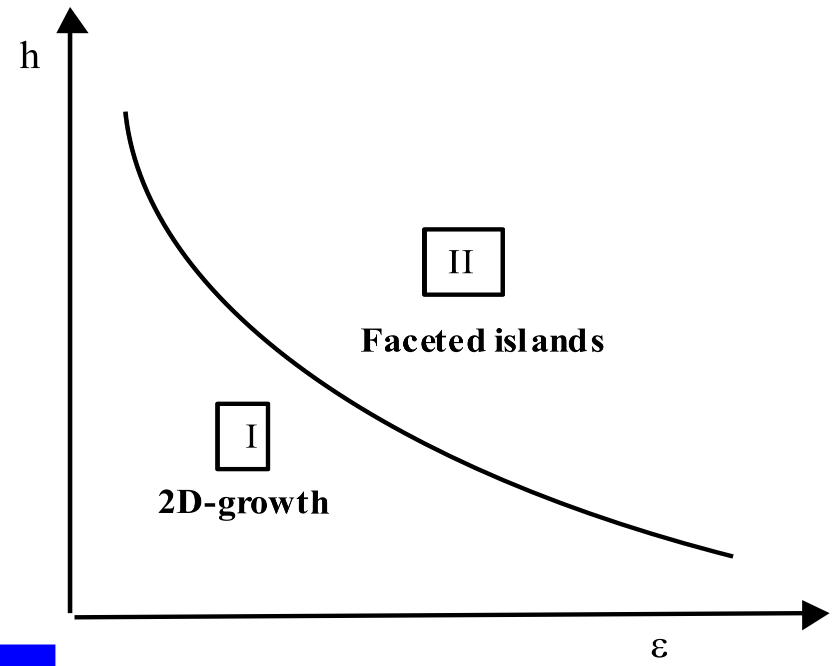
Scan : 20 µm

x = 50 % m = 2 %150 Å

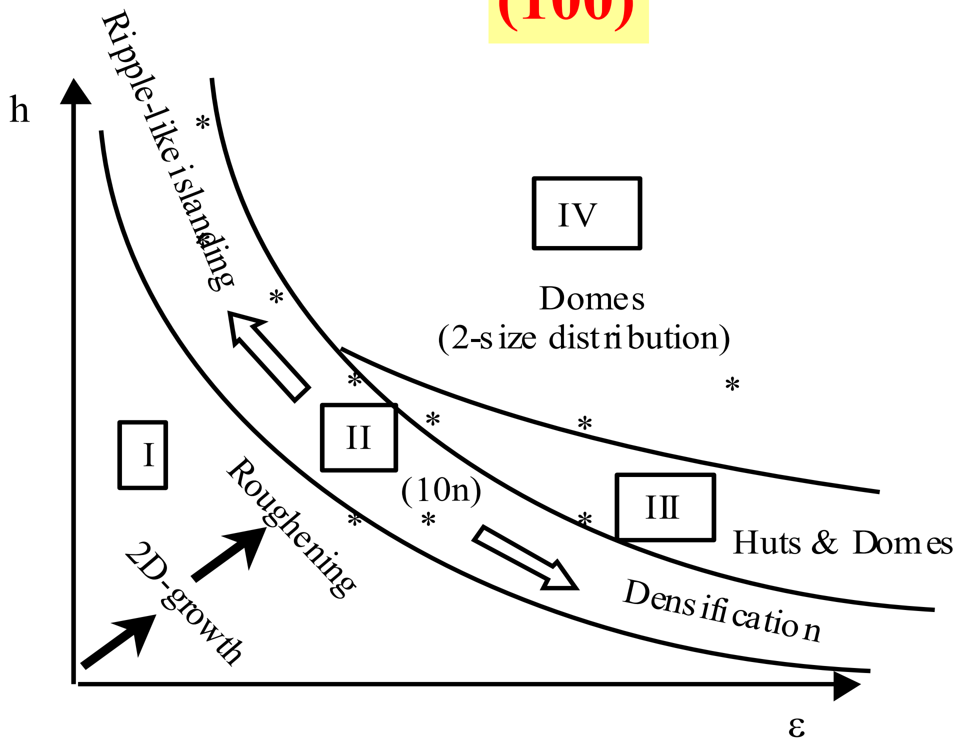
Again 2 levels of relaxation

KINETIC PHASE DIAGRAMS

(111)



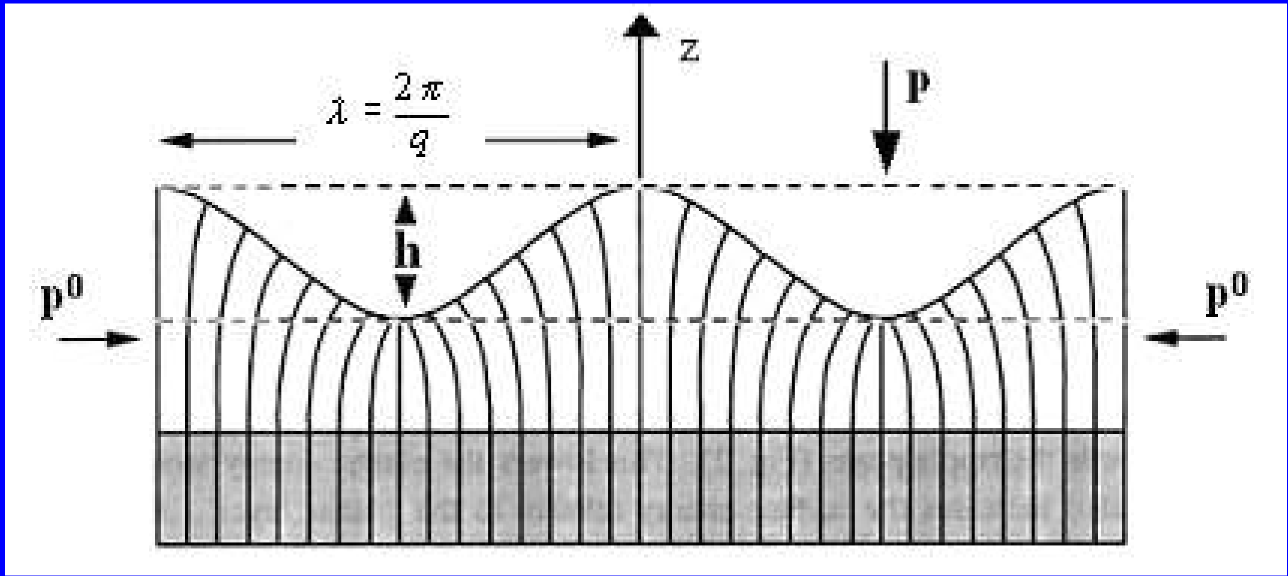
(100)



No kinetic instability
No strained islands

Regime II: growth instability
Regime III: islands
Morphological island transition explained by stress relaxation

Stress driven instability ???



Total surface free energy :

Capillarity energy:

$$\frac{\partial F_{cap}}{\partial A} = \frac{\sigma}{4} h^2 q^2$$

Elastic relaxation :

$$\frac{\partial F_{relax}}{\partial A} \approx -h p^0 \varepsilon$$

Strain fields gradients

$$\frac{\partial F_{el}}{\partial A} \approx \frac{C \varepsilon^2}{2q}$$

Macroscopic strain models cannot explain :

- **comparison (111) / (001)**
- **wires perpendicular to step edges**

New model

SK on (001) ≠ relaxation of elastic energy

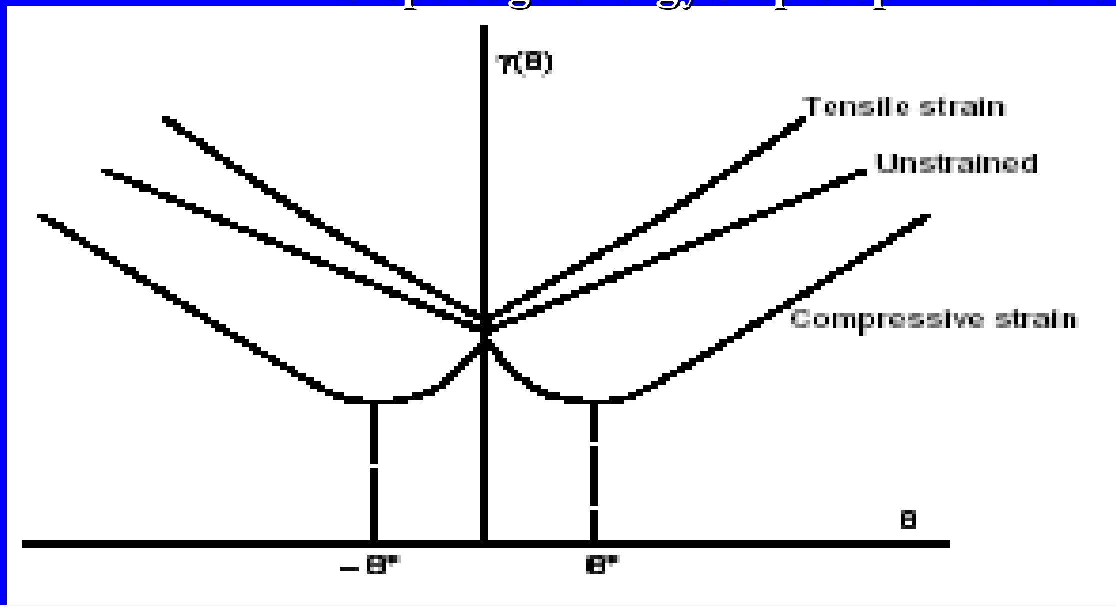
BUT : **SK instability does not form on Si(111)**
Stabilisation of (105) facets under stress

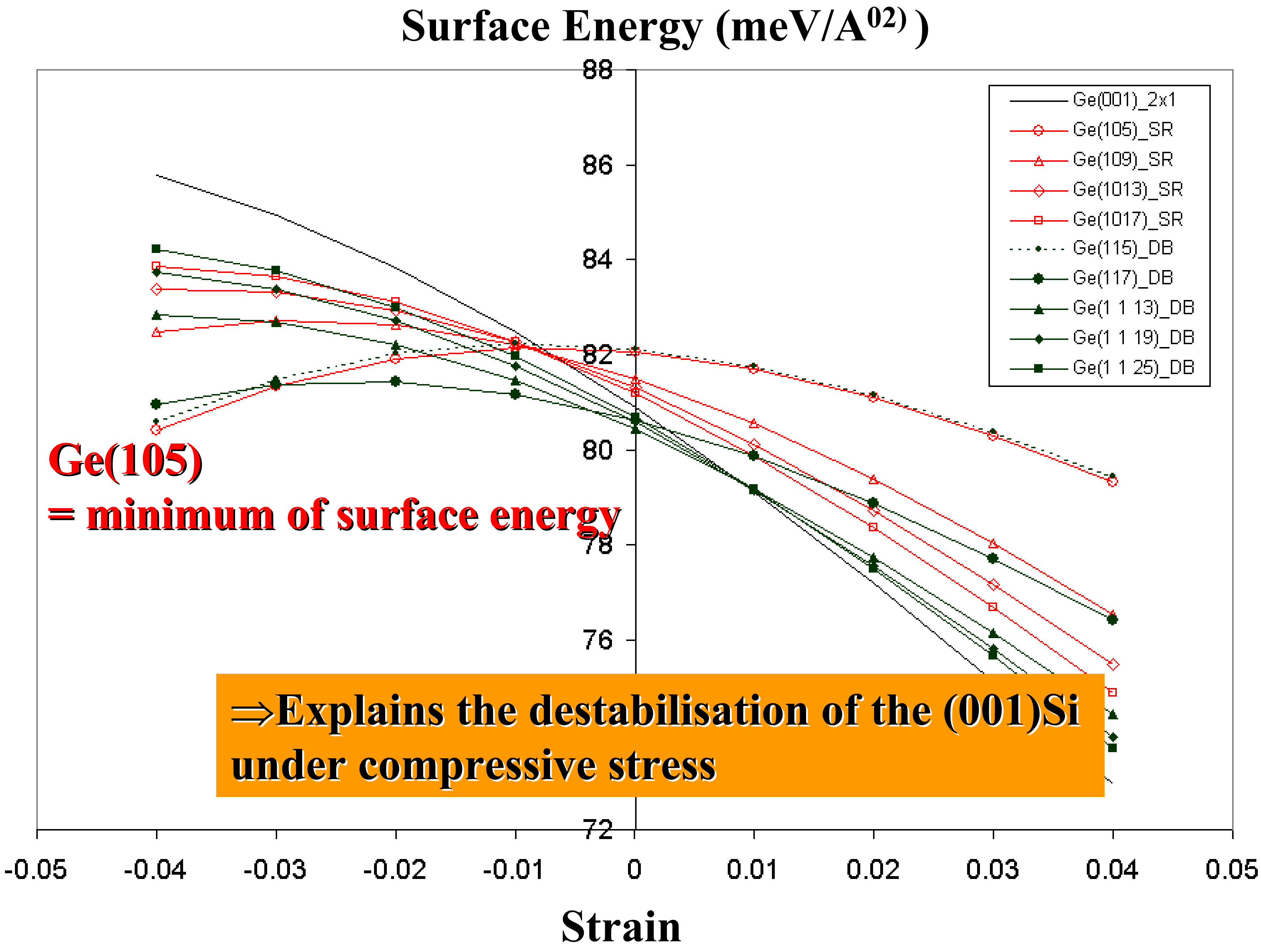
- Surface reconstruction (MD et ab initio) Raiteri, Migas, Miglio, Phys Rev. Lett. (2002)
Balance elastic energy and facet energy

-Sufrface energy of vicinal surface (continuum model)
Tersoff Phys Rev. Lett.; Shenoy, Freund (2002)

$$\gamma(\theta) = \gamma_0 \cos\theta + \beta_1 |\sin\theta| + \beta_3 \frac{|\sin\theta|^3}{\cos^2\theta}$$

Steps edge energy **Step-step Interaction**





Surface Energy (meV/A02))
88
86
84
82
80
78
76
72
-0.05
-0.04
-0.03
-0.02
-0.01
0
0.01
0.02
0.03
0.04
0.05
Strain
Ge(001)_2x1
Ge(105)_SR
Ge(109)_SR
Ge(1013)_SR
Ge(1017)_SR
Ge(115)_DB
Ge(117)_DB
Ge(1 1 13)_DB
Ge(1 1 19)_DB
Ge(1 1 25)_DB
Ge(105)
= minimum of surface energy
⇒Explains the destabilisation of the (001)Si under compressive stress

MORPHOLOGICAL EVOLUTION

Si(111): 2D layer by layer ⇨ 3D dislocated islands

THERMODYNAMIC EQUILIBRIUM SHAPE

Si(001) : 2D ⇨ instability ⇨ islanding ⇨ 3D dislocated islands

elongated islands ⊥ step deges

SURFACE ENERGY MINIMIZATION + KINETICS