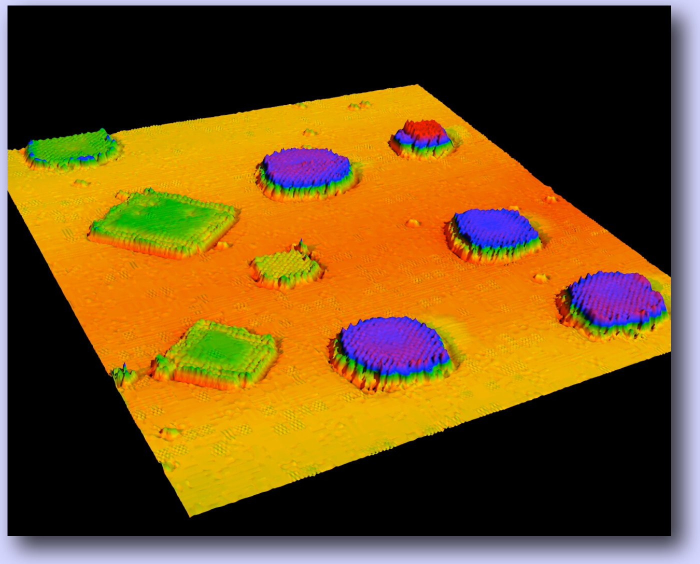
Hartmut S. Leipner: *Structure of imperfect materials*

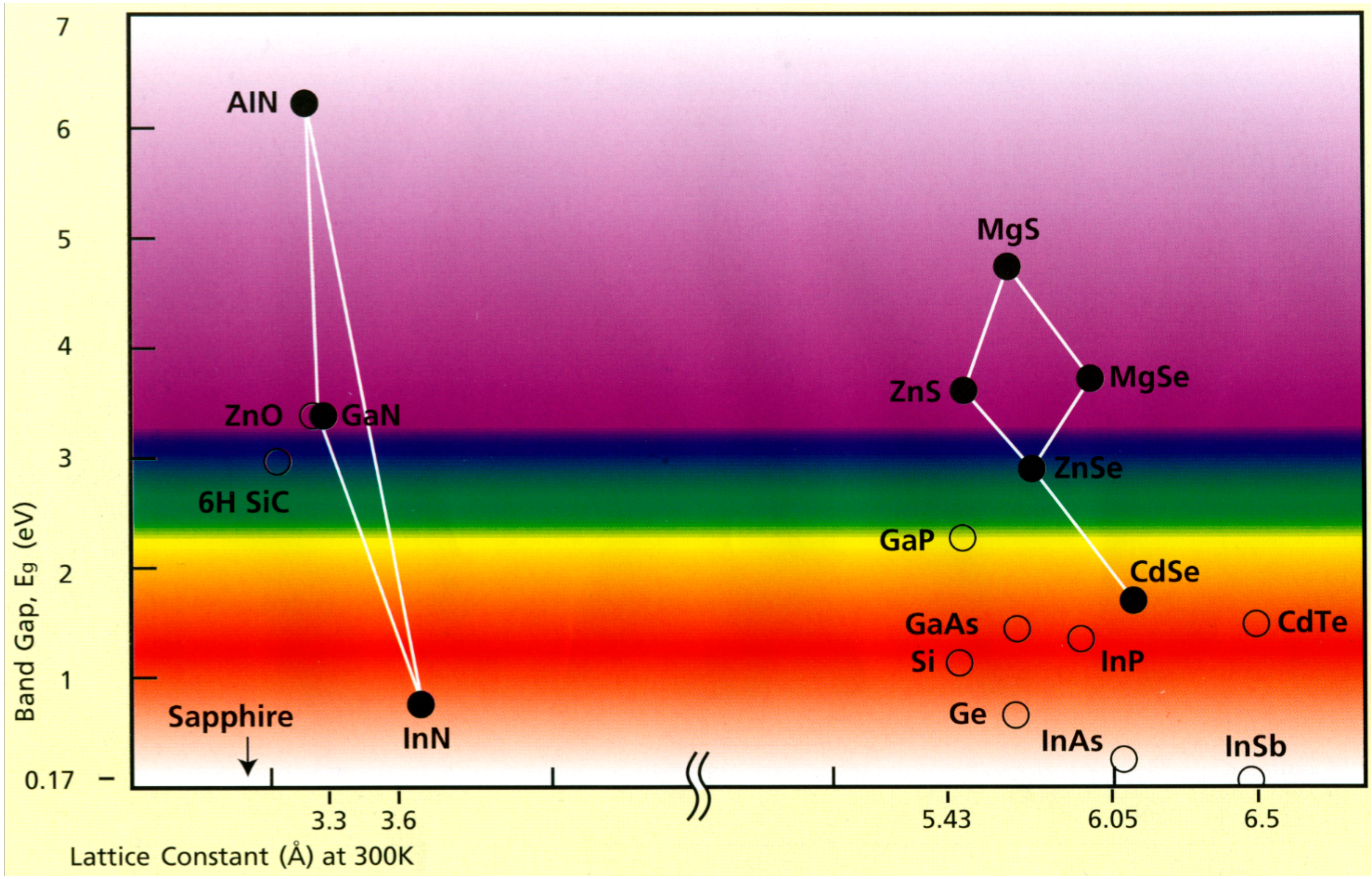
2. Epitaxy and interface defects



2.1 Basic models of epitaxy

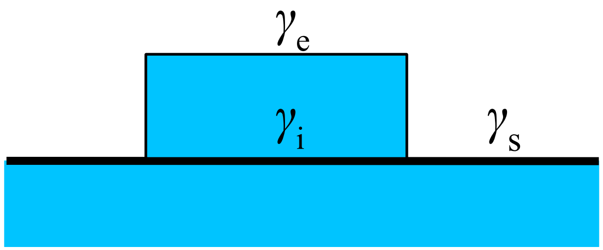
- Growth of a single crystal layer on a single-crystalline substrate
- *Homoepitaxy*: material identical to the substrate
- *Heteroepitaxy*: different material
- Why epitaxy?
  - No bulk material available
  - Layers with special properties
  - Only high-quality layers are required (semiconductor technology)

Lattice constants



Bandgap energy versus lattice constant for a range of elemental and compound semiconductors

Basic models of homoepitaxy

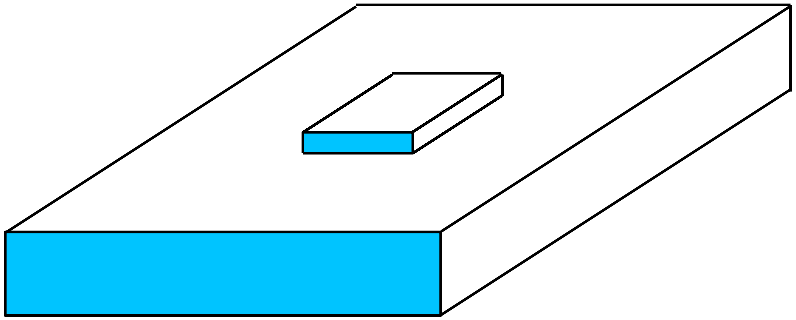


Energetic considerations:

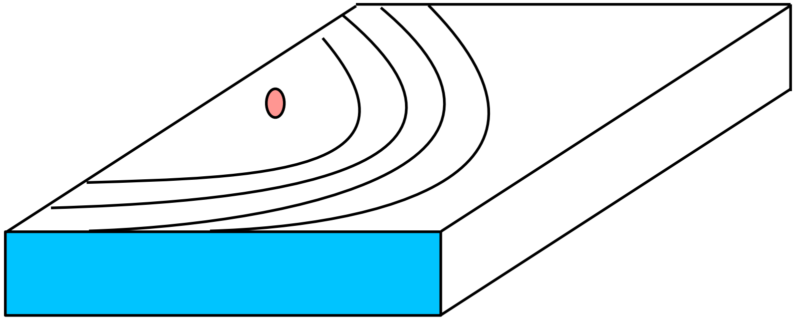
$\gamma_e + \gamma_i \leq \gamma_s$	Layer-by-layer growth (Frank–van der Merwe)
$> \gamma_s$	2D growth + coalescence (Volmer–Weber)

Kinetics of layer growth

Nucleation mechanism

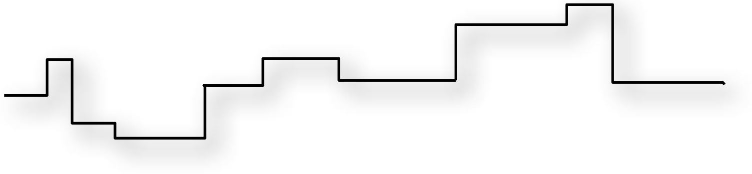


Homogeneous nucleation
(high supersaturation, non-continuous growth)

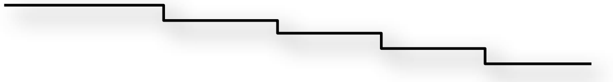


Heterogeneous nucleation at suitable defects – steps
(low supersaturation, continuous growth)

Surface morphology

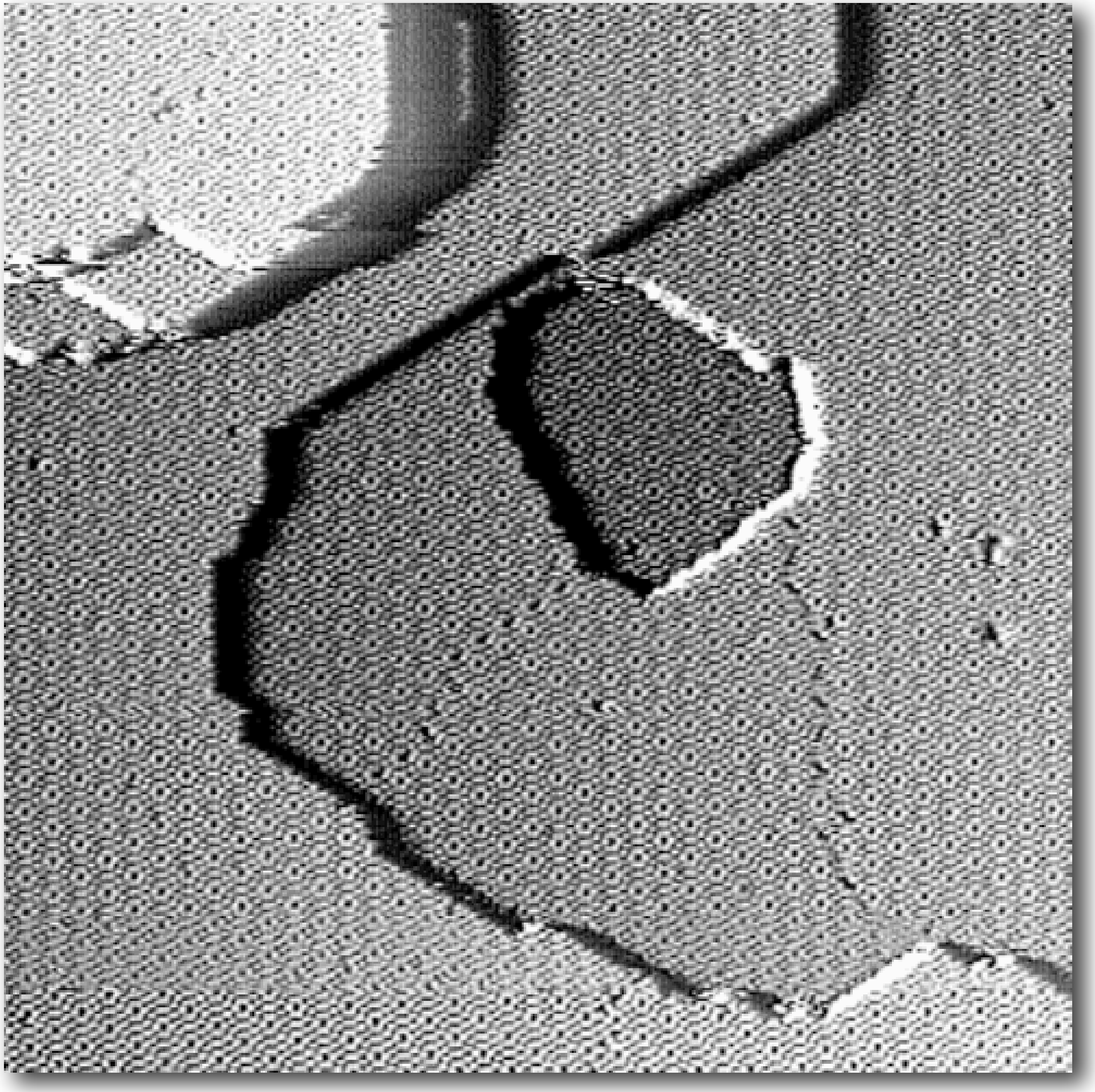


Bundling of steps, wavy surface
(topologically unstable)



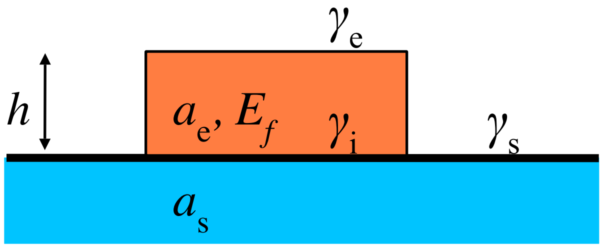
Step of monoatomic height in equal distances (topologically stable)

Surface steps



Scanning tunneling microscopy of surface steps on (111) Si.
$U = 2.2$ V, $I = 0.8$ nA, 95 × 95 nm.
[Kraus:2001]

2.2 Heteroepitaxy



Lattice misfit $f = \frac{a_e - a_s}{a_s}$

Strain energy (per unit thickness h) $E_f = 2G \frac{1+\nu}{1-\nu} f^2$

Pseudomorphic growth

Energetic considerations:

$\gamma_e + \gamma_i + E_f h \leq \gamma_s$ Growth of closed layers
(Frank–van der Merwe)

$> \gamma_s$ ▼

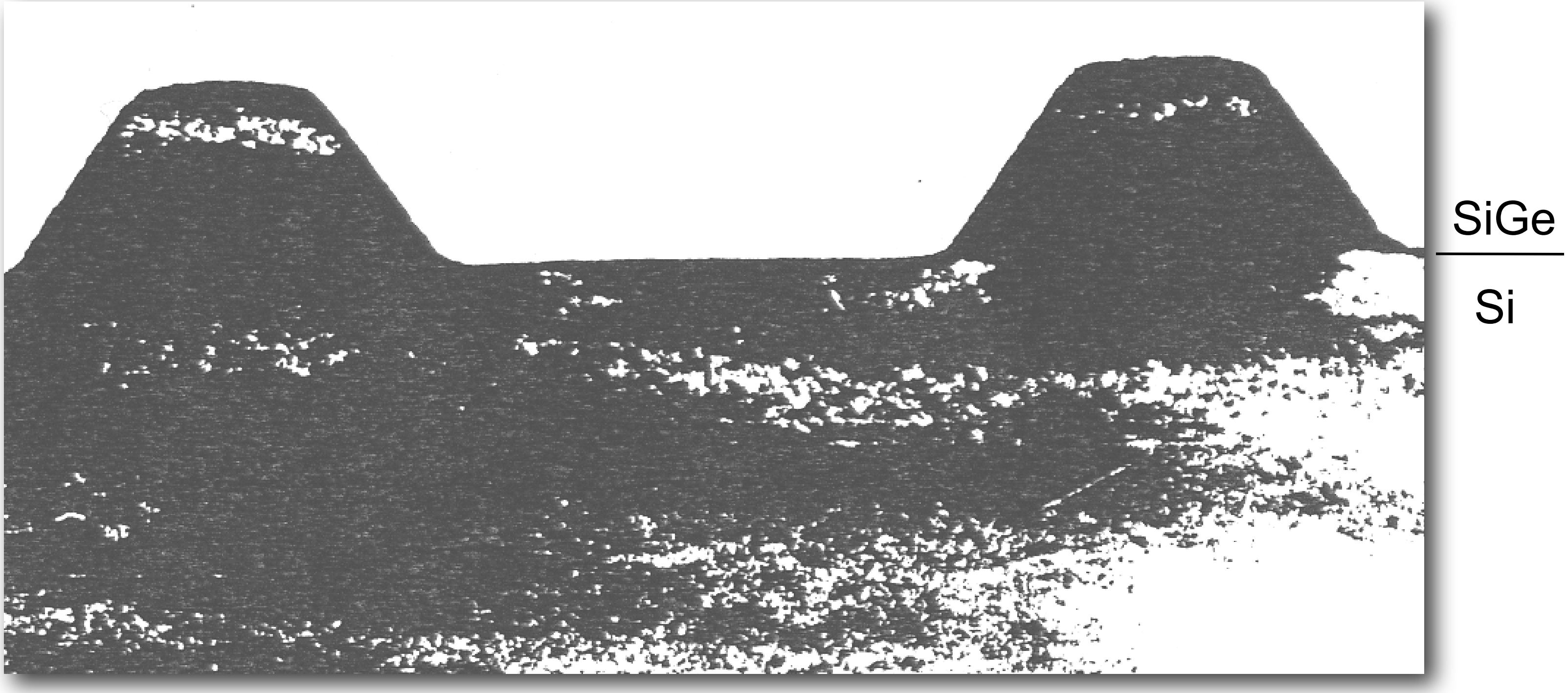
a) 2D growth + coalescence
(Volmer–Weber)
b) Island growth on top of a wetting layer
(Stranski–Krastanov)

Further growth:

a) Elastic relaxation

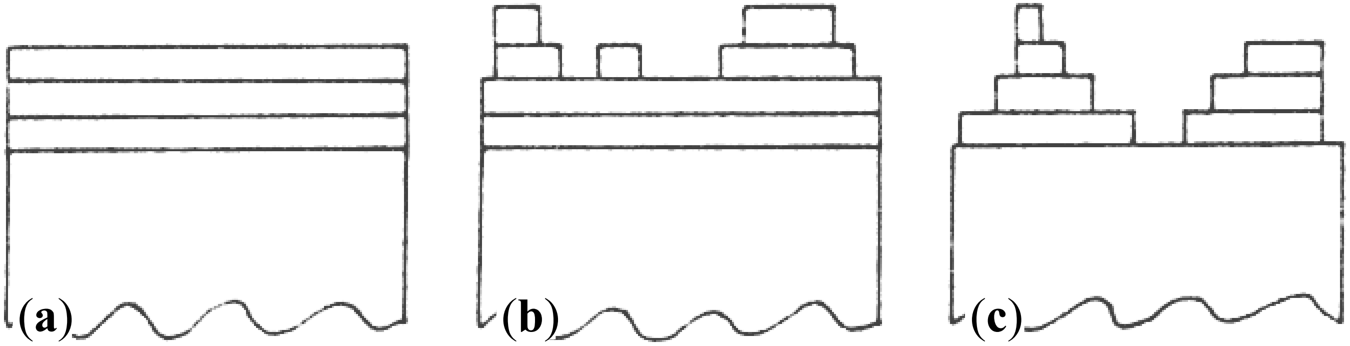
b) Plastic relaxation
($E_f h$ increases)

Stranski–Krastanov growth

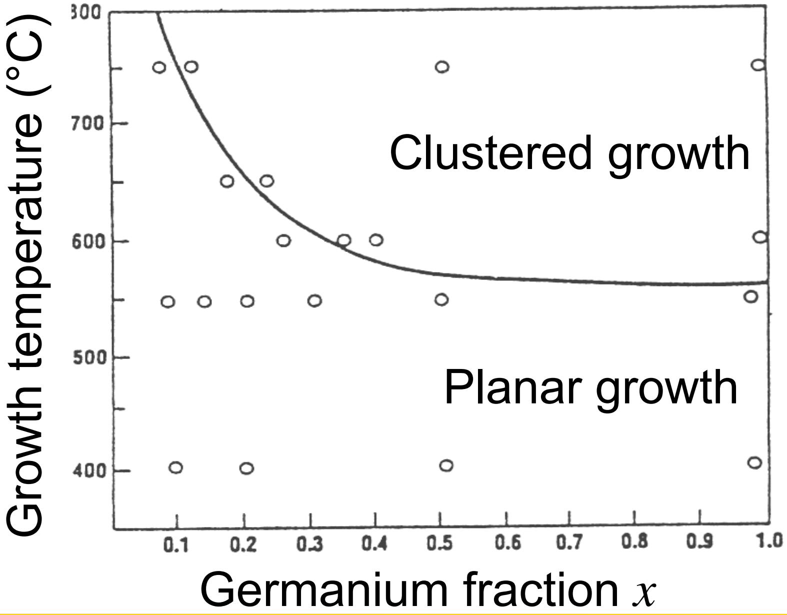


Stranski–Krastanov growth of SiGe on (001) Si.
Liquid phase epitaxy. Cross-section TEM image.
[Albrecht, Strunk: 1999]

Epitaxy modes



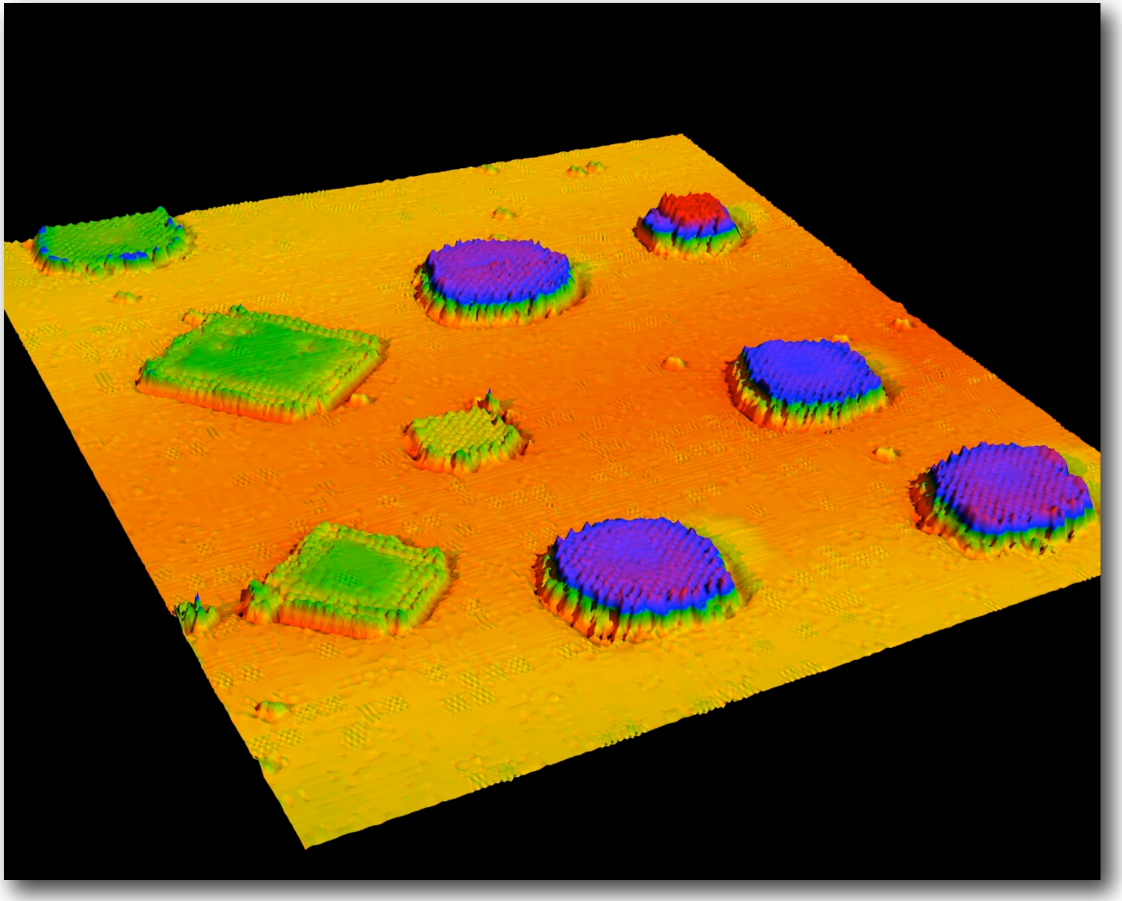
Epitaxial nucleation modes in heteroepitaxy:
a) layer-by-layer, *b*) Stranski–Krastanov, and *c*) clustered.



Measurements of clustered vs. layer-by-layer growth in the $Si_{1-x}Ge_x$/Si (001) system for molecular beam epitaxy.

[Bean *et al.* 1984]

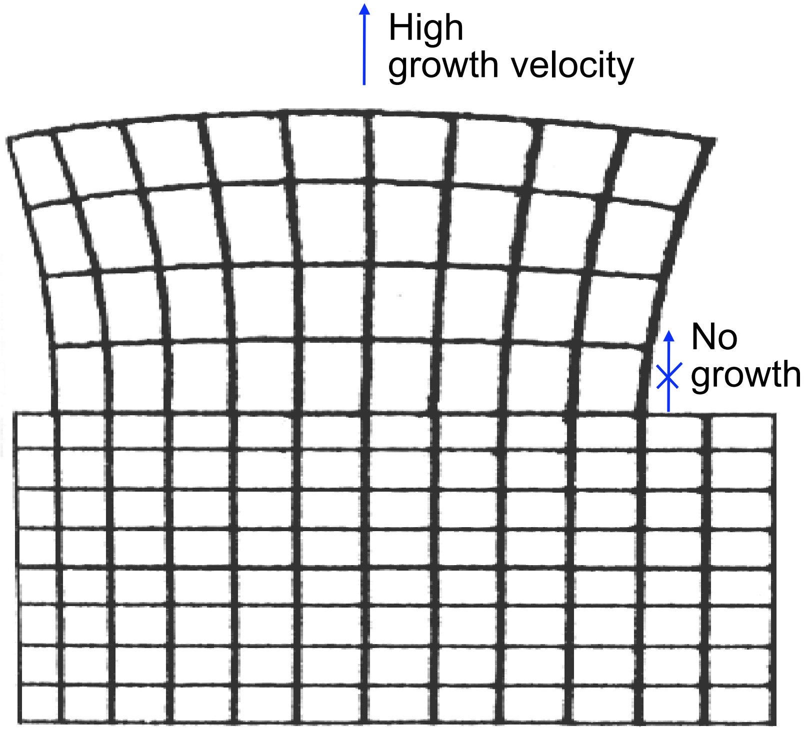
Islands



Scanning tunneling microscopy of CoO islands on a Ag substrate. The diameter of the island amounts to about 6 – 8 nm. The layer thickness corresponds to 1, 2, and 3 monolayers. Single atoms in the CoO can be resolved.

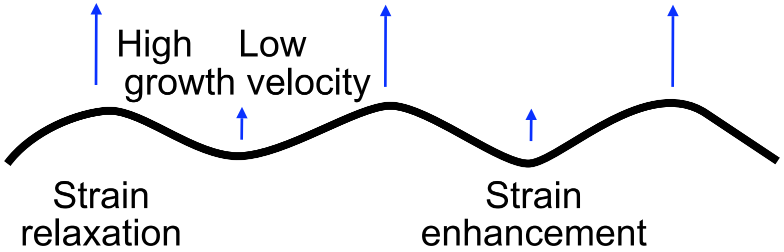
[Widdra 2004]

Elastic relaxation

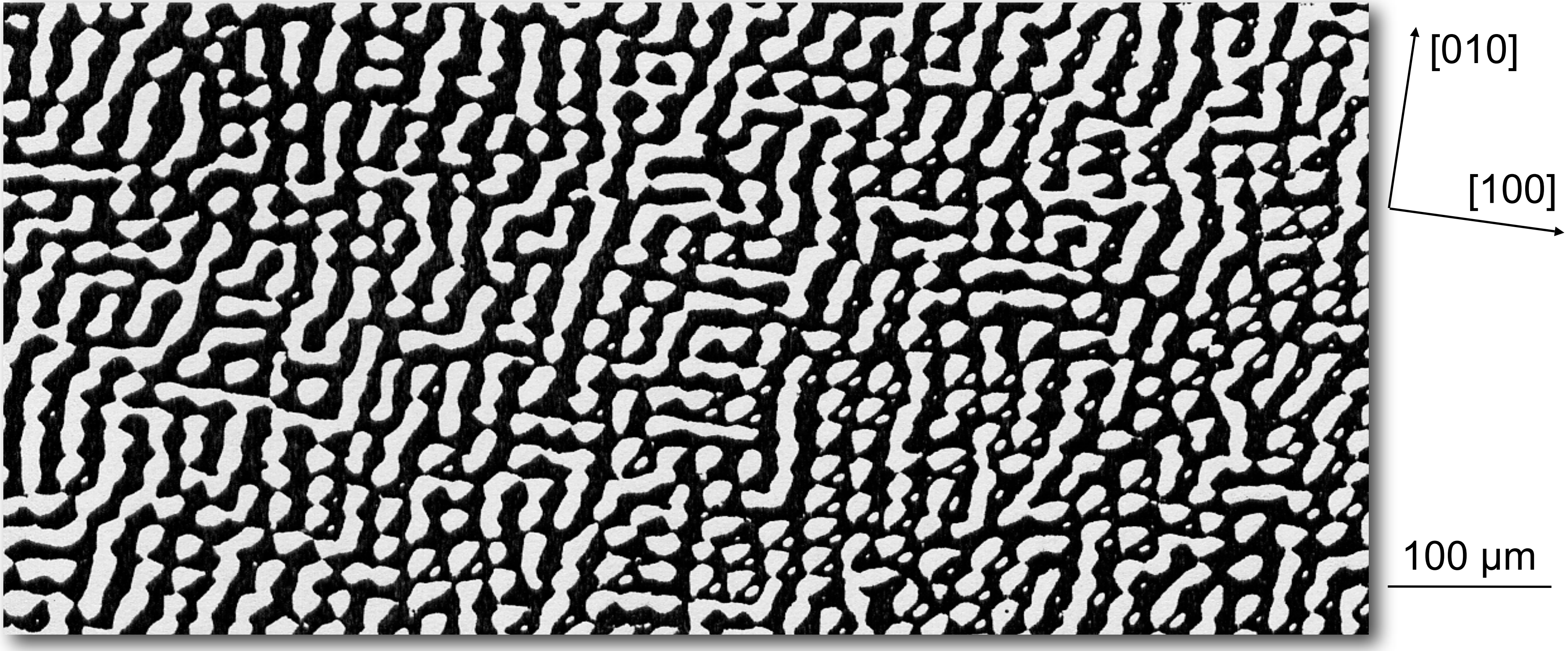


Elastic relaxation during island growth

Ripples = sinusoidal undulations



Ripples



Ripples in $Si_{0.97}Ge_{0.03}$ on (001) Si. Liquid phase epitaxy.
Light microscopy, Normarski differential interference contrast.
Ripple amplitude 5.4 nm, layer thickness 150 nm, wavelength 11.7 µm.

[Albrecht, Strunk: 1999]

2.3 Formation of misfit dislocations

Pseudomorphic layer

- Misfit stress
- Thermally unstable against plastic/diffusive relaxation

Relaxed layer

- Almost no elastic stress
- Rather stable
- Presence of lattice defects affects processing
- Recombination activity of defects

Modeling of misfit dislocations

- **What has to be considered?**

1. Generation of dislocations
2. Dislocation motion
3. Dislocation multiplication and interaction

- **Conditions**

1. Crystallography of the real system – combination of different lattice types
2. Slip geometry
3. Population of intrinsic defects

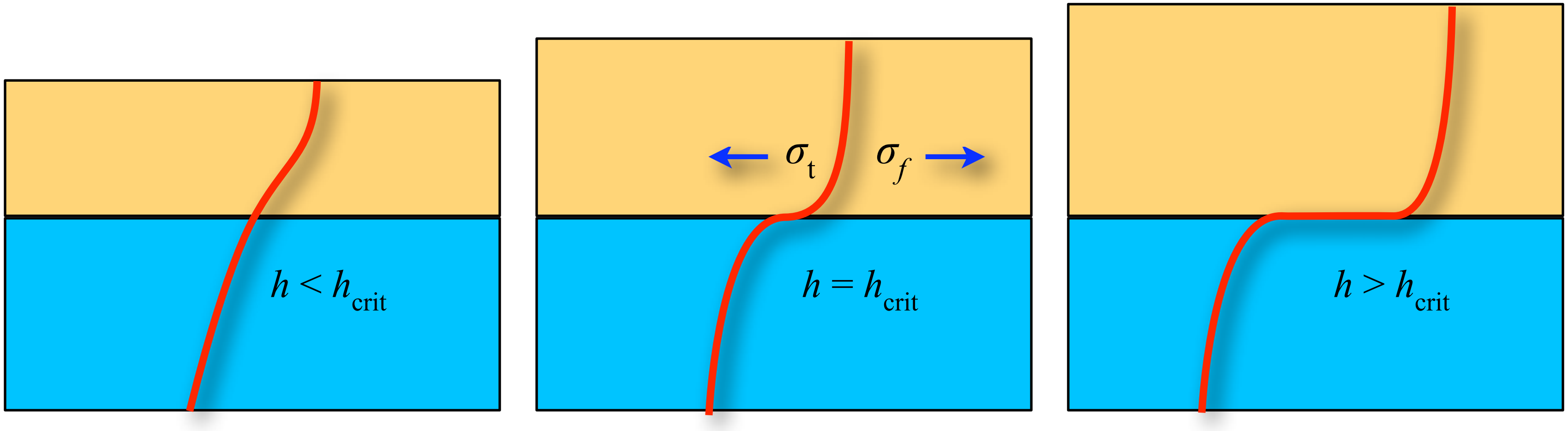
- **Consequence**

Restriction on simple systems

2.4 The concept of critical thickness

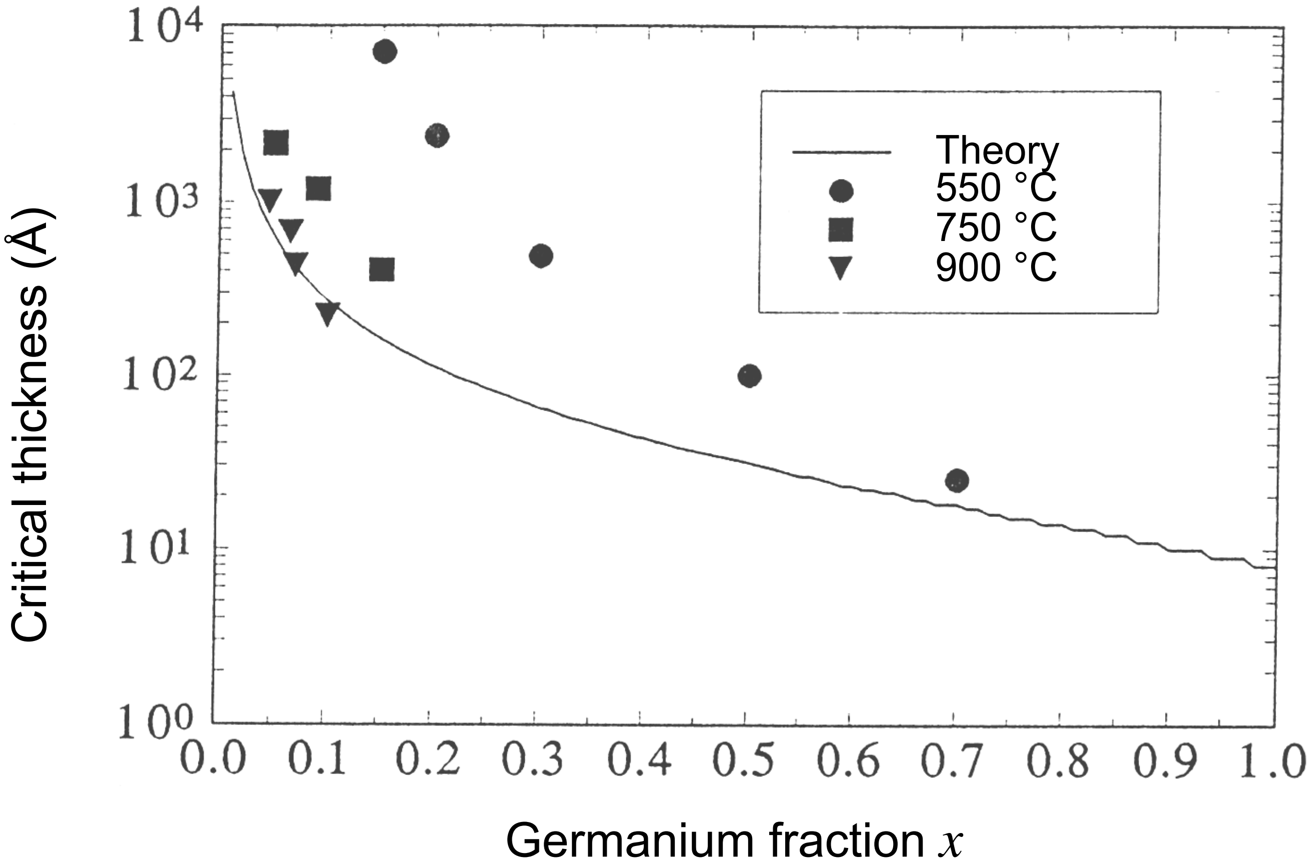
- h_{crit} thickness at which the self-energy of dislocation is equal to the strain energy
- Below h_{crit}, formation of dislocations energetically unfavorable
- **Frank–van der Merwe**: calculation of density of interface dislocation from mathematical analysis of interfacial energy
- **Matthews–Blakeslee**: consideration of the stress on pre-existing, threading dislocations
- **Dodson–Tsao**: strain relaxation rates are kinetically limited, *i.e.* dislocation nucleation and growth rates have to be considered

The Matthews–Blakeslee model



- Above the critical thickness, there is a driving force of dislocation motion in the interface due to the lattice mismatch.
- For $h = h_{\mathrm{crit}}$, $\sigma_{\mathrm{t}} = \sigma_f$
  (σ_{t} restoring stress due to the line tension of the dislocation, σ_f stress due to the lattice mismatch)

Measurement of critical thickness

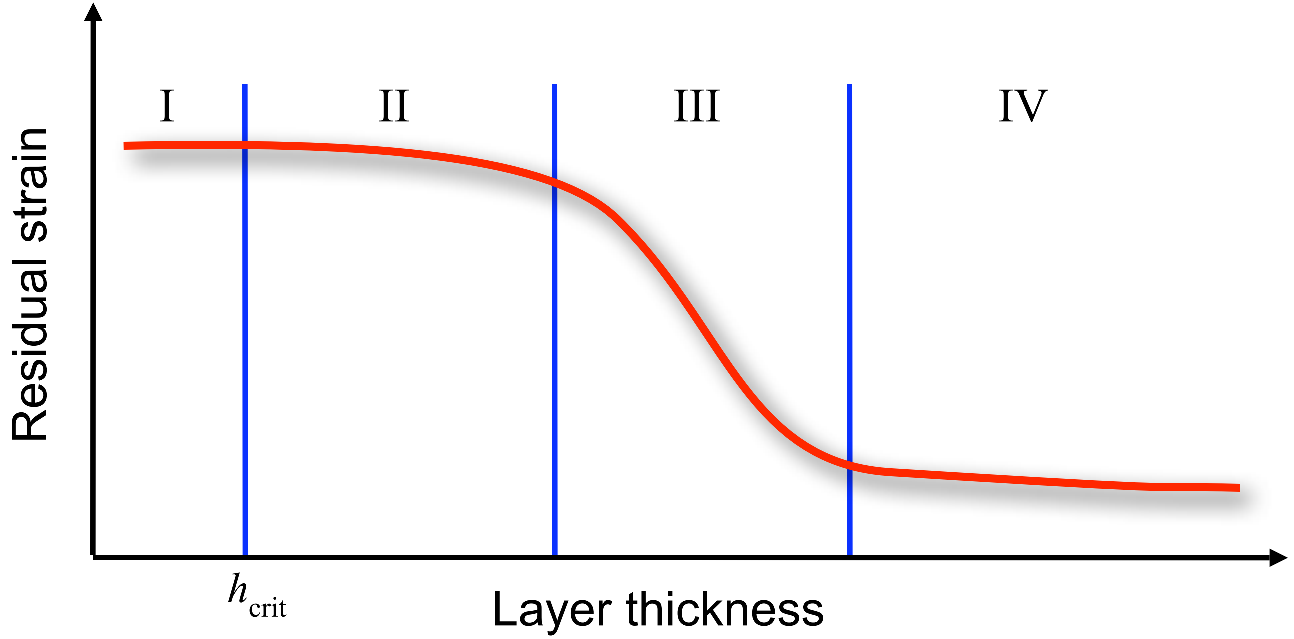


Measurement of critical thickness in the $Si_{1-x}Ge_x$/Si (001) system
for different growth temperatures vs. the prediction of the Matthews–Blakeslee model
[Hull:94]

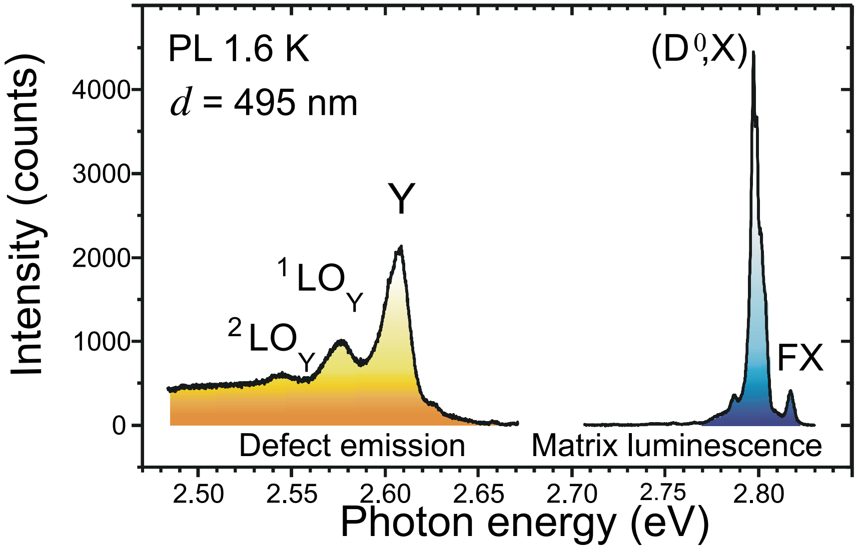
The Dodson–Tsao model

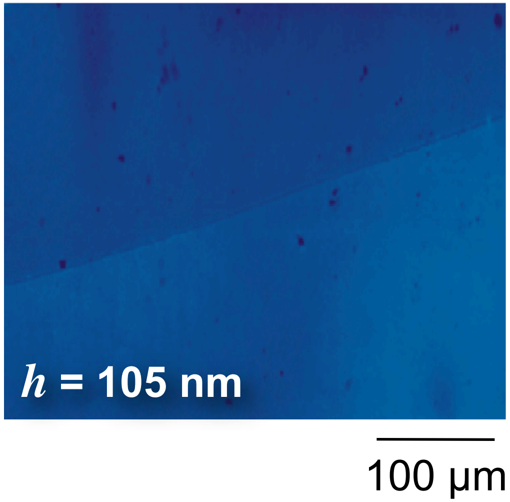
- Relaxation of the epitaxial layer is controlled by thermal activation of dislocation glide processes
- Dislocation velocity (analogous bulk material) $$\upsilon = \upsilon_0 \sigma_{\mathrm{eff}} \exp\left(-\frac{Q}{k_{\mathrm{B}} T}\right)$$

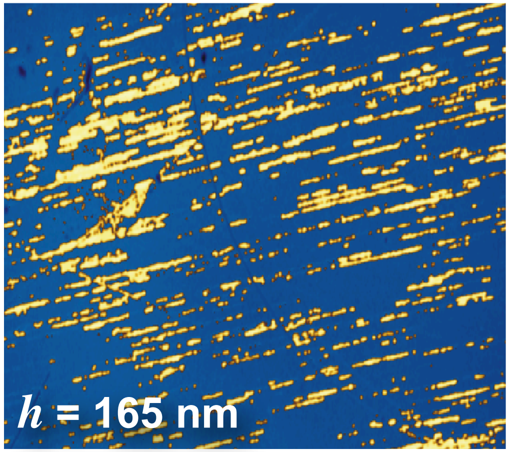
  (σ_{eff} effective driving stress in MPa, Q activation energy, υ_0 prefactor)
- Four stages of strain relaxation in the Dodson–Tsao model

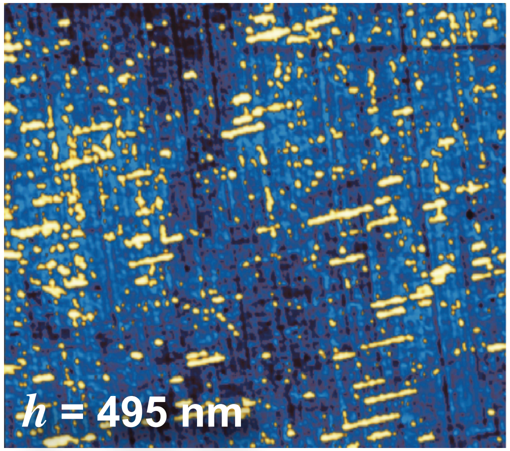


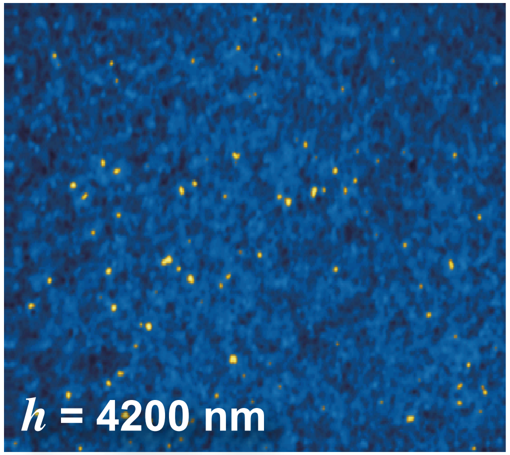
Anisotropic relaxation in compound semiconductors









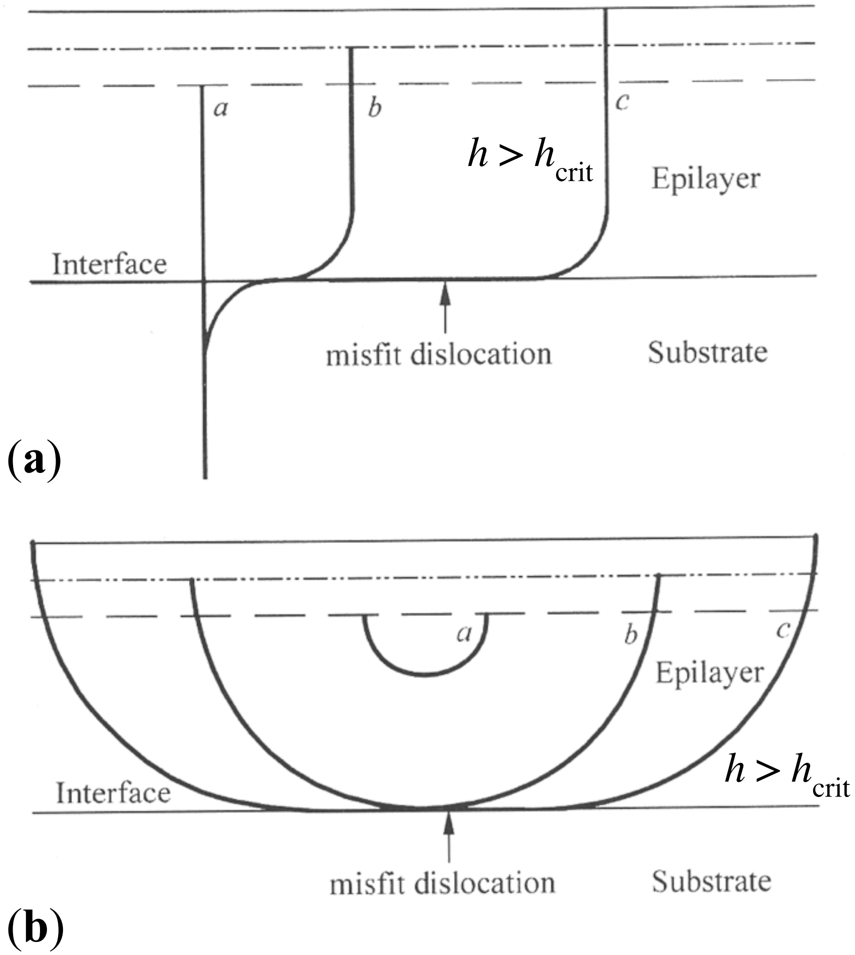


Cathodoluminescence investigation of plastic relaxation in ZnSe/GaAs(001) heterostructures

[Hilpert:2001]

2.5 Sources of misfit dislocations

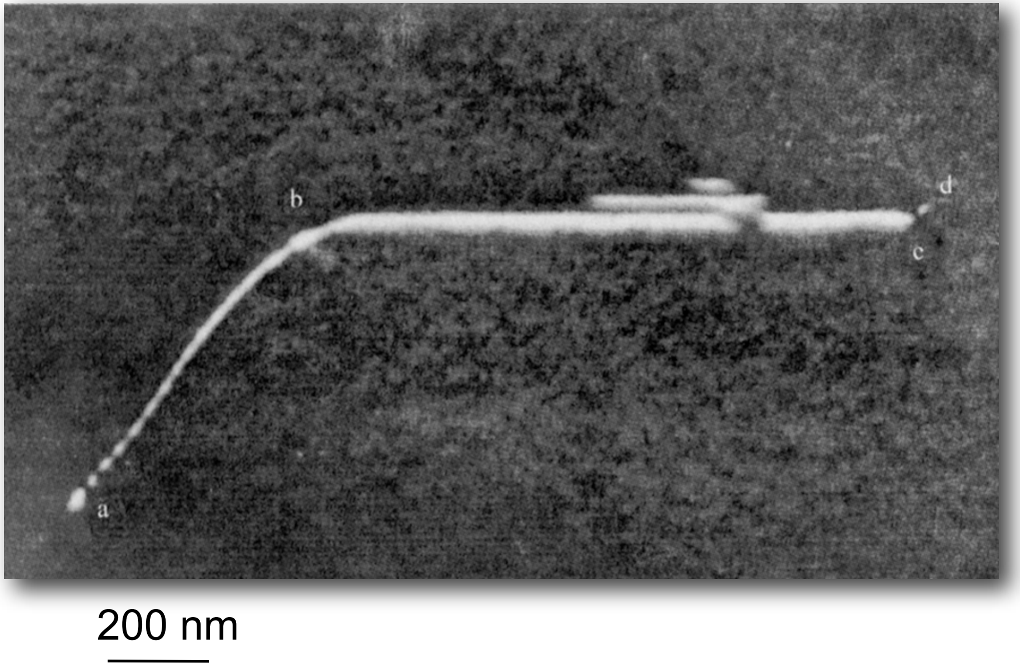
- Multiplication mechanisms arising from dislocation pinning or interaction
- Heterogeneous nucleation at specific local stress concentrations, *e.g.* growth artifacts or substrate defects
- Homogeneous (spontaneous) nucleation of dislocation loops



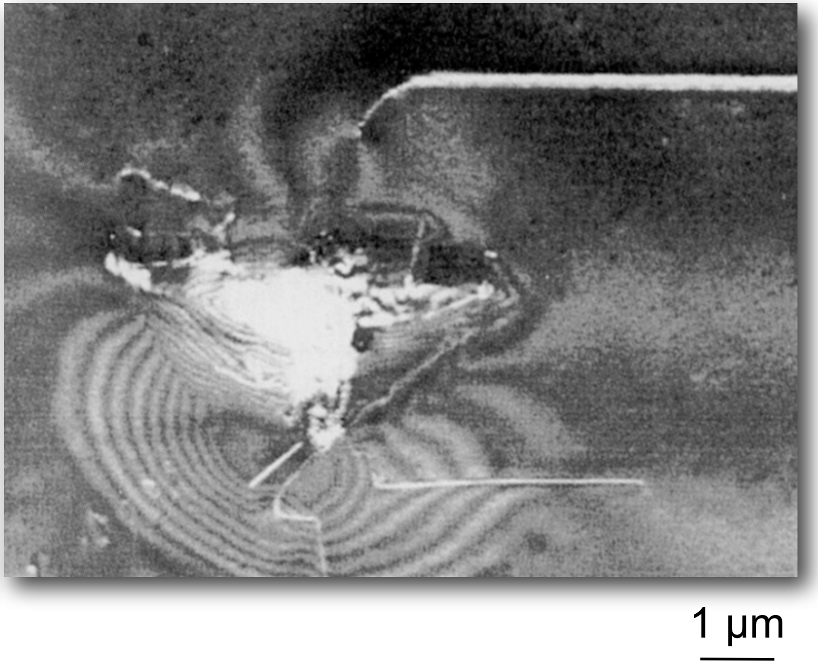
Generation of misfit dislocations from different sources: *a*) the pre-existing threading dislocation model and *b*) the half-loop generation from the free surface.

[Zou:01]

TEM examples



TEM weak-beam image showing the generation of a misfit dislocation bc from a threading dislocation ab. The short segment cd corresponds to the threading dislocation in the layer. InGaAs/GaAs single heterostructure.

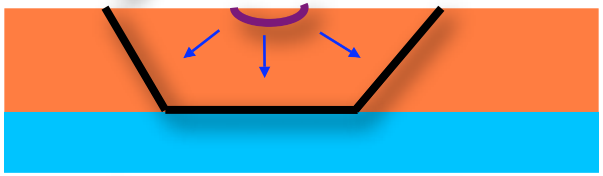
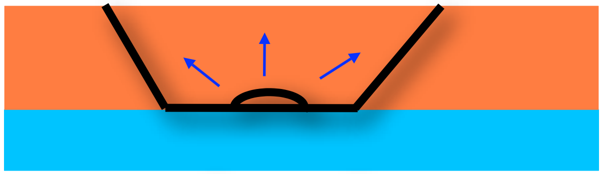
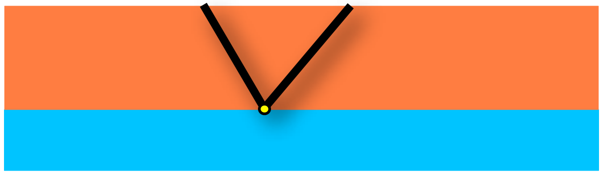


TEM weak-beam image of the generation of misfit dislocations at an inhomogeneous source. InGaAs/GaAs single heterostructure.

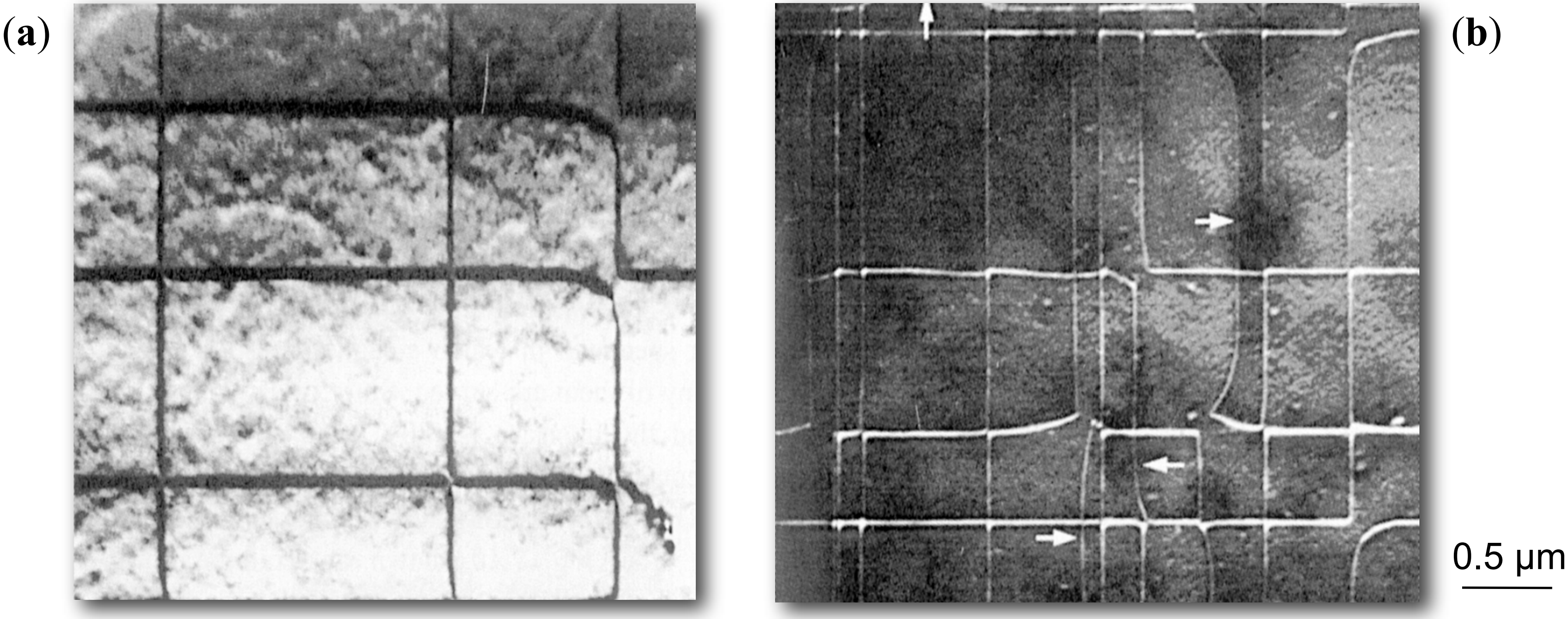
[Zou 2001]

Generation mechanisms

Compilation of Vdovin 1999

Dislocation behavior	Mechanism	Author
	Bending	[Matthews 1966]
	Surface generation	[Matthews *et al*. 1970]
	Interface generation	[Perovic, Houghton 1995]
	Interface precipitation	[Perovic *et al*. 1989, Fitzgerald *et al*. 1989, Eaglesham *et al*. 1989]

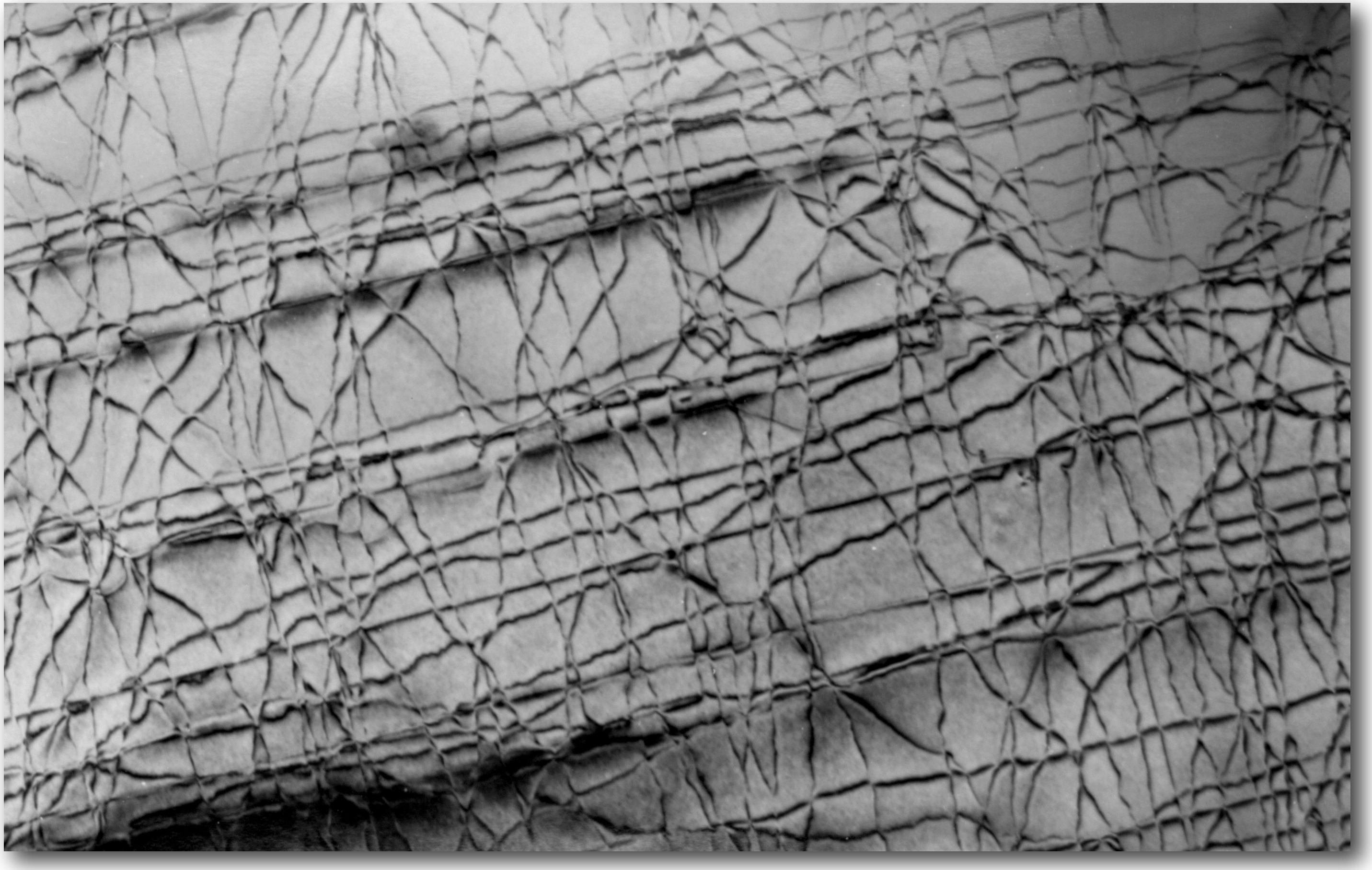
2.6 Configurations of misfit dislocations



TEM images from an (001) $In_{0.1}Ga_{0.9}As$ single heterostructure on (001) GaAs.
a) Layer thickness of 100 nm, *b*) 200 nm.

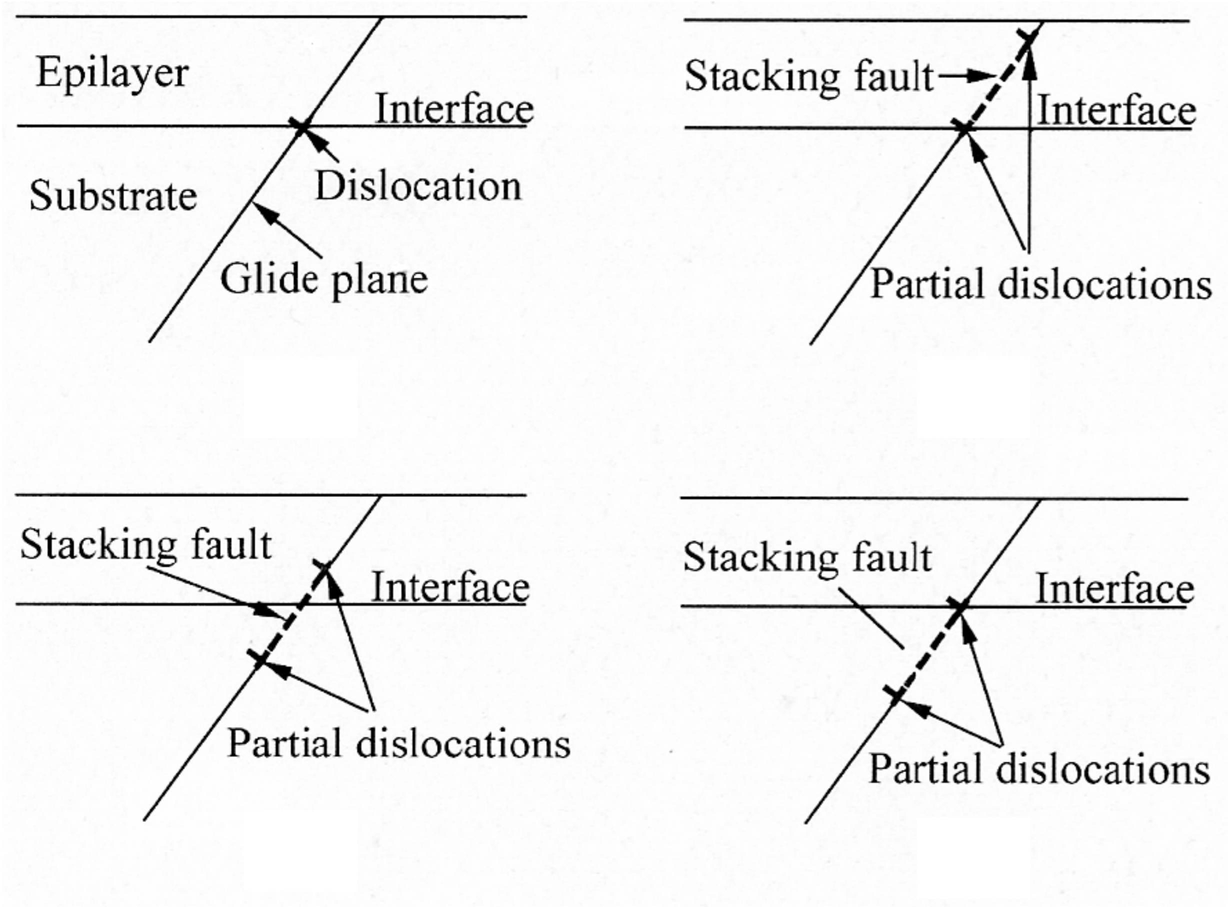
[Zou 2001]

Alignment of misfit dislocations



Misfit dislocations in (001) ZnSe/GaAs. MBE growth, layer thickness 495 nm.
TEM bright field image.

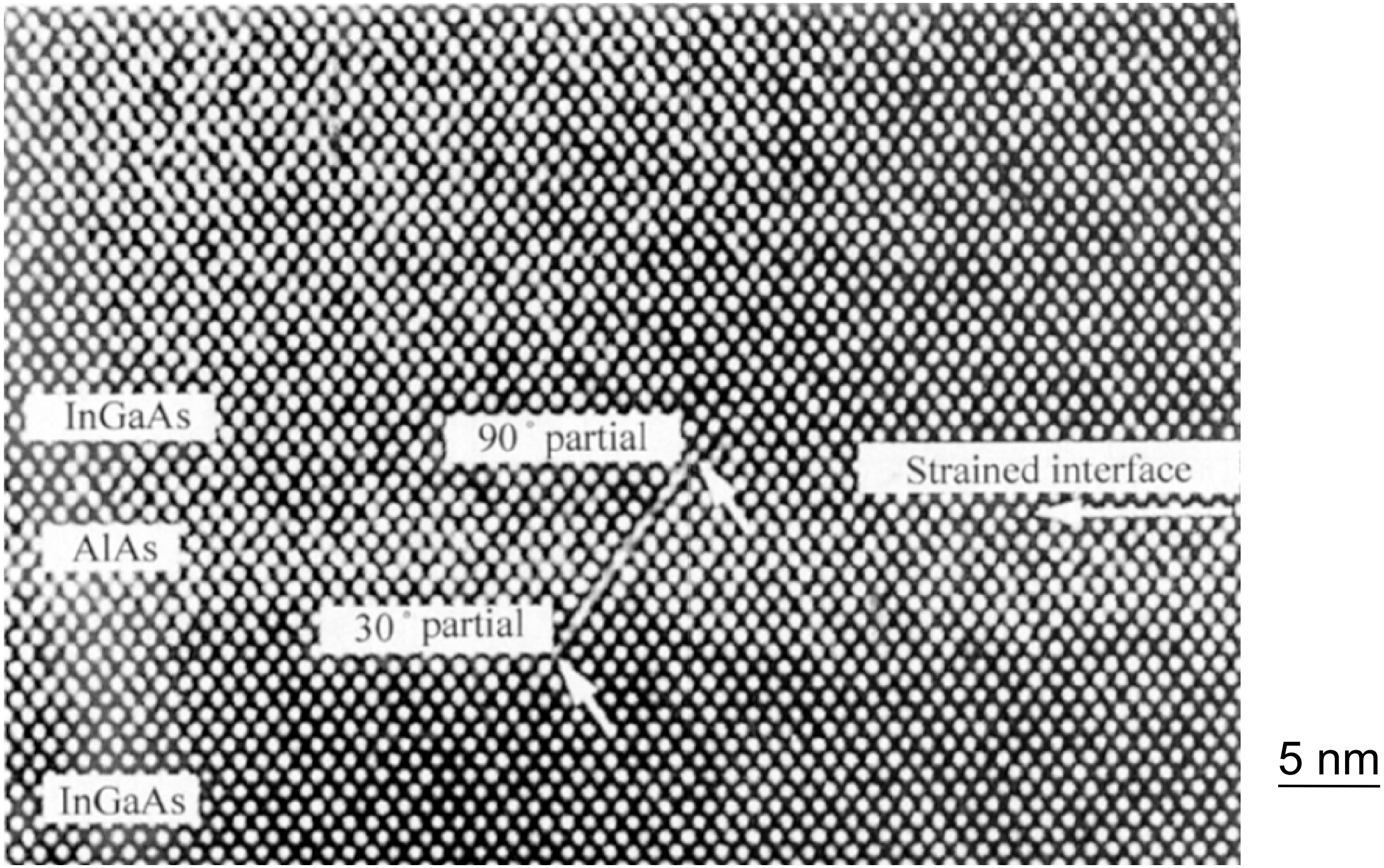
Dissociated misfit dislocations



Possible configuration of misfit dislocations

[Zou:01]

Configuration of a dissociated misfit dislocation in a heterostructure



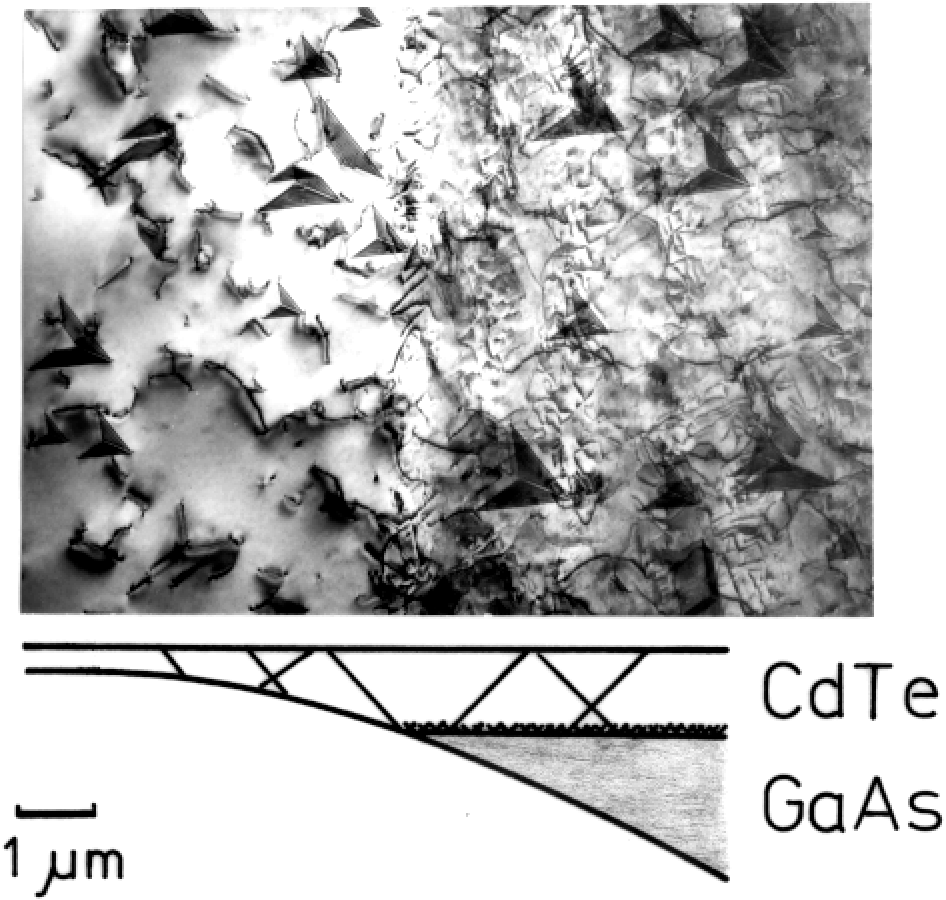
A high-resolution TEM image of a cross-section sample of a InGaAs heterostructure showing a dissociated 60° misfit dislocation. The 90° partial is near the strained interface, while the 30° is in the substrate.

[Zou 2001]

Stacking faults in the epitaxial layer

Stacking faults and threading dislocations in heteroepitaxial (111)CdTe/(001)GaAs. TEM bright field image, ***g*** diffraction vector.

Defects in CdTe/GaAs



Stacking fault tetrahedra, misfit and threading dislocations in heteroepitaxial (111)CdTe/(001)GaAs. Plane view transmission electron microscopy. The cross section of the TEM foil is shown below.

References

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