Epitaxy

Epitaxial Growth

- Epitaxy means the growth of a single crystal film on top of a crystalline substrate.
- For most thin film applications (hard and soft coatings, optical coatings, protective coatings) it is of little importance.
- However, for semiconductor thin film technology it is crucial.

Types of Epitaxy

- Homoepitaxy
  - The film and the substrate are the same material.
  - Often used in Si on Si growth.
  - Epitaxially grown layers are purer than the substrate and can be doped independently of it.
- Heteroepitaxy
  - Film and substrate are different materials.
  - Eg: AlAs on GaAs growth
  - Allows for optoelectronic structures and band gap engineered devices.

Heteroepitaxy

- Trying to grow a layer of a different material on top of a substrate leads to unmatched lattice parameters.
- This will cause strained or relaxed growth and can lead to interfacial defects.
- Such deviations from normal would lead to changes in the electronic, optic, thermal and mechanical properties of the films.

Lattice Strains

- For many applications nearly **matched** lattices are desired to minimize defects and increase electron mobility.
- As the mismatch gets larger, the film material may **strain** to accommodate the lattice structure of the substrate. This is the case during the early stages of film formation (pseudomorphic growth) and with materials of the same lattice structure. The Si-Ge system is an example.
- If strain accommodation is not possible then dislocation defects at the interface may form leading to **relaxed** epitaxy and the film returns to its original lattice structure above the interface.
- **Lattice misfit** is defined as:

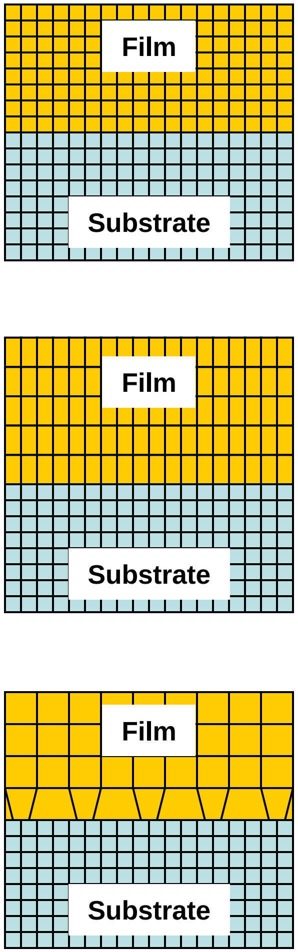
$$\underline{f} = \left[a_0(s) - a_0(f)\right] / a_0(f)$$

where $a_0(s/f)$ are the lattice constants of the substrate and the film.

Matched

Strained

Relaxed

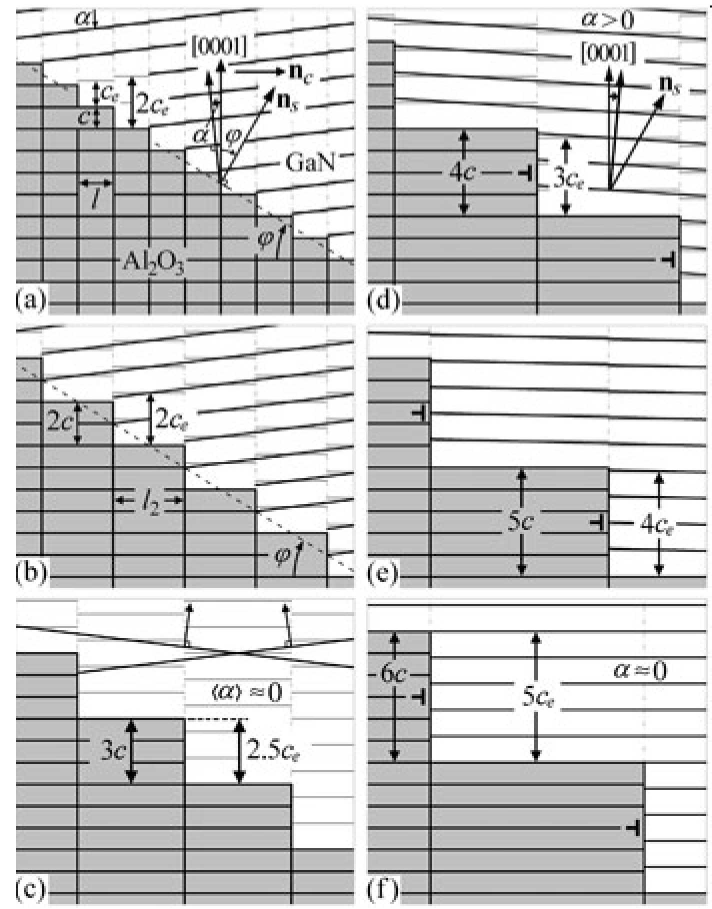


Metal-Semiconductor Heteroepitaxy

- Metal-semiconductor structures are used for contact applications.
- While not essential, epitaxial growth allows increased electron mobility through a junction.
- Examples:
  - $CoSi_2$ or $NiSi_2$ on Si. Since the lattice mismatch is small (all around 5.4 Å) and the crystal structures are similar, interfaces are remarkably defect free.
  - Fe on GaAs is similarly possible since the lattice size of Fe is about half of GaAs.
  - The lattice constants of Al and Ag are $\sim 1/\sqrt{2}$ of GaAs. In this case the crystal orientation of the film is rotated with respect to the substrate. A few layers of intervening metal (such as Fe or Ga) can be deposited to foster epitaxy.

Tilted Layer Epitaxy

- It is possible to have a misorientation between the crystal plane of the film and the substrate.
- As a result the surface breaks up in to an array of terraces of variable length and height.
- Then the film growth occurs by step advancement along the terraces (step - flow process).



Epitaxial Tilting of GaN Grown on Vicinal Surfaces of Sapphire (Huang, et.al.)

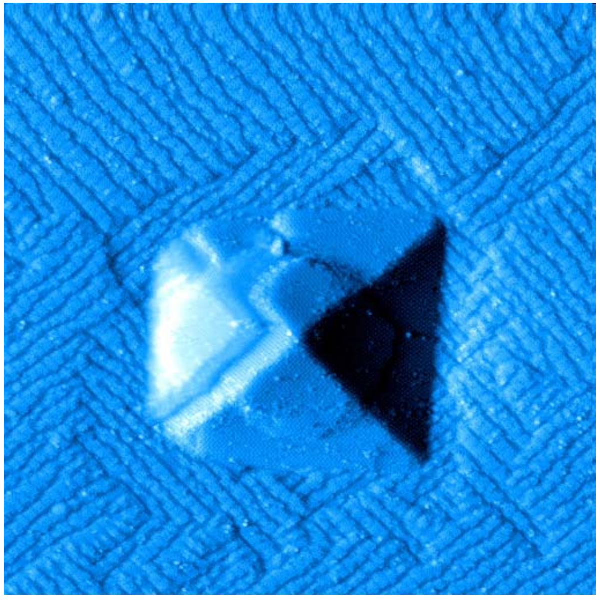
Lattice Misfits and Defects

- If the lattice mismatch is less than ~9%, the initial layers of film will grow pseudomorphically.
- Therefore very thin films strain elastically to have the same inter-atomic spacing as the substrate.
- As film thickness increases, the rising strain will eventually cause a series of misfit dislocations separated by regions of relatively good fit. As such they are equilibrium theories.
- There is a critical film thickness, d_c, beyond which dislocations are introduced.
- In most cases pseudomorphic growth occurs until

$\underline{f} d_c = b/2$,where b is the size of the film unit cell.

Defects Ge_xSi_{1-x}/Si Films

- The GeSi/Si system has a large lattice misfit built in and as such is not an equilibrium system.
- This results in a large number of dislocations with few regions of good fit and the theory breaks down.
- Rippled surfaces and pyramidal tips are typical.



Types and Sources of Defects

- Defects reduce electron mobility, carrier concentration and optical efficiency.
- Current levels in Si are 1-10 defects/cm^2.
- Defects can propagate from the substrate as a screw dislocations.
- Dopants and impurities can cause edge and point dislocations.
- Another type of defect is the stacking faults where the stacking order of successive layers do not follow a specific order.

Formation of Misfit Dislocations

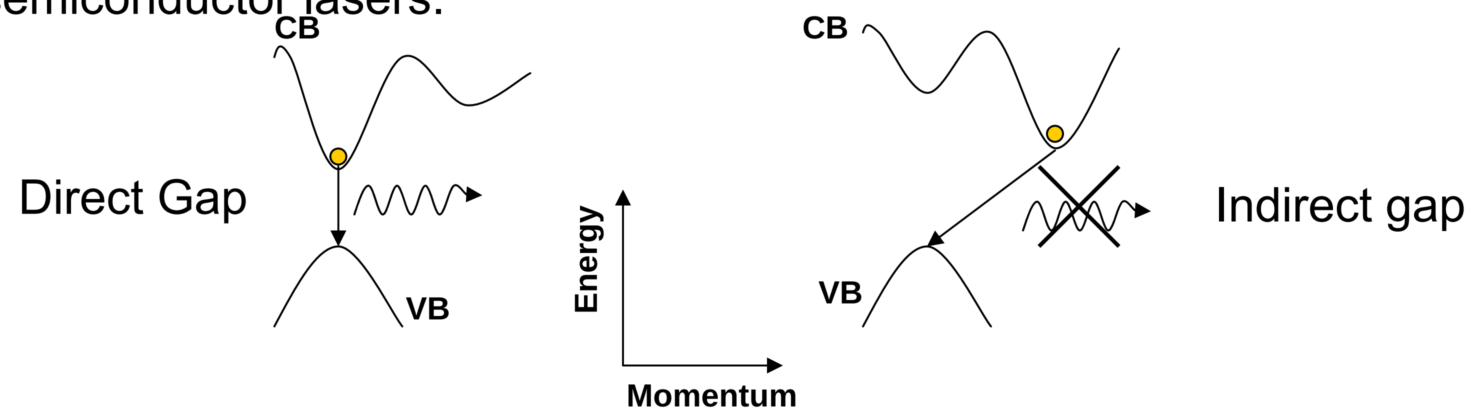
- They generally originate from threading dislocations at the film-substrate interface.
- The dislocation pierces through the substrate and the film.
- As it grows, it glides and bends in a slip plane.
- Above the critical thickness (d_c) the increasing strain allows a break and the film dislocation separates from the originating defect, leaving behind a stable misfit dislocation.

Epitaxy of Compound Semiconductors

- Most compound semiconductors are from the III-V group of materials (GaAs, InP, etc.) although II-VI materials are also used (ZnO, CdSe, CdS).
- Stochiometric adjustments allow control of the band structures and lattice constants.
- This affects both the electrical, thermal and optical properties and the epitaxial nature of the film.

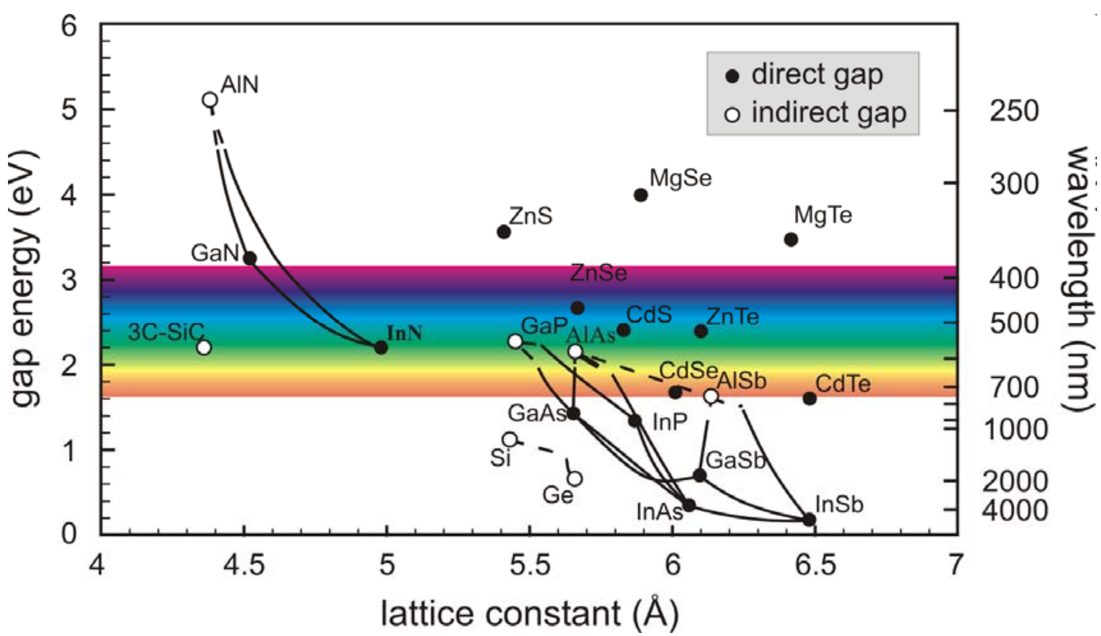
Optical Properties of Compound Semiconductor

- Optical emission from semiconductors requires energy and momentum conservation. While the energy of the emitted photon can come from an excited electron returning to its ground state, such a transition may require extra momentum which the photon can not supply (photons have minimal momentum).
- Materials that require extra momentum are called indirect semiconductors. Silicon and Germanium are examples (which is why we do not have Si lasers).
- In contrast direct gap semiconductors do not require a momentum change and can emit a photon efficiently. GaAs, ZnO, GaN and many of their alloys are in this class and are used in LEDs and semiconductor lasers.



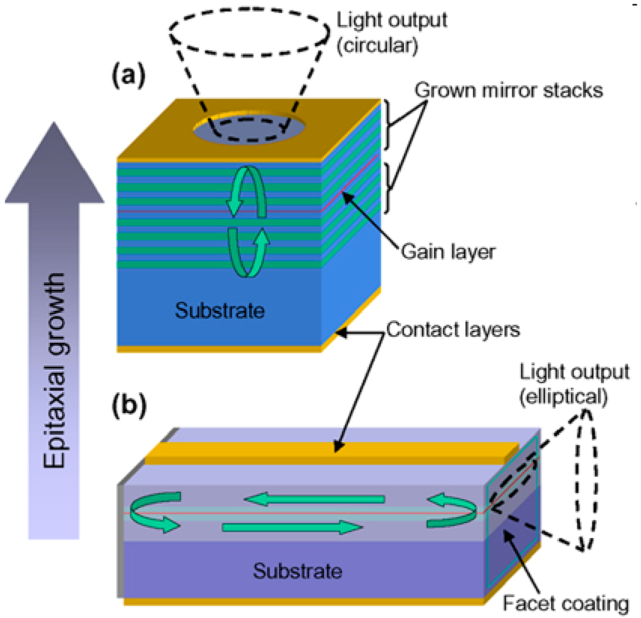
Other Properties of Compound Semiconductors

- For direct gap semiconductors, the band gap energy determines the wavelength (color) of the light that will be emitted. Various III-V alloys are used to cover most areas from the UV (GaN) to the NIR (GaAs) to the IR (InSb).
- The various alloys also offer a spectrum of lattice constants for lattice matching. GaAs and AlAs interfaces have minimal misfit and negligible dislocations.
- Thermal expansion coefficients are also comparable.



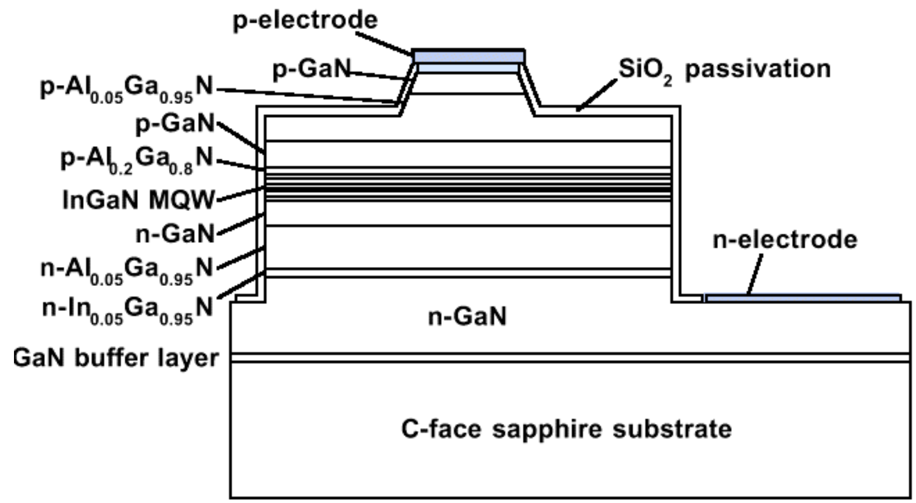
Devices and Applications

- Optoelectronic Devices
  - Using the direct gap nature for efficient light emission and the stochiometric flexibility for epitaxial purity, most lasers are made with compound semiconductors.
- High Speed Electronic Devices
  - The higher electron mobilities of compound semiconductors allow for operation in the microwave range (1 – 1000 GHz).
  - The heterojunction nature also increases the gain and efficiency of amplifiers made from these devices.



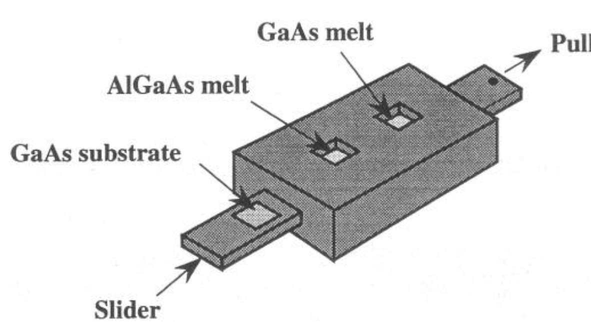
GaN Light Emitting Devices

- While materials with wide band gaps exist (AlN, GaN, ZnO) it has been difficult to get commercial blue/violet laser sources.
- Main difficulties lie in p-doping these materials and the high density of defects at the heterojunctions. Lack of suitable lattice matched substrates contribute to this problem.
- Current technology uses GaN for this region of the spectrum.
- p-doping was achieved using Mg. Also interface defects were reduced with a buffer layer over the sapphire substrate.



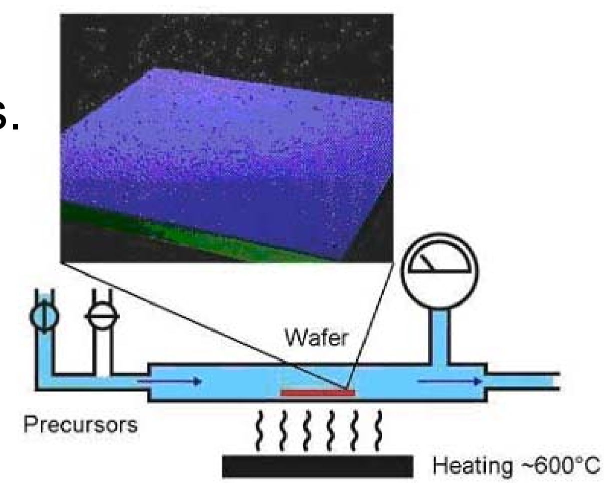
Liquid Phase Epitaxy (LPE)

- LPE involves the precipitation of a crystalline film from a supersaturated melt on to a substrate.
- The temperature is increased until a phase transition occurs and then reduced for precipitation.
- By controlling cooling rates the kinetics of layer growth can be controlled.
- Once can have either continuous reduction with the substrate (equilibrium cooling) or separate reduction in increments followed by contact with the substrate (step cooling).
- It is a low cost method yielding films of controlled composition, thickness and lower dislocation densities.
- Disadvantages are rough surfaces and poor thickness uniformity.



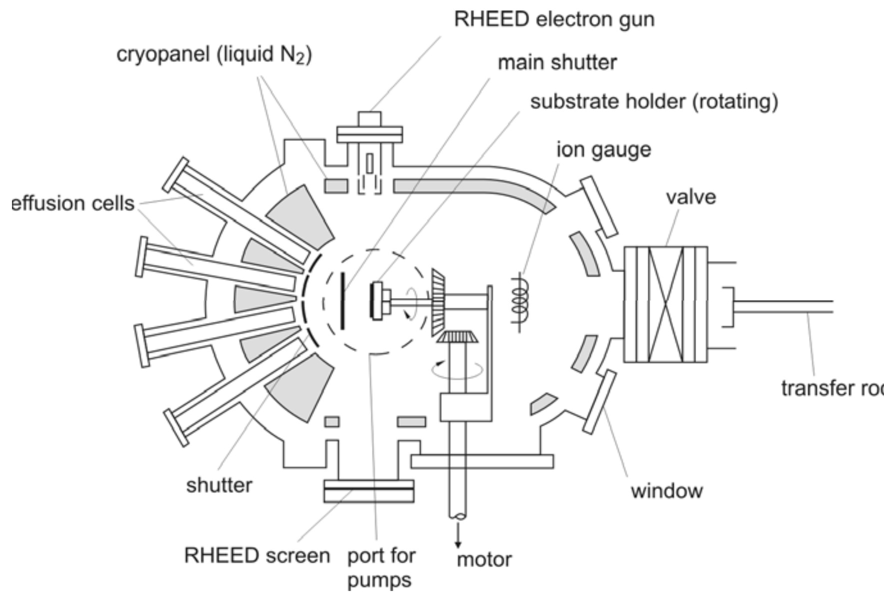
CVD Epitaxy (MOCVD)

- The CVD process is carried out a pressure around 0.5 – 760 torr and at temperatures hundreds of degrees lower than the substrate melt temperature.
- The precursors are metalorganic. The reactions can produce high quality epitaxial layers of III-V semiconductors with very good thickness control allowing quantum well structures to be manufactured.
- Examples:
  - TMGa + AsH_3 at 650 – 750 °C for GaAs.
  - TMGa + NH_3 at 800 °C for GaN.
  - TEIn + PH_3 at 725 °C for InP.



Molecular Beam Epitaxy (MBE)

- The environment is highly controlled ($P \sim 10^{-10}$ torr).
- One or more evaporated beams of atoms react with the substrate to yield a film.
- For epitaxial growth the surface diffusion-incorporation time has to be less than one layer's deposition time. This limits the technique to being a low temperature one.
- Semiconductor and dopant sources are arrayed around the substrate. Each source and the substrate can be individually heated. Shutters control exposure to each species.
- The sources can be solid source (for arsenide compounds) or gas source (for phosphorus compounds).



MBE vs. MOCVD

- Both techniques can produce highly epitaxial films with excellent abruptness, allowing thin layers to be formed.
- The UHV of MBE allows for better in situ diagnostic techniques to be employed.
- Substrate temperatures are lower in MBE.
- MBE is relatively safer.
- MOCVD has a higher growth rate and less downtime.
- It also has no issues regarding phosphor deposition.

Silicon Heteroepitaxy

- While Si is not the ideal material from an electronic and optical point of view, its abundance, ease of processing and availability of a good native oxide have made it the backbone of semiconductor industry.
- Combining Si substrates with compound semiconductor films would enable higher optoelectronic functionality and higher speeds.
- However, there are severe lattice mismatch and chemical compatibility issues between Si and most III-V alloys that preclude direct growth.
- Wafer Bonding
  - The III-V epi-layer is grown on a lattice matched substrate and bonded to a Si wafer by heat and pressure. The lattice matched substrate is then removed by etching leaving the Si/III-V structure behind.