Intermixing-promoted scaling of self-assembled island sizes : the Ge/Si(100) system.

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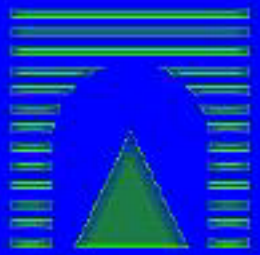


Outline

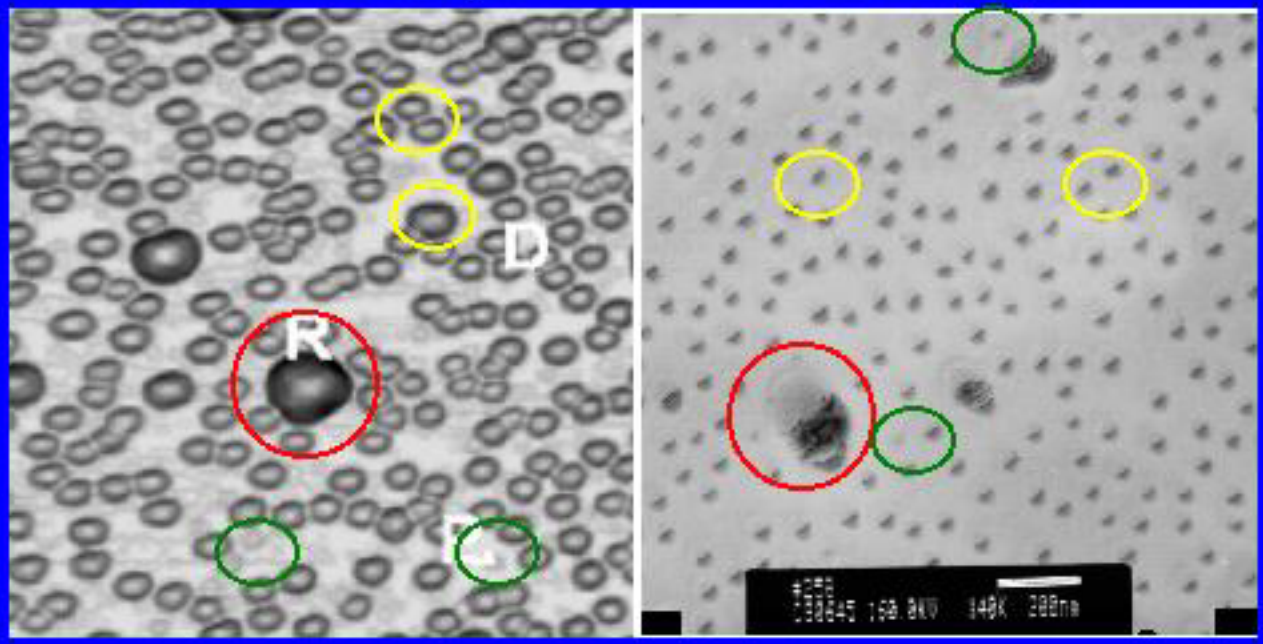
- Ge/Si(100) self assembling in the SK growth mode:
  - Evolution of morphology and strain
  - Parameter definitions
- The role of the deposition temperature:
  - Evidence for a Ge-Si intermixing
  - Island size scaling with the actual misfit

Ge/Si(100) self assembling

We can correlate the structural to morphological properties

Differential AFM 1× 1 μm²

TEM 1× 1 μm²



T_{dep}=600°C
θ=12 ML
UHV-CVD

Plastically relaxed domes (interrupted Moiré pattern)

Strained multifaceted domes (steeper)

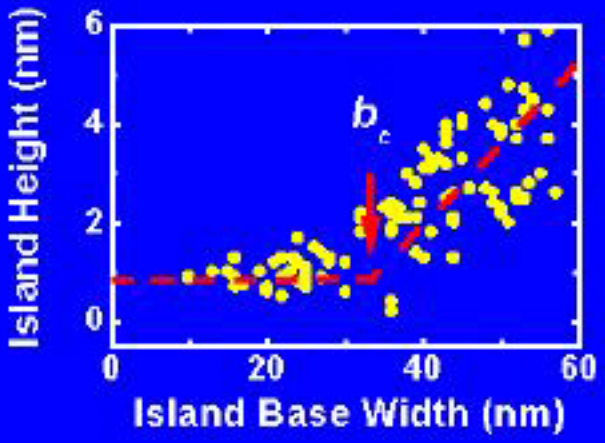
Strained pyramids

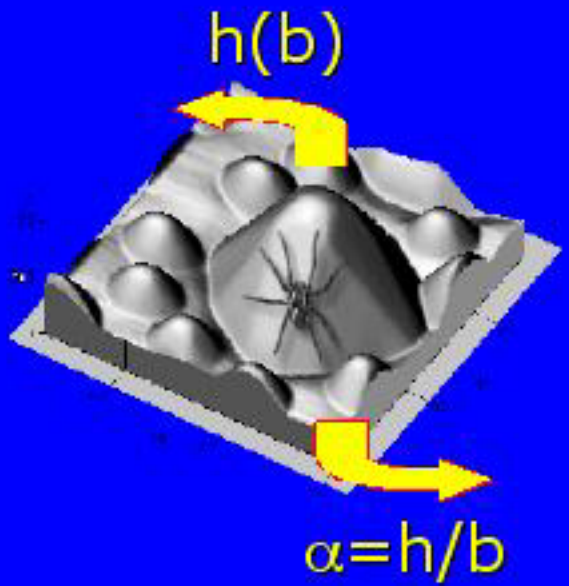
Platelets (precursors, not detectable this scale)

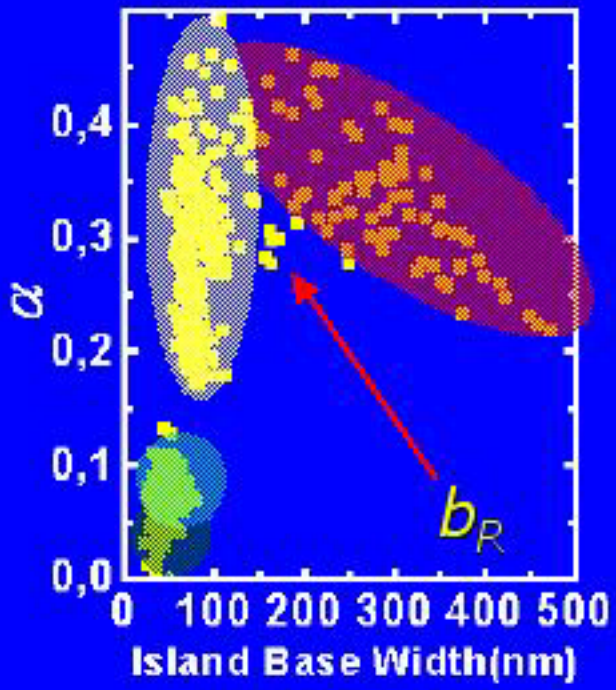
} Moiré pattern spacing Δ

Ge/Si(100) self assembling

Defining quantitative parameters of the growth







(F= 10 ML/min T_{dep}=600°C, 0-45 ML)

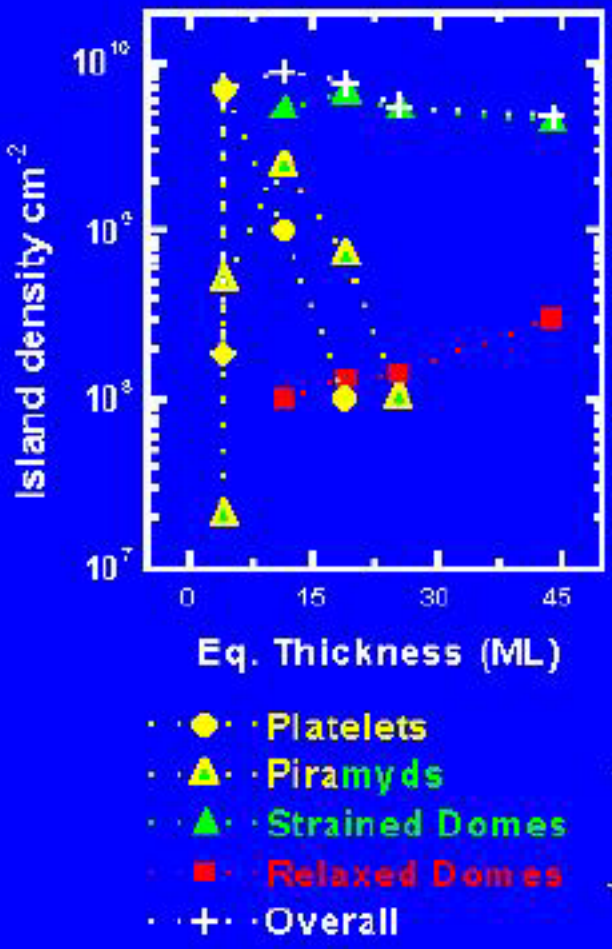
b_c: critical base for the 2D-3D transition (from platelets to pyramids)

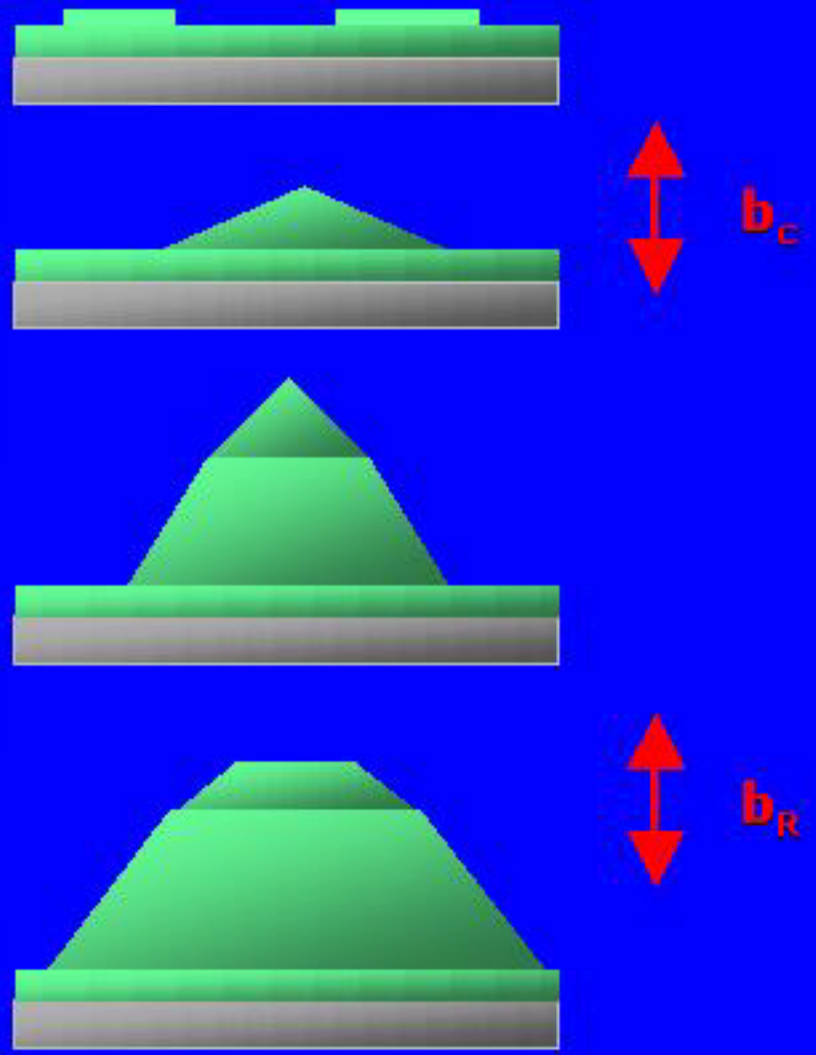
b_R: inversion of the aspect ratio α=h/b derivative with b

(from strained to relaxed domes)

Ge/Si(100) self assembling

The growth dynamics evolves through metastable states



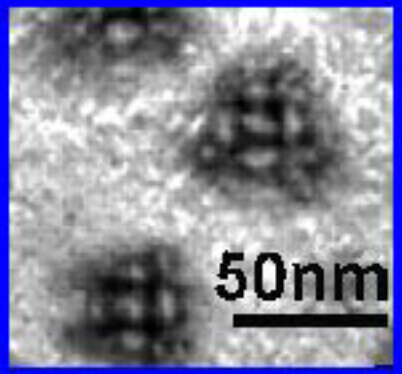


Ge/Si(100) self assembling

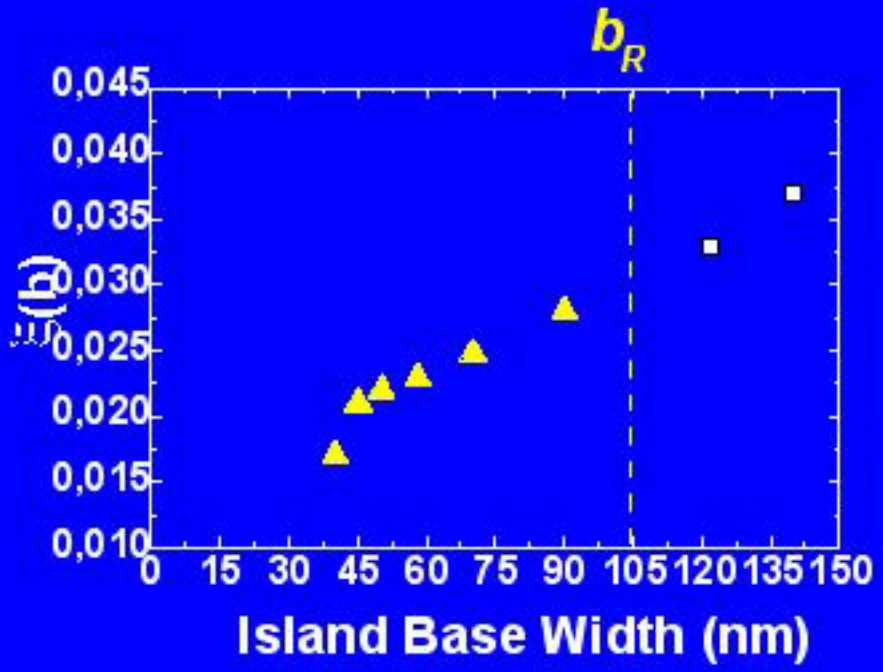
Searching for morphology-strain evolution during the growth: why the aspect ratio increases

From TEM
(two beams [220])

$\xi = d_{Si}/(\Delta - d_{Si})$: lattice mismatch



Measurement performed on a choice of individual island of a given size, no intermixing is assumed (verify later on: T=500°C)



Increasing the island size (i.e. α) the lattice planes are allowed to bend: nearly complete elastic relaxation $\xi = \varepsilon_o$

Ge/Si(100) self assembling

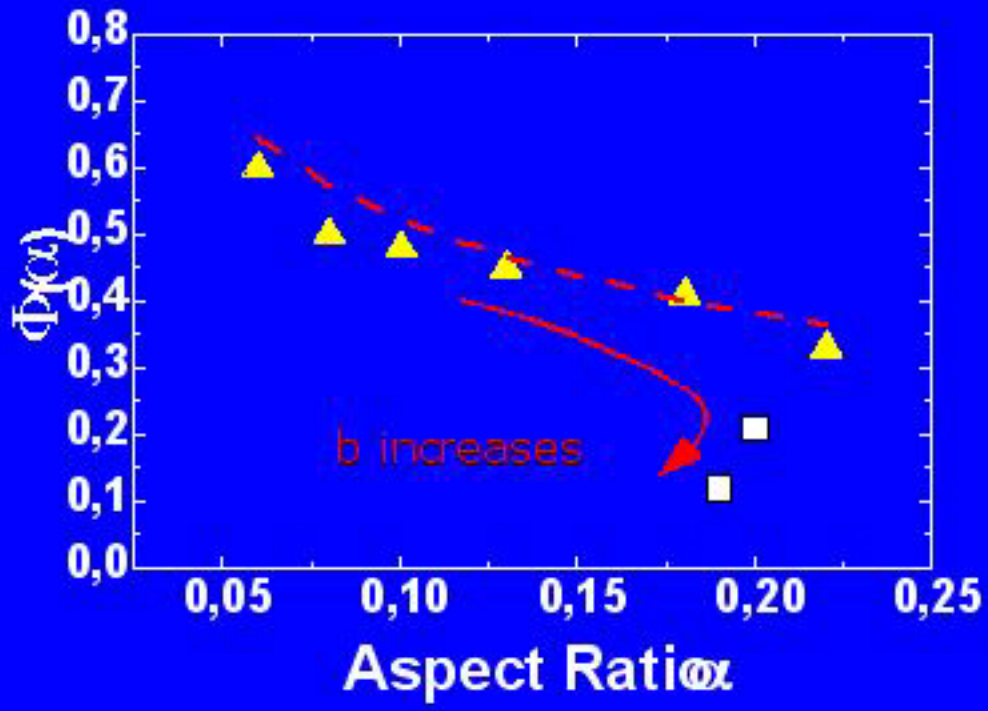
The 3D growth allows strain energy relaxation

$$E_{st}=C(\Phi(\alpha)*\varepsilon)^2$$

C:elastic constant
$\Phi(\alpha)$: relaxation function
ε : heterostructure misfit
(no intermixing then=4.2%)

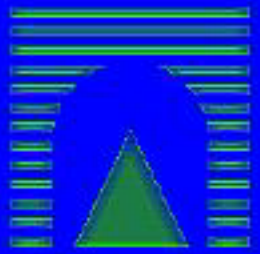
$$\Phi(\alpha) = 1 - \xi(b(\alpha)) / \varepsilon$$

$b(\alpha)$ obtained from AFM



Agreement with thetheory .
Christiansenet al., APL **66**, 574 (1995).

- We can derive the universal function$\Phi(\alpha)$ for strain relaxation.
- MDs insertion implies change in the α (b) behavior.
- The chosen b_R is the critical base for MD insertion



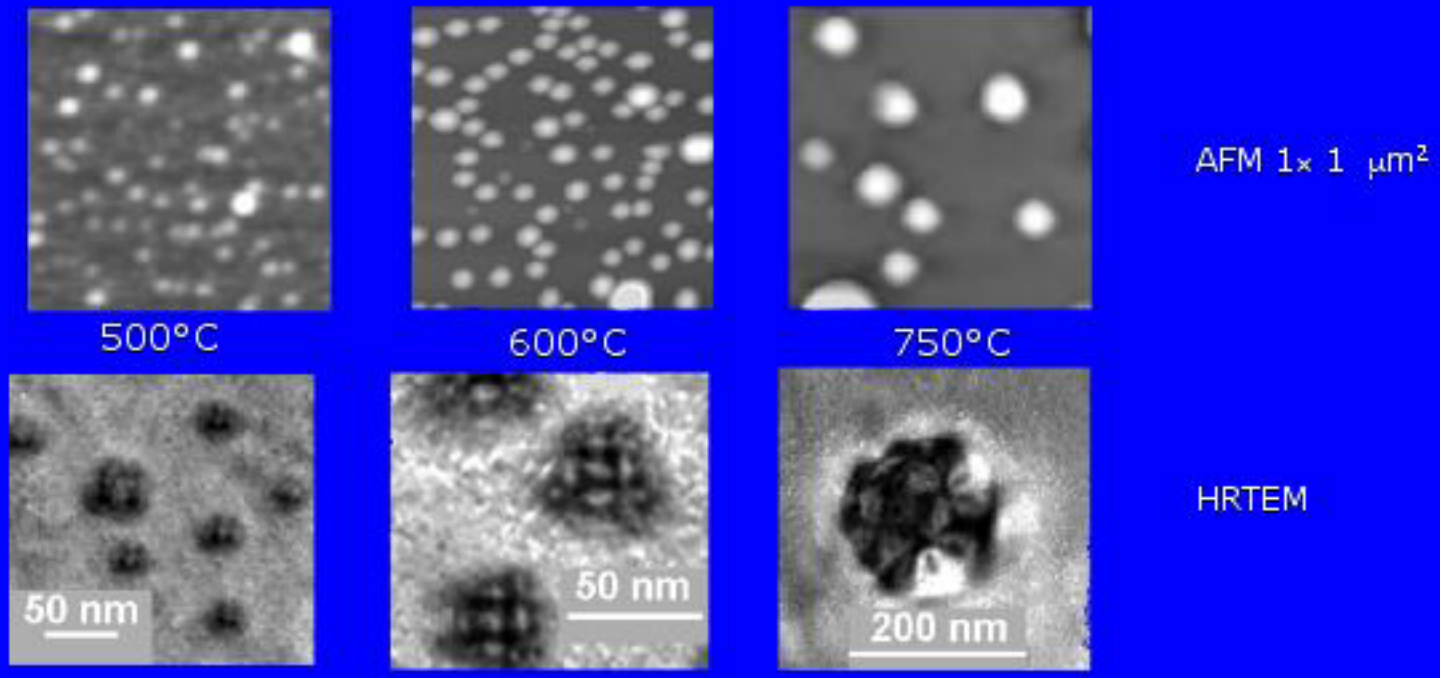
Ge/Si(100) self assembling

- Well defined pathway toward the equilibrium shape.
- Energy relaxation-shape evolution evidenced.
- Parameters b_c b_R have been defined.

The role of the deposition temperature

Constant growth rate and coverage, variable T_{dep}

(F= 10 ML/min, θ=12 ML, T=450-850°C)

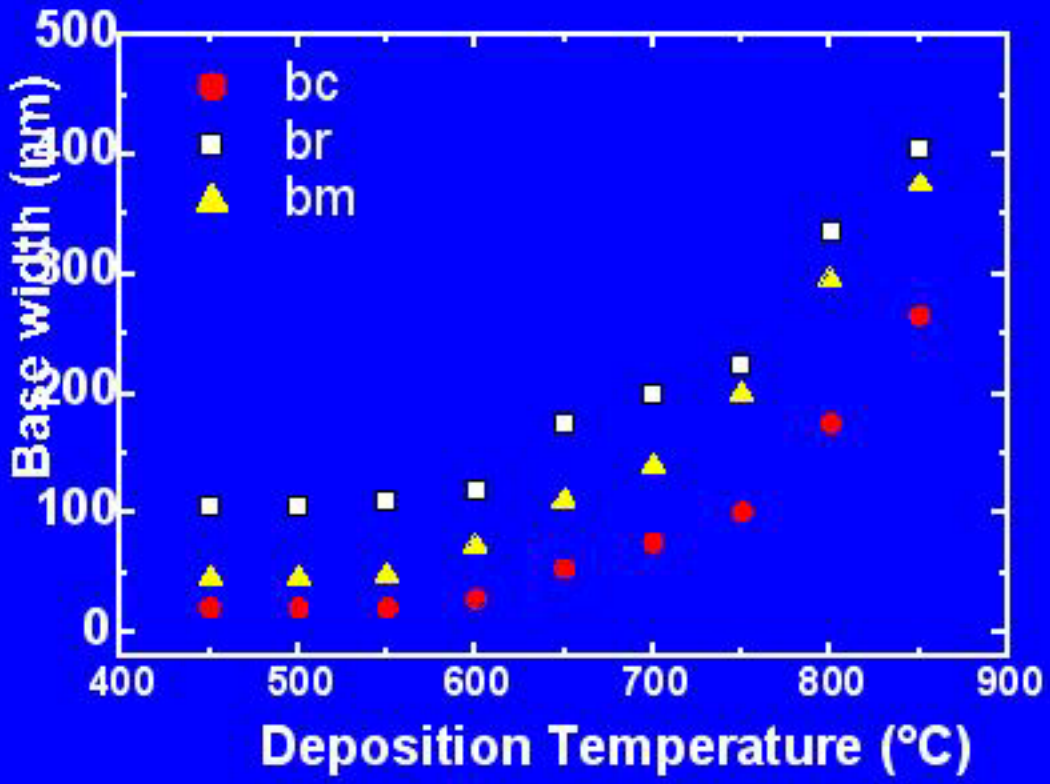


Upon increasing T_{dep} we observe:

- similar growth dynamics (b_c,b_R properly describe the system)
- typical sizes of each island family increases

The role of the deposition temperature

To be more quantitative.....



Above 550°C b_c, b_R, and the average strained island base b_m increase: why?

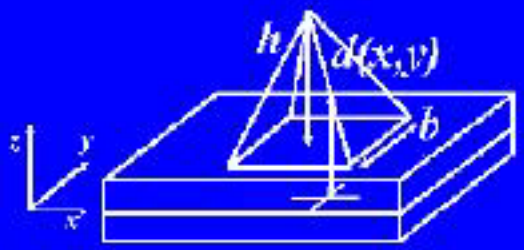
SiGe INTERMIXING

The role of the deposition temperature

A new technique to measure island composition

From AFM

Sample Morphology



From XPS

Ge, Si photoemitted currents

$$\int_{Sample} dI(x,y,z) = \int_{Sample} I_0 N_\gamma \sigma_\gamma e^{-\frac{d(x,y)-z}{\lambda_\gamma}} dxdydz$$

One can calculate the expected photoemitted current ratio R_{th} given the actual sample morphology

The role of the deposition temperature

We obtained

Capellini et al., Appl. Phys. Lett. **78,** 303(2001).

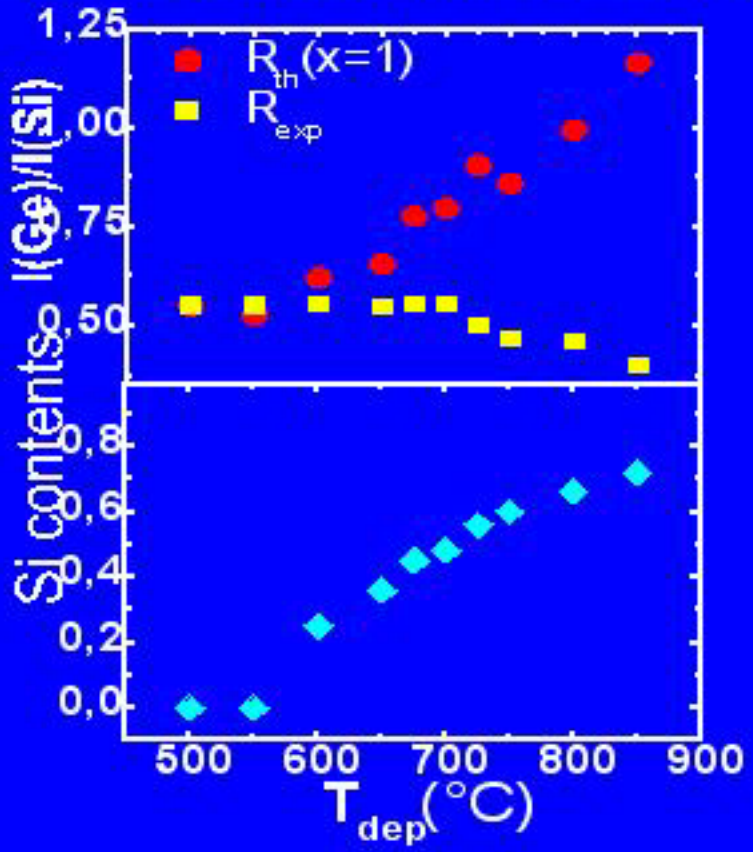
$$R_{Th} = \frac{\sigma_{Ge}}{\sigma_{Si}} \frac{x\left[1 - \frac{e^{-\frac{d_{wl}}{\lambda}}}{A}\left(\theta + 2\sum_i b_i^2\left(\frac{\lambda}{\alpha_i b_i} + \left(\frac{\lambda}{\alpha_i b_i}\right)^2\left(e^{-\frac{\alpha_i b_i}{\lambda}} - 1\right)\right)\right)\right]}{1 - x\left[1 - \frac{e^{-\frac{d_{wl}}{\lambda}}}{A}\left(\theta + 2\sum_i b_i^2\left(\frac{\lambda}{\alpha_i b_i} + \left(\frac{\lambda}{\alpha_i b_i}\right)^2\left(e^{-\frac{\alpha_i b_i}{\lambda}} - 1\right)\right)\right)\right]}$$

A: sample area
σ: atomic cross section
x : average Ge contents
λ: electron escape depth
b_i: i-th island base width
α_i: i-th island aspect ratio

The x Ge content is the only fitting parameter

The role of the deposition temperature

By comparing the experimental and the theoretical ratio one can obtain the actual sample composition



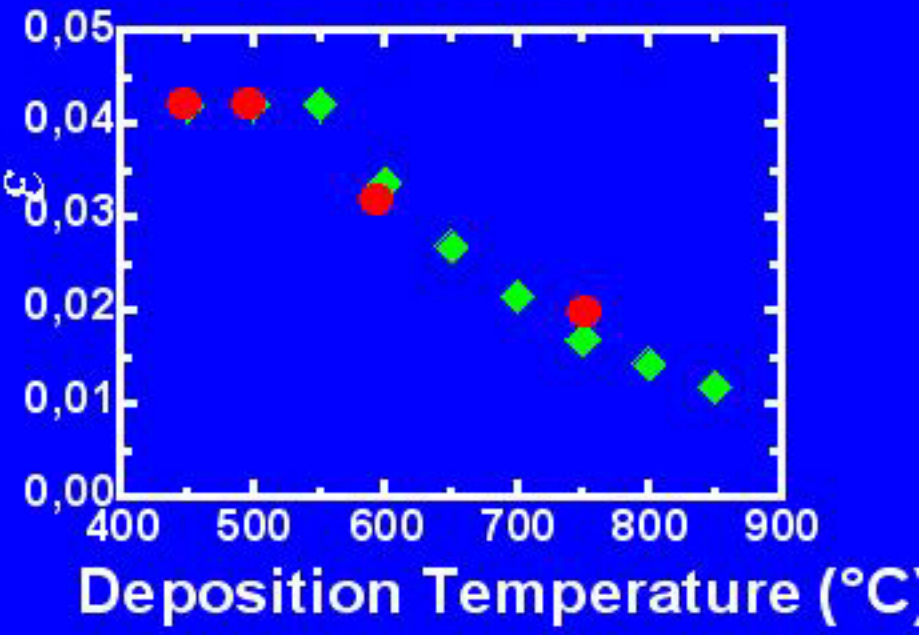
Strain driven, temperature enhanced intermixing is evidenced for $T_{dep} > 550°C$

The role of the deposition temperature

By means of a AFM/XPS technique we can evaluate the actual composition of the island layer and derive $\varepsilon = \varepsilon_0 * x$,

Given the universality of $\Phi(\alpha)$ obtained in the non-intermixed case (is only shape dependent), and measuring by TEM the lattice mismatch ξ, we can extract

$$\varepsilon = \xi / 1 - \Phi(\alpha)$$

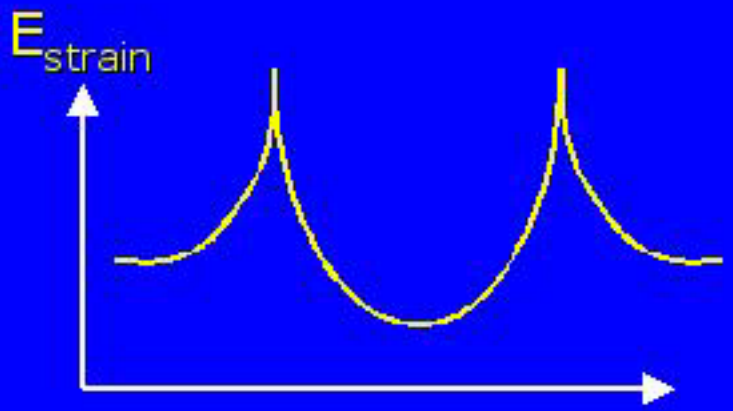


The main effect of the T_{dep} increase is to promote GeSi intermixing

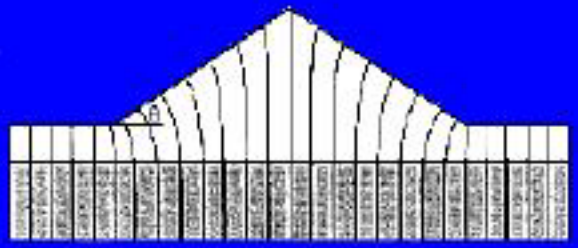
The higher the intermixing the lower the heterostructure effective misfit

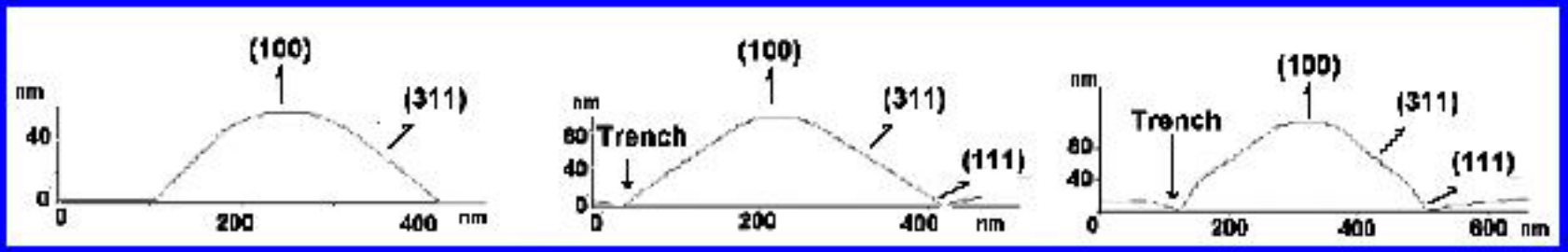
The role of the deposition temperature

The intermixing offer an alternate way to reduce the strain energy, atom dragging from the substrate is enhanced



Trenches surrounding the islands at $T_{dep} > 550°C$





500°C 600°C 750°C

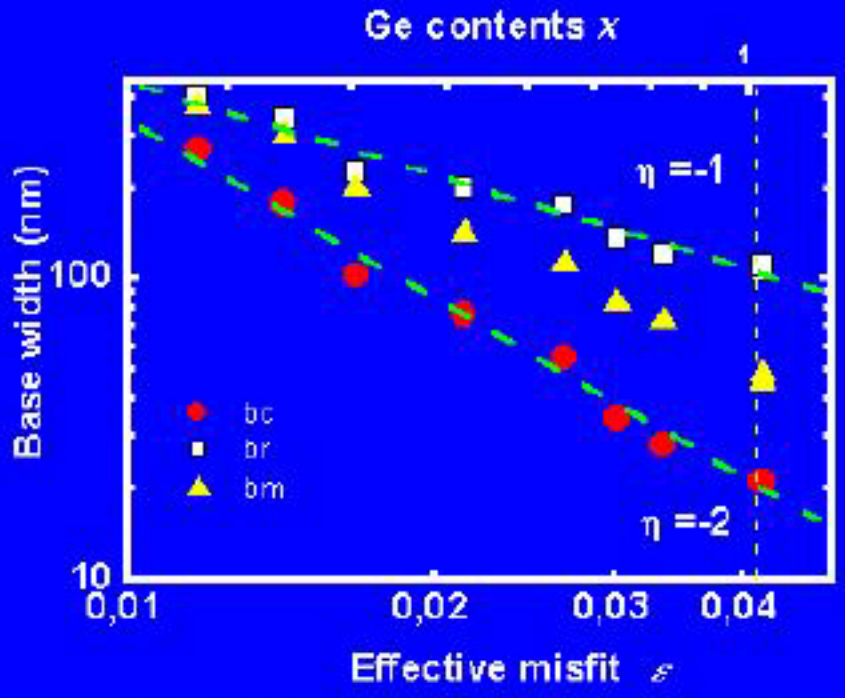
The role of the deposition temperature

Island sizes scaling behavior with the effective misfit $\varepsilon^{-\eta}$

CALCULATED

- $b_c \sim \varepsilon^{-2}$ K.E. Khor et al., JVSTB 15, 1051 (1997)
- $\langle b_m \rangle \sim \varepsilon^{-2}$ B. G. Orr et al, Ephys. Lett 19,33 (1992).
- $b_{cR} \sim \varepsilon^{-1}$ K. Tillmann et al., Th.Sol.F. 368, 93 (2000)

MEASURED



The island size enlargement is fully accounted by the measured intermixing driven misfit reduction

Conclusion

- Ge/Si(100) self assembling:

  Island growth dynamics described

  Strain energy relaxation function obtained

- The role of the deposition temperature:

  New technique to measure intermixing described

  The temperature-induced misfit reduction well account for the observed island size scaling behaviour