HOMEWORK
From Dieter
5-1, 5-4, 5-5, 5-9

Module #14

Dislocations in Common Crystal Structures

READING LIST

DIETER: Ch. 5, Pages 154-160

Chs. 5 and 6 in Hull & Bacon
Chs. 10-12 in Hirth & Lothe

Objective

- The objective of this module is to present some of the dislocations observed in FCC, HCP and BCC crystal structures.
- This section is intentionally brief. More details can be found by consulting the reading list.
- We will not address ceramics or intermetallics here. They will be addressed separately.

Plastic Flow in General

- Slip occurs via glide
- Slip occurs on close-packed planes in close-packed directions
- Slip system = Slip plane + Slip direction

Slip in FCC Crystals

Close-packed plane: $\{111\}$

Close-packed directions on $\{111\}$: $\langle 110 \rangle$

Shortest lattice vectors: $\dfrac{a_o}{2}\langle 110 \rangle$

Dislocations usually glide on the basal plane with $b = \dfrac{a_o}{2}\langle 110 \rangle$

Each unit cell contains 4 {111} planes

Each {111} plane contains 3 <110> directions

Thus, there are 12 slip systems in an FCC unit cell

RECALL: Dissociation of dislocations

- Because of energy considerations it is also possible for some dislocations to dissociate (split) into shorter segments. This is favorable in certain crystals (Ex., FCC).

Will the reaction $b_1 \rightarrow b_2 + b_3$ occur?

Yes if $b_1^2 > \left(b_2^2 + b_3^2\right)$

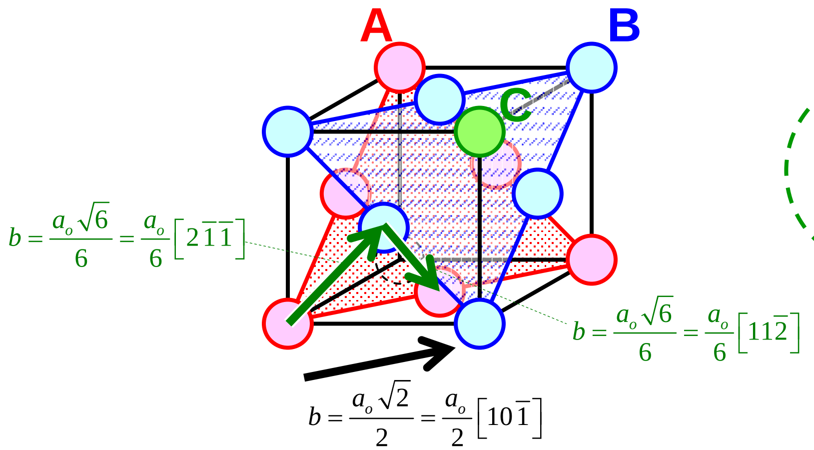
No if $b_1^2 < \left(b_2^2 + b_3^2\right)$

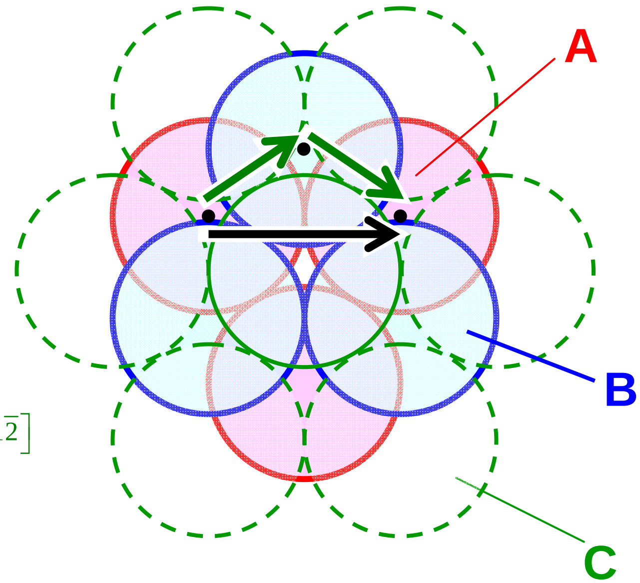
IMPORTANT
Elastic strain energy $\propto Gb^2$

- This is possible in *close-packed crystals* such as FCC and HCP where equilibrium positions are not the edges of the unit cell.

Shockley Partial Dislocations in FCC crystals

- In this example, the separation into partial dislocations is energetically favorable. There is a decrease in strain energy.

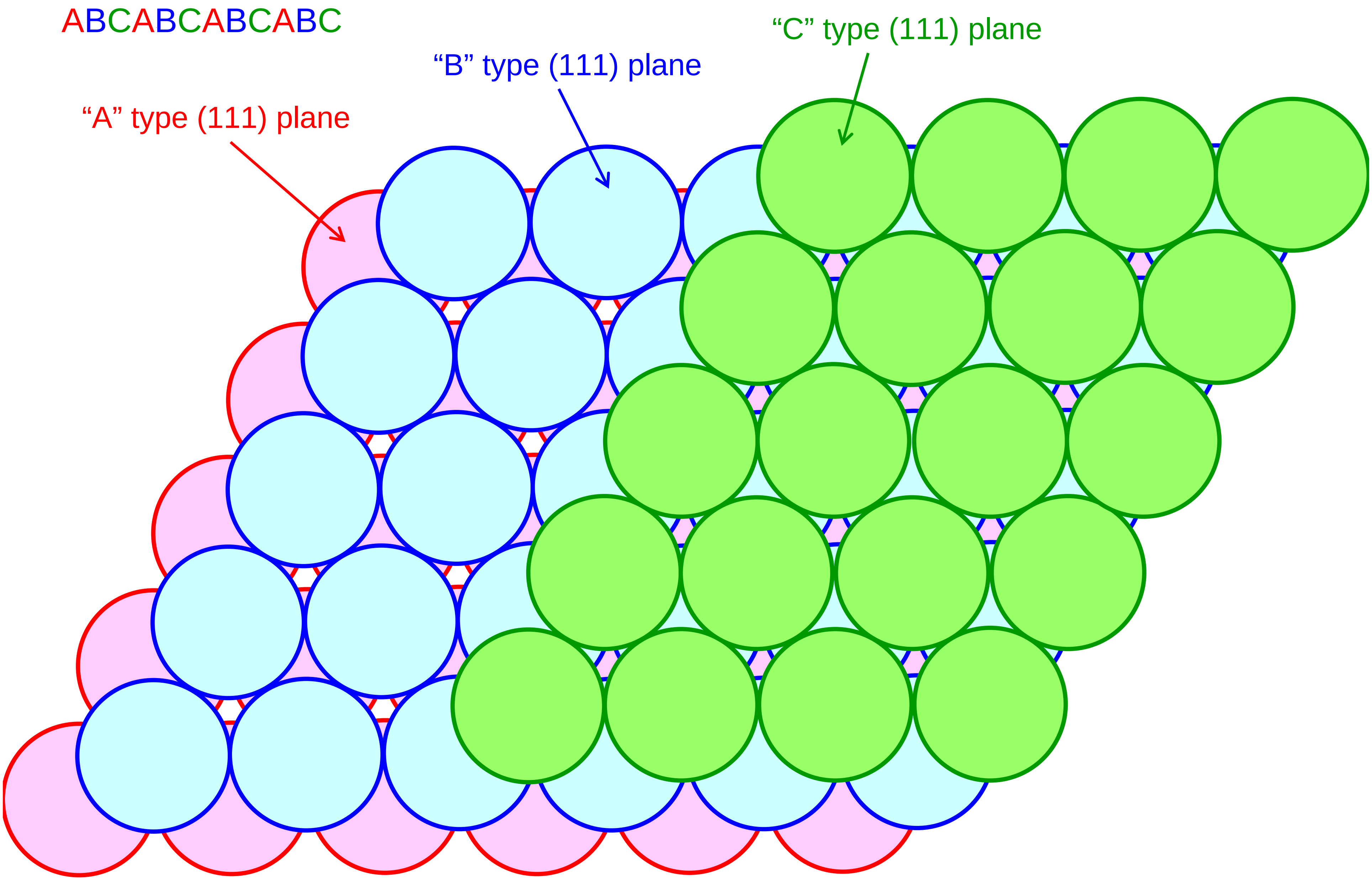




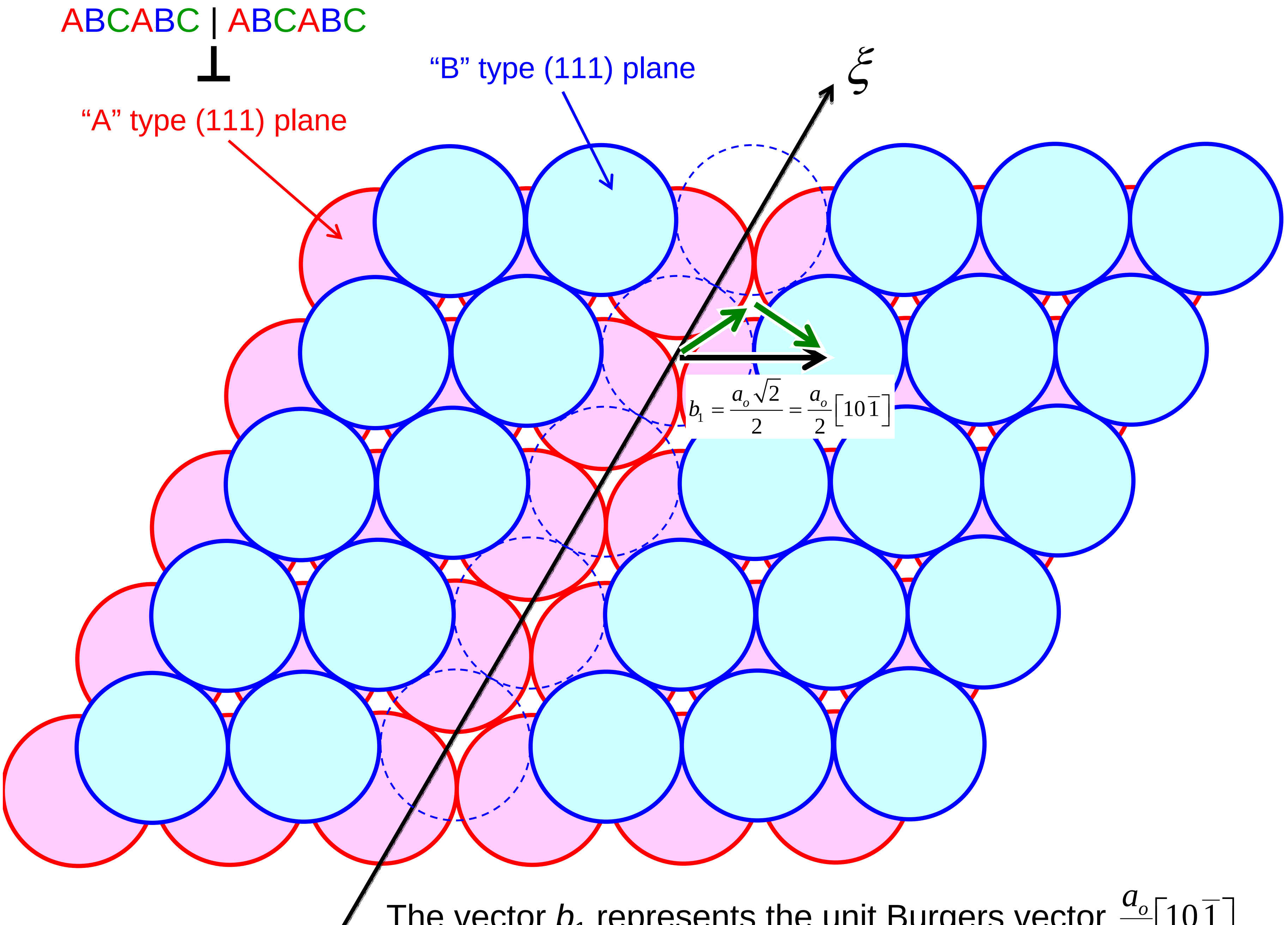
$$\frac{a_o}{2}[10\bar{1}] \rightarrow \frac{a_o}{6}[2\bar{1}\bar{1}] + \frac{a_o}{6}[11\bar{2}]$$

$$\frac{a_o^2}{2} > \frac{a_o^2}{6} + \frac{a_o^2}{6}$$

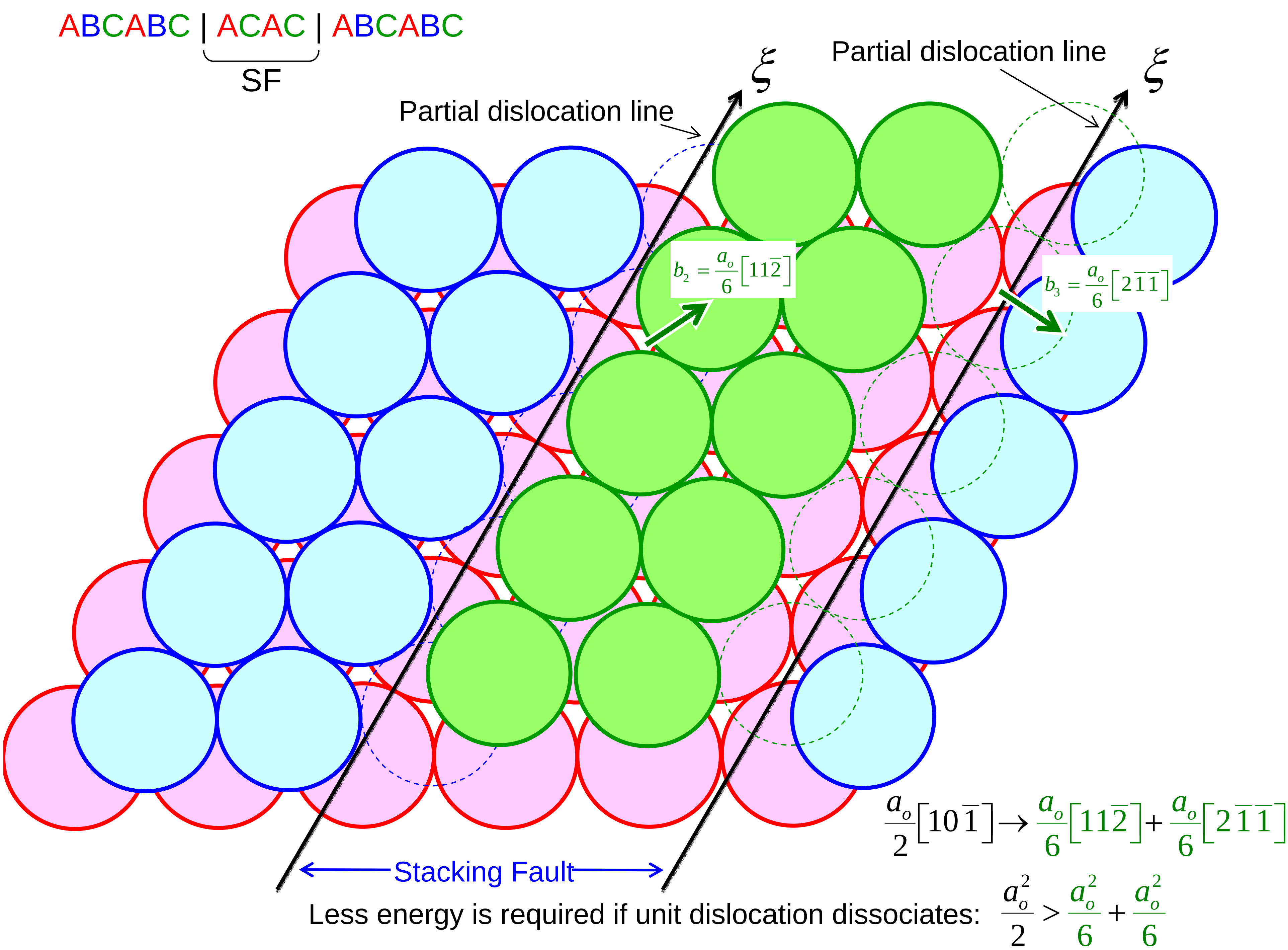
- Separation produces a *stacking fault* between the partials.



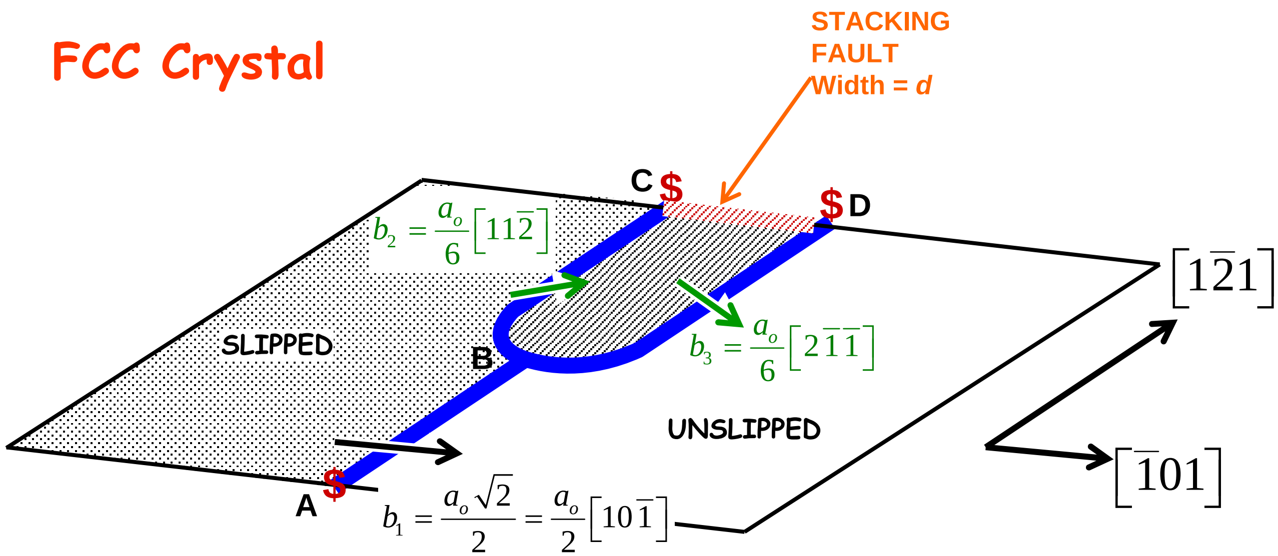
In an fcc lattice, slip occurs on (111) planes in <110> directions



The vector b_1 represents the unit Burgers vector $\frac{a_o}{2}[10\bar{1}]$
However, there is a "simpler" path.


ABCABC | ACAC | ABCABC
SF
Partial dislocation line
Partial dislocation line
ξ
ξ
$b_2 = \frac{a_o}{6}[11\bar{2}]$
$b_3 = \frac{a_o}{6}[2\bar{1}\bar{1}]$
$\frac{a_o}{2}[10\bar{1}] \rightarrow \frac{a_o}{6}[11\bar{2}] + \frac{a_o}{6}[2\bar{1}\bar{1}]$
Stacking Fault
Less energy is required if unit dislocation dissociates: $\frac{a_o^2}{2} > \frac{a_o^2}{6} + \frac{a_o^2}{6}$

FCC Crystal



$$SFE = \gamma_{SFE} = \frac{Gb_2b_3}{2\pi d}$$

$d =$ partial dislocation separation

$G =$ shear modulus

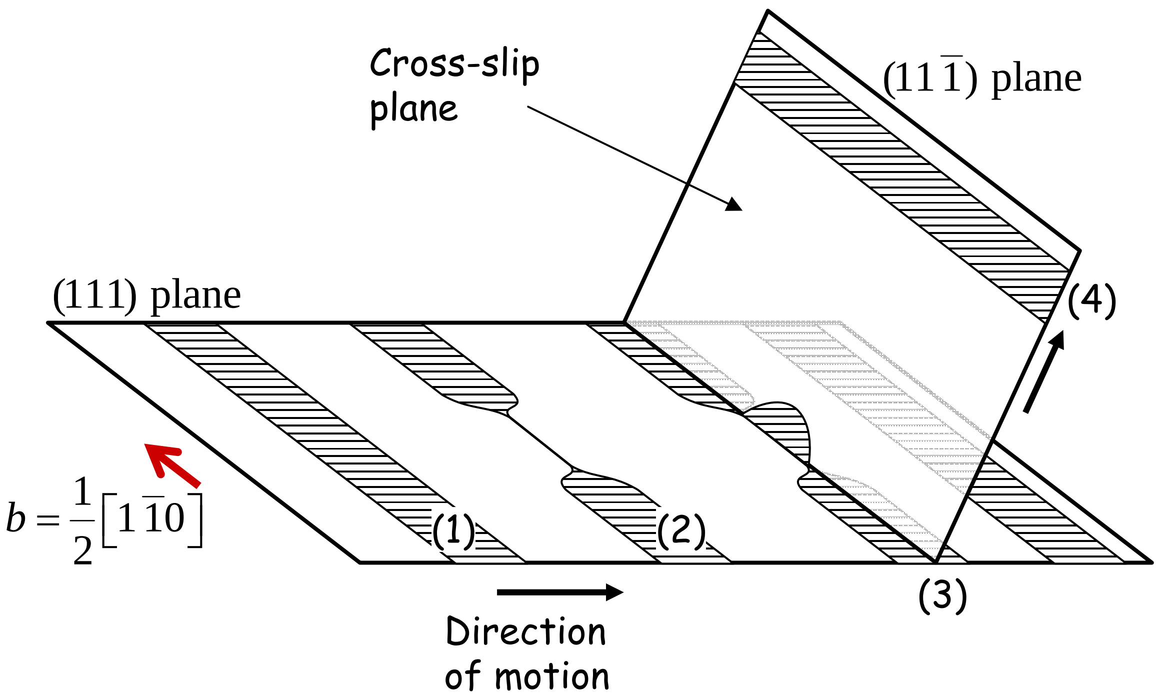
- AB represents a regular (un-extended) dislocation.
- **BC** and **BD** represent partial dislocations.
- The region between BC and BC represents the stacking fault. In this region, the crystal has undergone “intermediate” slip.
- BC + stacking fault + BD represents an *extended dislocation*.
- Extended dislocations (in particular screw dislocations) define a specific slip plane. Thus, *extended screw dislocations can only cross-slip when the partial dislocations recombine*. See the illustration on the next page.
- This process requires some energy.

Extended Dislocation

[Partial Dislocation + SF + Partial Dislocation]

- An extended screw dislocation <u>must</u> constrict before it can cross slip.

Schematic illustration



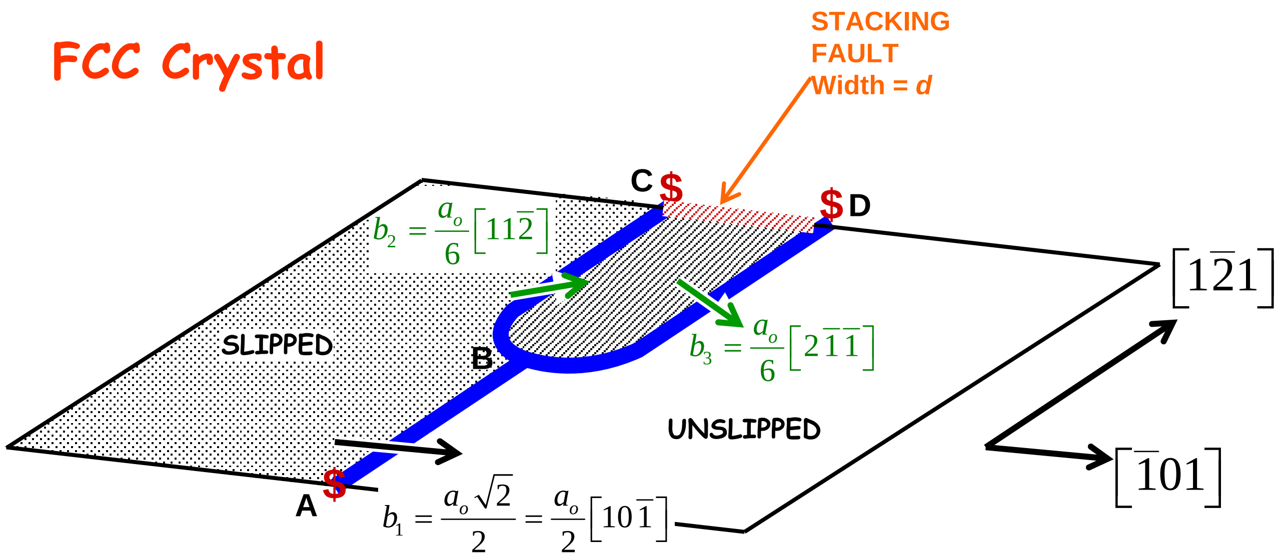
(1) Extended ⊥

(2) Formation of constricted segment

(3) Cross-slip of constricted segment and separation into extended ⊥

(4) Slip of extended ⊥ on cross-slip plane

FCC Crystal



$$SFE = \gamma_{SFE} = \frac{Gb_2b_3}{2\pi d}$$

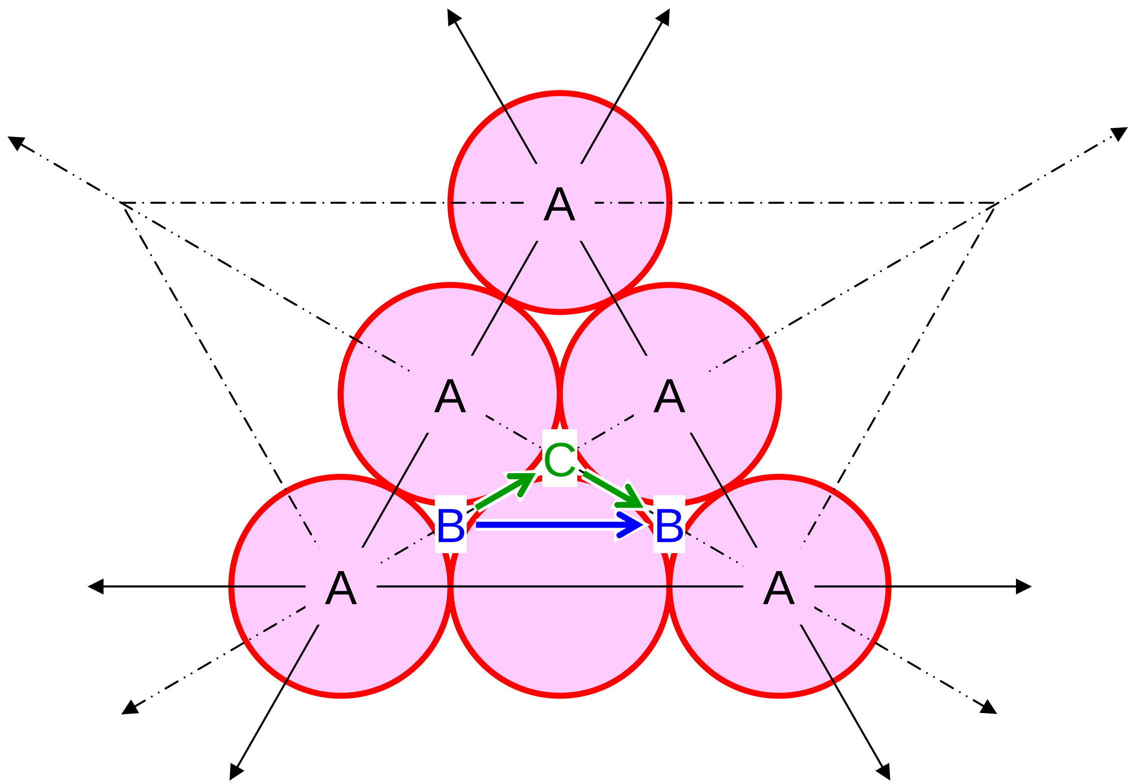
$d =$ partial dislocation separation

$G =$ shear modulus

- It is more difficult to re-combine wide stacking faults (i.e., those with large *d*).
- Cross-slip is more difficult in materials with low SFE. Thus high SFE materials will work harden more rapidly.
- We will address this in more detail when we discuss work hardening.

Material	SFE (mJ/m^2)	Fault width	Strain Hardening rate	REASONS
Stainless Steel	<10	~0.45	High	Cross slip is more difficult
Copper	~90	~0.30	Med	
Aluminum	~250	~0.15	Low	Cross slip is easier

See pages 74-79 in Hertzberg



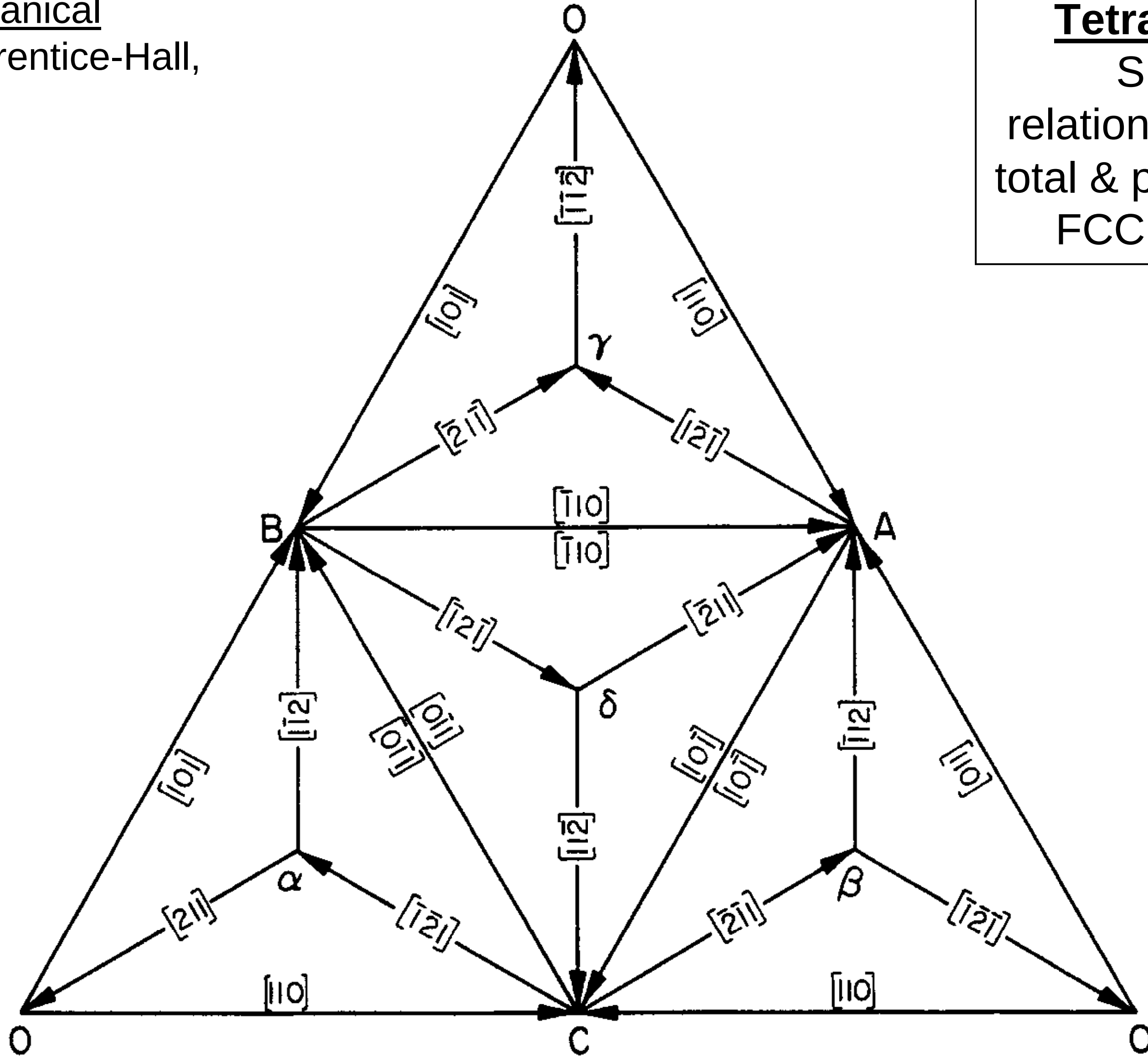
Geometry of close-packed planes appropriate for dissociation into Shockley partial dislocations. The large blue arrow corresponds to $\frac{a}{2}\langle 110 \rangle$ while the small green arrows correspond to $\frac{a}{6}\langle 211 \rangle$ and $\frac{a}{6}\langle 12\bar{1} \rangle$.

Figure adapted from R.C. Reed, Superalloys: Fundamentals and Applications, (Cambridge University Press, Cambridge, 2006) p. 56.

[M.A. Meyers and K.K. Chawla, Mechanical Metallurgy, (Prentice-Hall, 1984) p. 249]

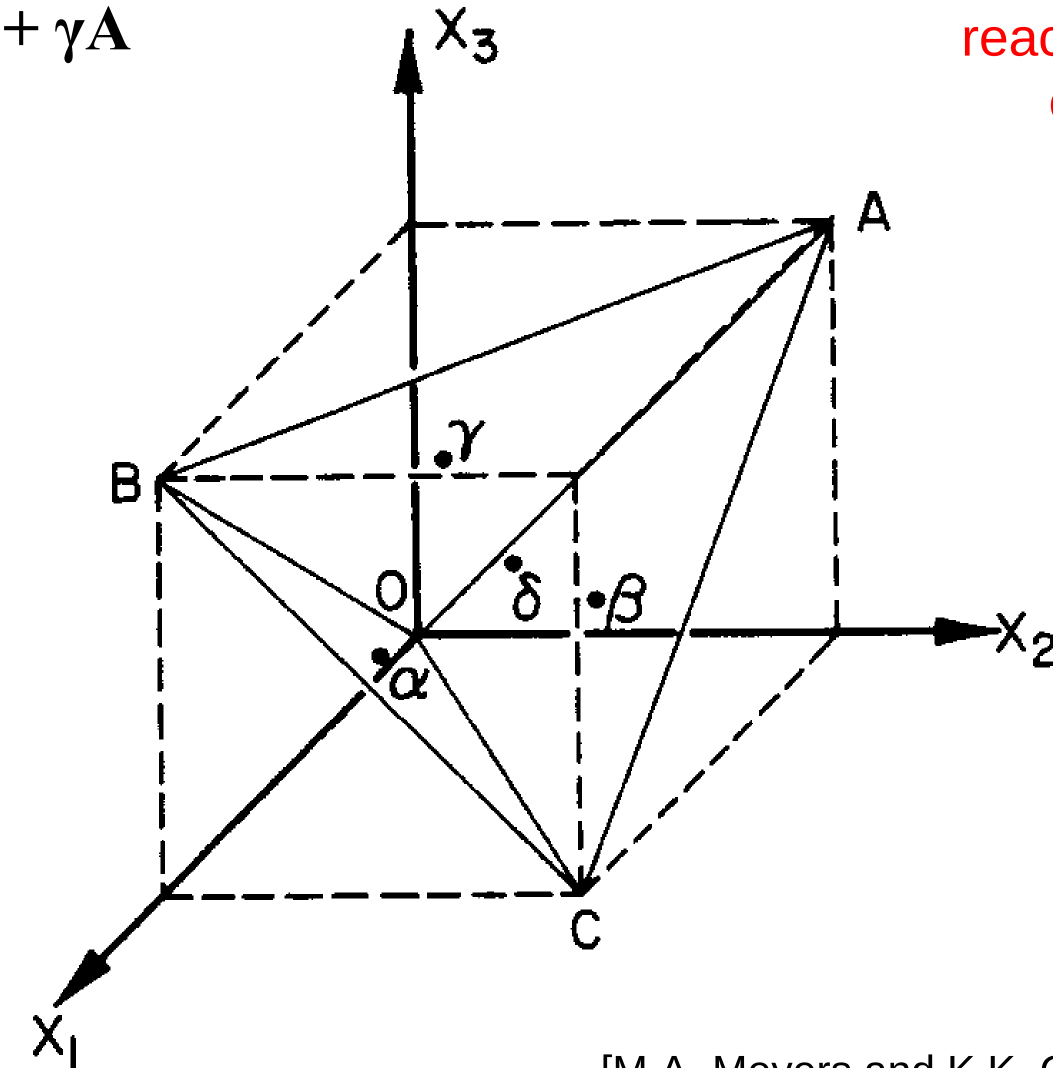
Thompson Tetrahedron

Shows relationships of all total & partial ⊥'s in FCC system.



BA = Bγ + γA

Convenient way to visualize dislocation reactions in fcc crystals



[M.A. Meyers and K.K. Chawla, Mechanical Metallurgy, (Prentice-Hall, 1984) p. 249]

Frank Partial dislocations in FCC crystals

- Formed by inserting or removing one close-packed {111} layer of atoms. This results in either an intrinsic or an extrinsic stacking fault.

- This results in an edge dislocation with a Burgers vector is normal to the {111} plane of the fault. This dislocation is sessile.

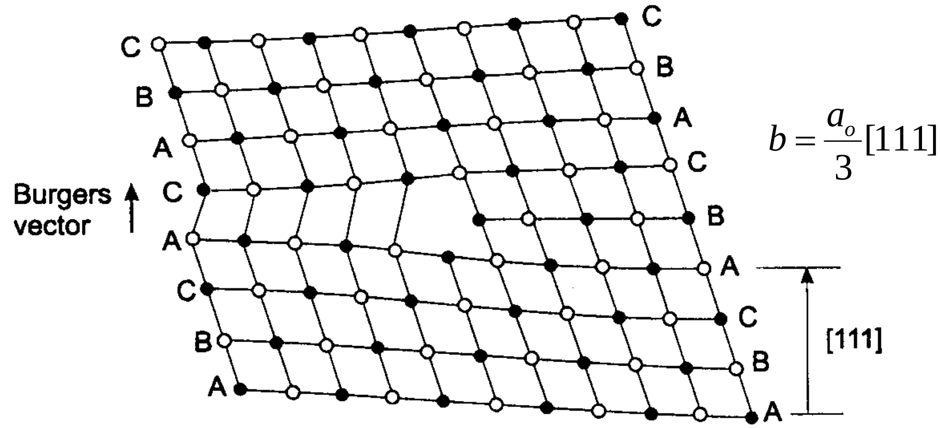


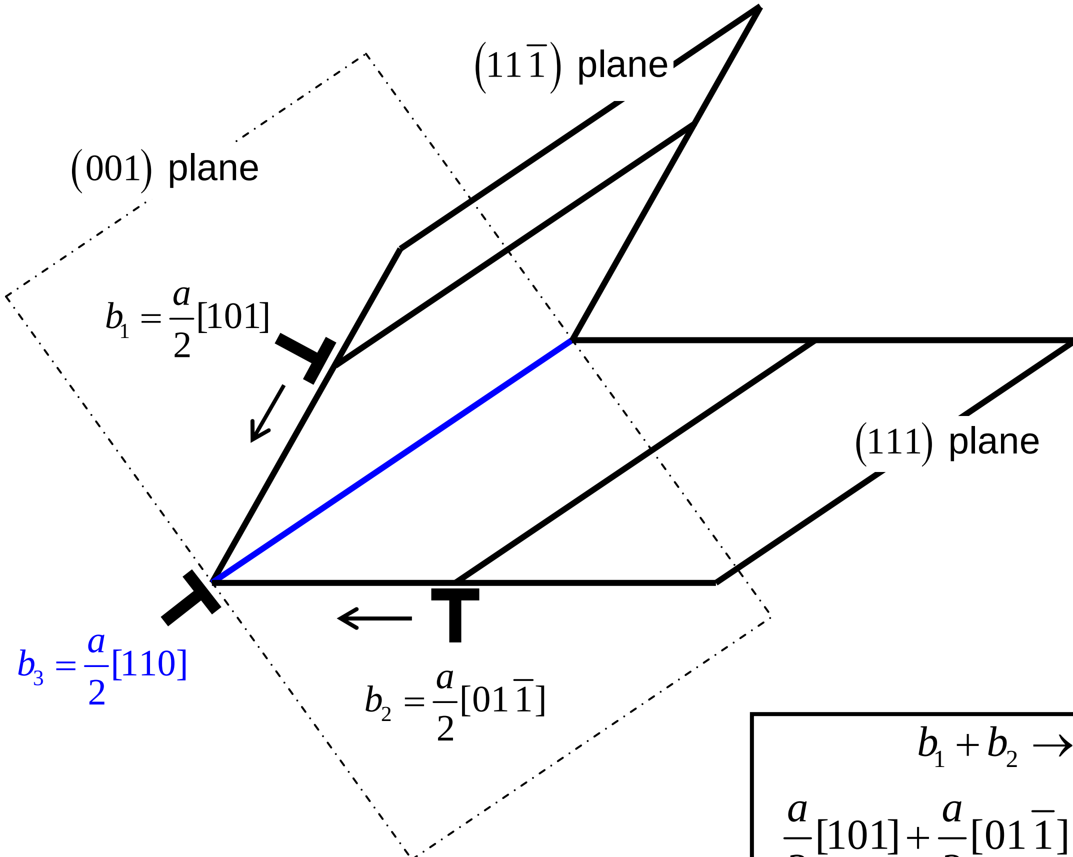
Figure 5.12 Formation of a $\frac{1}{3}$[111] Frank partial dislocation by removal of part of a close-packed layer of atoms. The projection and directions are the same as Fig. 5.2. (After Read (1953), *Dislocation in Crystals*, McGraw-Hill.)

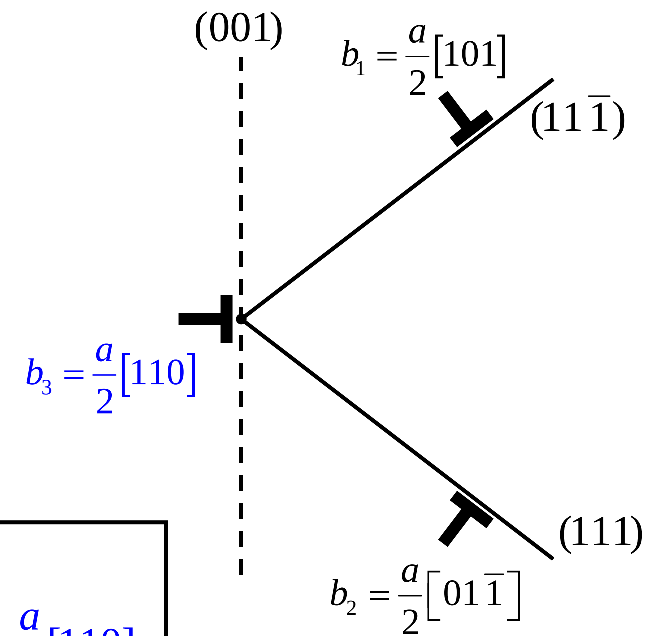
[Hull & Bacon]

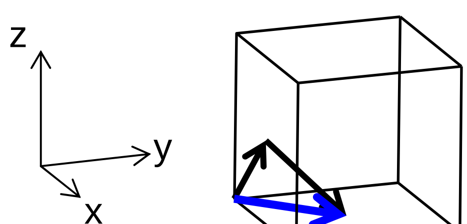
Interaction of dislocations on intersecting slip planes

- Consider intersection (111) slip planes in an FCC lattice

Lomer lock







$$b_1 + b_2 \rightarrow b_3$$

$$\frac{a}{2}[101] + \frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{2}[110]$$

on $(11\bar{1})$, on (111), on (001)

$$b_1^2 + b_2^2 > b_3^2$$

$$\frac{a_o^2}{4} + \frac{a_o^2}{4} > \frac{a_o^2}{4}$$

Interaction of dislocations on intersecting slip planes

- Consider intersection (111) slip planes in an FCC lattice.
- <110> dislocations can separate into Shockley partials.

on $(11\bar{1})$

$$b_1 \rightarrow b_{1a} + b_{1b}$$

$$\frac{a}{2}[101] \rightarrow \frac{a}{6}[2\bar{1}1] + \frac{a}{6}[112]$$

Lomer-Cottrell lock

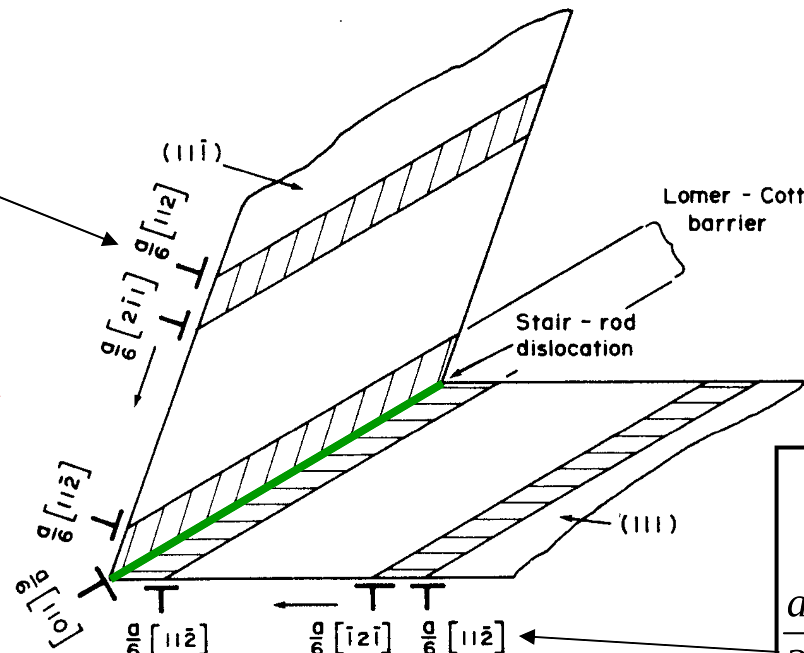


Figure adapted from I. LeMay, Principles of Mechanical Metallurgy, Elsevier (1981) p. 111

on (111)

$$b_2 \rightarrow b_{2a} + b_{2b}$$

$$\frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{6}[\bar{1}2\bar{1}] + \frac{a}{6}[11\bar{2}]$$

Fig. 4.24 A Lomer-Cottrell barrier formed by the meeting of Shockley partial dislocations on intersecting {111} planes

AT INTERSECTION

$$b_{1a} + b_{2a} \rightarrow b_{LC}$$

$$\frac{a}{6}[2\bar{1}1] + \frac{a}{6}[\bar{1}2\bar{1}] \rightarrow \frac{a}{6}[110]$$

This combination is known as a Lomer-Cottrell lock. It is termed a stair-rod dislocation and is sessile.

Dislocations in Hexagonal Close-Packed Crystals

Dislocations are similar to those in FCC crystals.

Close-packed plane: (0001)

Close-packed direction: $\langle 11\bar{2}0 \rangle$

Shortest lattice vectors: $\dfrac{a_o}{3}\langle 11\bar{2}0 \rangle$

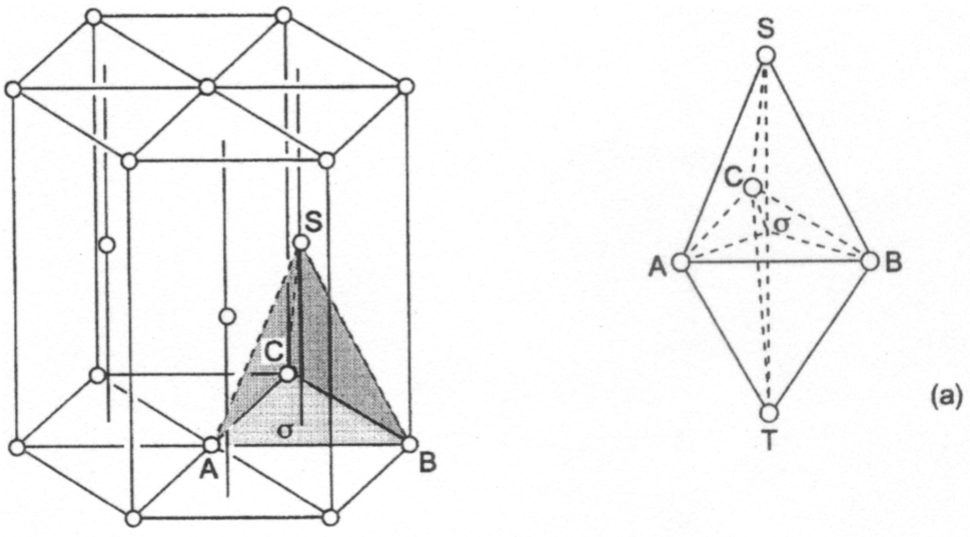
Dislocations usually glide on the basal plane with $b = \dfrac{a_o}{3}\langle 11\bar{2}0 \rangle$

Table 6.1 Properties of some hexagonal close-packed metals at 300 K

Metal	*Be*	*Ti*	*Zr*	*Mg*	*Co*	*Zn*	*Cd*
c/a ratio	1.568	1.587	1.593	1.623	1.628	1.856	1.886
Preferred slip	basal	prism	prism	basal	basal	basal	basal
Plane for $\mathbf{b} = \mathbf{a}$	(0001)	$\{10\bar{1}0\}$	$\{10\bar{1}0\}$	(0001)	(0001)	(0001)	(0001)

[Hull & Bacon, p. 102]

HCP



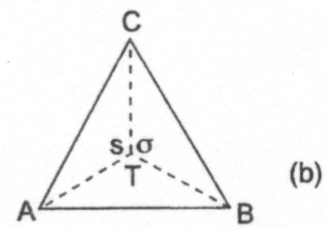


Figure 6.1 Burgers vectors in the hexagonal close-packed lattice. (Originally from Berghezan et al., *Acta Metall.*, v.9 (1961) p. 464. Scanned from Hull & Bacon, p. 103).

AB = perfect (unit) dislocation
Aσ = Shockley partial type

Table 6.2. Dislocations in HCP materials [adapted from Hull & Bacon, p. 104]

$Type$	AB	TS	SA/TB	$A\sigma$	σS	AS
$\boldsymbol{b}$	$\frac{1}{3}\langle 11\bar{2}0\rangle$	$[0001]$	$\frac{1}{3}\langle 11\bar{2}3\rangle$	$\frac{1}{3}\langle \bar{1}100\rangle$	$\frac{1}{2}[0001]$	$\frac{1}{6}\langle \bar{2}203\rangle$
b	a	c	$\sqrt{c^2+a^2}$	$a/\sqrt{3}$	$c/2$	$\sqrt{\frac{a^2}{3}+\frac{c^2}{4}}$
b^2	a^2	$\frac{8}{3}a^2$	$\frac{11}{3}a^2$	$\frac{1}{3}a^2$	$\frac{2}{3}a^2$	a^2

Non-basal slip

HCP

- Can occur. Burgers vector is still:

$$b = \frac{a_o}{3}\langle 11\bar{2}0\rangle$$

- In Be, Mg, Cd and Zn, perfect dislocations dissociate into Shockley partials.

$$\frac{1}{3}[11\bar{2}0] \rightarrow \frac{1}{3}[10\bar{1}0] + \frac{1}{3}[01\bar{1}0]$$

$$b^2: \quad a^2 \qquad a^2/3 \qquad a^2/3$$

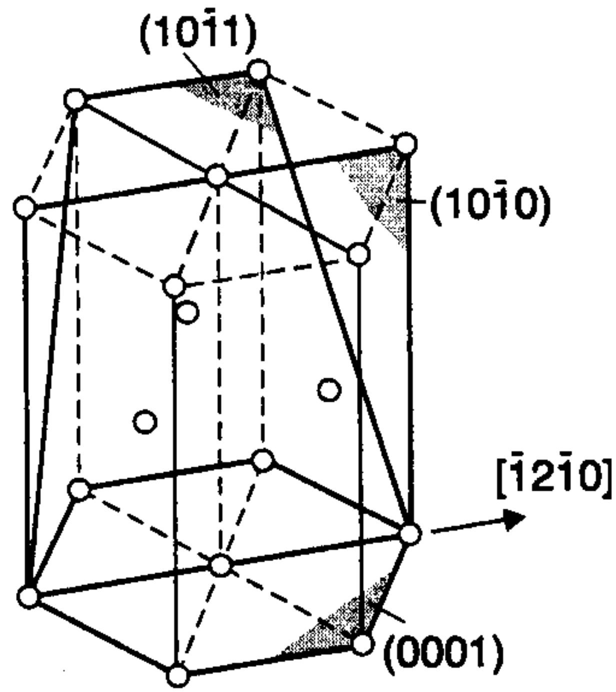


Figure 6.3 Planes in an hexagonal lattice with a common $[\bar{1}2\bar{1}0]$ direction.

[Hull & Bacon, p. 105]

Slip in BCC Crystals

Close-packed plane: $\{110\}$

Close-packed directions on $\{110\}$: $\langle 111 \rangle$

Shortest lattice vectors: $\frac{a_o}{2}\langle 111 \rangle$

Dislocations usually glide on the basal plane with $b = \frac{a_o}{2}\langle 111 \rangle$

Each unit cell contains 6 {110} planes

Each {110} plane contains 2 <111> directions

Thus, there are 12 {110}<111> slip systems in an BCC unit cell.

Slip in BCC Crystals – cont’d

In BCC slip can also occur on {112} and {123} planes in <110> directions

Each unit cell contains 12 {112} planes

Each {112} plane contains 1 <111> direction

Thus, there are 12 {112}<111> slip systems.

Each unit cell contains 24 {123} planes

Each {123} plane contains 1 <111> direction

Thus, there are 24 {112}<111> slip systems.

Thus there are a total of 48 possible slip systems in BCC crystals

Dislocations in Body-Centered Cubic Crystals

- Slip on {110} is most prevalent.
- However, {112}, and {123} planes, but
- Three {110} planes intersect a [111] direction. Unit screw dislocations can easily move from one {110} to {123} and/or {211} planes resulting in wavy slip lines.
- Extended dislocations are uncommon.