• Stacking sequence in simple crystals.

• Stacking faults (intrinsic, extrinsic)

• Twin boundaries

• Dislocations and Burgers Vectors

• Shockely and Franck partial dislocations.

• Thompson Tetrahedron.

• Dislocations in Hexagonal, Covalent and polar/nonpolar epitaxial crystals.

• Polar Materials on non-Polar Substrates.

Stacking Sequence (1)

• Stacking sequence: To describe the arrangement of lattice sites within a crystal structure, we refer to the order or sequence of the atom layers in the ‘stack’ as ‘stacking sequence’.

Simple cubic structure:
- Lattice sites are identical when projected normal to the (100) plane → AAA... stacking
- Lattice sites are displaced by $a/2^{1/2}$ in the [-110] direction → ABABAB... stacking

Body Centered Cubic:
Stacking Sequence (2)

Face centered cubic structure:

(111) plane in one lattice

Arrangement of atoms in (111) plane

Stacking sequence

Close packed (111) plane

(110) $\rightarrow$ ABABAB...

(111) $\rightarrow$ ABCABCABC...

Fcc cell

View along diagonal \(<111>\)

Si

J.W. Morris, UC Berkeley

Dayeh, SST 25, 02424 2010.

Yoo & Dayeh, APL, 2013.
Stacking Sequence (3)

Hexagonal crystal structure:

[Diagram of hexagonal crystal structure]

http://www.hardmaterials.de/html/diamonds__ionsdaleite.html
Stacking Faults

- Are planar defects where the regular sequence in the crystal has been interrupted.
- Cannot occur with $ABAB$ stacking but can occur in $ABC$ stacking because layers in $A$ have alternative position in close packed layers to rest in either $A$ or $B$ positions.
- Two types:
  - Intrinsic
  - Extrinsic

Fault energy: $1 – 1000 \text{ mJ/m}^2$

- Usually occur with composition change, high doping levels, and non-optimal growth conditions.
Twin Boundaries

- Deformation twinning is a process in which a region of a crystal undergoes homogeneous shear that produces the original crystal structure in a new orientation.
- Atoms of the original crystal (‘parent’) and those of the product crystal (‘twin’) are mirror images of each other by reflection in a composition plane.

http://www.ece.umn.edu/groups/nsfret/TEMpics.html

- Usually occur with composition change, and at surfaces. Roughening of surfaces in heterostructures generally occurs by grains and twins.
Dislocations

- Is one of the most usual types of defects that are generated during heteroepitaxy which occurs in two types: (i) edge, (ii) screw, and a mixed dislocation constituting both edge and screw dislocations is often observed.

\[ \tau = \frac{G b}{2 \pi a} \sin \frac{2 \pi x}{b} \]

- \( \tau \) is the applied shear stress.
- \( G \) is the shear modulus.
- \( b \) is the spacing of atoms in the direction of the shear stress.
- \( a \) is the spacing of the rows of atoms.
- \( x \) is the translation of the two rows away from the low energy equilibrium position.

- For small strains: \[ \tau = \frac{G b}{2 \pi a} \sin \frac{2 \pi x}{b} = \frac{G b}{2 \pi a} \cdot \frac{2 \pi x}{b} = \frac{G x}{a} \] (Hooke’s Law)

- Maximum shear stress (theoretical critical shear stress): \[ \tau = \frac{b G}{a 2 \pi} \]

- The shortest lattice vectors in FCC are \( \frac{1}{2}<110> \) and \( <100> \). Energy of dislocation depends on \( b^2 \), therefore, \( \frac{1}{2}<110> \) are more energetically favored.

- The \( \frac{1}{2}<110> \) is a translation vector for the lattice and glide of a dislocation with this Burgers vector leaves behind a perfect crystal \( \rightarrow \frac{1}{2}<110> \) is a perfect dislocation.
Introduction to Edge and Screw Dislocations

A Burgers circuit is any atom-to-atom path taken in a crystal containing dislocations which forms a closed loop.

Burgers Circuit for edge dislocation

The difference between the two enclosures above is the Burgers vector (clockwise circuit).

Burgers Circuit for screw dislocation

- The Burgers vector of an edge dislocation is normal to the line of the dislocation.
- The Burgers vector of a screw dislocation is parallel to the line of the dislocation.

Burgers Vector for a Mixed Dislocation

In the viewing direction of the dislocation, make a clockwise loop around the dislocation and the extra vector to close the loop is the Burger’s vector.

For a given dislocation, there is only one Burgers vector, no matter what shape the dislocation line has.

A dislocation must end on itself, thus forming a loop, or on other dislocations, thus forming a (3D) network, or on surfaces/grain boundaries.

The sum of the Burgers vectors at the node or point of junction of the dislocation is zero.

The slip (or glide) plane of a dislocation contains the dislocation line and its Burgers vector.

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Burgers Vector for a Mixed Dislocation

Components of the mixed dislocation at P

- **Screw Component**
  - $\vec{b} \cos(\theta)$
- **Edge Component**
  - $\vec{b} \sin(\theta)$

**Diagram Notes:**
- Pure screw
- Pure Edge
- Curved Dislocation Line
- 'Extra half-plane'

**Equations:**
- $\vec{b} \cos(\theta)$
- $\vec{b} \sin(\theta)$
Shockley Partial Dislocations

- When the Burgers vector is not a lattice vector, it leaves behind an imperfect crystal containing a stacking fault which separates the faulted region from the perfect region of the crystal by a partial dislocation.

**Shockley partial:**

\[ b = \frac{a}{6} <112> \Rightarrow b = \frac{a}{6} \sqrt{1+1+4} = \frac{a}{6} \sqrt{6} \]

**Perfect dislocation:**

\[ b = \frac{a}{2} <110> \Rightarrow b = \frac{a}{2} \sqrt{1+1+0} = \frac{a}{2} \sqrt{2} \]

**Splitting of perfect dislocations into partials:**

\[ \frac{1}{2} [110] \rightarrow \frac{1}{6} [211] + \frac{1}{6} [121] \]

\[ \frac{1}{2} [101] \rightarrow \frac{1}{6} [211] + \frac{1}{6} [112] \]

\[ \frac{1}{2} [011] \rightarrow \frac{1}{6} [121] + \frac{1}{6} [112] \]

**Slip**

Movement of atoms in FCC crystals occurs on slip planes which are the close-packed \{111\} atomic planes, and slip occurs in \langle110\rangle direction. Atoms slide over one another by dissociating a \langle110\rangle transition into two \langle112\rangle transitions.
Thompson Tetrahedron

- The Thompson tetrahedron is a convenient notation to describe all important dislocations and dislocation reactions in FCC materials.

\[ \mathbf{A} \mathbf{B} = \mathbf{A} \mathbf{\gamma} + \mathbf{\gamma} \mathbf{B} \quad \text{(on slip plane } \mathbf{ABD}) \]

- Dislocations happen on \{111\} planes.
- Perfect dislocations on tetrahedral sides.
- Partial Shockley dislocations are bisectors of tetrahedral faces.

Which crystal direction should orient the crystal to visualize edge dislocations?

FCC: \( \frac{1}{2} <110> \{111\} \) slip system

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/i5_4_5.html
Frank Partial Dislocations

- Formed at the Boundary line of inserting or removing one close-packed \{111\} layer of atoms.

\[ b = \frac{a}{3} <111> \]

\[ \frac{1}{6} [112] + \frac{1}{3} [111] \rightarrow \frac{1}{2} [110] \]

\[ B\alpha \quad \alpha A \quad BA \]

Shockley partial  Frank partial  Perfect dislocation

\[ \frac{1}{6} [\bar{2}1\bar{1}] + \frac{1}{6} [2\bar{1}1] + \frac{1}{3} [111] \rightarrow \frac{1}{2} [110] \]

\[ \alpha C \quad \alpha D \quad \alpha A \quad BA \]
Dislocations in Hexagonal Crystals

- The (0001) basal plane is close-packed and close-packed directions are $<11\bar{2}0>$ with $b = 1/3 <11\bar{2}0>$ generally occurring on prismatic {10-10} planes.

- Important dislocations:
  - Perfect dislocations with one of six Burgers vectors in Basal plane along ABC sides (AB, BC, CA, BA, CB, and AC).
  - Perfect dislocations with one of two Burgers vectors perpendicular to basal plane (c-axis), ST and TS.
  - Perfect dislocations with one of twelve Burgers vectors such as SA and TB.
  - Imperfect basal dislocations of Shockley partial type (Aσ, Bσ, etc.)
  - Imperfect dislocations with Burgers vectors perpendicular to basal plane (σS, σT, etc).
  - Imperfect dislocations that combine previous two (Aσ, Bσ, etc.).
Dislocations in Covalent Crystals

- Perfect dislocations have $\frac{1}{2}<110>$ Burgers vectors and slip on {111} planes.
- They typically lie at 0° (pure edge) or 60° with $<110>$ direction (mixed dislocation, more commonly observed).

![Diagram of perfect dislocations]

- Perfect dislocations can dissociate into partial dislocations.

$$b = \frac{1}{6} <112>$$

at 30° to the line direction.
Defects in Heteroepitaxial Interfaces

reference crystals, $\lambda$ and $\mu$

with misfit dislocation

(a)

(b)
Growth of Polar on non-polar Substrates (III-V on Si)

The problem of anti-phase boundaries on (001) surfaces

Anti-phase boundaries in GaAs
Ga-Ga and As-As bonds

Single steps on Si lead to anti-phase boundaries at step edges

Alternative surfaces/interfaces that eliminate anti-phase boundaries

Growth on off-cut Si(100) and surface reconstruction to eliminate anti-phase boundaries

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Fig. 1. Two sublattices in a Si crystal, distinguished only by bond orientation in space.

Fig. 2. Anti-phase boundary (APB) formation in the zincblende structure, containing (in the case of GaAs) both Ga-Ga and As-As bonds. The configuration shown is the simplest possible case, a perfectly (110)-oriented APB, with alternating Ga-Ga and As-As bonds.

Fig. 3. Mechanism of APB formation during polar-to-non-polar growth due to the presence of single-height steps on the substrate surface.