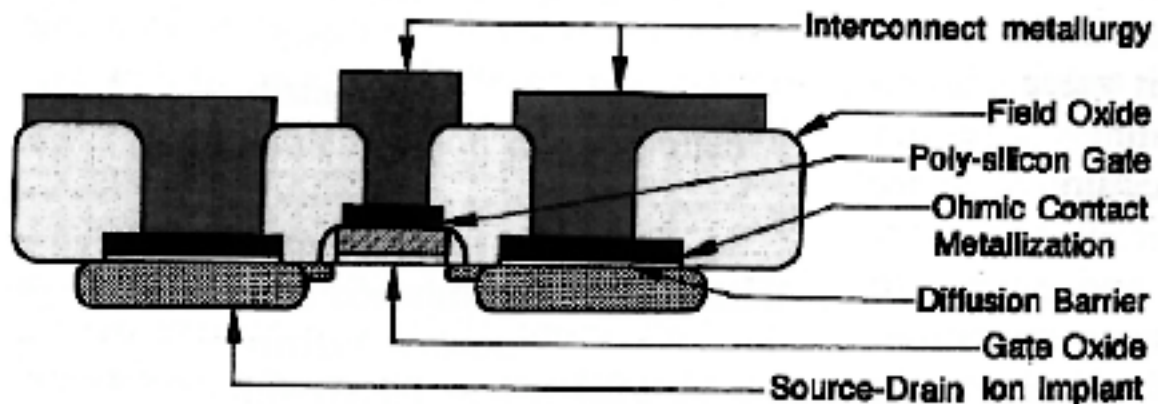


HETERO-INTERFACES

Significance

- integration of different semiconductor materials, metals, insulators
- example: field-effect transistor



- regions of different conductivity
- modification of regions near the surface via
 - diffusion
 - ion implantation
 - oxidation (\square SiO_2)
 - deposition of materials (!)

\square many processing steps

- deposition of materials \square hetero-interfaces
 - \square structural defects (misfit dislocations, stacking faults, ...)

- stresses, □ segregation of impurities
 - ohmic resistance (metal/semiconductor interfaces)
- problem: interfaces are often difficult to control
 - inhomogeneities along the interfaces
 - “accidental“ agglomeration of impurities
 - diffusion-controlled processes, “stochastisch“
 - example: Schottky barrier of 0.8 eV can typically only be controlled with a precision of 0.1 eV owing to the lateral variation of the interface structure
 - problems associated with lateral variation of properties increase with downscaling
- fabrication of interfaces under *controlled* conditions is crucial
- downscaling requires increasingly better layer deposition techniques
- particularly high quality can be achieved by “epitaxy”
 - meaning: growth of a crystalline layer with unique orientation relationship to the (crystalline) substrate
 - substrate “replicates” the atomistic structure of the substrate
- variety of techniques:
 - gas-phase epitaxy (chemical vapor deposition)
 - liquid-phase epitaxy
 - molecular-beam epitaxy

- select according to desired properties of the layer and the interface, as well as boundary conditions imposed by the fabrication process, for example
 - temperature window
 - growth rate
 - impurities
- layer composition can be varied along the growth direction
 - multi-layers
 - “artificial” periodicities
 - tailor electron bandstructure
 - atom layer by atom layer...
 - atomically sharp interfaces...
 - however: often requires low growth temperatures
- most common form of epitaxy: **homo-epitaxy**
- example: epitaxial Si layer on Si substrate
 - doping
 - enables particularly steep (atomically sharp?) doping profiles
- dissimilar materials: **hetero-epitaxy**
- example: epitaxial layer of $\text{Ge}_{1-x}\text{Si}_x$ solid solution on Si substrate
 - abrupt change of electron band structure

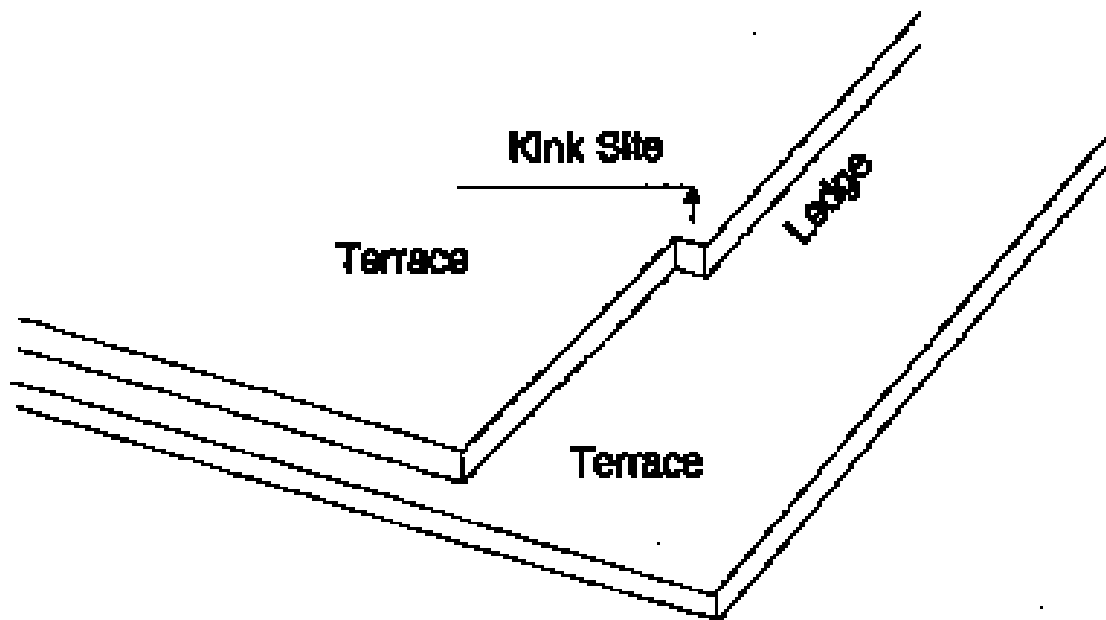
- particularly important semiconductor hetero-systems:
 - $\text{Ge}_{1-x}\text{Si}_x/\text{Si}$
 - $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$
 - $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}/\text{InP}$
- many novel electronic devices
 - quantum-well laser
 - hetero-bipolar transistors
(current amplification++, high-frequency response++)
 - highly-sensitive photodetectors

General Aspects of Epitaxy

- crystal growth on a *surface*
 - structure?
 - composition?
 - atomistic mechanisms at the growth front?
- not in thermodynamic equilibrium, but:
 - growth rate typically slow compared to atomistic relaxation processes
- epitaxy can take place under *near* equilibrium conditions
- atomistic structure of a surface in thermodynamic equilibrium?

Thermodynamics and Equilibrium Structure of Surfaces

- surface atoms see different environment than bulk atoms:
 - less neighboring atoms, broken bonds
 - surface *phase*
 - surface *energy* and *tension*, always positive
- consequences:
 - facets (terraces), ledges, and kinks
 - “TKL” structure
 - configuration entropy
- approximation for energy balance:
add TKL components



- three important cases:

1. surface plane with special *crystallographic* orientation

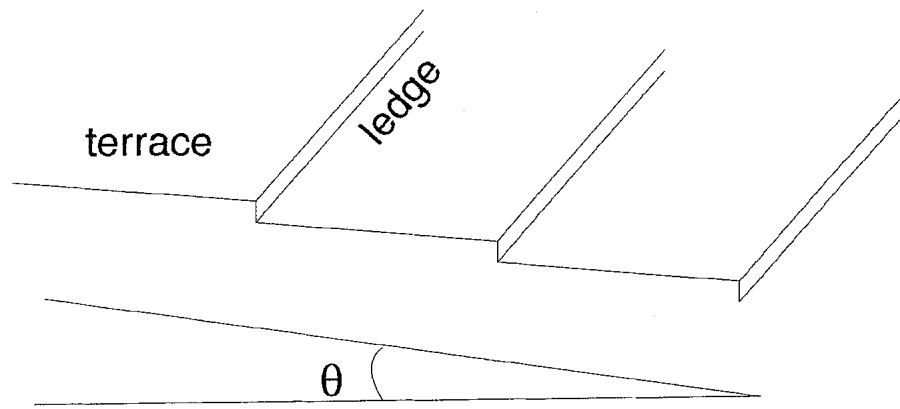
surface exactly parallel to a low-indexed plane of the crystal lattice

equilibrium: no ledges

2. surface slightly “off-axis”

surface plane slightly inclined against a low-indexed plane of the crystal lattice

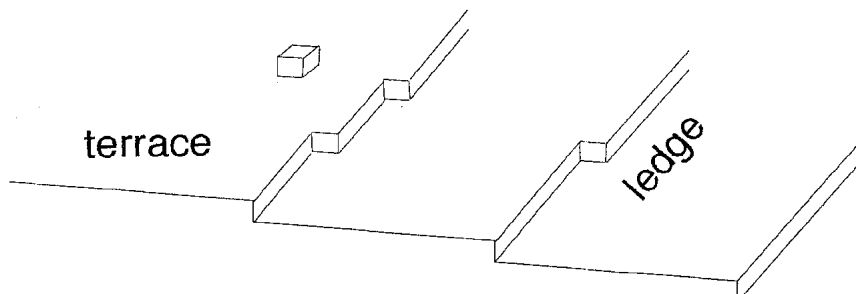
equilibrium: ledges with regular spacing



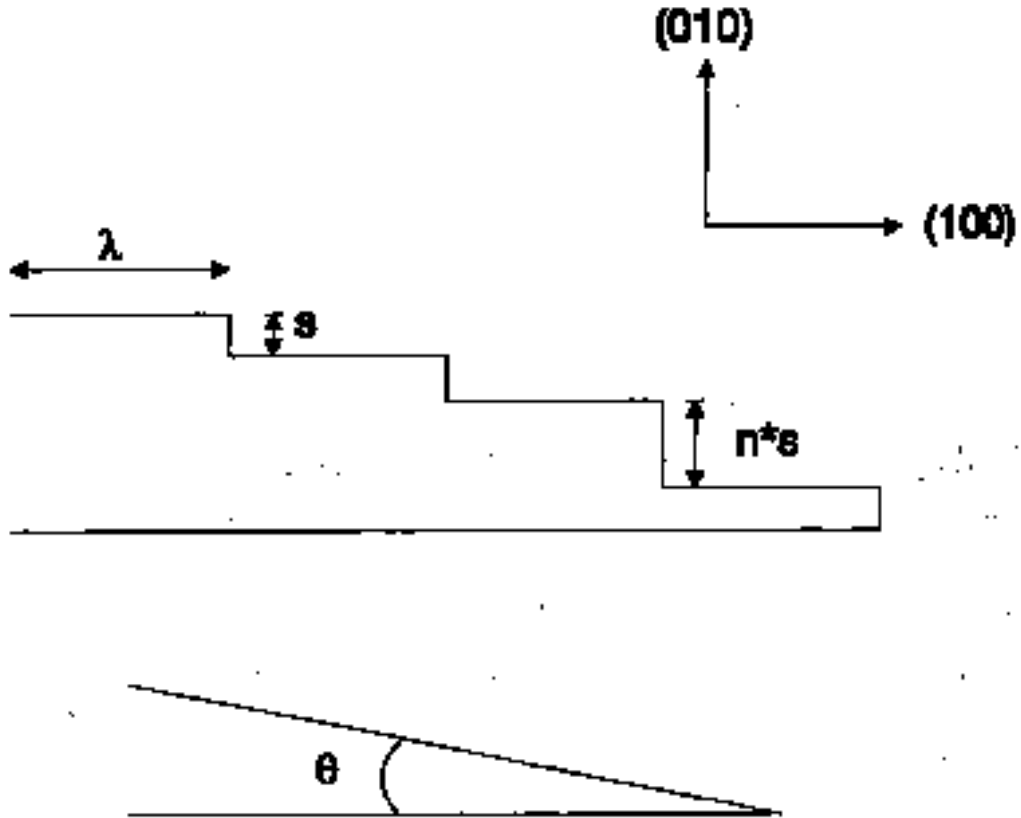
3. surface “randomly” oriented

- surface plane corresponds to high-indexed plane of the lattice

ledges with *kinks*



- frequently: surface plane *nearly* parallel to low-indexed plane
 □ exploit ledges for controlling epitaxial growth
- example: Si surface with an inclination of $\varphi \leq 4^\circ$ versus (001)



- equilibrium at 0 K:
 - mono-atomic ledges of height s
 - density of these ledges:

$$\frac{\text{Tan}[\varphi]}{s}$$

□ average width of terraces between the ledges:

$$\lambda = \frac{s}{\tan[\theta]}$$

– energy balance:

$$E[\theta] = E[0] \cos[\theta] + \frac{\lambda}{s} \sin[\theta]$$

$E[\theta]$: energy of surface inclined by θ ; $E[0]$: energy of surface parallel to low-indexed plane; λ line energy of ledges (energy per unit length); s : ledge height; $\cos[\theta]$: relative amount of terraces with respect to total area.

– temperature > 0 K:

- entropy contribution to the free energy
- particularly: configuration entropy

□ irregular arrangement of kinks and ledges

□ surface structure more complex

– imaging of the surface structure down to atomic resolution is possible by scanning tunneling microscopy (STM)

- example: STM of a Si surface 4° off (001)

□ TLK structure

– alternating contrast indicates *reconstruction* of the atom positions at the surface

□ surface structure \neq crystal structure

– cut a crystal in two halves □ dangling bonds

□ reconstruction:

- saturation of dangling bonds
- covalent bonding with neighboring atoms