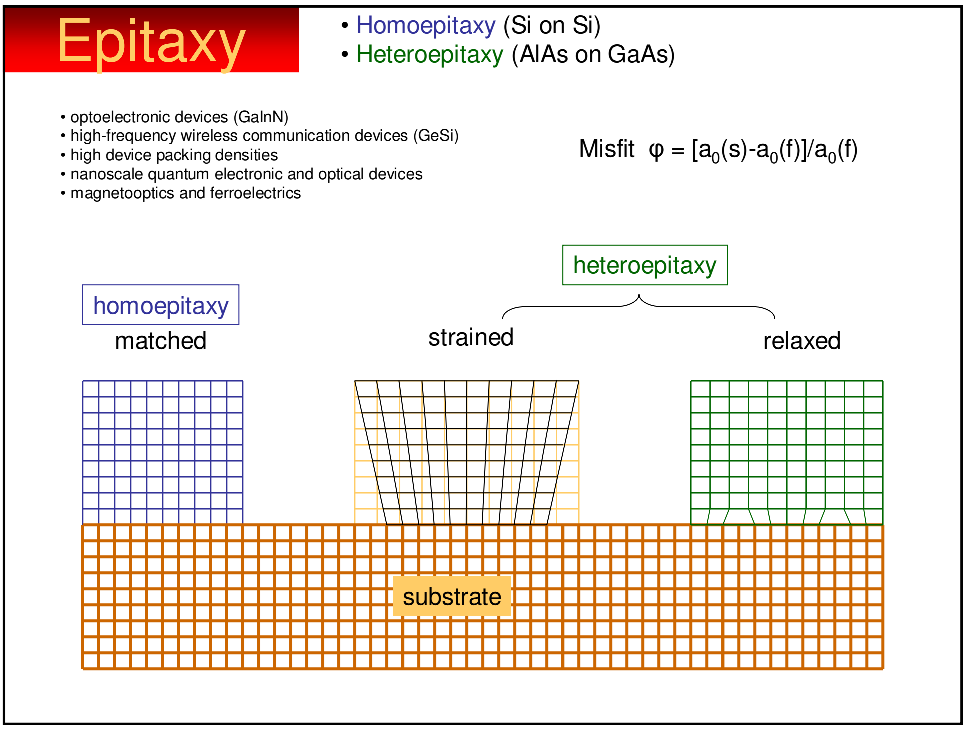
επιταξιζ

extended single-crystal film formation on top of a crystalline substrate



Epitaxy

- Homoepitaxy (Si on Si)
- Heteroepitaxy (AlAs on GaAs)

- optoelectronic devices (GaInN)
- high-frequency wireless communication devices (GeSi)
- high device packing densities
- nanoscale quantum electronic and optical devices
- magnetooptics and ferroelectrics

Misfit $\varphi = [a_0(s)-a_0(f)]/a_0(f)$

homoepitaxy

matched

heteroepitaxy

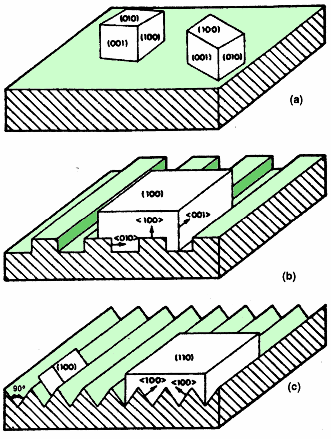
strained

relaxed

substrate

Epitaxy

Graphoepitaxy: films can be oriented even in the presense of a large misfit strain and absence of any bonding between the film and substrate



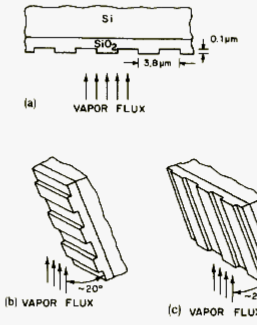


FIG. 2. Configurations for crystallization experiments in which Cr, Au, and Ge were evaporated (a) normal to the substrate, (b) at 70° from normal and perpendicular to the grating axis, and (c) at 70° from normal and along the grating lines.

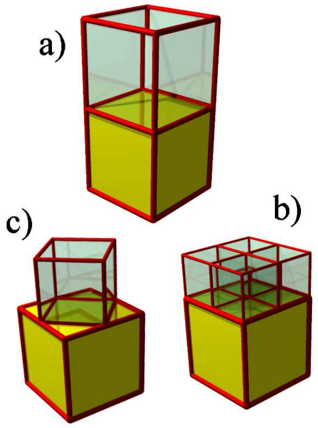
Graphoepitaxy of germanium on gratings with square-wave and sawtooth profiles
M. W. Geis, B-Y. Tsaur, and D. C. Flanders

Applied Physics Letters Vol 41(6) pp. 526-529. September 15, 1982

Epitaxy

Heteroepitaxy: coupled orientations of the thin film and substrate

Notation: $\underbrace{(001)\text{Ni}}_{\text{thin film}}$ // $\underbrace{(001)\text{Cu}}_{\text{substrate}}$: [100]Ni // [100]Cu



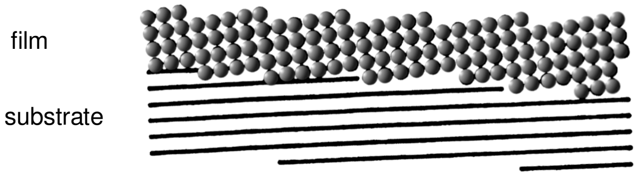
a)
Si: a_0=5.431 Å
CoSi_2: a_0=5.365 Å
NiSi_2: a_0=5.406 Å

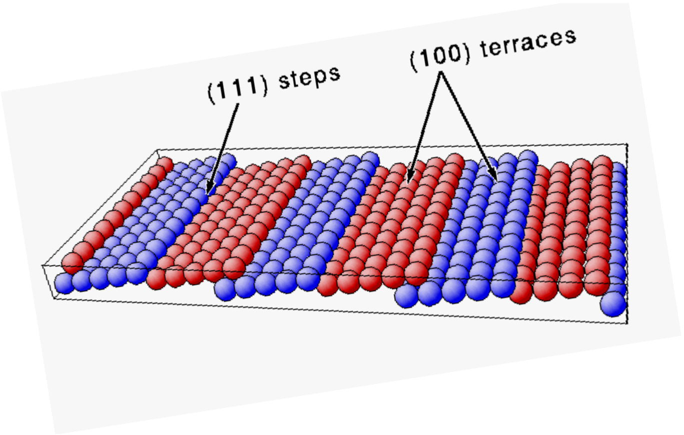
b)
GaAs: a_0=5.654 Å
Fe: a_0=2.866 Å
(110)Fe // (110)GaAs:
[200]Fe // [100]GaAs

c)
SrRuO_3: a_0=5.567 Å;
b_0=5.530 Å
$\text{YBa}_2\text{Cu}_3\text{O}_7$: a_0=3.82 Å
b_0=3.88 Å
(001)YBCO // (001)SRO:
[100]YBCO // [110]SRO

Epitaxy

Tilted-Layer: growth on vicinal-cut substrates





Epitaxy

Lattice Misfit
and Defects in Epitaxial Films

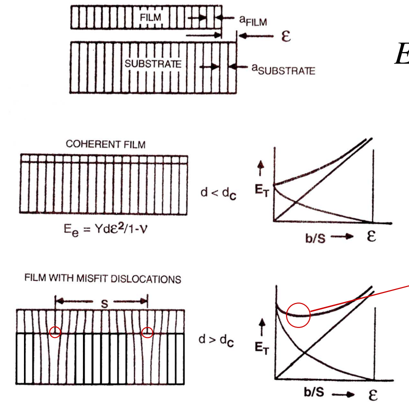


Figure 8-7 Illustration of the Matthews–Blakeslee equilibrium theory of misfit-dislocation formation. (Top) Coherent film is produced when $d < d_c$. (Bottom) Film with misfit dislocations result when $d > d_c$. (From Ref. 18. Reprinted with permission of W. D. Nix.)

elastic dislocations

$$E_T = \frac{Yd(\varphi - b/S)^2}{1-\nu} + \frac{2\mu b^2 \ln(\beta d/b)}{4\pi(1-\nu)S}$$

minimum

$$\frac{\mathrm{d}E_T}{\mathrm{d}(b/S)} = 0$$

$$\mu = \frac{Y}{2(1+\nu)}$$

Critical thickness

$$d_c = \frac{\mu b}{4\pi Y \varphi} \ln\left(\frac{\beta d_c}{b}\right) = \frac{b}{8\pi(1+\nu)\varphi} \ln\left(\frac{\beta d_c}{b}\right)$$

Epitaxy

Lattice Misfit
and Defects in Epitaxial Films

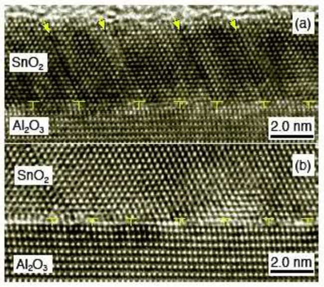
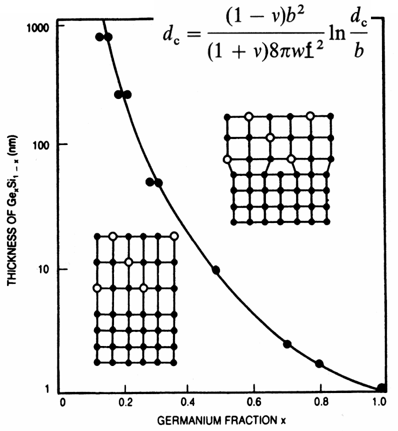


Figure 1: Cross-section high-resolution TEM images of epitaxial SnO$_2$ films with a thickness of 5 nm (a) and 100 nm (b), grown on R-cut sapphire. The interface is viewed along SnO$_2$ [010]. Note that the film with a small thickness consists of a number of planar defects (APBs) indicated by arrows. Misfit dislocations are marked by T.

Abs. 638, 204th Meeting, © 2003 The Electrochemical Society, Inc.

Structure-Property Relationships of Interfaces in Epitaxial SnO$_2$ Thin Films
Xiaoqing Pan, Juan E. Dominguez, Wonwoo Kim, and Haiping Sun
Department of Materials Science and Engineering,
University of Michigan, Ann Arbor, MI 48109

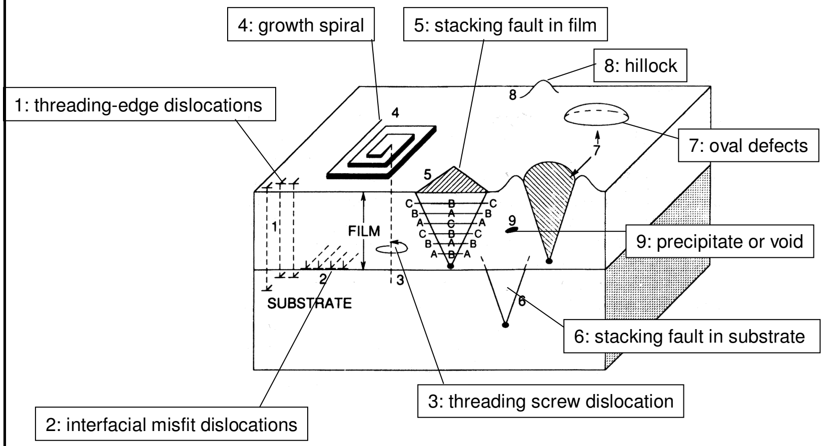


$$d_c = \frac{(1-\nu)b^2}{(1+\nu)8\pi w f^2}\ln\frac{d_c}{b}$$

Figure 8-8 Experimentally determined limits for defect-free strained-layer epitaxy of Ge$_x$Si$_{1-x}$ on Si. Note that f is proportional to Ge fraction J.C.Bean, *Physics Today* **39**, 2 (1986)

Epitaxy

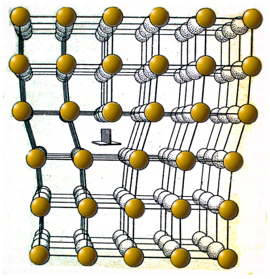
Dislocation Types
in Epitaxial Films

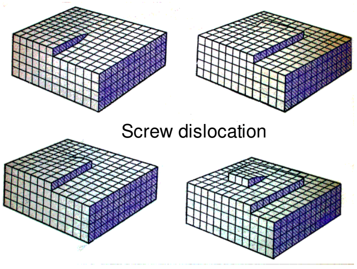


Epitaxy

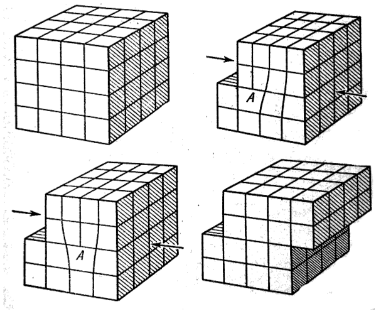
Dislocation Types
in Epitaxial Films

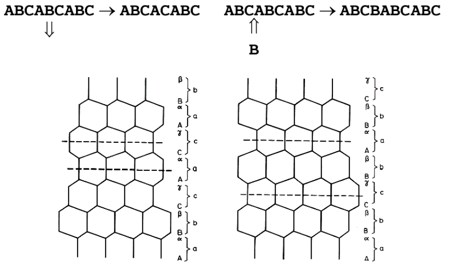
Edge dislocation





Dislocation motion (plasticity)





Intrinsic and extrinsic stacking faults in the projection onto the (110) plane

---

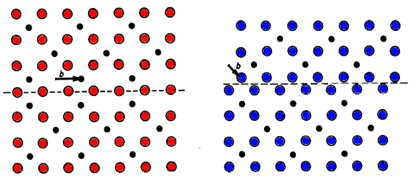
Epitaxy

Dislocation Types
in Epitaxial Films

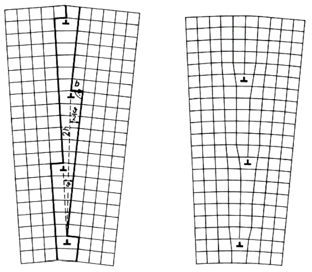
Stacking faults as translation boundaries between the crystals with parallel orientation
Twin boundaries with a certain difference in the orientation between the crystals
Grain boundaries between regions of the crystal with arbitrary orientations
Phase boundaries between regions of different structure

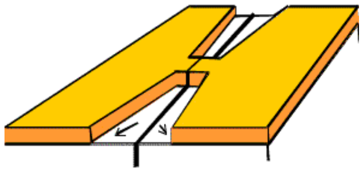
From: Hartmut S. Leipner : *Structure of imperfect crystals*

Stacking fault as the deviation in the ordered sequence of atomic layers



Physical and chemical stacking faults as translation boundaries

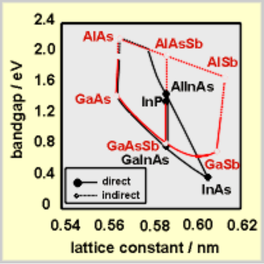




Epitaxy

Compound-Semiconductor Materials: Designing Film-Substrate Match

- direct and indirect energy bandgaps
- bangap energies
- lattice match; thermal expansion



http://www.hhi.fraunhofer.de

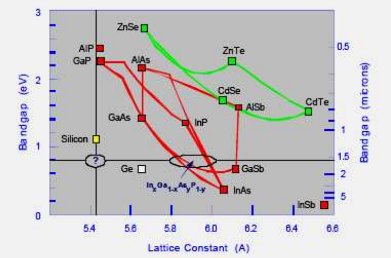


Figure 1. Band gaps and lattice constants for various traditional semiconductor materials. The III-V's are shown as red squares, and the II-VI's are shown as green squares. The color-shaded areas denote possible alloyed materials. The InxGa1-xAsyP1-y alloy has a bandgap near 1.5 microns and is the current industry standard. The large lattice constant mismatch with Si prohibits monolithic integration. An ideal material would have a lattice constant and bandgap lying in the region containing the question mark.

14 — **Surfaces and Interfaces** – Semiconductor Surface Studies — 14
RLE Progress Report 143

Semiconductor Surface Studies

Academic and Research Staff
Professor John D. Joannopoulos, Dr. Niko Moll

Graduate Students
Tairan Wang

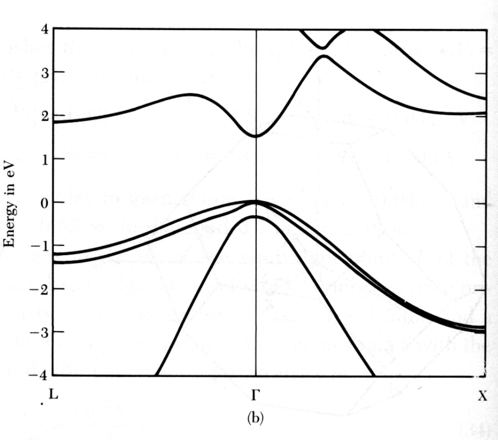
Technical and Support Staff
Margaret O'Meara

http://rleweb.mit.edu/Publications/pr143/chapter14-web.pdf

Epitaxy

Compound-Semiconductor Materials: Designing Film-Substrate Match

In direct gap semiconductors such as GaAs the top of the valence band and the bottom of the conduction band occur at the same k-vector.



(b)

k = 0

Epitaxy

Compound-Semiconductor Materials: Designing Film-Substrate Match

Indirect Bandgap Semiconductors

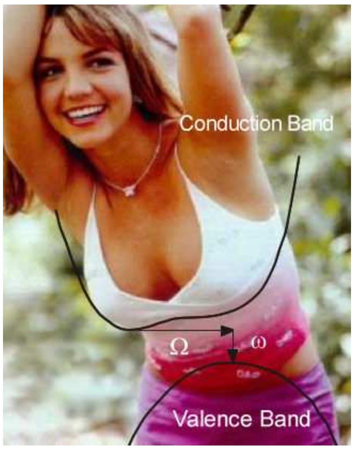
Not all semiconductor materials have the minimum of the conduction band above the top of the valence band in the E-k bandstructure. These materials are known as indirect semiconductors. Examples include **Si, Ge** and **AlAs**. For indirect bad gap semiconductors, the conduction band can be crudely approximated by the following equation near the conduction band minimum.

$$E(k)=E_g+h^2(k-k_0)^2/(2m_e)$$

where k_0 is the offset in the conduction band minimum. For light emitting devices, indirect band gap semiconductors are not at all promising.

To see why, consider the band edge diagram of an indirect band gap semiconductor. The momentum of an electron in the conduction band is different from a hole in the valence band.

For a transition to occur, requires both a photon of frequency ω and also a phonon of frequency Ω.Clearly, the probability of these two events happening is less likely than an electron making a single direct transition, as occurs in direct bandgap semiconductors.



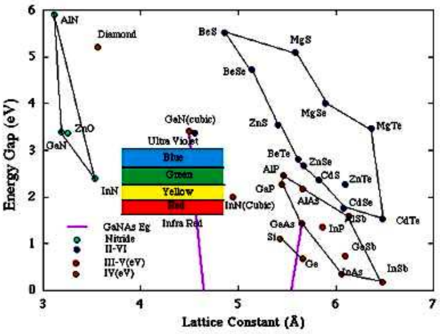
from Britney Spears Guide to Semiconductor Physics: **Indirect-gap ...** : http://britneyspears.ac/physics/indirect/indirect.htm

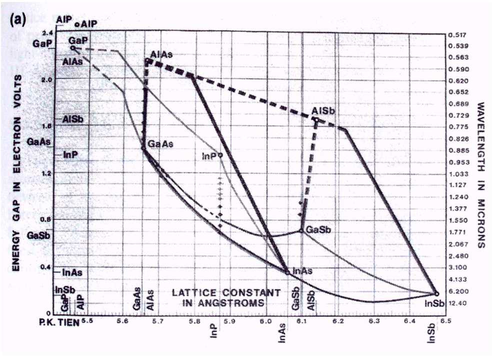
---

Epitaxy

Compound-Semiconductor Materials: Designing Film-Substrate Match

- direct and indirect energy bandgaps
- bangap energies
- lattice match; thermal expansion





Relationship between energy gaps and lattice constants of representative semiconductors. Energy gap of GaNAs is shown in this figure as a representative of III-V-N nitrides. The solid line is an extrapolation of the experimental results close to GaAs and cubic GaN based on the dielectric model, and negative energy gap is expected in-between from this extrapolation. **http://opmac06.es.hokudai.ac.jp/opres/resthe/r2/res2e.html#res2_1**

Epitaxy

Compound-Semiconductor
Materials

- direct and indirect energy bandgaps
- bangap energies
- lattice match; thermal expansion

$$\lambda_c(\mu\mathrm{m}) = \frac{1.24}{E_g(\mathrm{eV})}$$

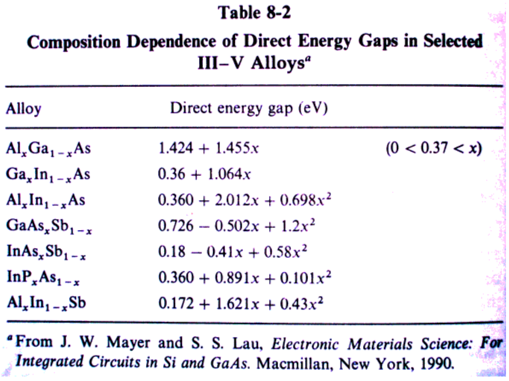
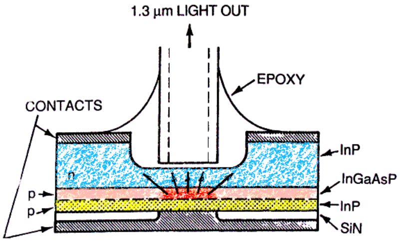


Table 8-2

Composition Dependence of Direct Energy Gaps in Selected III–V Alloys[a]

Alloy	Direct energy gap (eV)	
$Al_xGa_{1-x}As$	$1.424 + 1.455x$	$(0 < 0.37 < x)$
$Ga_xIn_{1-x}As$	$0.36 + 1.064x$	
$Al_xIn_{1-x}As$	$0.360 + 2.012x + 0.698x^2$	
$GaAs_xSb_{1-x}$	$0.726 - 0.502x + 1.2x^2$	
$InAs_xSb_{1-x}$	$0.18 - 0.41x + 0.58x^2$	
InP_xAs_{1-x}	$0.360 + 0.891x + 0.101x^2$	
$Al_xIn_{1-x}Sb$	$0.172 + 1.621x + 0.43x^2$	

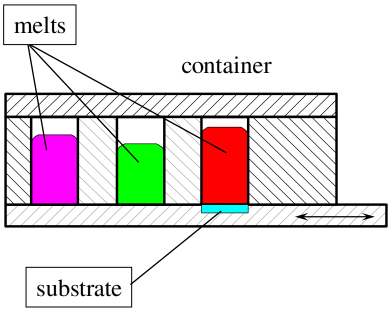
[a] From J. W. Mayer and S. S. Lau, *Electronic Materials Science: For Integrated Circuits in Si and GaAs.* Macmillan, New York, 1990.

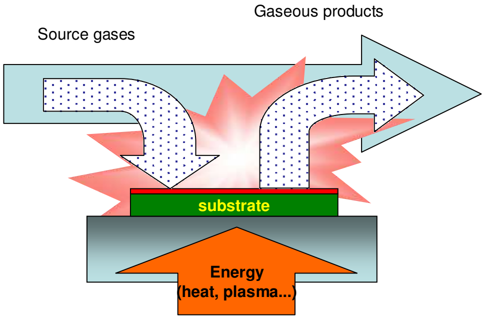


Epitaxy

High-Temperature
Deposition Methods

- Liquid-Phase Epitaxy (70% of light-emitting diods)
- CVD-Based Epitaxy

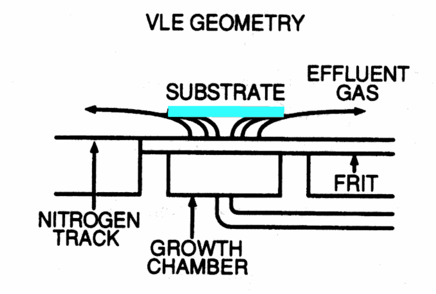


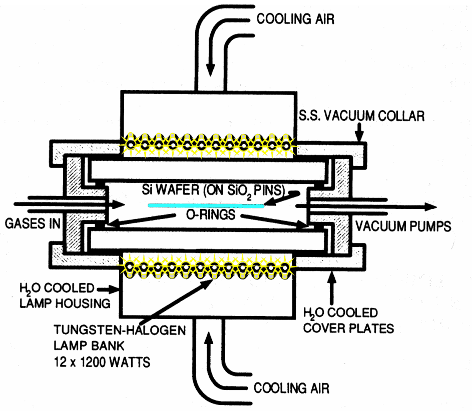


Epitaxy

High-Temperature Deposition Methods

CVD-Based Epitaxy: vapor levitation & rapid-thermal processes





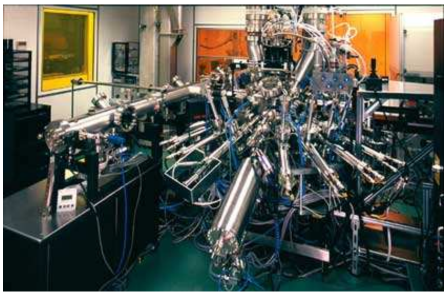
Epitaxy

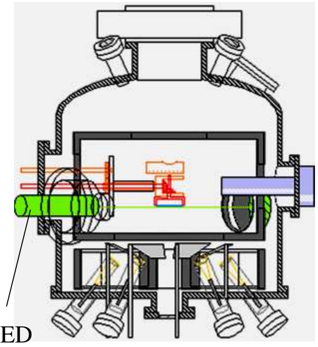
Low-Temperature Deposition Methods

- MBE

- **evaporation** at very low deposition rates
- typically in ultra-high vacuum
- very well controlled
- grow films with good crystal structure
- expensive
- often use multiple sources to grow alloy films
- deposition rate is so low that substrate temperature does not need to be high

OXXEL, Germany



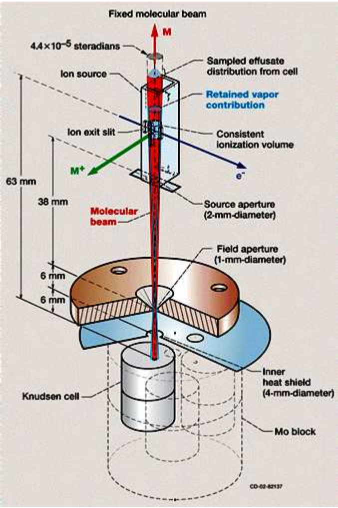


Knudsen cell sources

Epitaxy

Low-Temperature
Deposition Methods

- MBE sources; effusion

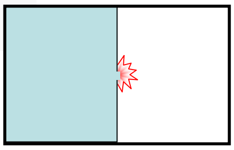


Knudsen cell source

http://www.grc.nasa.gov

Knudsen's effect

$$\frac{P_1}{\sqrt{T_1}} = \frac{P_2}{\sqrt{T_2}}$$



effusion rate (1/s) ~ Snv $\quad n = P/k_B T, \quad v \sim \sqrt{k_B T / m_0}$

effusing gas will be enriched with lighter molecules
(isotope rectification)

Epitaxy

Low-Temperature
Deposition Methods

- MBE sources; RHEED

5-100 keV

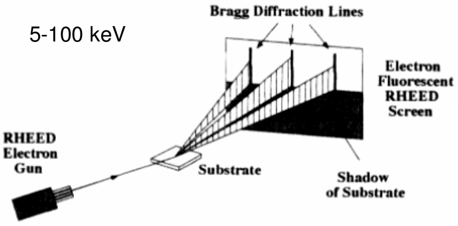
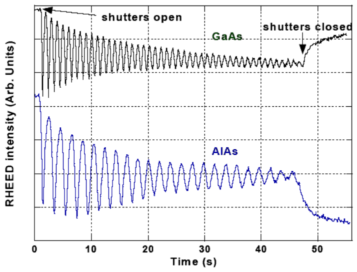


Figure 4. Schematic diagram illustrating the principle of RHEED.



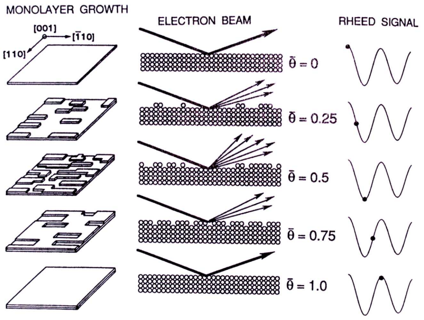


Figure 8-36 Real space representation of the formation of a single complete monolayer. $\bar{\theta}$ is the fractional layer coverage. Corresponding RHEED oscillation signal is shown.

Epitaxy

Less Common
Epitaxy Processes

- MBE Allotaxy
- Mesotaxy

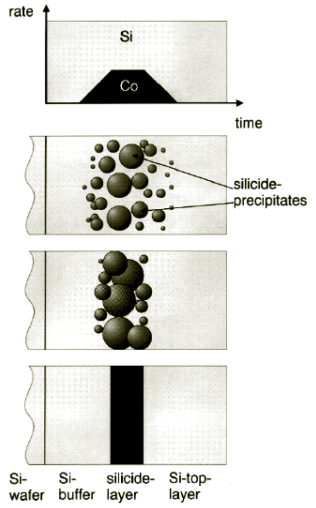
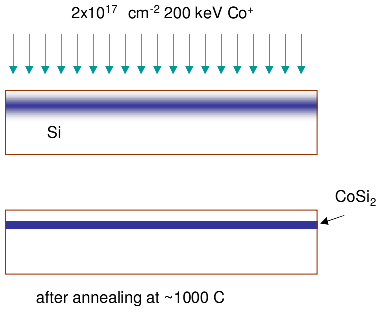


Figure 2. An illustration of the molecular beam allotaxy (MBA) method for the fabrication of heterostructures: (a) deposition rates of Si and Co versus time, (b) a cross sectional view of the schematic microstructure of the as-grown film, (c) an illustration of Ostwald ripening and coalescence of the precipitates during annealing and (d) a buried silicide layer after high-temperature annealing.

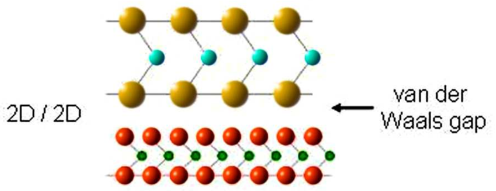


J. Phys. D: Appl. Phys. **31** (7 January 1998) 1-17
Molecular beam allotaxy: a new approach to epitaxial heterostructures
Siegfried Mantl

Epitaxy

Less Common
Epitaxy Processes

- van der Waals epitaxy



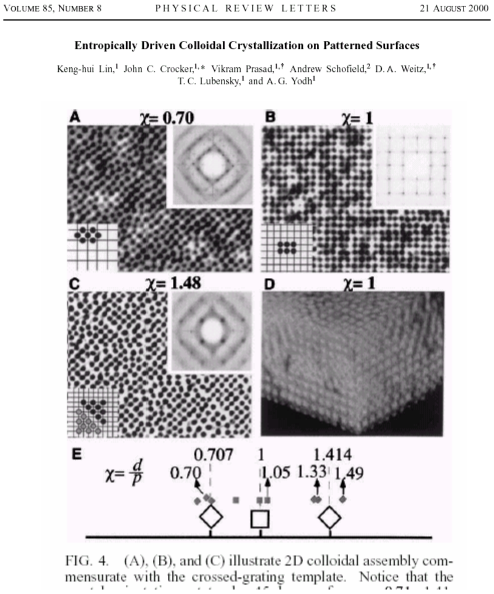
Se/Te; [(Mo,Nb,)(S,Te,Se)$_2$]/(mica,SbS$_2$,S-GaAs);
GaSe/Se-GaAs; GaSe/H-Si

- large lattice mismatch
- still an epitaxial growth

Epitaxy

Less Common
Epitaxy Processes

- Colloidal epitaxy



Volume 85, Number 8 PHYSICAL REVIEW LETTERS 21 August 2000

Entropically Driven Colloidal Crystallization on Patterned Surfaces

Keng-hui Lin,[1] John C. Crocker,[1,*] Vikram Prasad,[1,†] Andrew Schofield,[2] D. A. Weitz,[1,†]
T. C. Lubensky,[1] and A. G. Yodh[1]

FIG. 4. (A), (B), and (C) illustrate 2D colloidal assembly commensurate with the crossed-grating template. Notice that the

Solid particles in a liquid->colloid (paint, ketchup). The particles are usually very small, often less than 10μm in diameter.