# Structure and Morphology of Silicon-Germanium Thin Films

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# Island Formation

- **Significance:**

  - Critical to growth of multilayer stacks

  - Of interest as self-assembling arrays

# Island Formation

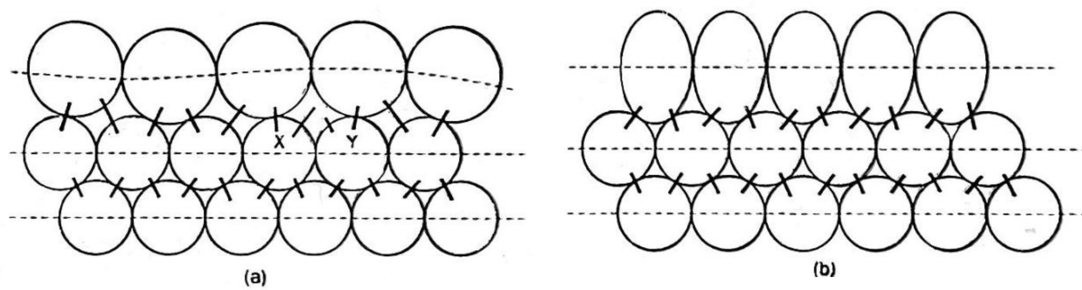
- **Interest Areas:**

  - Growth under tensile and compressive strain

  - Growth on (Si, Ge) (001) and (111)

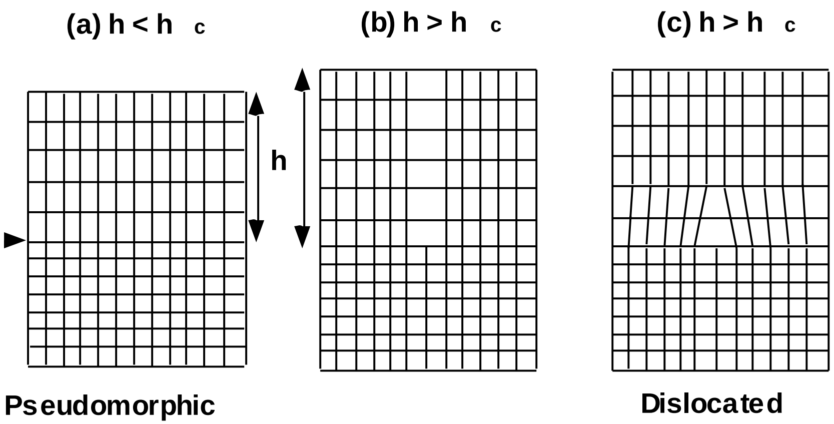
  - Local lattice deformation in film

# SiGe Strained Layer




adapted from Reference 1

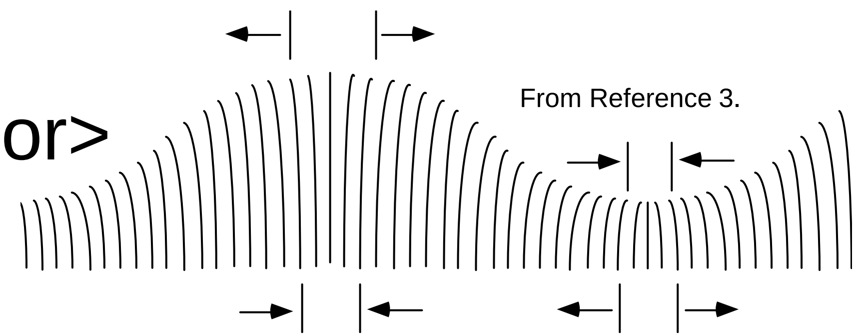
↓grows as↓




From Reference 2.

**Planar w/dislocations.**
**$h_c$ = critical thickness for dislocation formation =(b/f)[ln(hc/b) + 1],**
(b = Burger's vector)

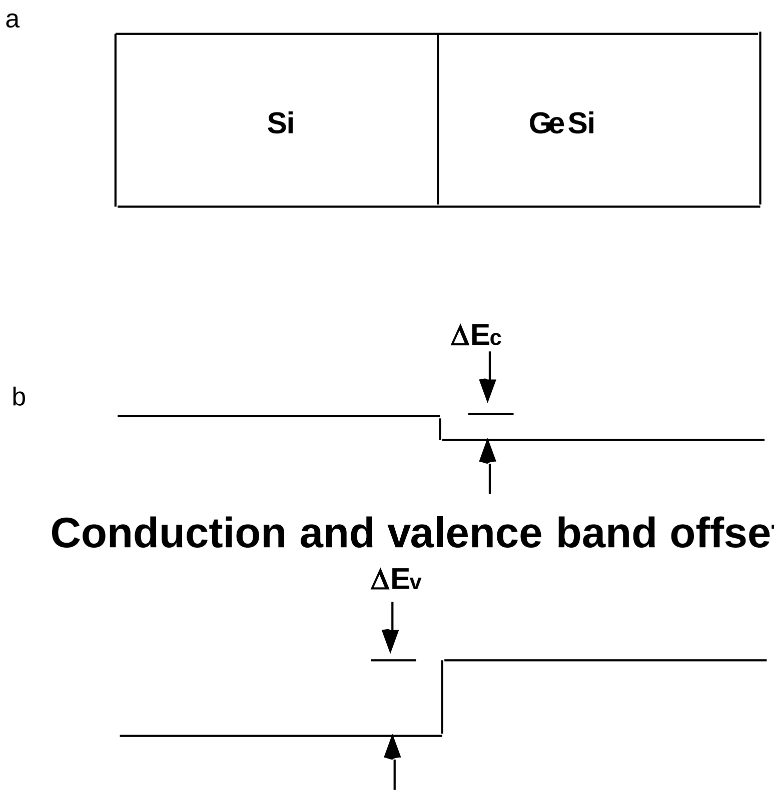
<or>



From Reference 3.

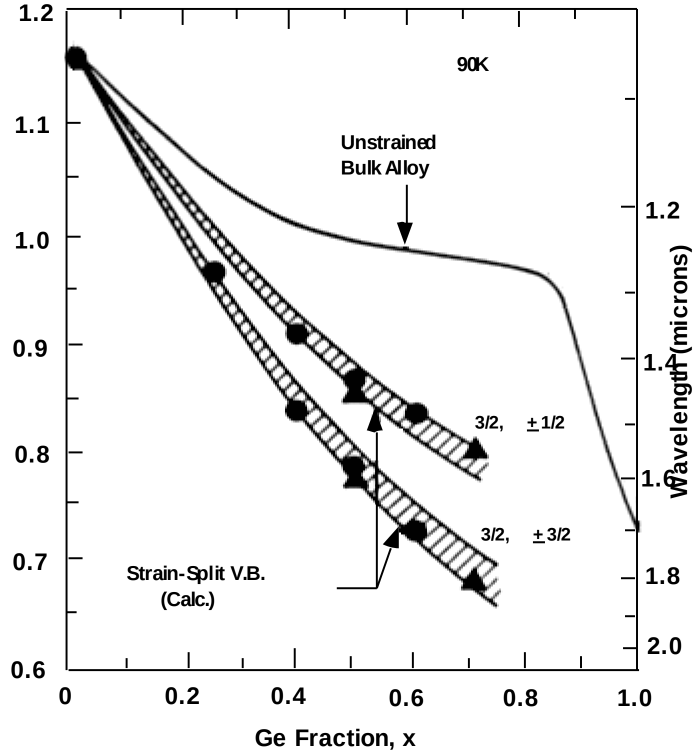
**Strain-free islands**

# Band Offset



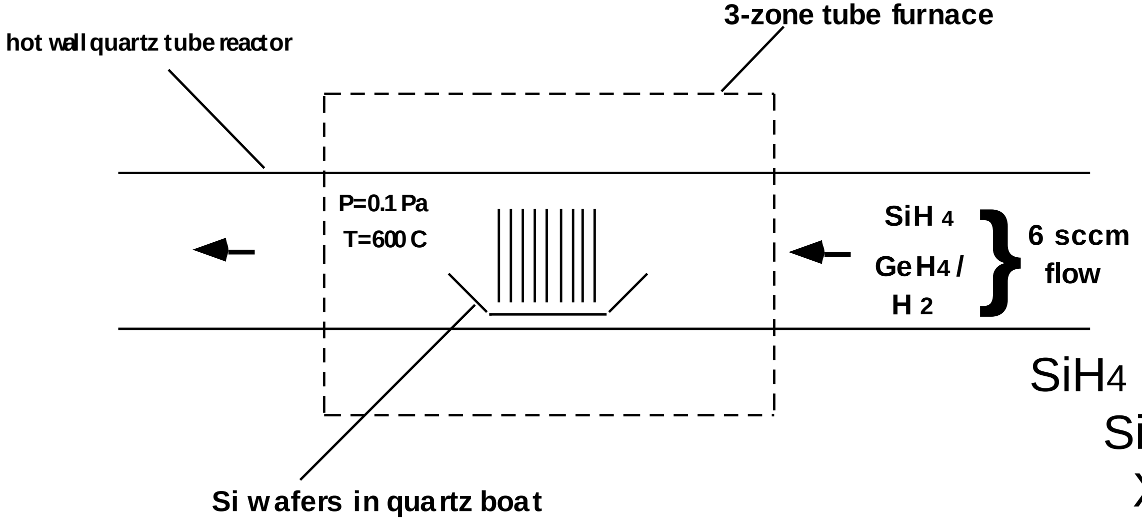

**Conduction and valence band offsets.**

adapted from Reference 4.




From Reference 5.

# Thin Film Growth: UHVCVD




For Silicon:

$SiH_4 + 2^* \rightarrow SiH^* + SiH_3^*$

$SiH^* \rightarrow Si^* + \frac{1}{2} H_2$

X = surface site

x* is species, x, bound to surface site

Gas (low pressure) Kinetics:,

$$Z_i = N_a/2\pi M_i\, k_b T)^{-1/2}\, p_I$$

$Z_i$ = flux of species, i,

$p_i$ =partial pressure

$M_i$ = molar mass of species, i

$N_a$ = Avogadro’s number

$k_b$ = Boltzman’s constant

T = absolute temperature

**Depositions Made:**

substrates: Si and Ge (100) and (111)

compositions: Si, Ge and $Si_{0.5}Ge_{0.5}$

substrate $T_s$ = 600 C

thickness ~ 100 nm

# Alloy Thin Film Synthesis: Kinetics

**Fluxes, Z:**

$$Z_{SiH4} = A(M_{SiH4}\,T)^{-1/2}\,p_{SiH4}$$

$$Z_{GeH4} = A(M_{GeH4}\,T)^{-1/2}\,p_{GeH4}$$

**N = active site density,**
**k = decomposition rate constant**
**$M_i$ = molar mass**
**p = partial pressure**
**A = constant**

**Growth rate, R:**

$$R \sim N(k_{Si}\,Z_{SiH4} + k_{Ge}\,Z_{GeH4})$$

**Germanium fraction, x:**

$$x = R_{Ge}/(R_{Ge} + R_{Si}) = [1 + ((M_{GeH4}/M_{SiH4})^{1/2}(s_{SiH4}/s_{GeH4})\,(p_{SiH4}/p_{GeH4}))]^{-1}$$

$$= 1/[(1 + 1.545)\,(s_{SiH4}/s_{GeH4})(p_{SiH4}/p_{GeH4})]^{-1}$$

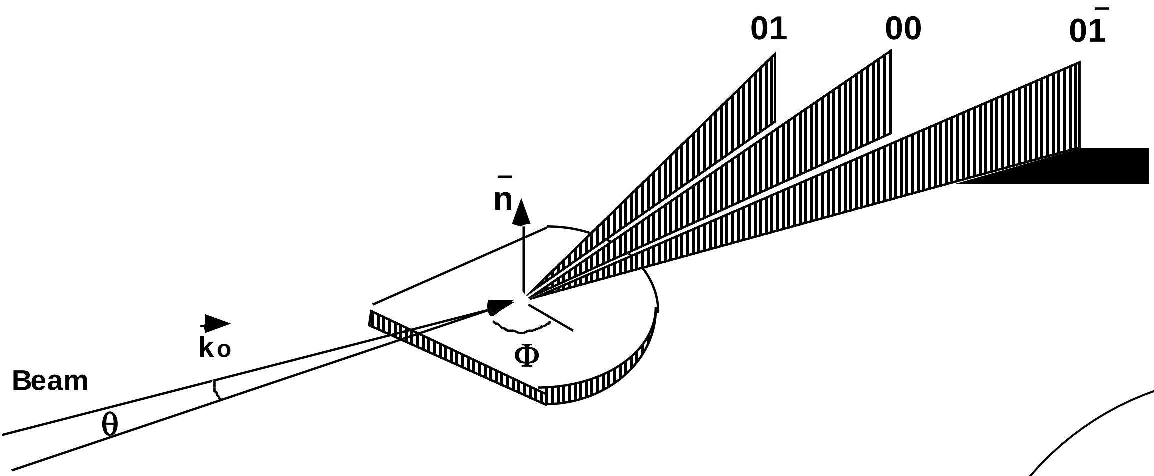
$$1.545 = (M_{GeH4}/M_{SiH4})^{1/2}$$

empirical, from Reference 4

# Technique Summary

| | | | |
|---|---|---|---|
| **Sampling Regime:** | ~1 μm | 100 nm | 1-10 nm |
| **Technique:** | AFM | RHEED | EM/HREM |
| **Gauges:** | 3D asperity size | Crystal “quality” | Character of interface |
| ***via*:** | Surface roughness | In-plane spacing | Local lattice parameters |

# RHEED Basics

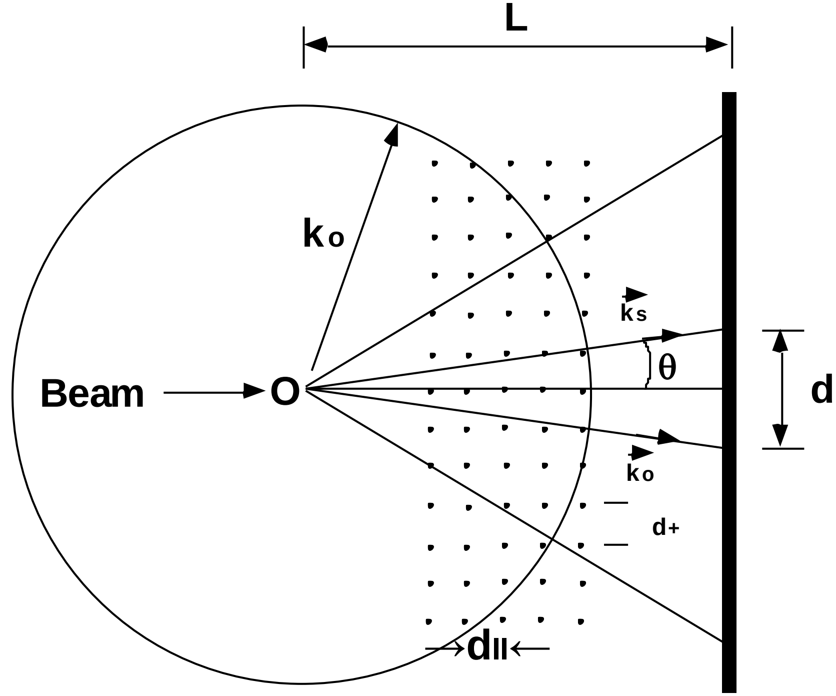



**Basic Geometry ↑**

adapted from Reference 6

**Reciprocal Lattice↓**

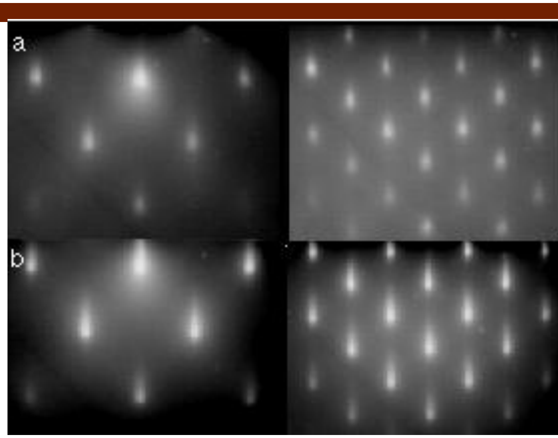
adapted from Reference 7




$$d_{II} = \lambda L/d$$

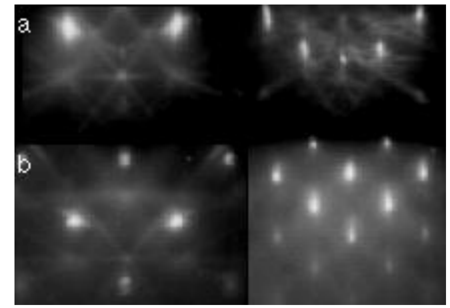
# (Si,Ge) Surface- (001)

Ge/Si(001) → Si/Ge(001)



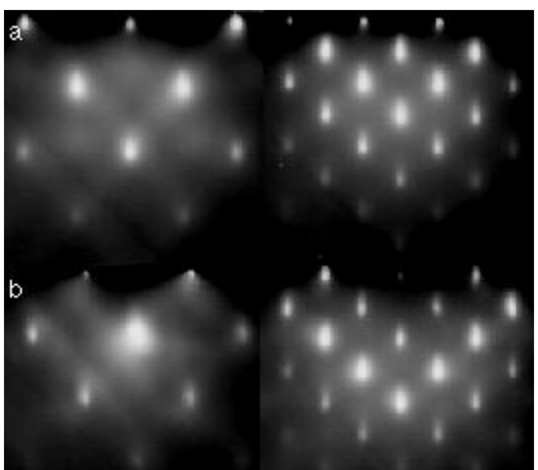
Si/Si(001) → Ge/Ge(001)

<001> <110>



<001> <110>

SiGe/Si(001) → SiGe/Ge(001)



**-"smoother" ( streaks) along <110>**

**- spacings: <110> "symmetric" a/4,**
**<100> asymmetric √2/2**

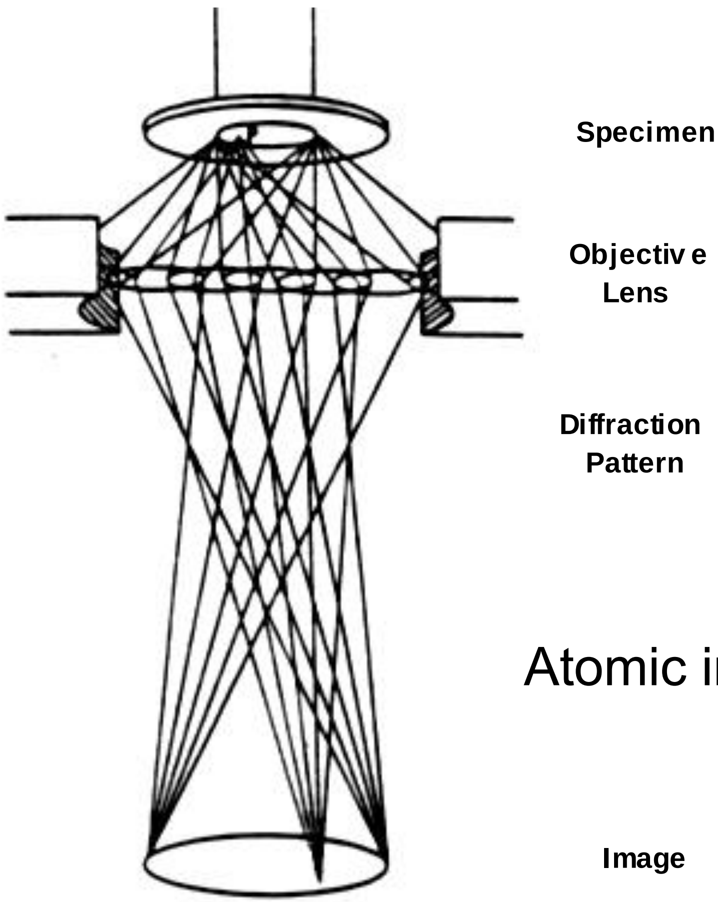
**- Si/Si(001): less rough**

**- Si/Ge(001): <110> elongated spots**

**- Ge/Si(001): maxima more discrete than Ge/Ge(001)**

**- Alloy films: elongated spots**

# HREM Fundamentals




**Schematic Representation**
after Reference 8

***In-Situ***

F (specimen periodic potential)

↓

diffraction pattern

Inverse F

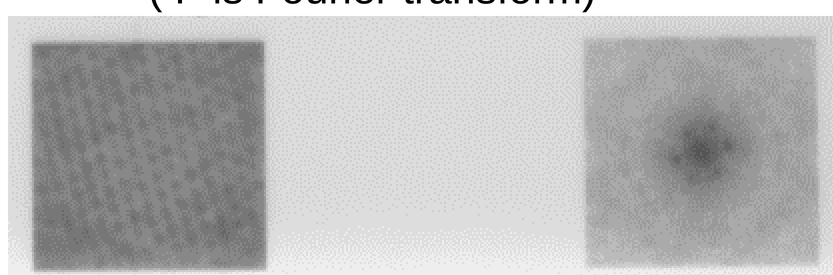
↓

structure (atomic) image

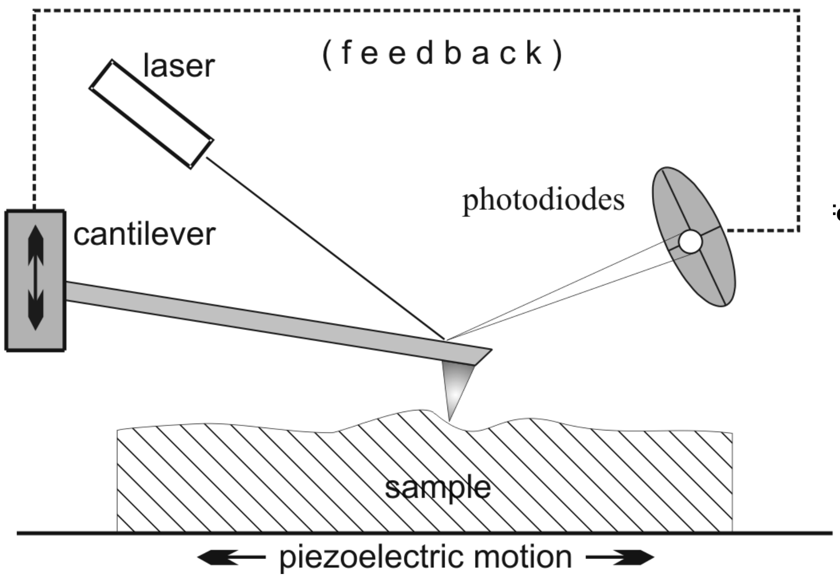
***Ex-Situ***

Atomic image → CCD Camera →Diffraction pattern

( F is Fourier transform)

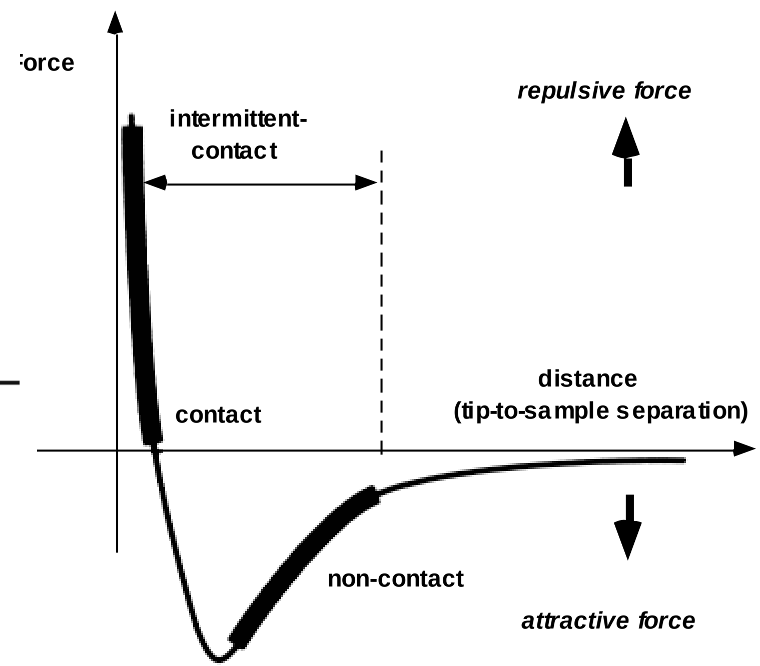


# AFM Basics




**Schematic Representation**

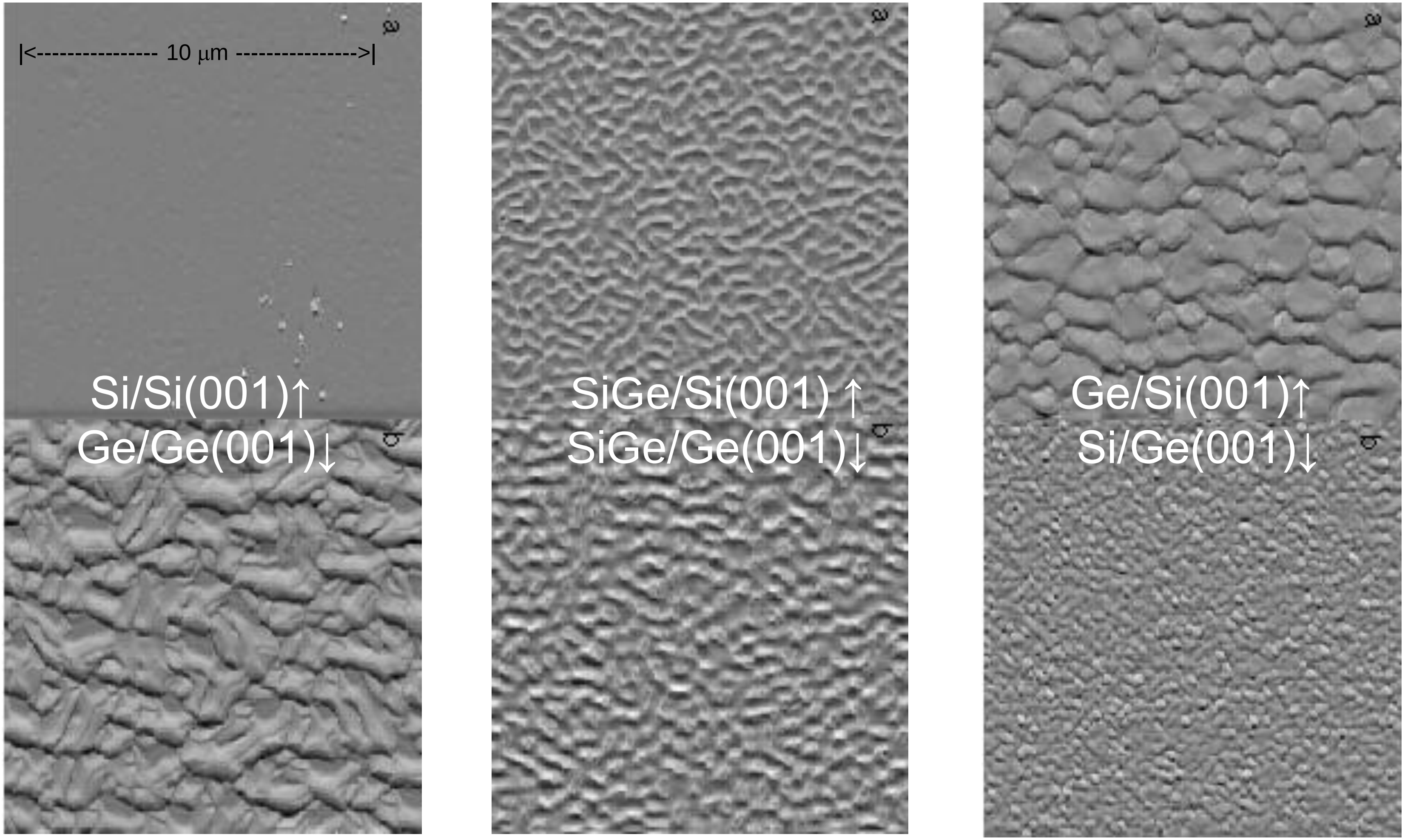
After reference 9



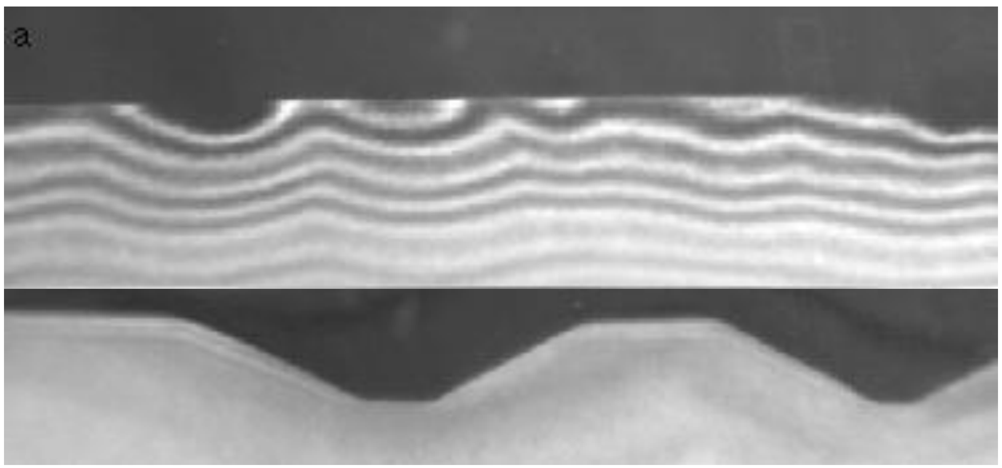

**Intermolecular Force vs. Separation**

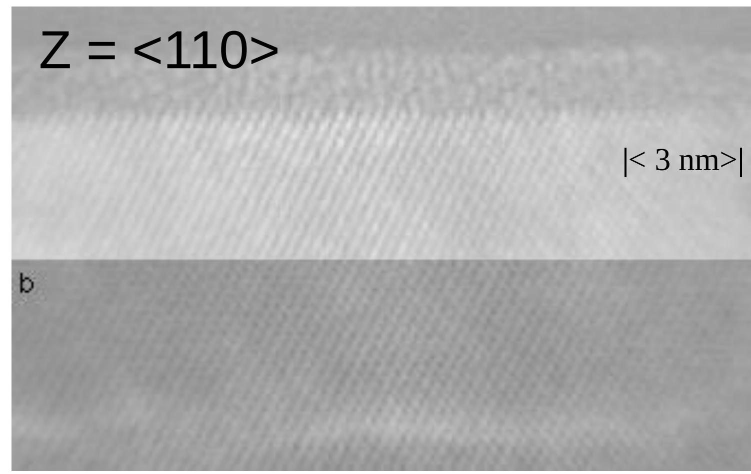
After Reference 10

# (Si,Ge) Morphology- (001)



# Interface-Zero Strain-(001)

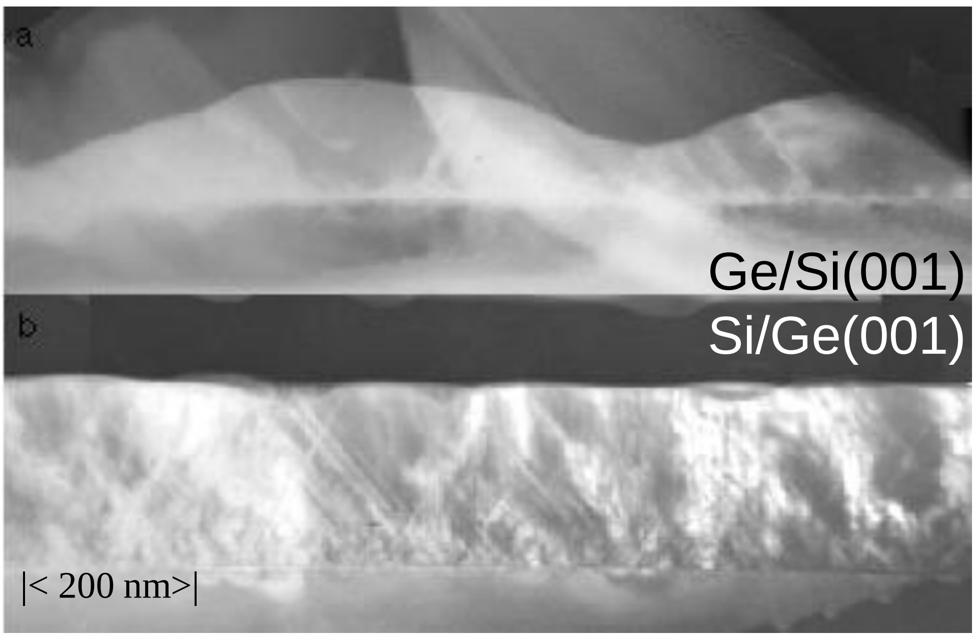


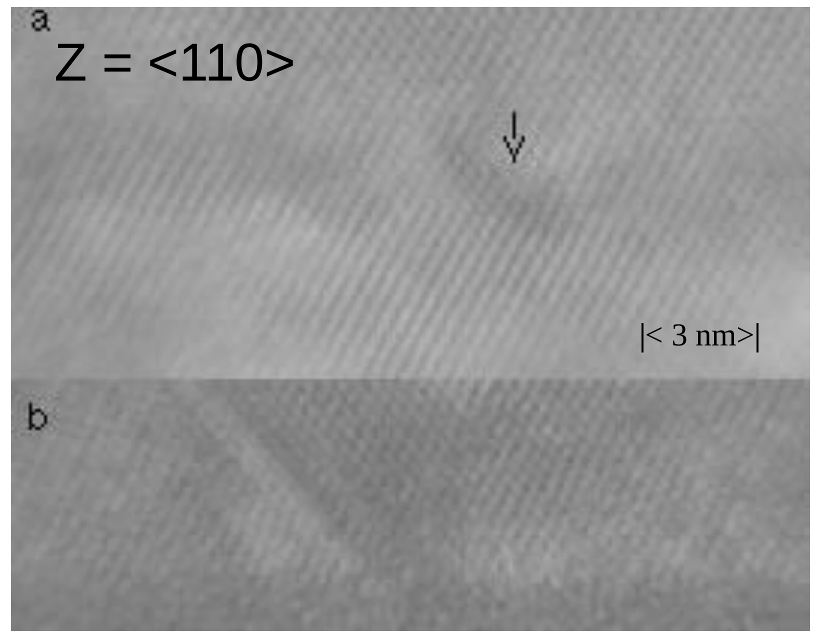




defect-free

# Interface-Maximum Strain-(001)

films in compression →surface undulations



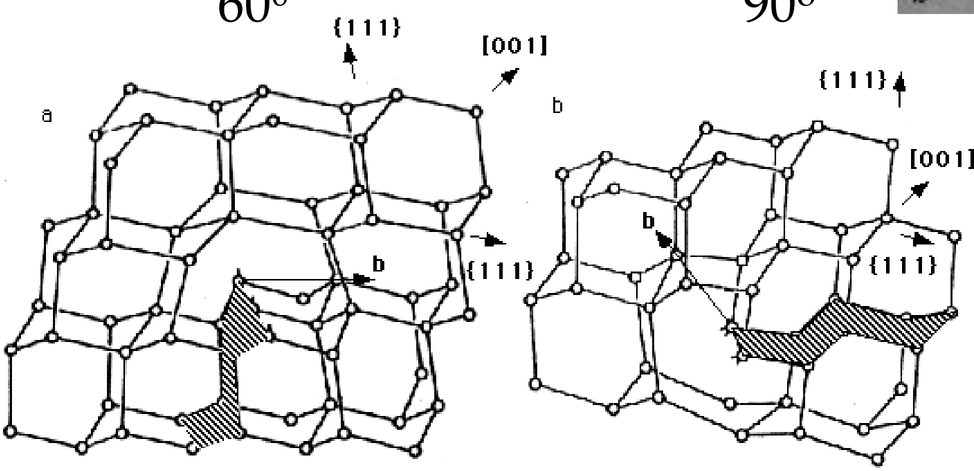

films in tension →more defects-

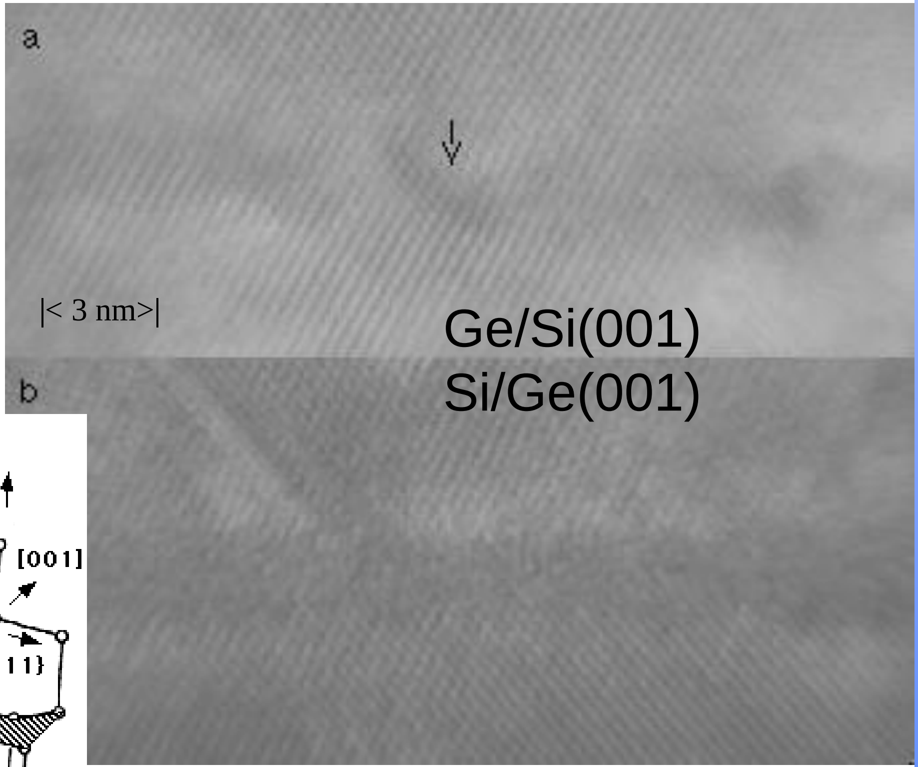
# Details of Strained (001) Interface

Roughness related to the presence of dislocation structures.

Dislocation structures in diamond cubic lattice .↓
from Reference 11.

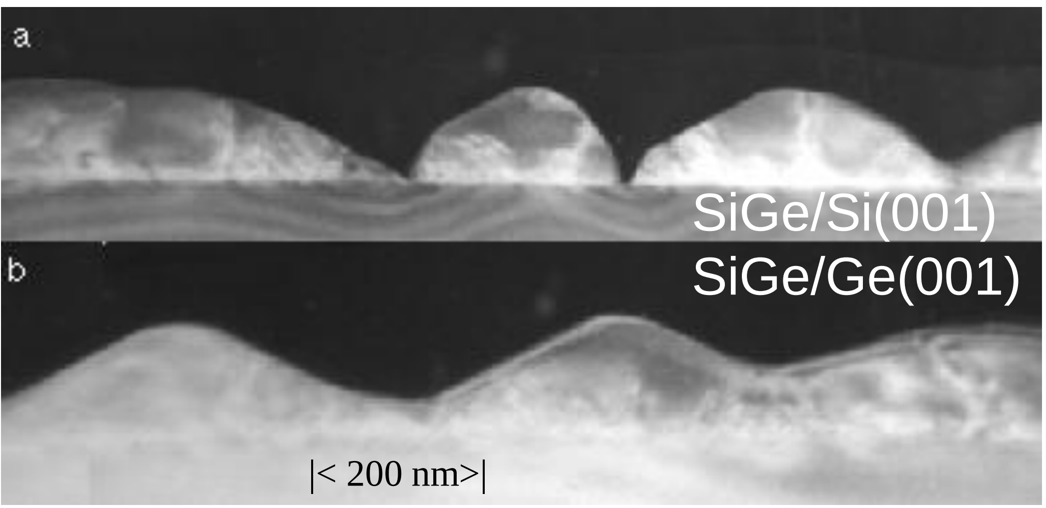
$60^0$ $90^o$

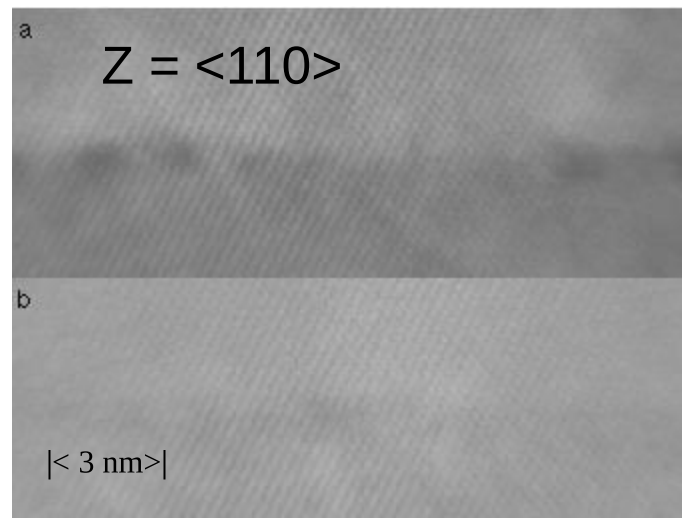


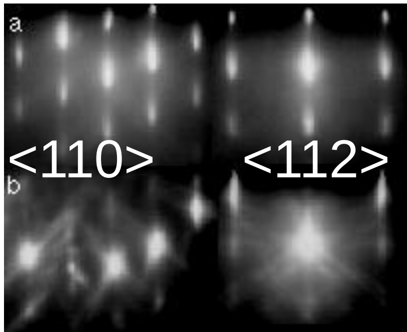
# Interface-SiGe- (001)

## steeply faceted islands



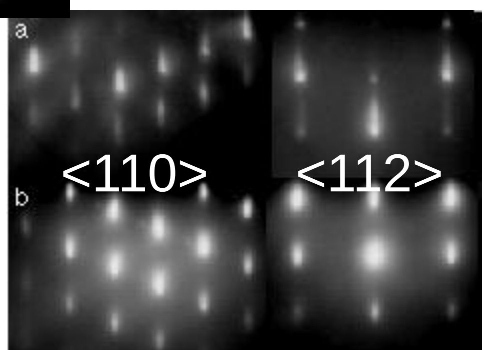



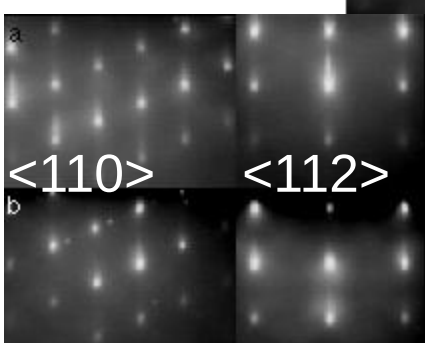
# (Si,Ge) Surface-(111)




Si/Si(111)
←
Ge/Ge(111)

Ge/Si(111)
→
Si/Ge(111)




SiGe/Si(111)
←
SiGe/Ge(111)

**Ge/Ge(111): streaked RHEED maxima**

**Si/Si(111): general surface roughness**

**Ge/Ge(111): large scale mesa coverage**

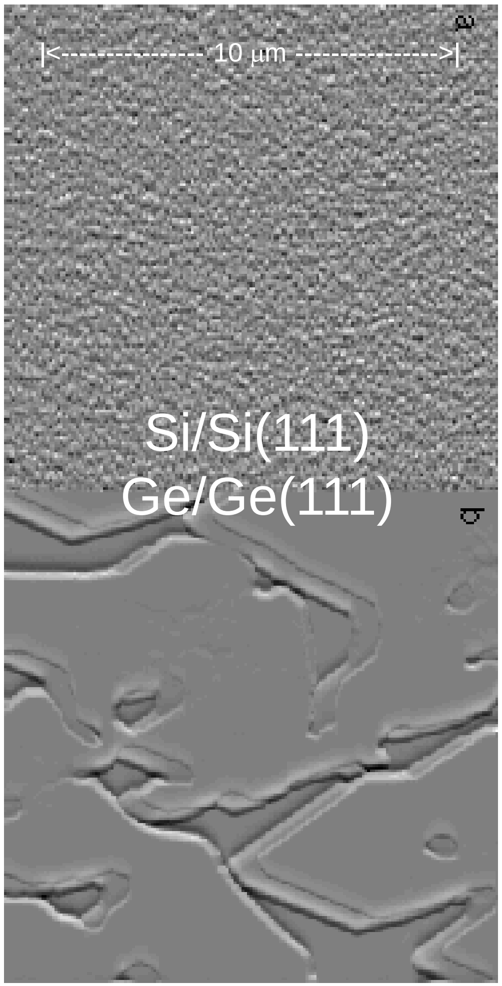
- **$R_a$ larger since RHEED samples the smooth <u>mesa</u> surface**

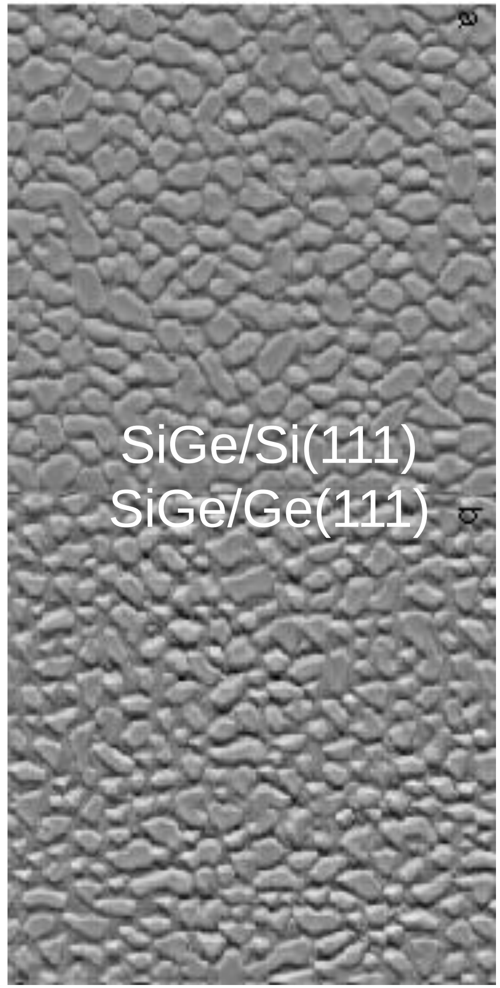
**(Ge/Si (111)): smoother than Si/Ge(111)**

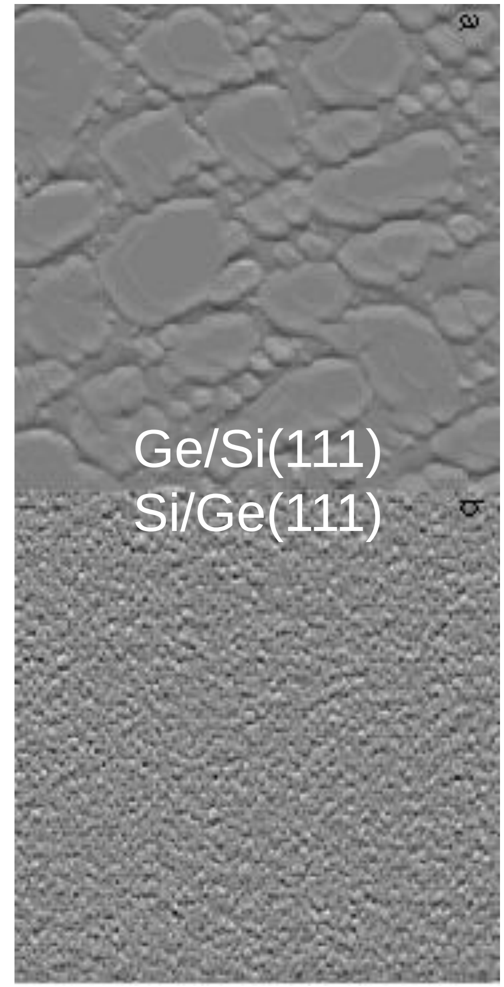
- **Ge/Si(111) consists of large scale plateaus,**
- **Si/Ge(111) displays general surface roughness**

**Alloy films on Si (111) and Ge(111)) are virtually indistinguishable**

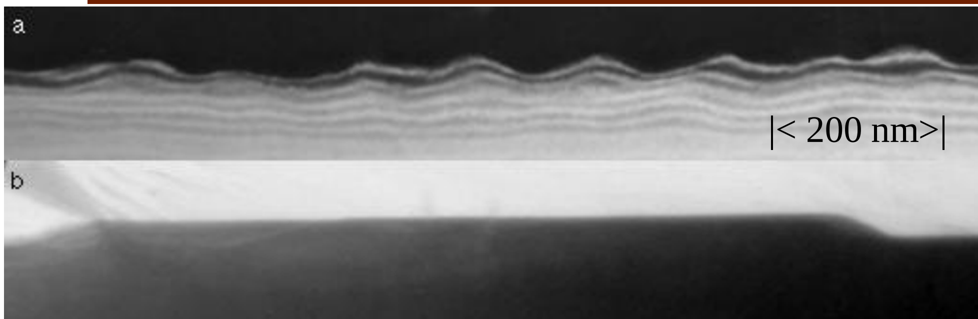
# (Si,Ge) Morphology–(111)



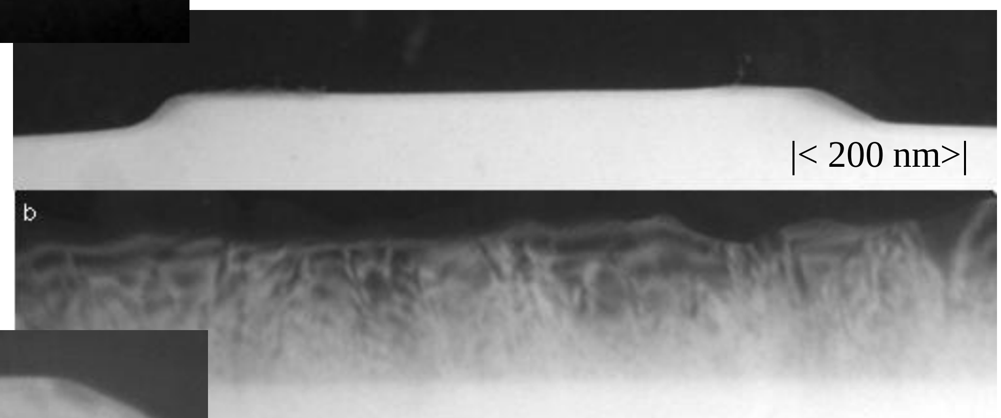



# (111) Substrates

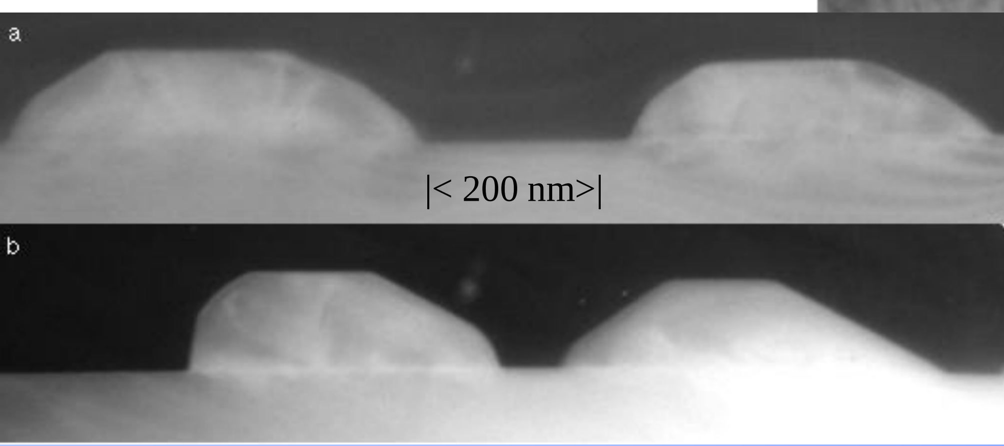



Si/Si(111)
Ge/Ge(111)

Z = <110>



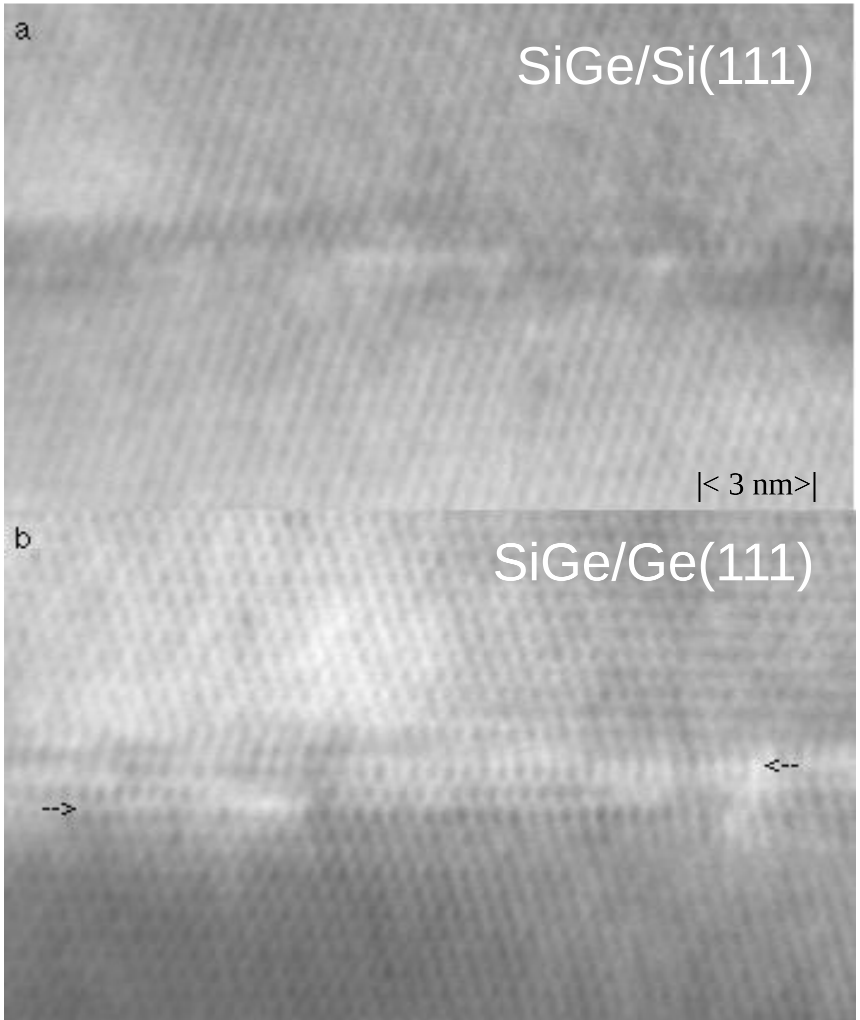

Si/Ge(111)
Ge/Si(111)

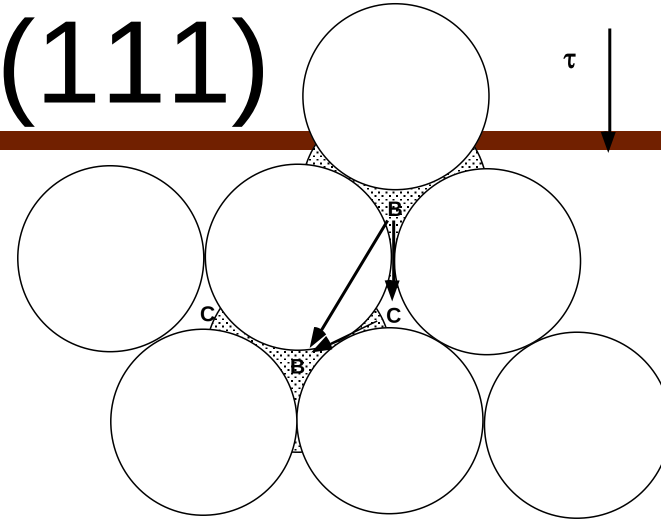



SiGe/Si(111)
SiGe/Ge(111)

broad plateaus

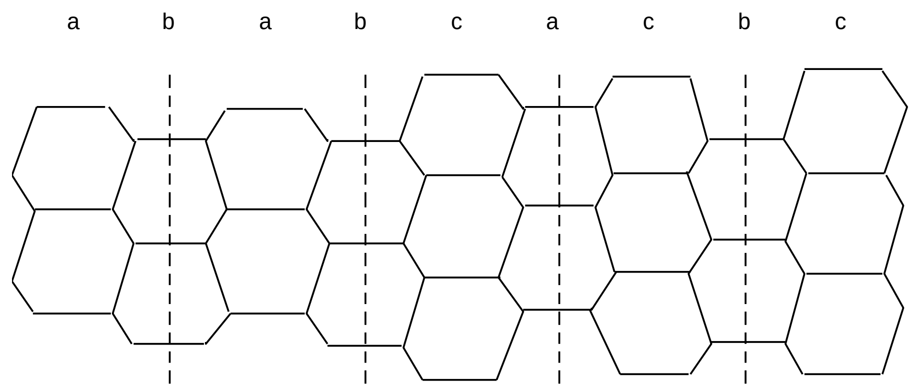
# Interface -SiGe on (111)




Schematic of slip mechanism of 60$^{o}$ dislocation on (111)

From Reference 12




Stacking faults in DC lattice

From Reference 11

# HREM Film-Substrate Mismatch of (Si,Ge) Films

**lattice parameter ↑ from substrate to bulk deposit value within islands**

| | (001) Substrates | (111) Substrates |
|---|---|---|
| Zero Strain Samples | | |
| Ge/Ge | .007 | |
| Maximum Strain Samples | | |
| Ge/Si | .045 | |
| Si/Ge | .032 | |
| Alloys | | |
| SiGe/Si | .041 | .035 |
| SiGe/Ge | .012 | .011 |

# Summary of Observations: Substrate Mismatch of (Si,Ge) Films

**Ge/Si(001): higher strain (4.5%) than the Si/Ge(001) (3.2%)**
**→ tetragonal strain (film constrained to match the substrate along the interface.**

**Si/Ge(001): high density of defects, which relieve a portion of the 4.5% strain**

**Alloy films: same mismatch on both (100) and (111)**

**Larger mismatches for alloys deposited on Si (3.5-4%), than Ge (~1%)**
**→evidence for a Ge-rich alloy composition at start of growth (stress-driven diffusion)**

| | | |
|---|---|---|
| Si/Si | Ge/Si (I) | Alloy/Si (I) |
| | | |
| Si/Ge (P) | Ge/Ge | Alloy/Ge (I) |
| | | |
| Si/Alloy (P) | Ge/Alloy (P) | Alloy/Alloy (I or P) |

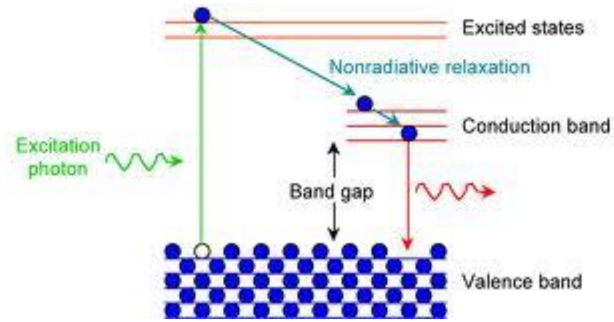
I-island formation
P-planar layer

# RHEED Surface Mismatch (e) with Bulk of (Si,Ge) Films

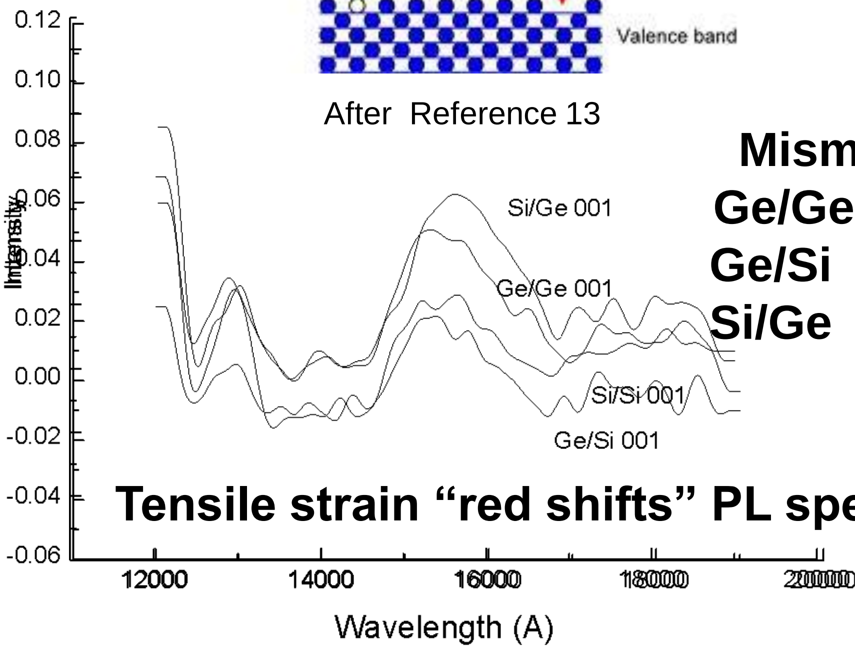
**- films adopt equilibrium spacings irrespective of substrate or orientation (completely relaxed)**

| | (001) Substrates | | (111) Substrates | |
|---|---|---|---|---|
| | $e_{Si}$ | $e_{Ge}$ | $e_{Si}$ | $e_{Ge}$ |
| Zero Strain Samples | | | | |
| Ge/Ge | ---- | -.009 | ---- | -.010 |
| Maximum Strain Samples | | | | |
| Ge/Si | .052 | -.007 | .036 | -.006 |
| Si/Ge | -.012 | -.052 | -.006 | -.047 |
| Alloys | | | | |
| SiGe/Si | .017 | -.024 | .036 | -.006 |
| SiGe/Ge | .026 | -.015 | .025 | -.016 |

# Photoluminescence




After Reference 13



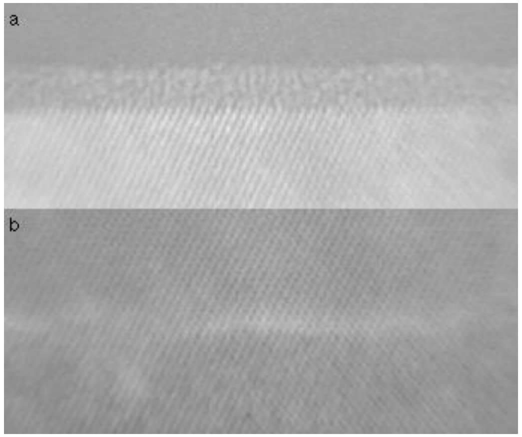

**Tensile strain "red shifts" PL spectra.**

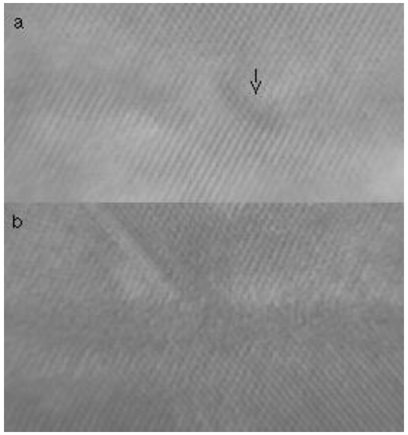
The insertion of an extra half plane on the Si side of the interface leaves it in a state of compression and this is manifested in the PL spectrum

**Mismatch:**

| | |
|---|---|
| **Ge/Ge** | **.007** |
| **Ge/Si** | **.045** |
| **Si/Ge** | **.032** |

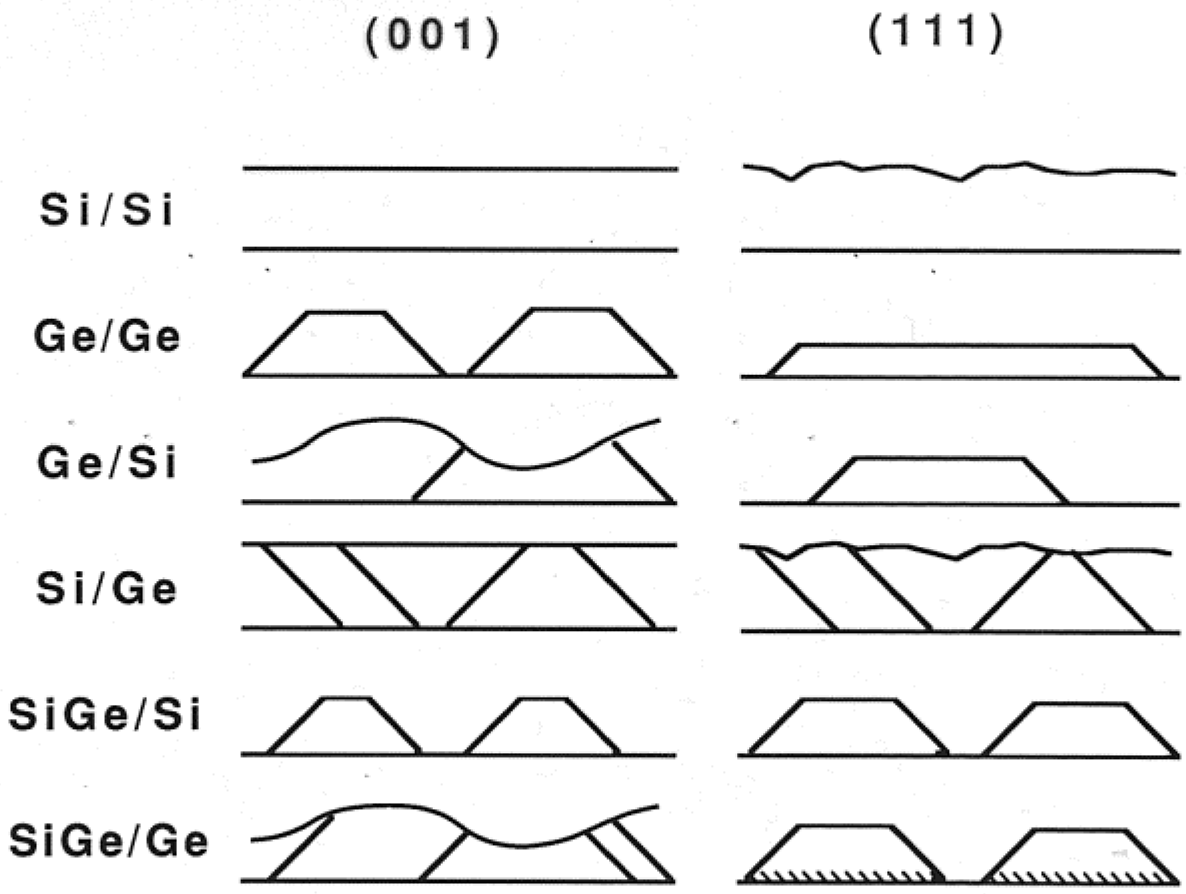
Si/Si(001)
Ge/Ge(001)



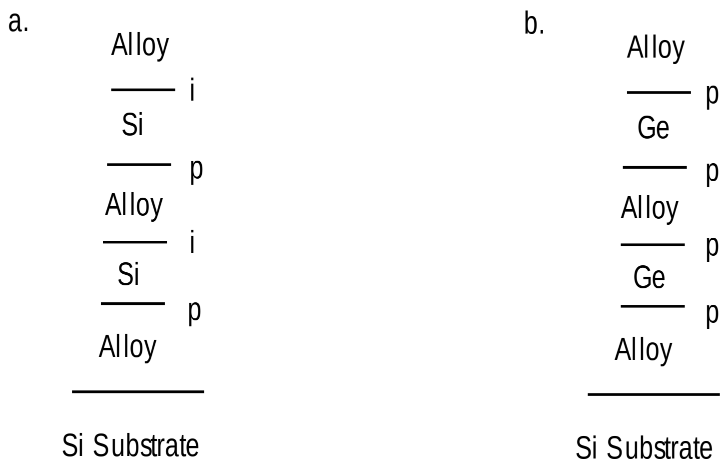




Ge/Si(001)
Si/Ge(001)

# Morphologies Observed

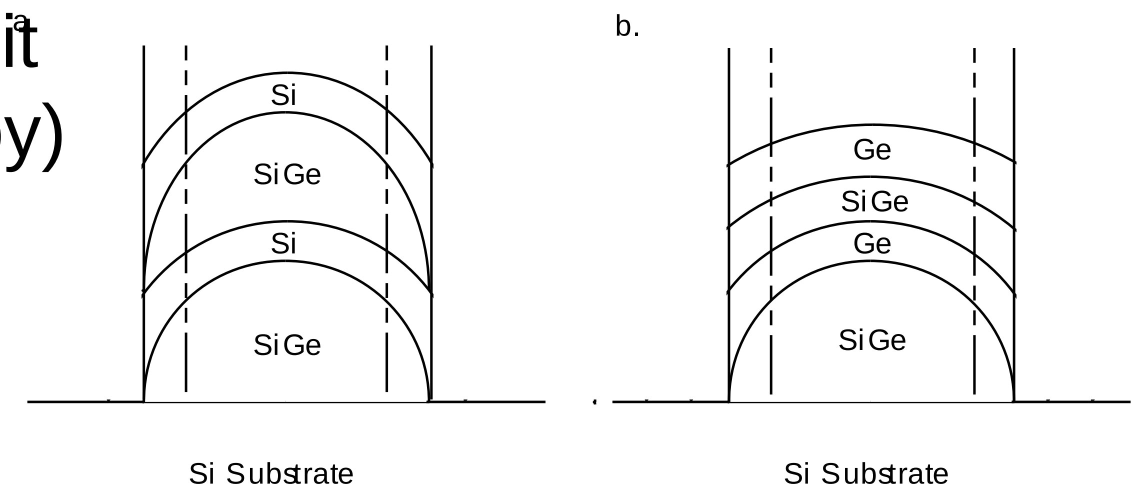


# Proposed SiGe Multilayer Quantum Dot




Promote dislocation -free, island growth in materials with bandgaps of interest

*Via a* low σ deposit (Ge or a SiGe alloy) grown on Si (or alloy on Ge), forming islands (σ is surface energy)



# Figure References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# Summary-SiGe Growth

- minimization of surface energy controls initial film coverage of substrate
  → *(111) surface area maximized*

- islands relieve strain
  → *lattice parameters ↑ near top of island*
  → *compete with dislocation formation*

- islands reduce surface energy
  → *form even with zero strain*

- tensile stress favors dislocations

- 2D to 3D growth transition depends on: energy difference, misfit & modulus

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