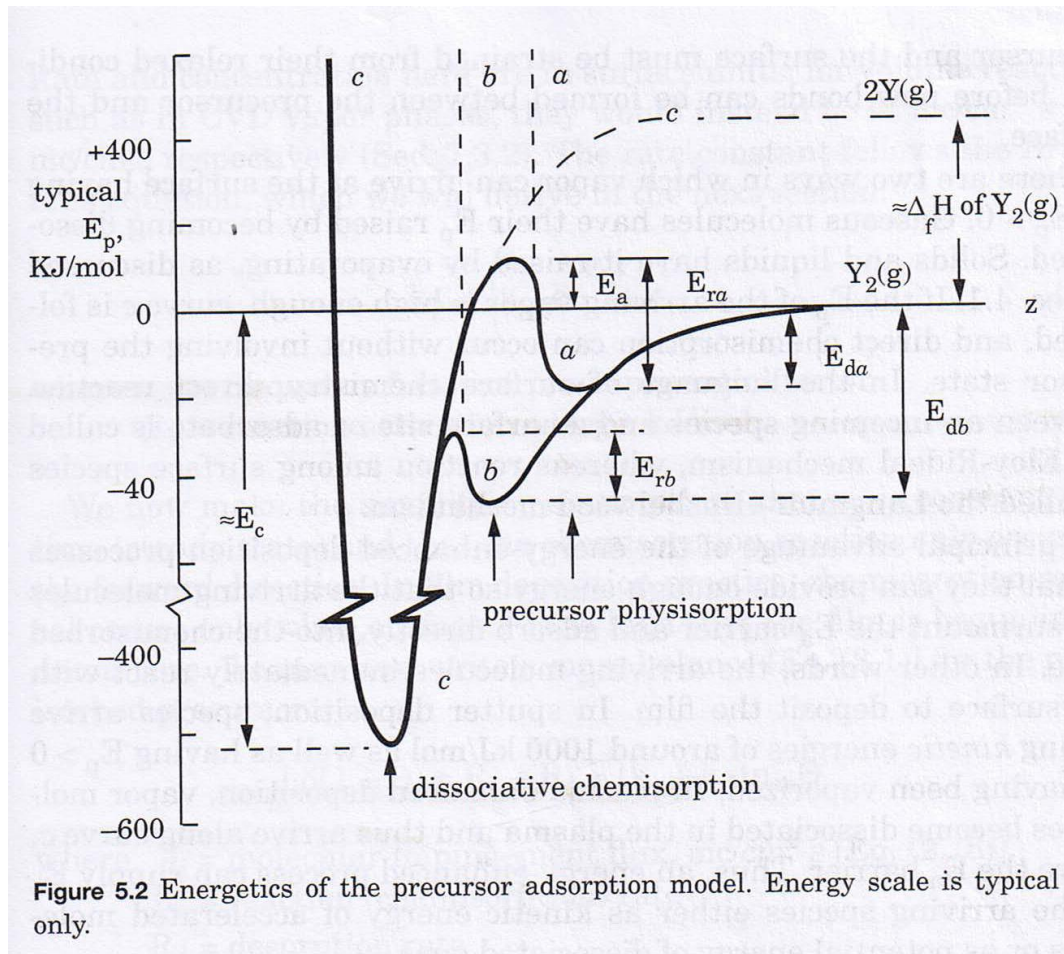


Chapter 6

Epitaxy

6.1. Symmetry

Crystal structures are determined by the specific type of bonding between atoms. Crystals are common in nature because their symmetry provides a bonding environment of minimum ϵ_p for every atom. This is so both from the point of view of bond length as in Fig. 5.2 and that of nearest neighbor environment in 3-D, i.e., bonding angles.



At temperatures below T_m , ϵ_p is the major component of U and G . The contribution from $-TS$ becomes significant only when T comes close to T_m . Any disruption of crystal symmetry increases ϵ_p . This includes surfaces, interfaces, grain boundaries, dislocation, vacancies, and interstitials.

6.1.1. Bonding Types: metallic, ionic covalent and van der Waals;

Symmetry: Body centered cubic (BCC), face centered cubic (FCC), diamond (Si, Ge) and Zinc-Blend: GaAs, ZnS, etc. Note the difference between symmetry and bonding, i.e., a cubic crystal composed of tetrahedral bonding in Si.

6.1.2. Homoepitaxy and Heteroepitaxy

Heteroepitaxy refers to epitaxy of dissimilar materials of compatible symmetry, e.g., cubic on cubic or hexagonal close packed (hcp) on cubic. The differences could be in many physical properties including lattice constants.

- A. Covalent bonding: highly directional, can be further divided into polar and non-polar with shared electron-pairs that are highly localized, e.g., Si, GaAs;
- B. Ionic bonding: the extreme of polar covalent bonding with complete electron transfers. Atoms are held together by electrostatic force, e.g., NaCl. Bondings are non-directional.
- C. Metallic bonding: originating from electrons losing affiliation to their host atoms and free to roam around the crystal, e.g., Fe. This type of bonding is non-directional.

Extreme case: graphene epitaxy with highly anisotropic bond strengths.

Lattice Mismatch:

$$f = \frac{a_e - a_s}{(a_e + a_s)/2} \approx (a_e - a_s)/a_s$$

where “e” refers to epilayer and “s” refers to substrate.

There exists a critical layer thickness for each materials combination (depends on bonding strength, etc) at which significant density of lattice imperfections appear.

Epitaxy can proceed when a subgroup of atoms at the interface match (see Fig. 6.1).

However, these kinds of interfaces have **higher interface energy γ_i** .

Epitaxy can also proceed via tilting (Fig. 6.2).

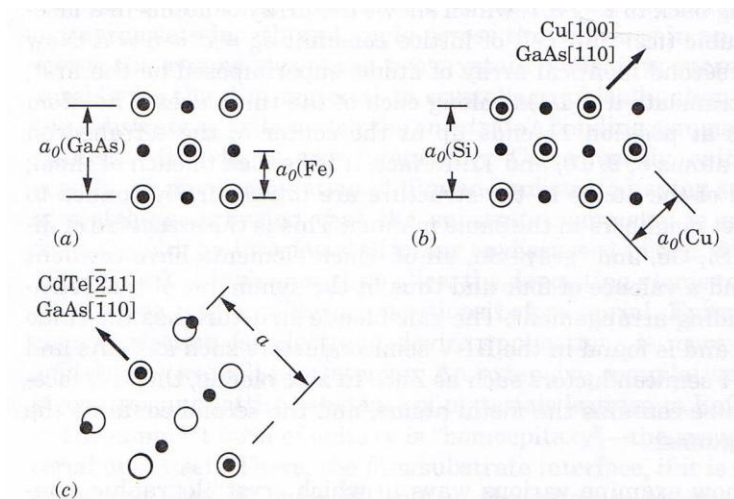


Figure 6.1 Variations on heteroepitaxial symmetry: (a) $a_0 \times 2$, (b) 45° rotation, and (c) CdTe(111) on GaAs(001). o = substrate surface atoms, • = first monolayer of epitaxy.

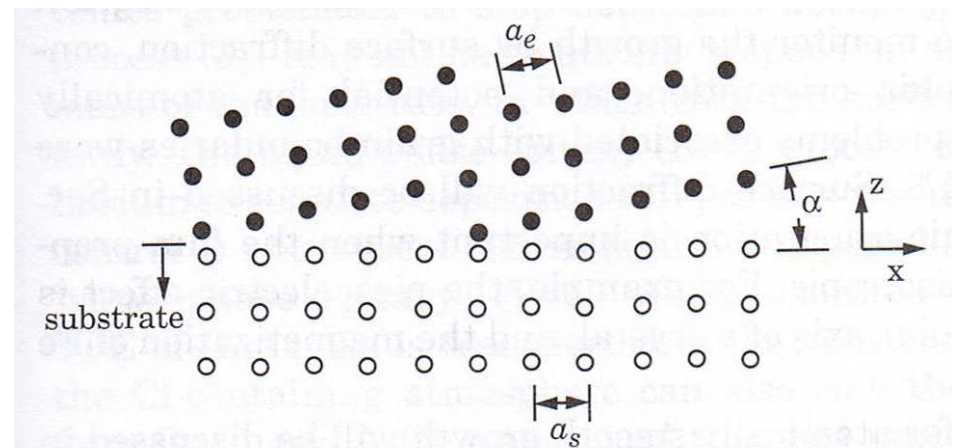


Figure 6.2 Cross-sectional view of misfit accommodation by epilayer tilt.

GaN

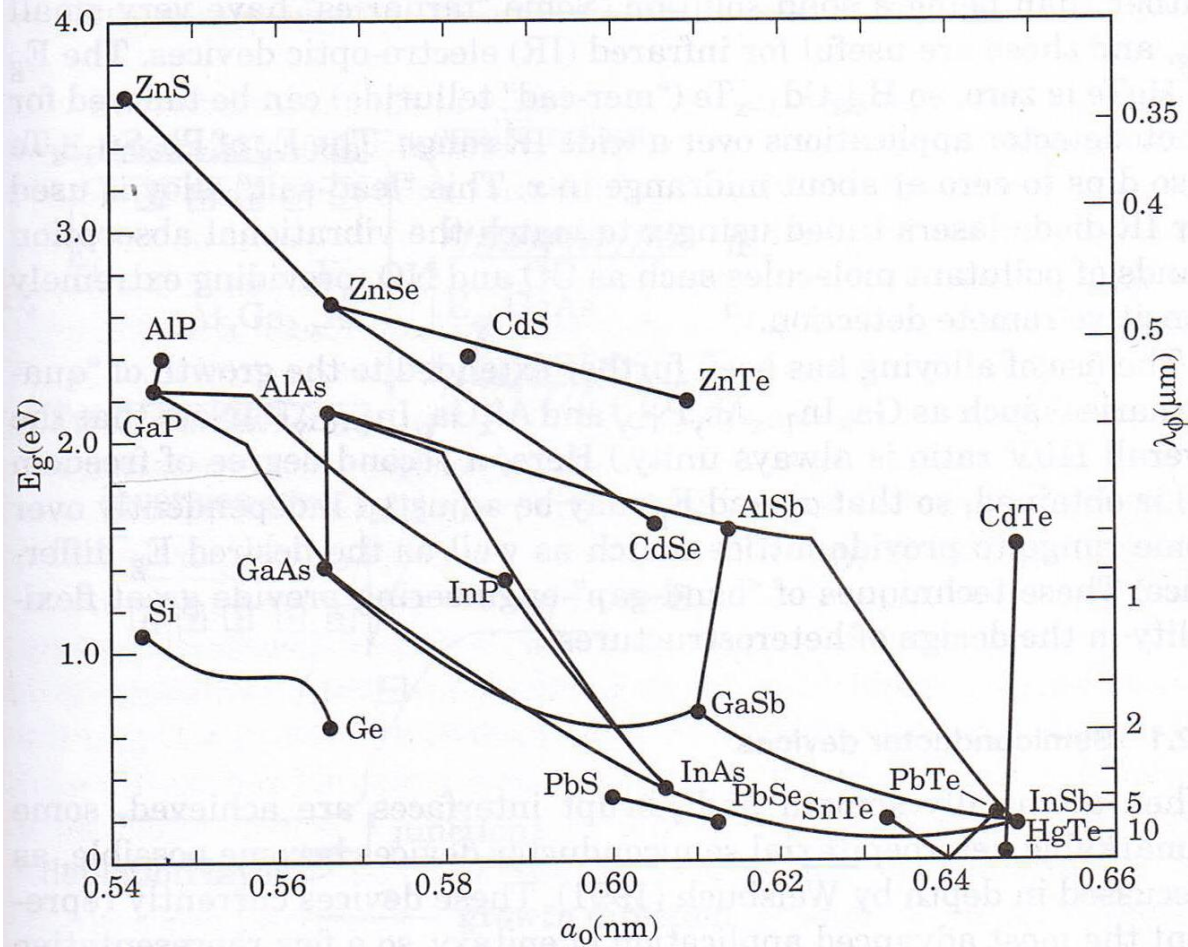


Figure 6.3 Band-gap energy vs. lattice constant at 300 K for various cubic semiconductors. (Based on an unpublished figure by H. Goronkin of Motorola Corp.; used by permission.)

6.4.1 Definition of insulator, semiconductor and conductor

The width of the energy band gap

6.4.2 Vegards law: interpolation

It is generally valid for both E_g and the lattice constant when dealing with **alloys**. There are **exceptions** to Vegard's law, e.g., SiGe, GaInP (see Fig. 6.3). Such exceptions are usually associated with shift of energy minima; e.g., from L to X valleys in the SiGe case.

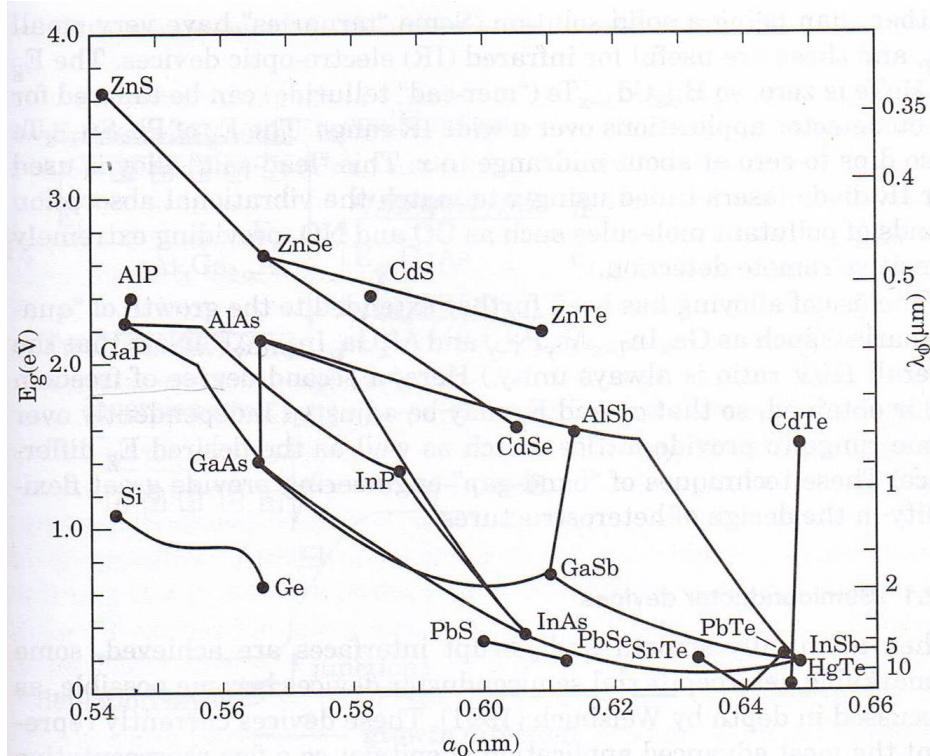
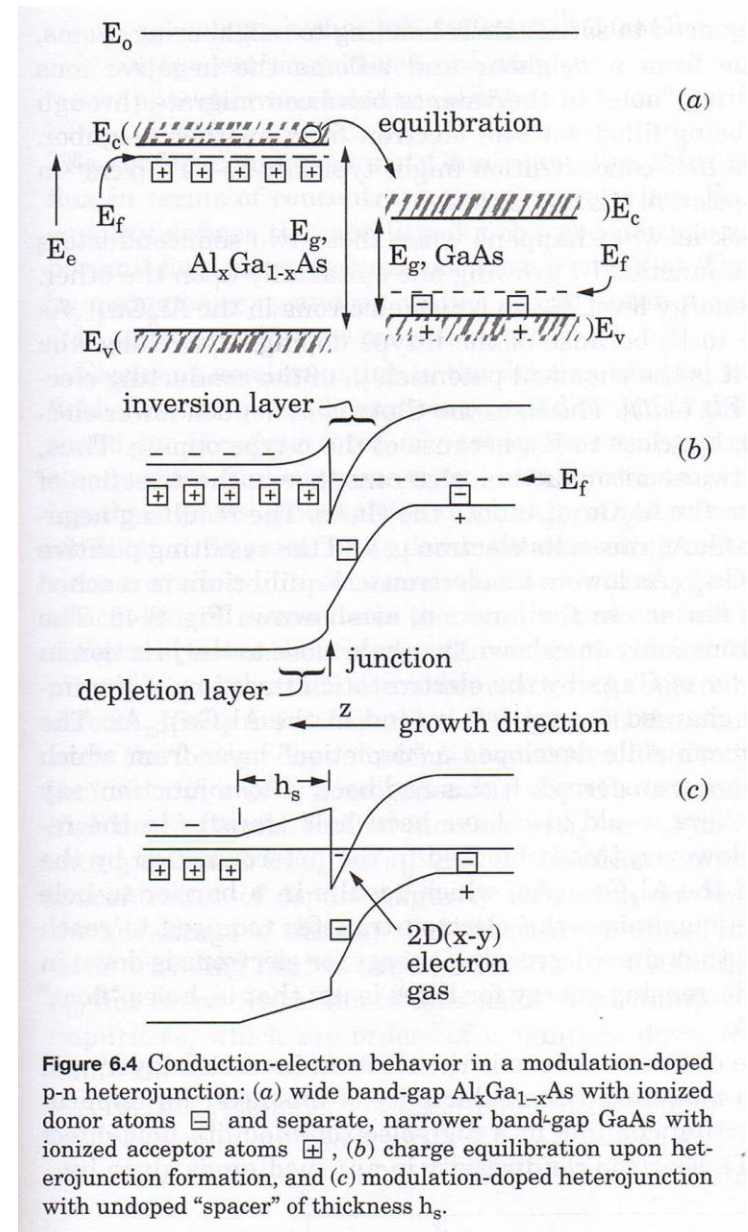
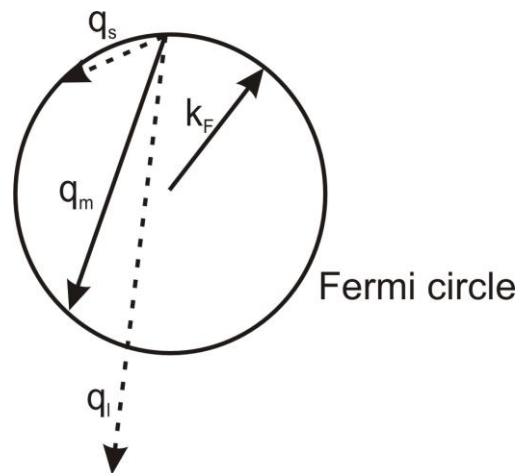


Figure 6.3 Band-gap energy vs. lattice constant at 300 K for various cubic semiconductors. (Based on an unpublished figure by H. Goronkin of Motorola Corp.; used by permission.)

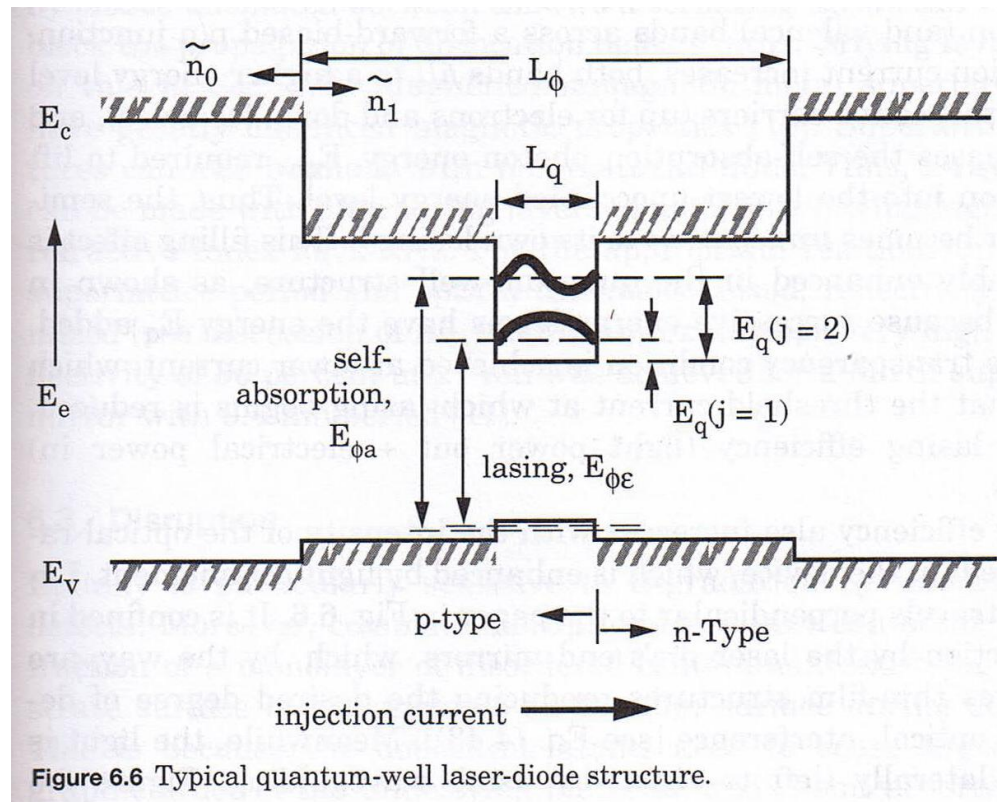
6.4.3. Two-dimensional electron gas (fig. 6.4)

- real space transfer of electrons
- reduction of Coulomb scattering with a spacer layer
- interface scattering
- Fermi circle and low temperature scattering



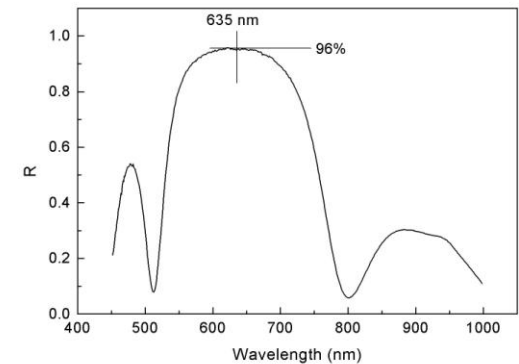
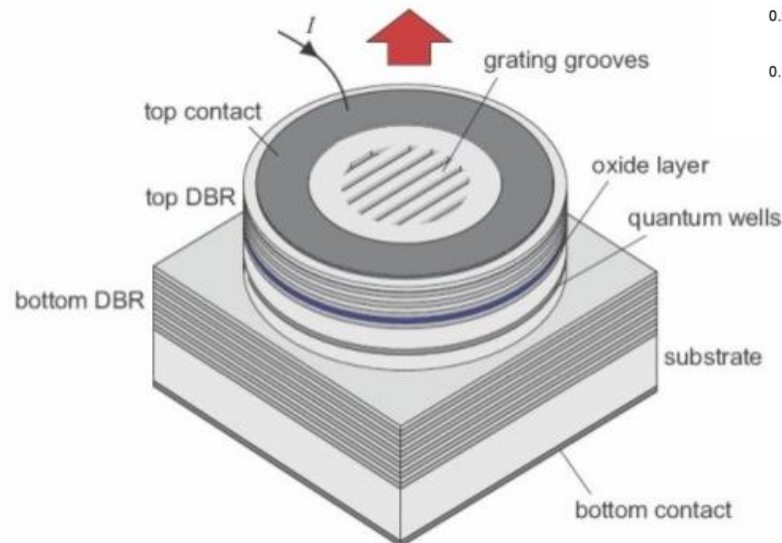
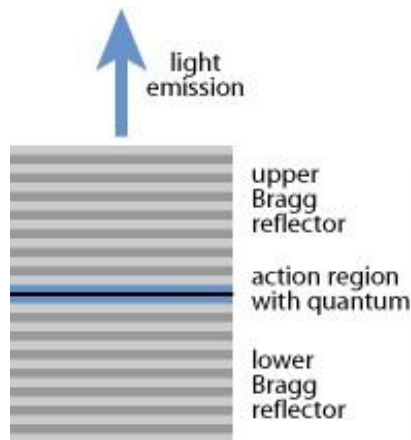
6.4.4. Quantum well Laser-Diode (fig. 6.6)

- Quantized energy levels
- Quantum well has lower E_g than the surrounding layers
- Band filling effect and transparency of the quantum well requires uniform well width



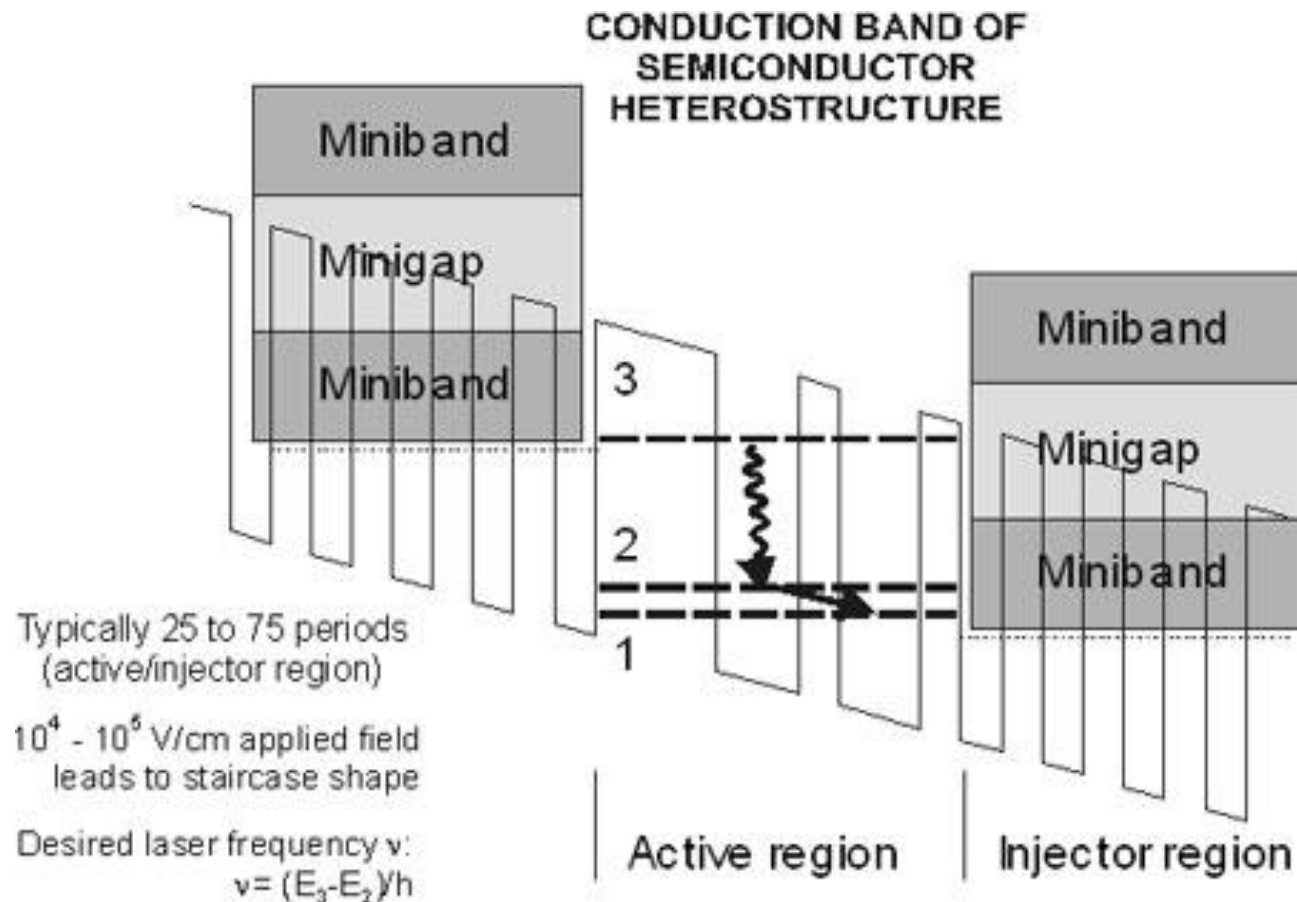
6.4.5. Vertical Cavity Surface Emitting Lasers (VCSELs);

- Single longitudinal mode operation because of the large mode spacing;
- Capable of fabricating 2D arrays of lasers;
- The Q of the cavity is determined by the n-contrast, the number of periods, and the preciseness of the thickness of each layer.



6.4.6. Quantum Cascade Laser

- For far IR and THz applications such as pollution monitoring;
- The extreme case of stringent requirement on interface flatness and layer thickness: $\pm 1\text{\AA}!!$
- Majority carrier laser



6.6.3.7. Reflection high-energy electron diffraction (RHEED) grazing incident. (see fig. 6.15)

- rods in reciprocal space because of the sampling depth.
- the grazing incidence geometry allows simultaneous deposition and monitoring.

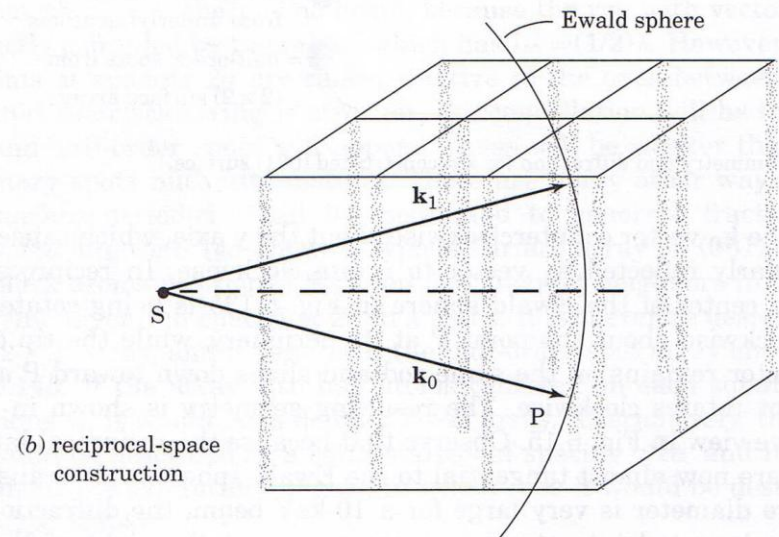
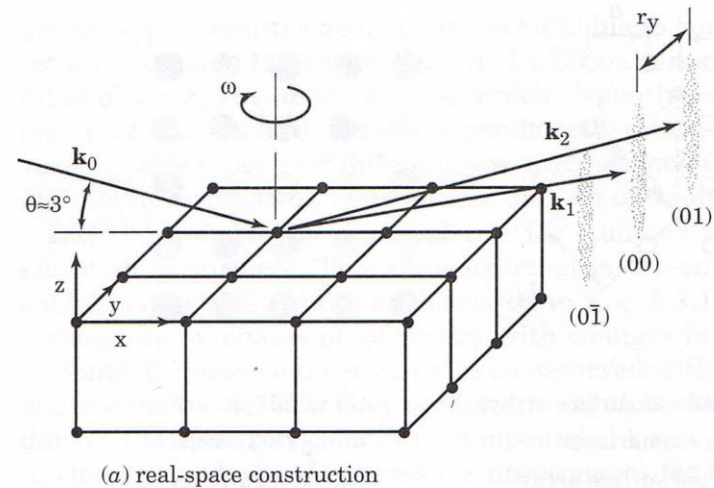
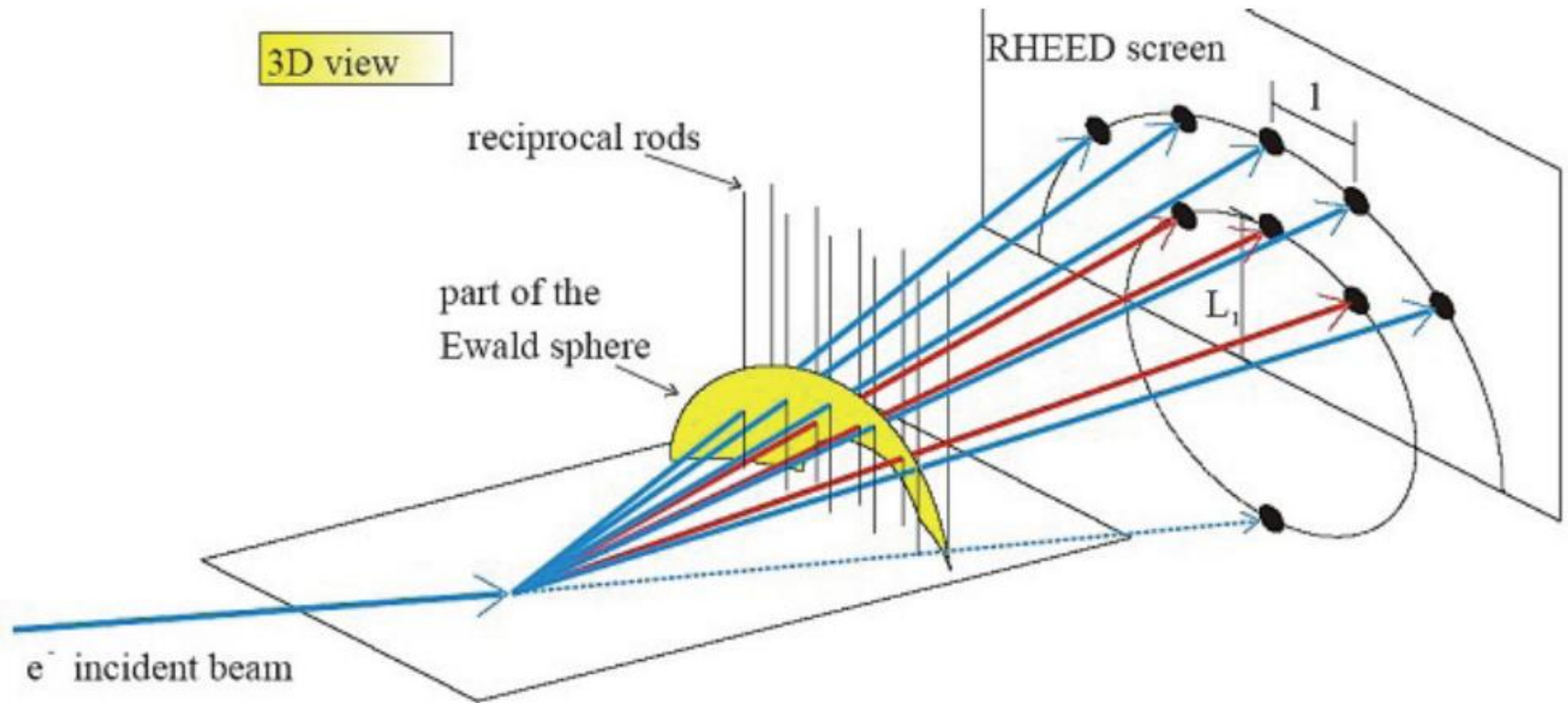


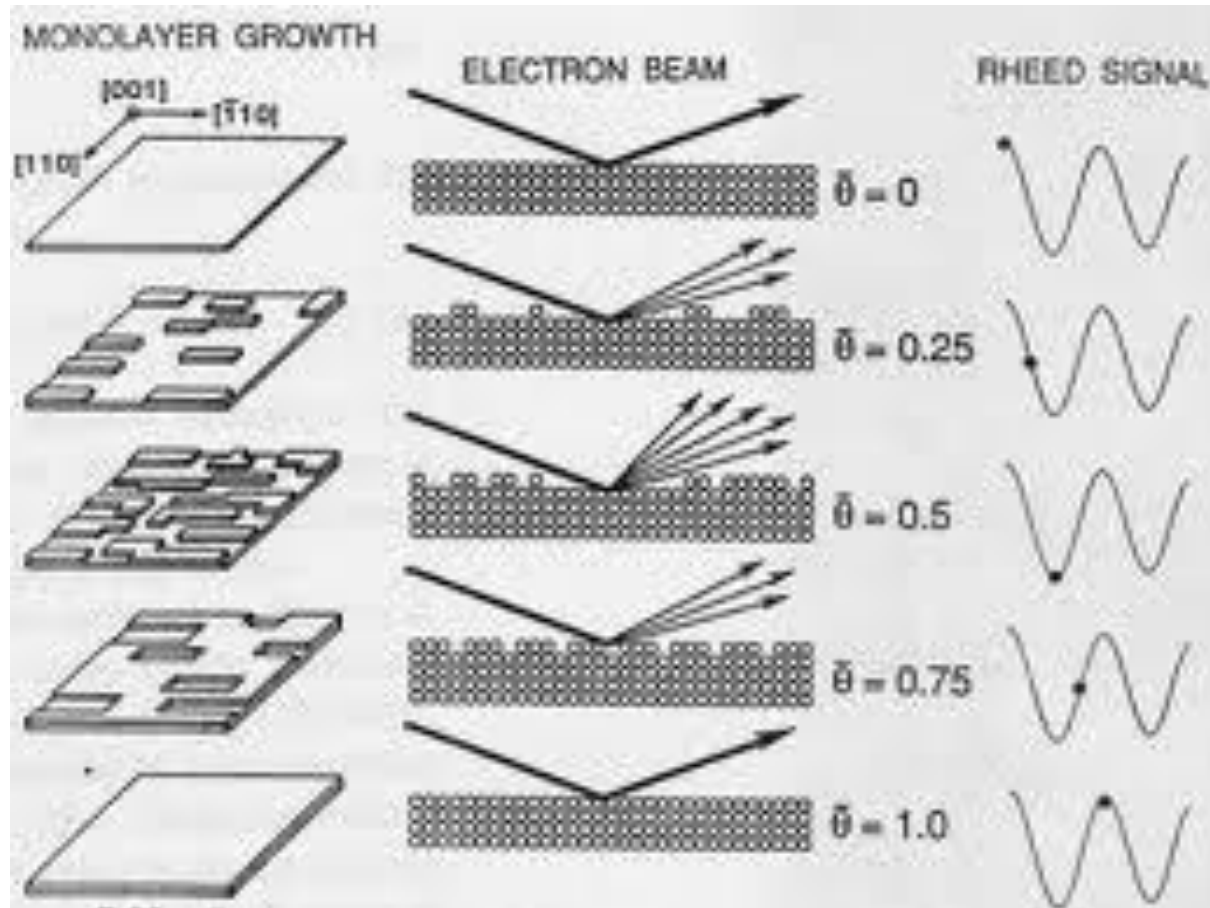
Figure 6.15 RHEED geometry.

RHEED



6.6.3.8. RHEED intensity oscillation

It happens when the epitaxial growth is carried out in the layer-by-layer mode via 2-D island nucleation. It is a technique to monitor the density of step edges in real time.



Which of the 3 growth modes are expected to lead to RHEED oscillation and why?

6.8. Lattice Mismatch

6.8.1. Five modes of heteroepitaxy:

- a) commensurate without strain (lattice matched, FvdM mode)
- b) in-commensurate with weak interaction (VW mode)
- c) commensurate with strain (coherently strained, pre-SK mode)
- d) discommensurate (relaxed with dislocations)
- e) elastic strain relaxation (surface morphological change, SK mode)

6.8.2. Calculation of coherent strain energy

$$\varepsilon_z = \frac{1}{Y} (\sigma_z - \nu \sigma_x - \nu \sigma_y)$$

$$\because \sigma_z = 0; \quad \text{and} \quad \sigma_x = \sigma_y \equiv \sigma_{x,y}$$

$$\therefore \varepsilon_z = -\frac{2\nu}{Y} \sigma_{x,y}$$

$$\text{Further,} \quad \because \varepsilon_x = \varepsilon_y = \varepsilon_{x,y} = \frac{\sigma_x}{Y} - \nu \frac{\sigma_y}{Y} = \frac{1-\nu}{Y} \sigma_{x,y}$$

$$\therefore \varepsilon_z = -\frac{2\nu}{1-\nu} \varepsilon_{x,y}$$

where $\left(\frac{1-\nu}{Y}\right)^{-1}$ is known as the biaxial elastic modulus.

Define tetragonal train ε_T :

$$\varepsilon_T \equiv \varepsilon_z - \varepsilon_{x,y} = -\frac{2\nu}{1-\nu} \varepsilon_{x,y} - \varepsilon_{x,y}$$

$$\therefore \varepsilon_T = -\frac{1+\nu}{1-\nu} \varepsilon_{x,y}$$

note the opposite sign between ε_T and $\varepsilon_{x,y}$

The strain energy:

$$\begin{aligned} U_{\varepsilon} \left(\frac{J}{m^2} \text{ or } \frac{N}{m} \right) &= 2U_x (\because \text{biaxial}) \\ &= 2 \int_0^x F_x \frac{dx}{L_x} = 2 \int_0^{\varepsilon} \frac{Y}{1-\nu} \varepsilon_x \cdot h \cdot d\varepsilon_x = \frac{Y}{1-\nu} h \varepsilon_x^2 \\ \therefore U_{\varepsilon} &\propto h \quad \text{and} \quad U_{\varepsilon} \propto \varepsilon_x^2 \end{aligned}$$

where F_x is the force per unit length in the direction perpendicular to x, i.e., y, and h is the film thickness.

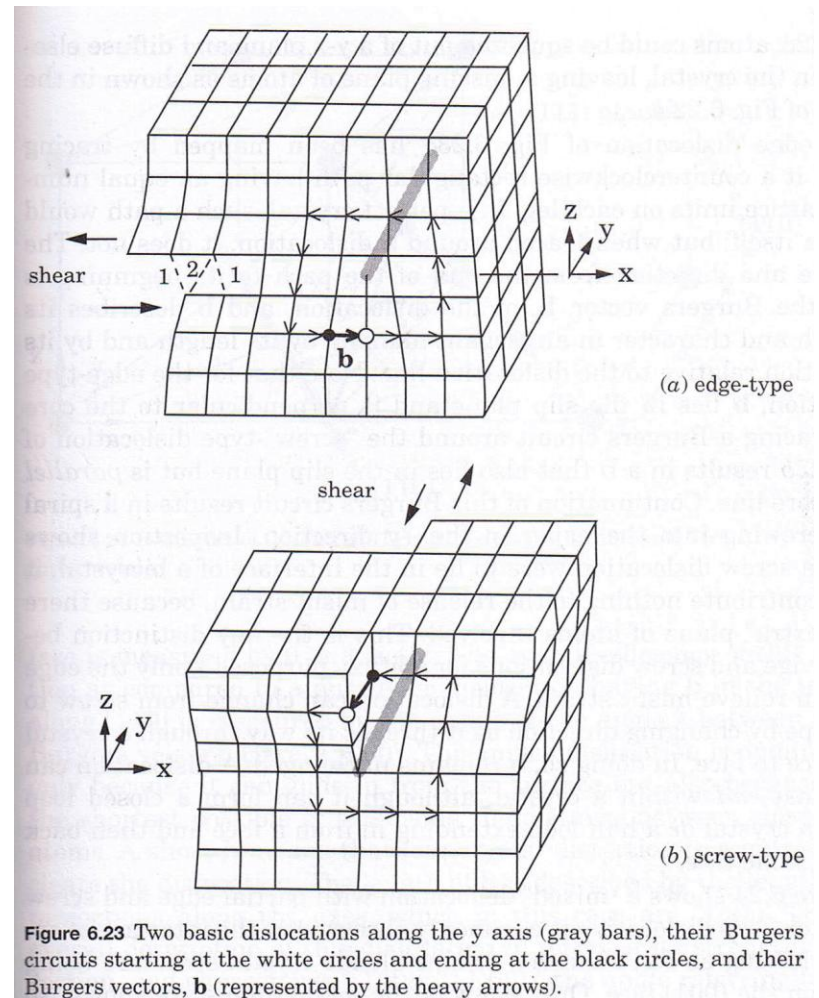
6.8.3. Plastic deformation: strain energy reduction via dislocation

There are two basic types of dislocations: edge-type and screw-type (fig. 6.23). They are defined by the angle between the Burger's vector and the dislocation line direction (fig. 6.23).

Edge-type: $\vec{b} \cdot \vec{\ell} = 0$

Screw-type: $\vec{b} \cdot \vec{\ell} = |\vec{b}| \cdot |\vec{\ell}|$

In addition to plastic deformation, elastic deformation is often encountered, e.g. in the fabrication of self-assembled quantum dots via S-K growth mode.



6.8.4. Dislocation introduction: another “critical” phenomenon (see fig. 6.27(d))

- a. Threading vs. misfit dislocations. One contributes to misfit strain relaxation and the other doesn't.
- b. Dislocation cannot terminate inside a crystal.
- c. Burger's vector is constant along a given dislocation.
- a. Nucleation of dislocation half-loops: the existence of critical radius that decreases with increasing stress.

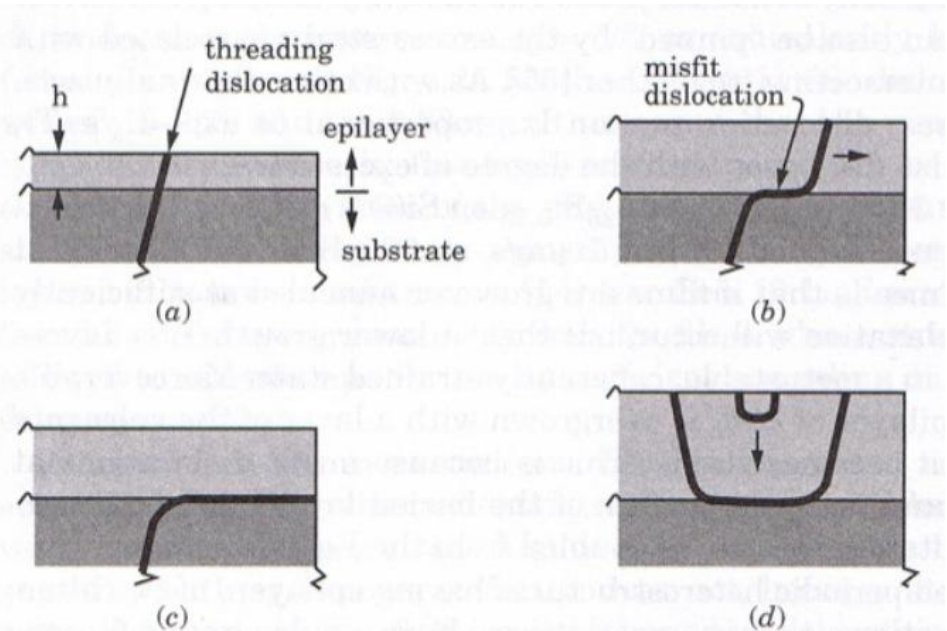
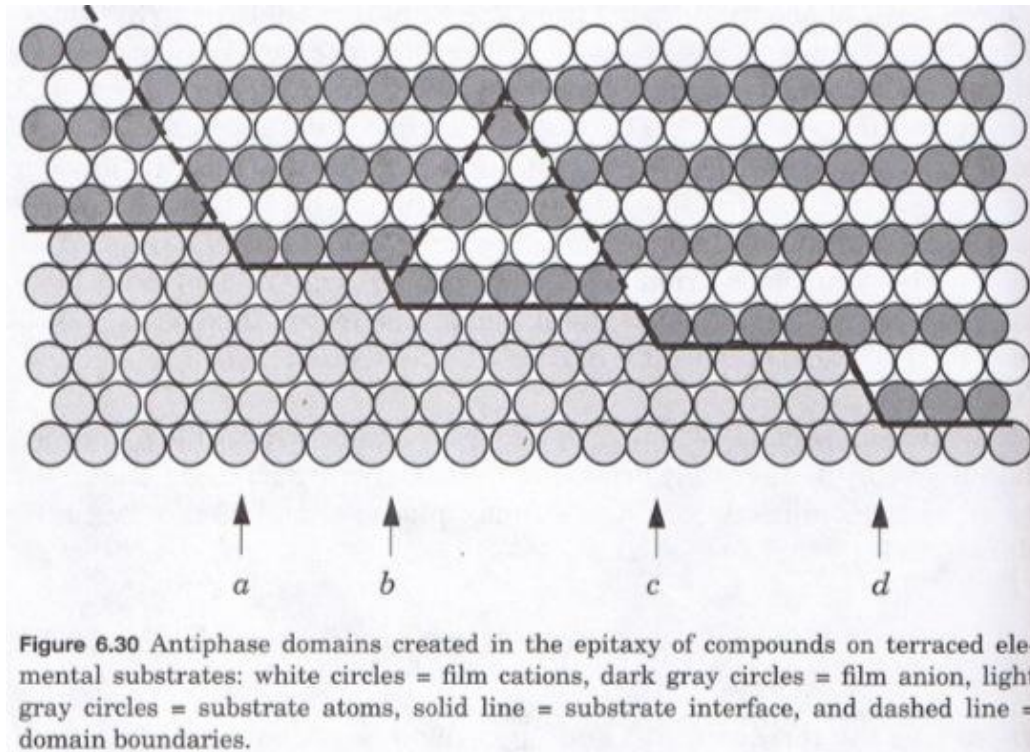


Figure 6.27 Dislocation motion in strained epilayers: (a) propagation through epilayer having $h < h_c$, (b) lateral motion for $h > h_c$, (c) termination at edge of substrate, and (d) nucleation of half-loops.

6.8.5. Anti-phase domain boundary (APB). [see fig. 6.30]

Happens for polar-on-nonpolar hetero-epitaxy. The associated surface charge.



The above discussion touches the three major families of crystalline defects: point defect and extended defects (line and area).