Theory of Semiconductor Devices (반도체 소자 이론)

Lecture 10

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Contents

Crystal Imperfections

Impurities

- One of the most important technological properties of semiconductors is the ability to make substantial changes in ***conductivity*** and ***other physical processes*** by the ***addition of impurity atoms***.

-The controlled addition of impurities to alter the properties of a semiconductor is called ***doping***.

- To determine how an impurity affects certain properties, it is necessary to consider several factors;

1. Does the impurity atom ***replace*** an atom of the host crystal, or does it take up an ***interstitial position*** in the host lattice? The former are referred to as *substitutional* impurities and the latter as *interstitial* impurities.

2. If the impurity is substitutional, what is its ***valence*** relative to the host atom it replaces? The valence is also important for an interstitial impurity.

3. If a substitutional impurity has the same valence as the host atom, what is its ***electro negativity*** relative to the host atom it replaces? Although these impurities are commonly referred to as *isoelectronic*, the proper terminology is *isovalent*. The effect of such impurities in an otherwise perfect crystal is most easily seen in the bond picture.

Impurities

- One of the most important technological properties of semiconductors is the ability to make substantial changes in ***conductivity*** and ***other physical processes*** by the ***addition of impurity atoms***.

-The controlled addition of impurities to alter the properties of a semiconductor is called ***doping***.

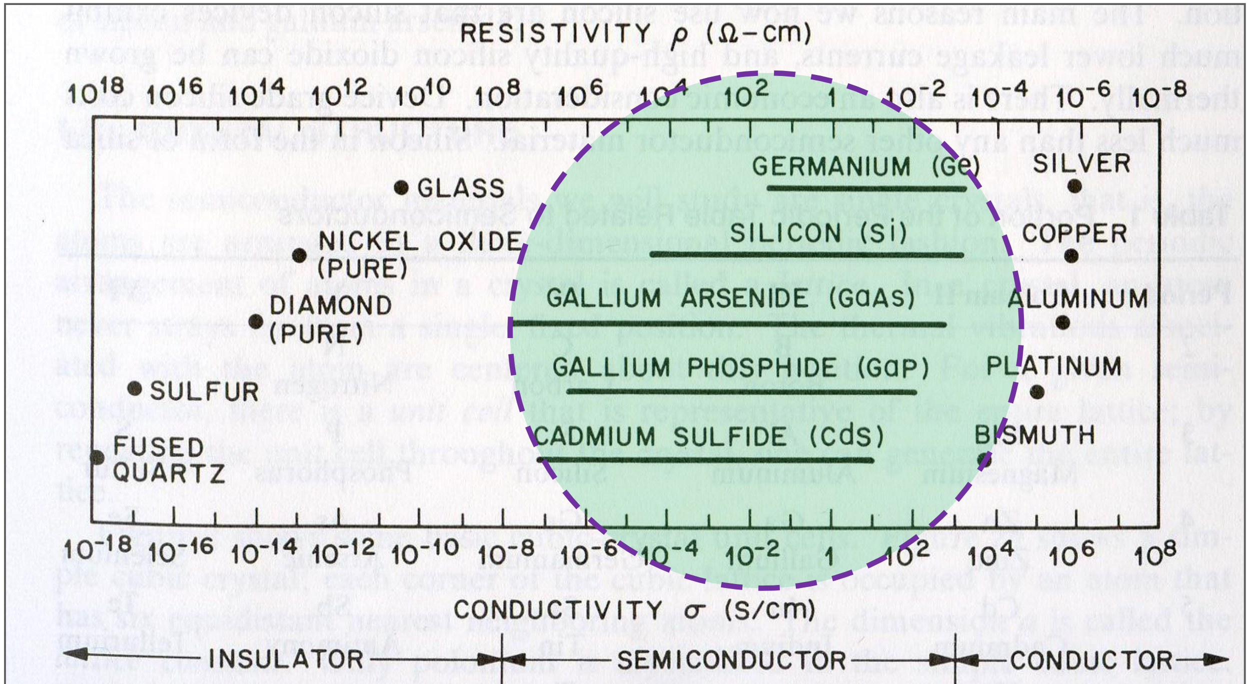
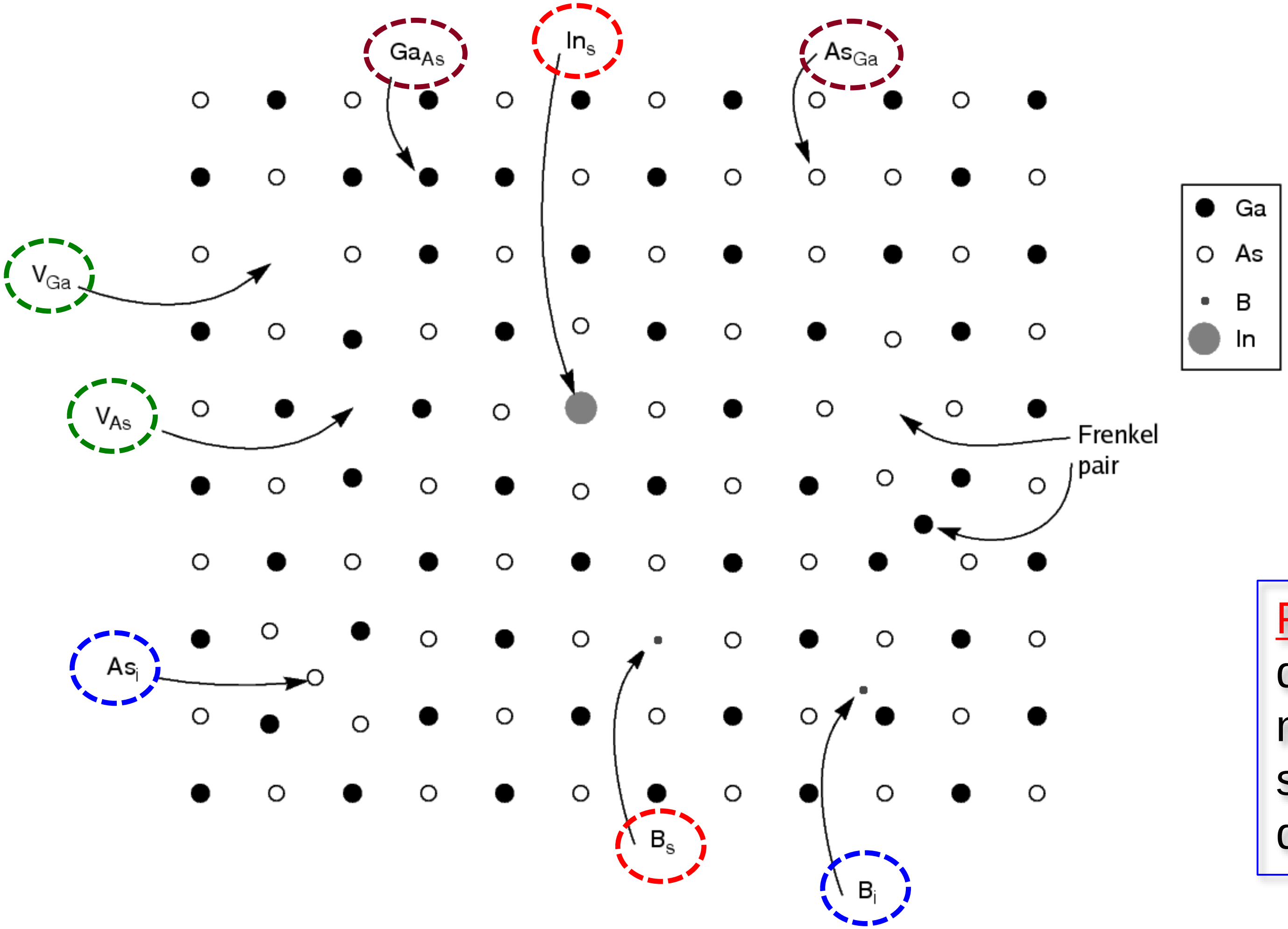


Fig. 1 Typical range of … rs, and conductors.

‘ranges’ instead of ‘points’

Various Point Defects

- Schematic Diagram of ***Point Defects* in GaAs**



substitutional

interstitial

vacancy

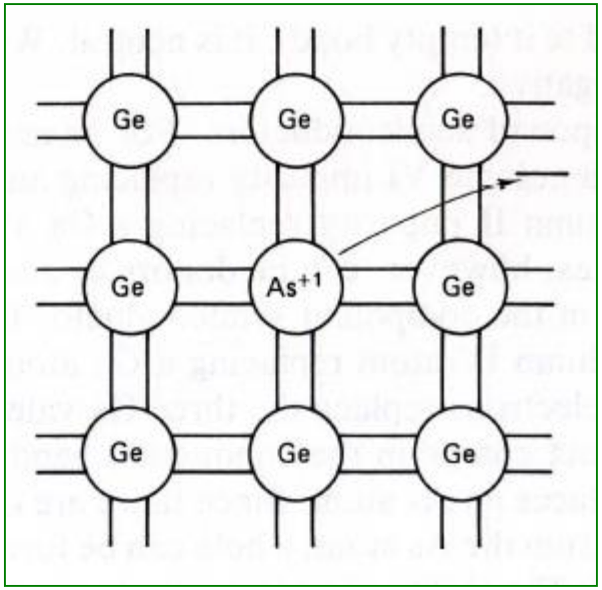
antisite

Point Defects:
defects which are not extended in space in any dimension

Bonding Concepts

- When a column V impurity substitutes for a column IV Ge atom in the diamond structure as in Fig. 3.6(a), four of the five valence electrons from the impurity replace the four electrons of the Ge atom to complete the bonding arrangement.

- Since all valence bonds or valence band states are filled, the ***fifth electron*** must go into conduction band states. However, the fifth electron is attracted to the net positive charge in the impurity core, and this produces a series of allowed energy levels ***in the forbidden bandgap*** just ***below*** the conduction band.



- The energy separation between these levels and the conduction band is sufficiently small that at room temperature, the attraction ***can be overcome*** and the electron will be free to move in the conduction band.

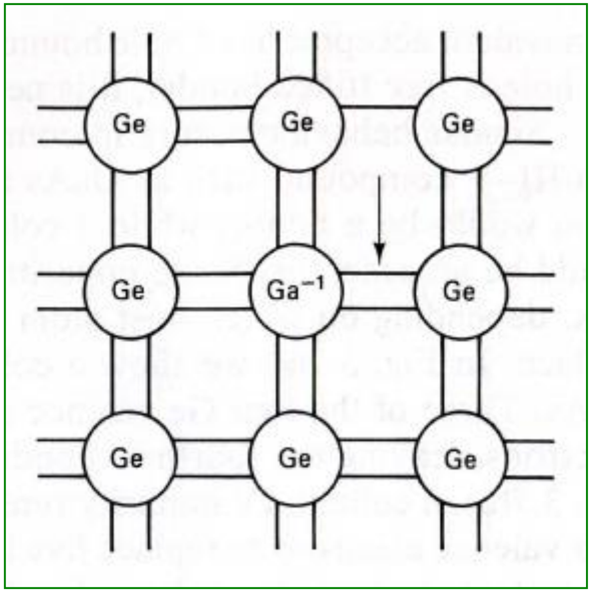
- Since this column V impurity can donate one electron to the conduction band, it is referred to as a monovalent ***donor***.

- When the conductivity of a semiconductor is controlled by donor impurities, it is called ***n-type***. Such a donor impurity can exist in two charge states; When the electron is bound to the impurity, it is ***neutral***; when the electron is ionized to the conduction band, it is ***positive***.

Bonding Concepts

- With the column III impurity shown in Fig. 3.6(b), the situation is significantly different. There are only three valence electrons to replace the four valence electrons of the Ge atom, so that ***one valence bond is empty***.

- If an electron is removed from a valence bond elsewhere to complete the bonding arrangement around the impurity atom, the missing electron elsewhere is a positively charged hole and the impurity atom has a net negative charge from the extra electron it *accepted* to complete its bonds.



- The attraction between the hole and the negatively charged ***acceptor*** impurity produce bound states for valence band electrons in the forbidden bandgap ***just above*** the valence band.

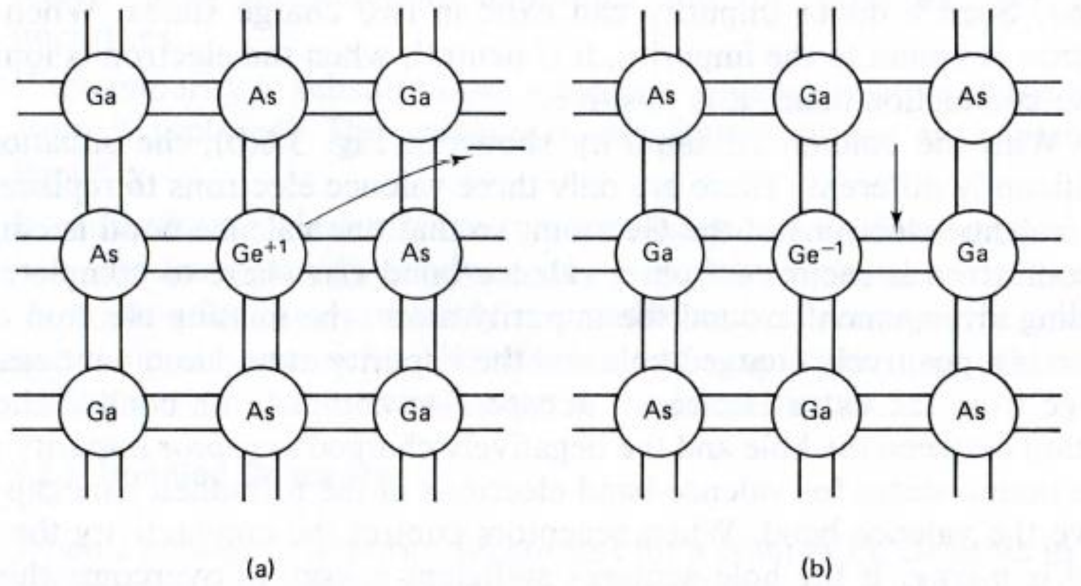
- When acceptors control the conductivity the material is ***p-type***. If the hole acquires sufficient energy to overcome this attraction, it is free to conduct net charge in the valence band.

- When this monovalent acceptor has a hole bound to it (empty bond), it is ***neutral***. When the hole is free (filled bonds), it is ***negative***.

Bonding Concepts

- Similar behavior occurs in compound semiconductors. For example, in a III-V compound such as GaAs a column VI impurity replacing an As atom would be a donor, while a column II impurity replacing a Ga atom would be an acceptor. Some impurities, however, can be donors or acceptors, depending on which host atom in the compound semiconductor they replace.

- In Fig. 3.7(a) we show a column IV atom replacing a Ga atom in GaAs. Three of the four Ge valence electrons replace the three Ga valence electrons, leaving the fourth to conduct charge in the conduction band . In Fig. 3.7(b), a column IV impurity replaces an As atom.



(a) (b)

Figure 3.7 Column IV impurity in GaAs can be (a) a donor on a Ga lattice site and (b) an acceptor on a As lattice site.

- Since there are only four valence electrons to replace five from the As atom, a hole can be formed to conduct charge in the valence band.

- The ability of an impurity to produce either *n*- or p-type conductivity is referred to as ***amphoteric*** behavior. For Ge in GaAs it is possible to make a *p*-*n* junction utilizing only this single dopant!

Bonding Concepts

- When an impurity atom differs in valence from the host atom it replaces by more than one, it can donate more than one electron to the conduction band or accept more than one electron from the valence band. Figure 3.8 shows the effects of a column VI donor in Ge. In this case there are two electrons left over after the bond is completed. If one electron is removed to the conduction band as in Fig. 3.8(a), the impurity has a net charge of + 1.

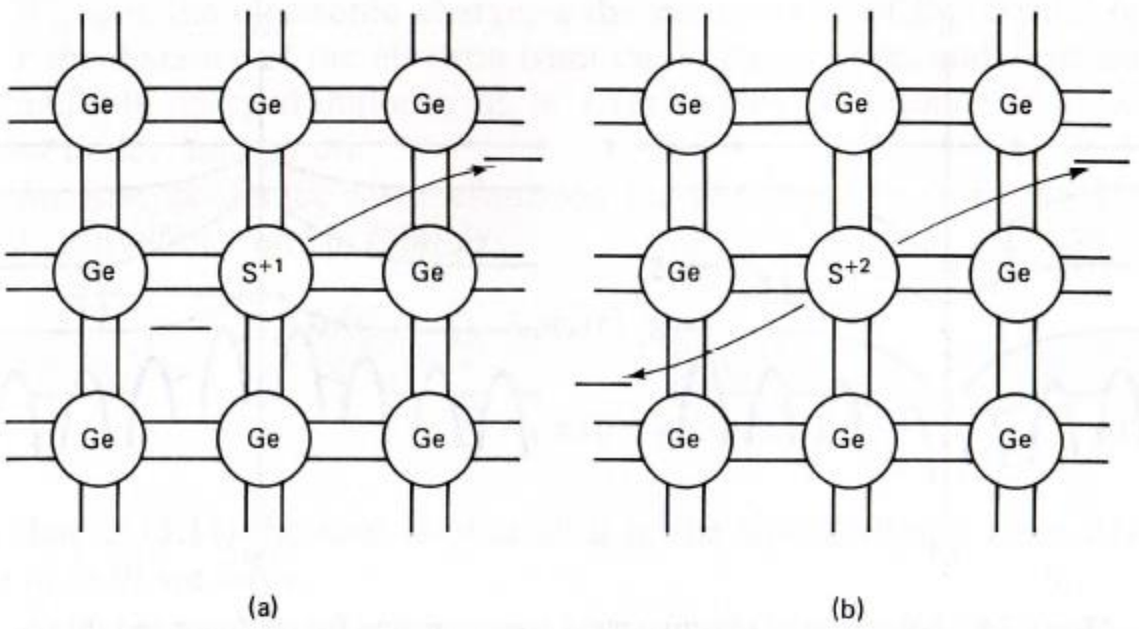


Figure 3.8 A column VI donor for Ge in (a) its first and (b) second ionization states.

When the second electron is removed as in Fig. 3.8(b), the impurity has a net charge of + 2. This impurity would be a ***divalent donor.***

Effective Mass Approx.

- If the binding energy of an electron or hole to a donor or acceptor impurity is ***relatively small***, the energy levels can be determined by considering the impurity potential energy as a perturbation on the periodic potential energy of an otherwise perfect lattice. This calculation is called an *effective mass approximation* .

- For the ***unperturbed*** lattice. The one electron Schrödinger equation is given by (2.1) as

$$\mathbf{H}\psi_k(\mathbf{r}) = \mathscr{E}\psi_k(\mathbf{r}) \tag{3.6}$$

where

$$\mathbf{H} = \frac{-\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) \tag{3.7}$$

From (2.10) the unperturbed wavefunction has the form

$$\psi_k(\mathbf{r}) = A \exp(i\mathbf{k}\cdot\mathbf{r})u_k(r) \tag{3.8}$$

The problem for the lattice perturbed by an impurity atom is set up in a similar manner.

$$\mathbf{H}_i\psi_i(\mathbf{r}) = \mathscr{E}_i\psi_i(\mathbf{r}) \tag{3.9}$$

$$\begin{aligned} \mathbf{H}_i &= \frac{-\hbar^2}{2m}\nabla^2 + U(\mathbf{r}) - \frac{Zq^2}{4\pi\epsilon r} \\ &= \mathbf{H} - \frac{Zq^2}{4\pi\epsilon r} \end{aligned} \tag{3.10}$$

Effective Mass Approx.

- The result is a series of hydrogenic impurity energy levels given by

$$(\mathscr{E}_c - \mathscr{E}_{in}) = \frac{q^4 Z^2 m^*}{2n^2(4\pi\epsilon\hbar)^2} \tag{3.32}$$

where *n* has all positive integer values. For a donor associated with the conduction band minimum at Γ, (3.32) gives a series of donor ionization energies,

$$\begin{aligned}\Delta\mathscr{E}_{dn} &\equiv \mathscr{E}_c - \mathscr{E}_{dn} \\ &= 13.6\left(\frac{Z}{n\epsilon_r}\right)^2\left(\frac{m^*}{m}\right)\text{eV}\end{aligned} \tag{3.33}$$

where ε_r is the dielectric constant of the semiconductor.

For materials with nearly spherical conduction bands at Γ such as GaAs, this hydrogenic model gives results that are in very good agreement with experiment.

In materials with ellipsoidal indirect conduction band minima, such as Si and Ge, or with an ellipsoidal direct conduction band minimum, such as wurtzite II-VI compounds , (3.25) must be modified to take into account the anisotropic effective masses.

Contents

Crystal Imperfections

Dislocations

-The crystal imperfections we have examined so far are classified as point defects.

-***Dislocations*** are linear defects which can extend throughout large regions of the crystal. Although they play an important role in the strength and fracture of metals, dislocations serve mainly to degrade the properties of semiconductors.

- If the dislocation has dangling bonds, they can act as a linear array of acceptors that scatter mobile carriers. The dangling bonds can also attract impurities and interstitials or act as an internal source and sink for vacancies.

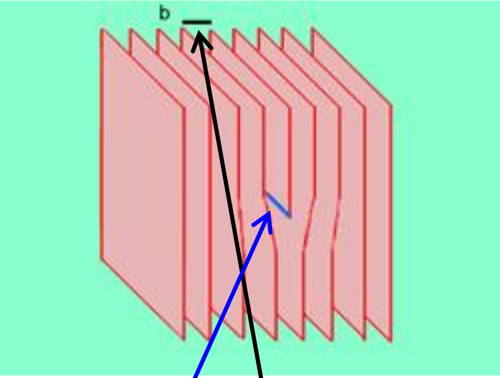
- In practical applications, dislocations can degrade the performance of semiconductor devices in a number of ways .

- As a result, a substantial amount of effort has been expended in the semiconductor industry to minimize the number of dislocations introduced into a material during crystal growth and subsequent device processing.

Dislocations - Examples

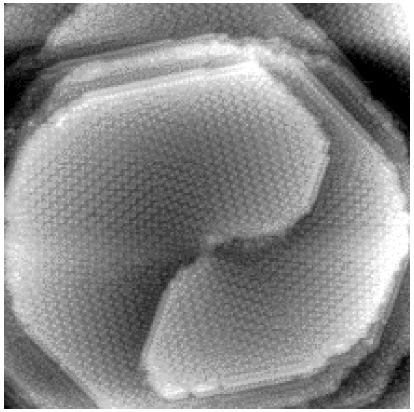
- Dislocations: edge dislocation, screw dislocation

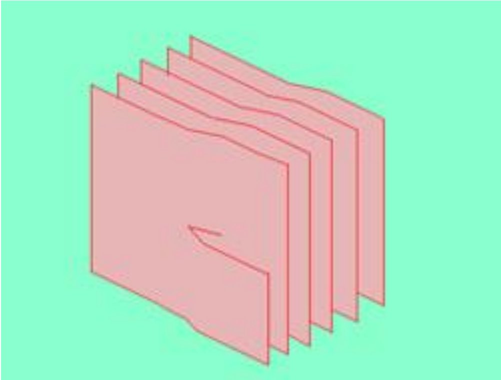
edge dislocations

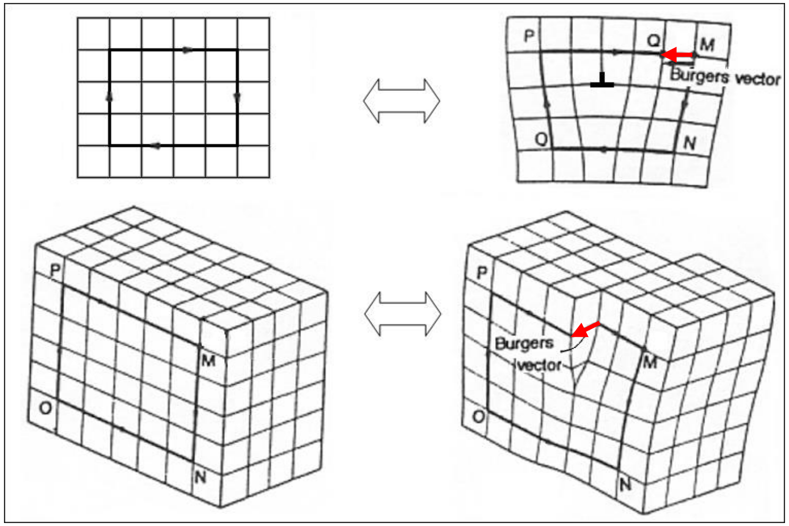


Schematic diagram (lattice planes) showing an edge dislocation.
Burgers vector in black, dislocation line in blue.

screw dislocations







Dislocations

- Figure 3.14 shows an edge dislocation in the sphalerite crystal structure.
- Dislocations are characterized by their ***axis***, **a**, ***Burgers vector***, **b**, and ***slip plane***.
- The axis indicates the direction along which the deviation from crystal periodicity occurs. This dislocation has a set of ***two*** dangling bonds in each atomic plane along the direction of its axis.
- The Burgers vector represents the direction and displacement of the dislocated region compared to a perfect crystal.

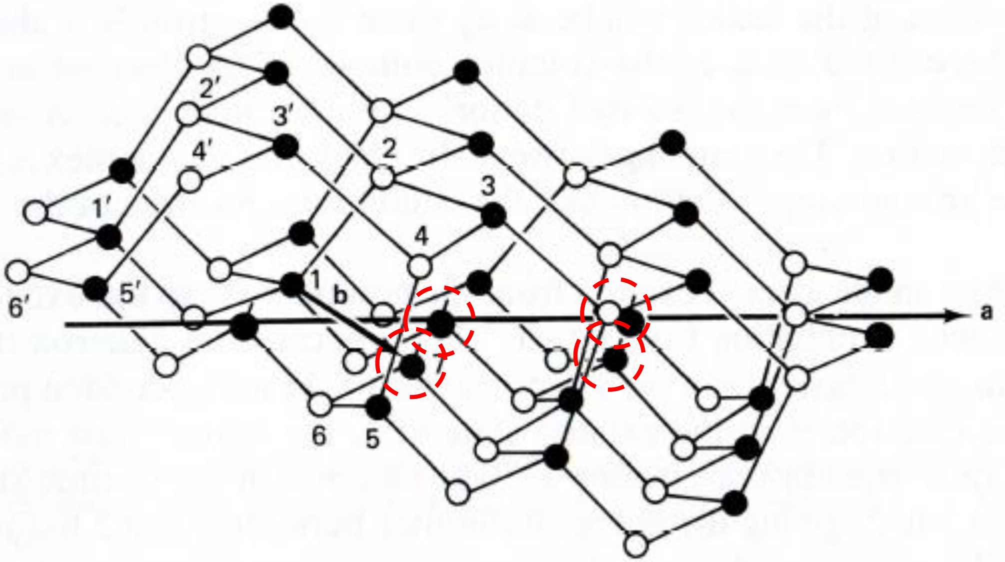


Figure 3.14 An edge dislocation in the sphalerite structure. The axis is along ⟨211⟩ and the Burgers vector is along ⟨110⟩. The slip plane is {111}.

- It can be determined by ***first*** taking a closed circuit around the bonds in a perfect region of the crystal and then taking the same circuit around a dislocated region.

- The vector required to close the circuit around the dislocated region is the Burgers vector.

Dislocations

- For example, in Fig. 3.14, the circuit 1' to 2' to 3' to 4' to 5' to 6' to 1 ' represents a circuit in a ***perfect*** region.
- The same circuit around a ***dislocated*** region would be 1 to 2 to 3 to 4 to 5 to 6 to 7. The vector required to close the circuit from 1 to 7 is the Burgers vector.
- Notice that the Burgers vector is a direct lattice vector.
- The slip plane is the plane along which the dislocation can move under applied stresses, so it ***must*** contain both the axis and the Burgers vector.

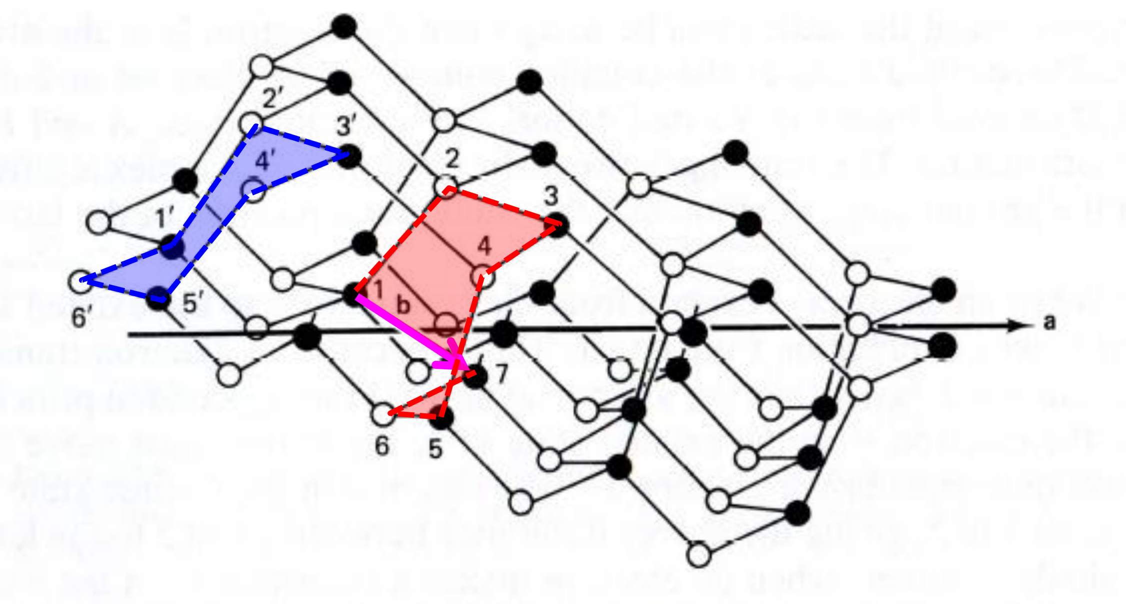


Figure 3.14 An edge dislocation in the sphalerite structure. The axis is along ⟨211⟩ and the Burgers vector is along ⟨110⟩. The slip plane is {111}.

-For this dislocation a is along ⟨211⟩, **b** is along ⟨110⟩, and the slip plane is {111}.

- Since the angle between **a** and **b** is **90°**, this dislocation is referred to as an ***edge dislocation***.

http://www.youtube.com/watch?v=xS7RXQPmCoc&NR=1

http://www.youtube.com/watch?v=OpKxyeU2dc0&feature=related

Dislocations

- When the angle between a and b is **zero**, the dislocation is called a ***screw dislocation***.
- If we take a circuit similar to that taken in Fig. 3.14 for the dislocation in Fig. 3.15, we find that **b** is in the same direction as **a**.
- Notice that this screw dislocation has no dangling bonds, but perturbs the lattice by a spiral rearrangement of bonds around its axis .

- Since **a** and **b** are in the same direction, a ***unique*** slip plane is ***not*** defined for this dislocation.

- Although the dislocations we have seen so far were either pure edge or screw, most dislocations have both edge and screw components. to edge, and so on.

http://www.phy.mtu.edu/~jaszczak/si%20seminar/screw_growth.gif

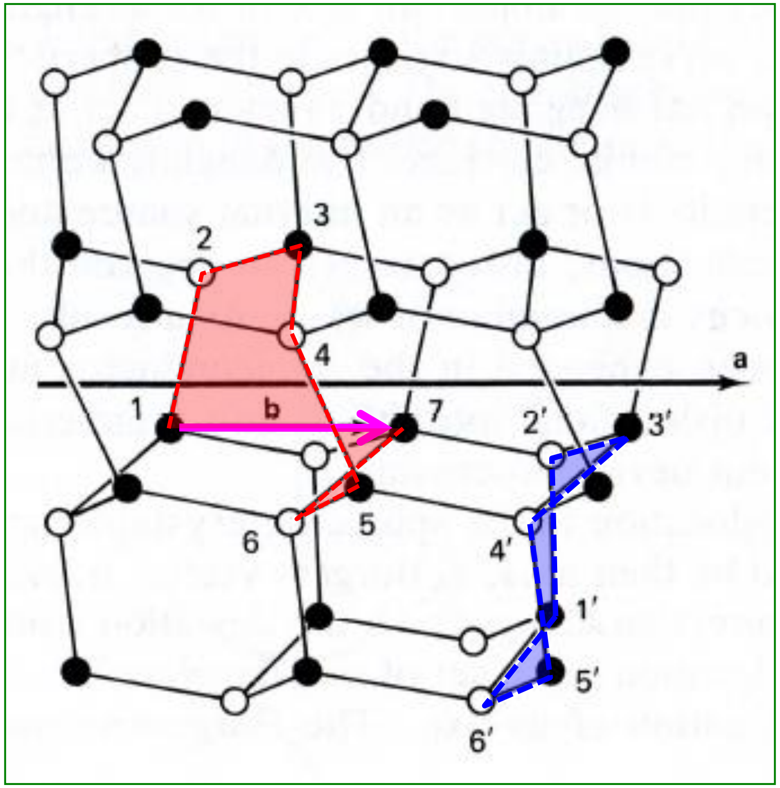


Figure 3.15 A screw dislocation in the sphalerite structure. The axis and Burgers vector are along ⟨110⟩. The slip plane is not defined.

Dislocations

- Although the dislocations we have seen so far were either pure edge or screw, most dislocations have **both edge and screw** components.
- Figure 3.16 shows a dislocation in the sphalerite structure in which the angle between **a** and **b** is 60°, so it has partially edge and partially screw properties .
Other dislocations of this nature are possible in the sphalerite structure [J. Hornstra, *J. Phys. Chern. Solids* 5, 129 (1958)].
- Dislocations ***must*** either extend throughout a crystal with each end terminated at a surface or form a closed loop within the crystal. Generally, the dislocation axis will twist and turn as it winds its way through the crystal, going from edge to screw to edge, and so on.

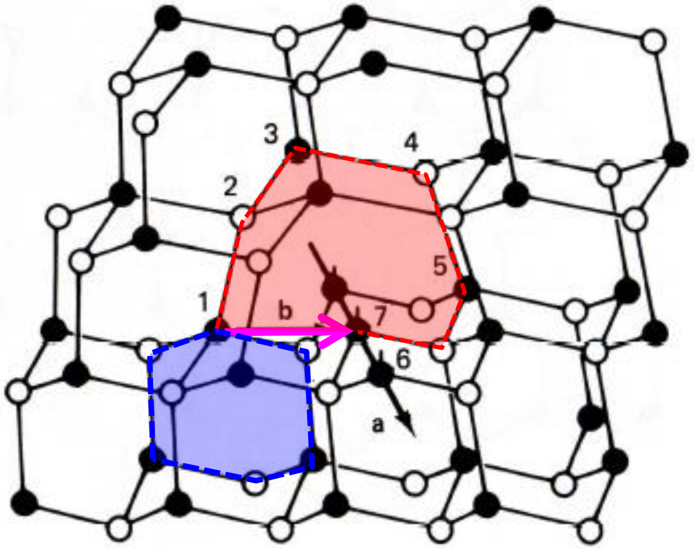
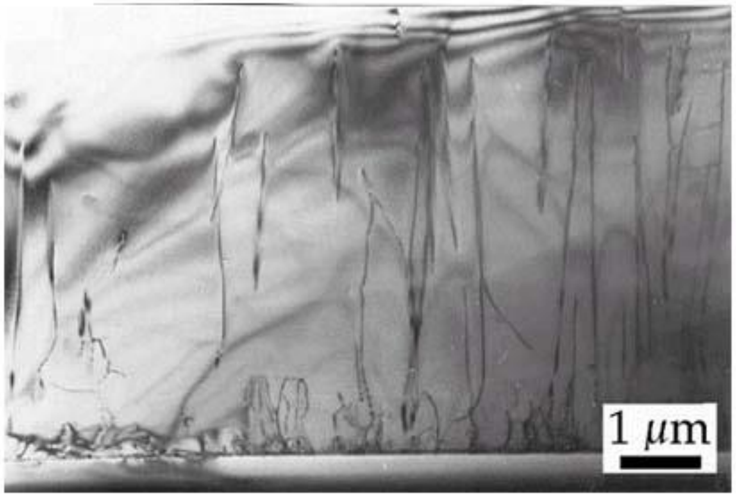
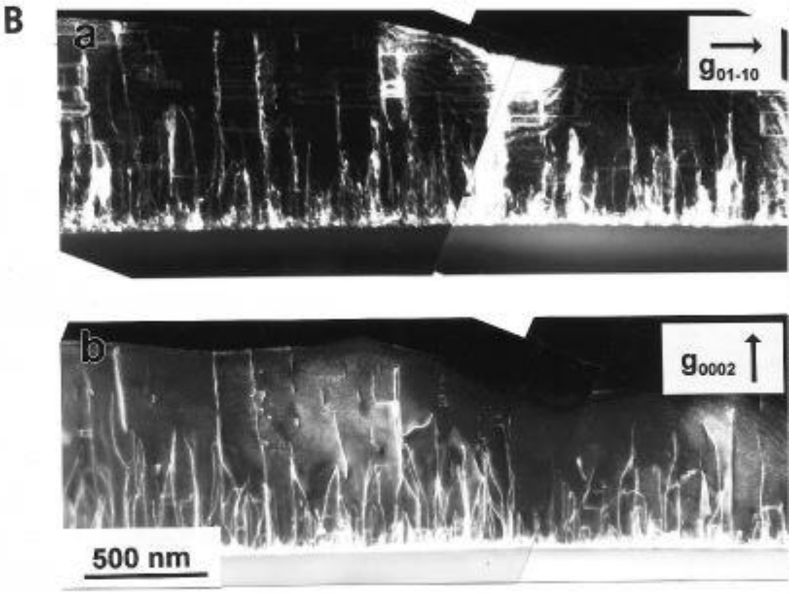


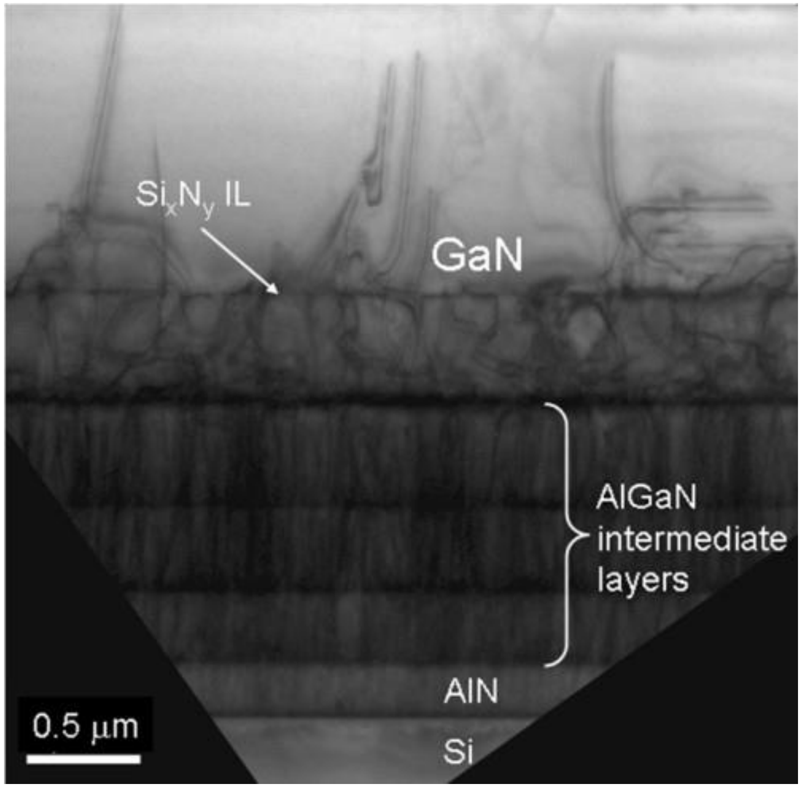
Figure 3.16 A 60° dislocation in the sphalerite structure. The axis and the Burgers vector are along different ⟨110⟩. The slip plane is {111}.

Dislocations observed by TEM

http://awsch-web.physics.ucsb.ed...ndex.php



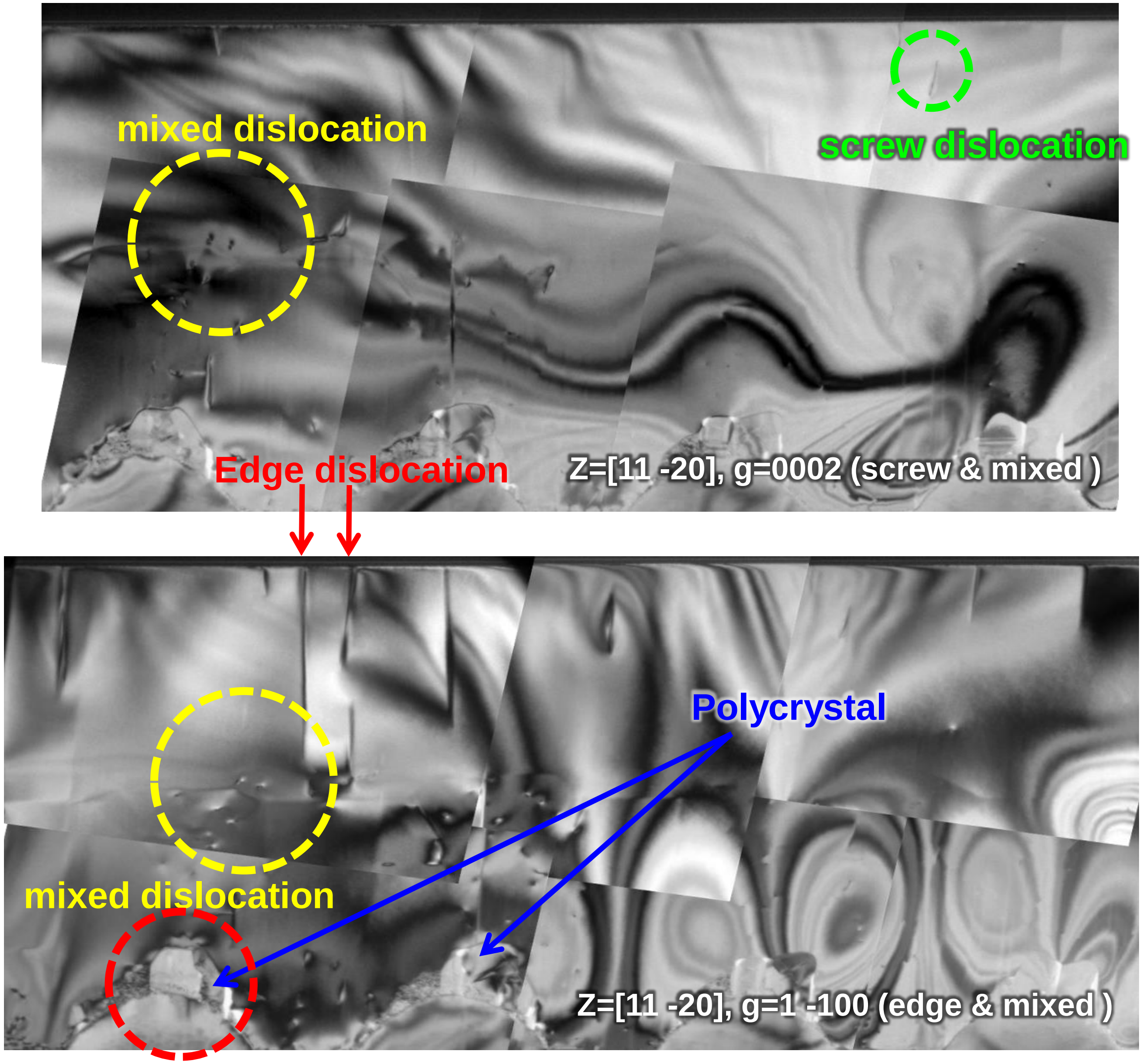




http://www.imec.be/ScientificRep...184.html

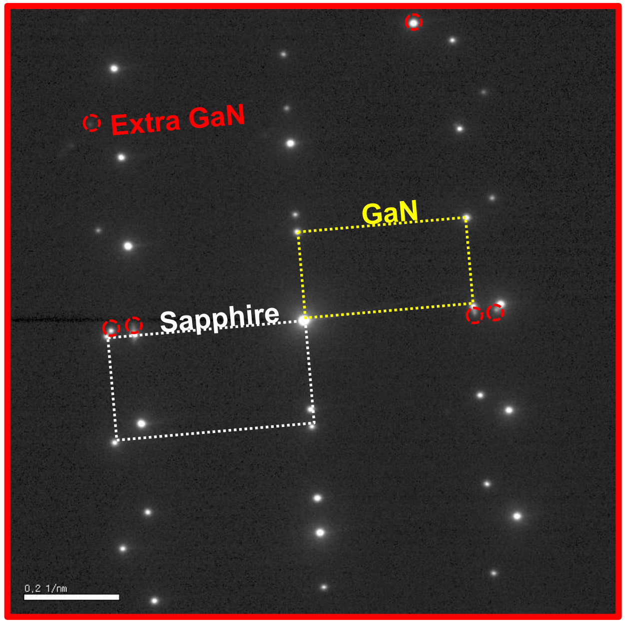
http://nsr.mij.mrs.org/1/19/comp...sym.html

Dislocations observed by TEM



More dislocation density than GaN Templates

Polycrystal formation



Contents

Crystal Imperfections

Planar Defects

- ***Two*** planar defects often observed in semiconductors can be *most easily* examined by first looking at the ***projections*** of the sphalerite and wurtzite crystal structures on a {110} and a {1100} surface, respectively.
- As can be seen in Fig. 3.17, there is a *distinct* difference between the hexagonal arrangement of atoms in the two projections. This is because the **six** atoms in the hexagonal projection for the sphalerite structure are arranged in a ***chairlike*** configuration in three dimensions (Fig. 1.10), whereas these six atoms in the wurtzite structure are arranged in a ***boatlike*** configuration (Fig. 1.12).

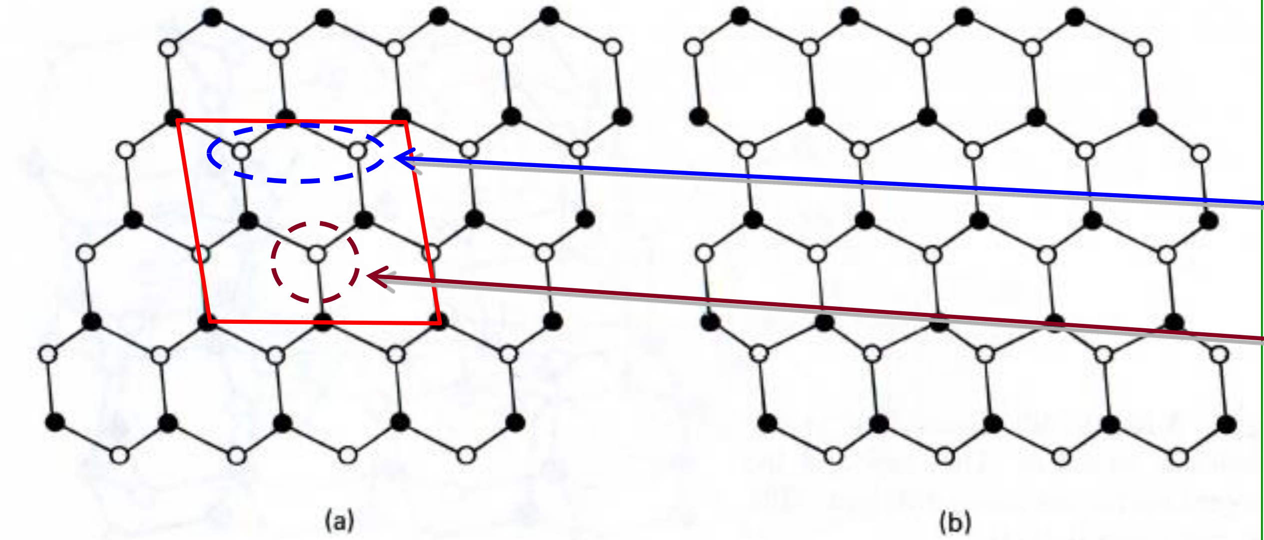
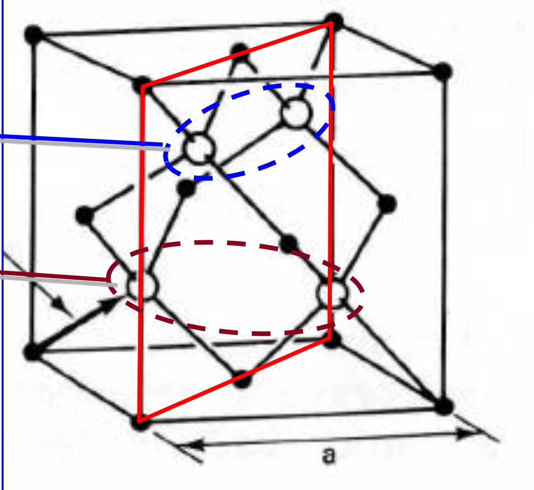


Figure 3.17 (a) Projection of the sphalerite structure on a {110} surface. (b) Projection of the wurtzite structure on a {1100} surface.

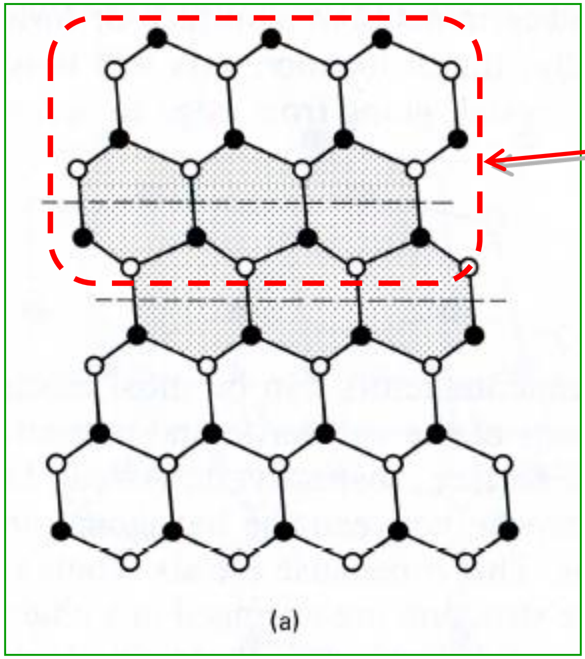


Planar Defects

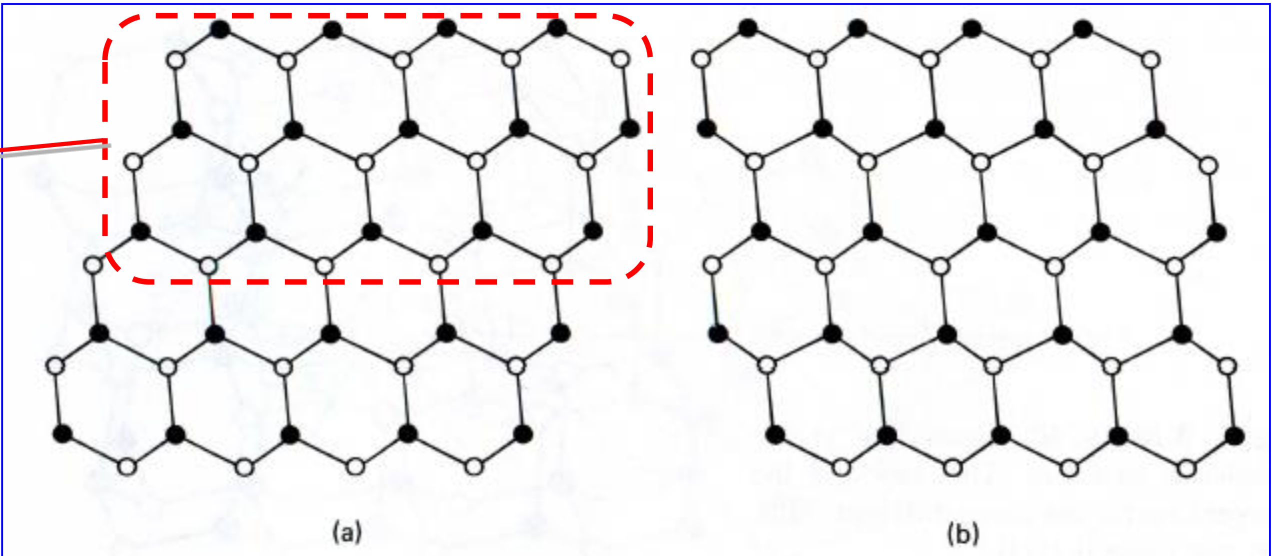
- With these two projections in mind, let us examine the ***intrinsic stacking fault*** shown in Fig. 3.18(a) for the sphalerite structure.

- The top row of six atom sets has the sphalerite structure. The next two rows of six atom sets (shaded region) *fits in the structure nicely* but have a wurtzite configuration. The bottom two rows have the sphalerite structure.

- Thus an *intrinsic* stacking fault *in the* ***sphalerite*** structure is an included wurtzite region. Conversely, an intrinsic stacking fault in the wurtzite structure is an included sphalerite region.



(a)



(a) (b)

Figure 3.17 (a) Projection of the sphalerite structure on a {110} surface. (b) Projection of the wurtzite structure on a {1100} surface.

Planar Defects

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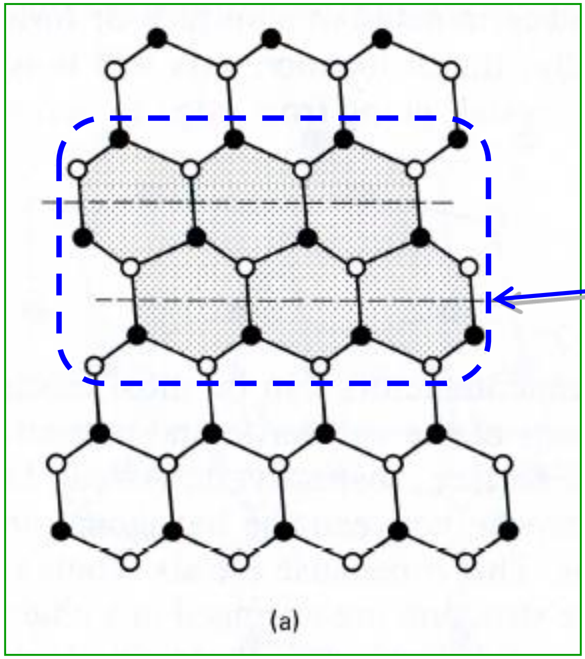


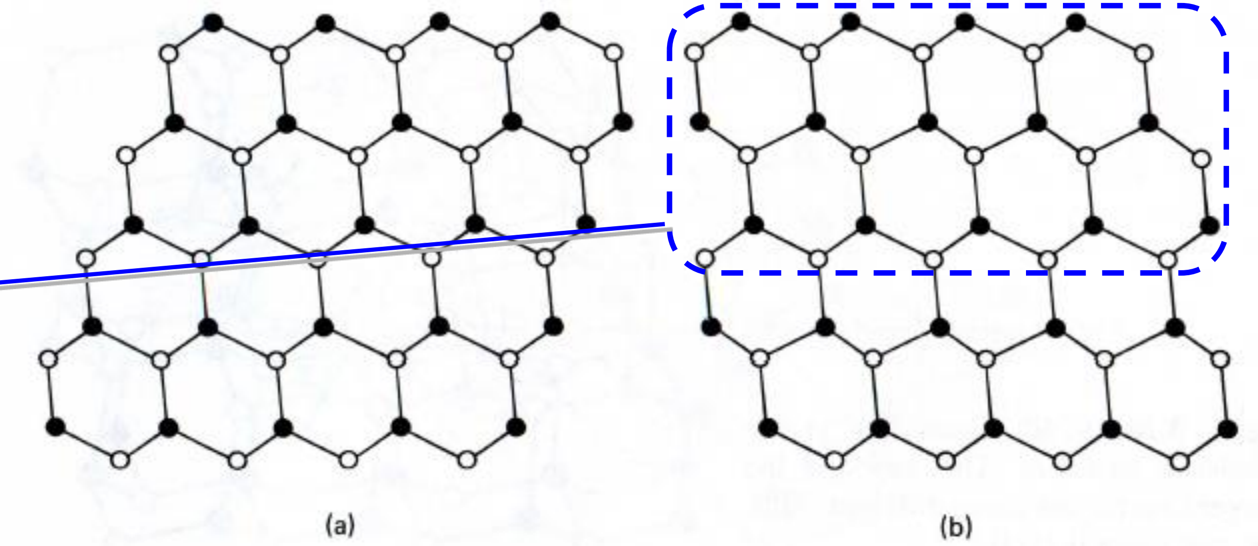


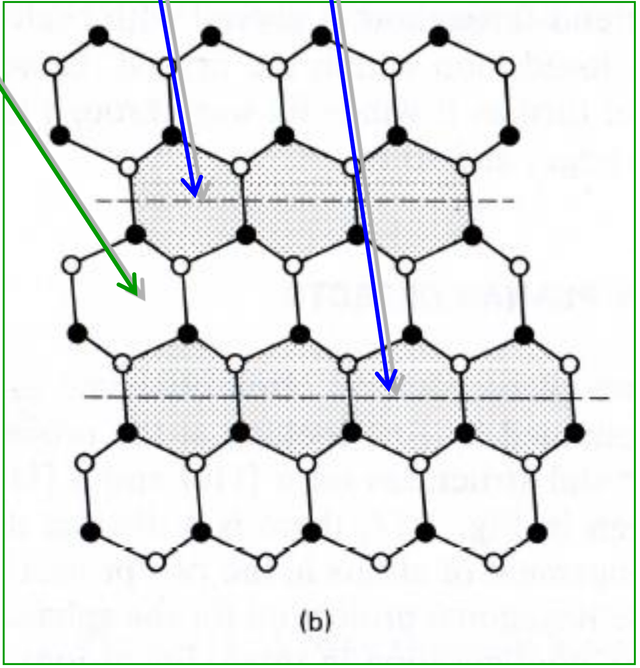
Figure 3.17 (a) Projection of the sphalerite structure on a {110} surface. (b) Projection of the wurtzite structure on a {1100} surface.

Planar Defects

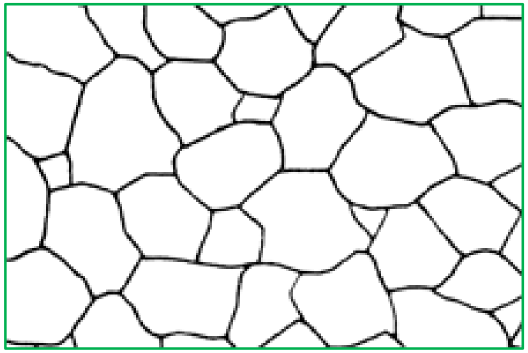
- Figure 3.18(b) shows an ***extrinsic stacking fault***, which has two rows of wurtzite-type bonding (shaded region) separated by a sphalerite region.

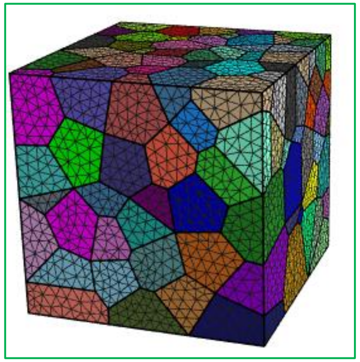
-Notice that for both the *intrinsic* and *extrinsic* stacking faults, two rows of included wurtzite region is required to return the crystal to its original structure. Stacking faults can terminate *on the surface* of a crystal or *on dislocations* referred to as partial dislocations.

-The dashed lines in Fig. 3.18 indicate ***twin*** planes. It can be seen that the crystal structure on one side of a twin plane is a mirror image of the other side. If a sphalerite crystal has only one row of included wurtzite, the entire crystal on one side of the twin plane will be a mirror image of the other side.



- Another planar defect that is often observed in semiconductors is the low-angle grain boundary or polygonization wall. This defect is formed as a low-energy configuration for a random field of dislocations.





Grain Boundaries - Example