INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONE: 2240-1
CABLE: CENTRATOM - TELEX 460392 - I

SMR/208 - 15

SPRING COLLEGE IN MATERIALS SCIENCE

ON

"METALLIC MATERIALS"

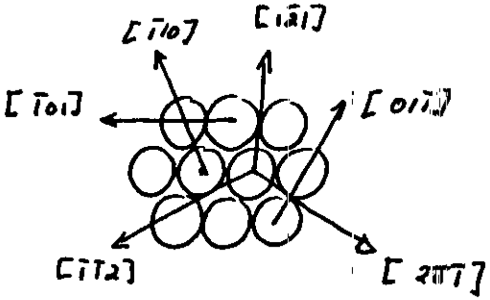
(11 May - 19 June 1987)

DISLOCATIONS (Part II)

J.Th.M. DE HOSSON
Department of Applied Physics
University of Groningen
9747 AG Groningen
The Netherlands

5. Dislocations in face-centred cubic metals

Slipplane $\{111\}$



smallest $\vec{b}$-vector: $\vec{b}_I = \frac{1}{2}[110]$

next-smallest $\vec{b}$: $\vec{b}_{II} = [100]$

$$E^{el}_{II} = 2\,E^{el}_{I}$$

Dislocations of the type $\frac{1}{2}[110]$ that lie on (111) planes may lower their energy by combining among themselves or by splitting into several new dislocations.

Two dislocations on the same (111) plane. $\pm\vec{b}_1, \pm\vec{b}_2, \pm\vec{b}_3$

$\vec{b}_1 = \frac{1}{2}[01\bar{1}]$

$\vec{b}_2 = \frac{1}{2}[\bar{1}01]$

$\vec{b}_3 = \frac{1}{2}[\bar{1}10]$

$$\vec{b}_1 + \vec{b}_2 = \tfrac{1}{2}[01\bar{1}] + \tfrac{1}{2}[\bar{1}01] \rightarrow \tfrac{1}{2}[\bar{1}10] = \vec{b}_3$$

$$\vec{b}_1 - \vec{b}_2 = \tfrac{1}{2}[01\bar{1}] - \tfrac{1}{2}[\bar{1}01] = \tfrac{1}{2}[11\bar{2}]$$

first reaction is favoured, total energy is halved.

second reaction disallowed.

Two dislocations on different (111) planes

(111) and $(11\bar{1})$ plane.

The two dislocations can combine at the intersection found by taking cross product. $\vec{i}+\vec{j}+\vec{k}$ and $\vec{i}+\vec{j}-\vec{k}$. Intersection runs parallel to $[\bar{1}10]$.

(111) $\pm\vec{b}_1 = \pm\frac{1}{2}[01\bar{1}]$, $\pm\vec{b}_2 = \pm\frac{1}{2}[\bar{1}01]$, $\pm\vec{b}_3 = \pm\frac{1}{2}[\bar{1}10]$

$(11\bar{1})$ $\pm\vec{b}_4 = \pm\frac{1}{2}[\bar{1}10]$, $\pm\vec{b}_5 = \pm\frac{1}{2}[101]$, $\pm\vec{b}_6 = \pm\frac{1}{2}[011]$

$\vec{b}_3$ and $\vec{b}_4$ parallel to the intersection of $(111)/(11\bar{1})$ planes. If these dislocations have $\vec{b}$'s of opposite sign they will annihilate each other upon combination. If the dislocations are of similar sign, their combination would result in an increase of the total energy. Mutual repulsion will therefore take place.

The only other combination that lead to lowering of $E^{el}_{tot} = \vec{b_1} + \vec{b_5}$

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

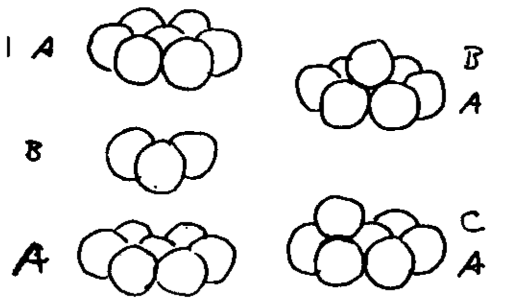
when they meet, the resulting dislocation is pure edge: dislocation line parallel to the intersection $(111)/(11\bar{1})$: $[\bar{1}10]$

$\Rightarrow$ slipplane $\stackrel{?}{=}$ (001) plane.

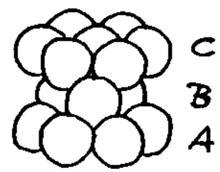
Since (001) plane is not a usual slip plane, the new dislocation is immobile. It would serve as a barrier to other dislocations and is called "Lomer lock".

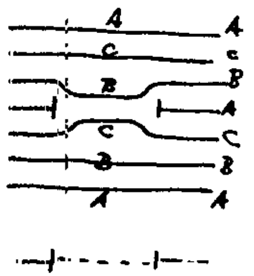
In order to obtain further reduction to E^{el} through dislocation reactions, it is necessary to consider imperfect dislocations.

Frank sessile dislocations.

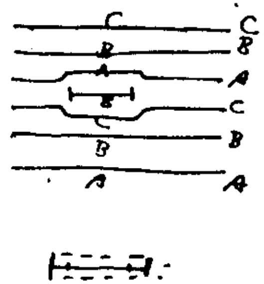


h.c.p.: ABABABA   f.c.c.: ABCABCABC





single stacking fault
S-Fault on (111)



D- Frank stacking fault

ABC/BC.A
intrinsic

ABC/B/ABC
extrinsic

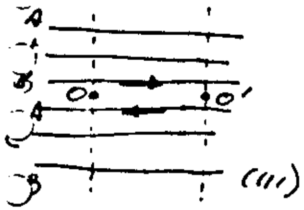
$\vec{b} = \frac{1}{3}[111]$ Frank sessile dislocation

Imperfect dislocations are not necessarily sessile !!

Extra energy associated with the stacking fault.

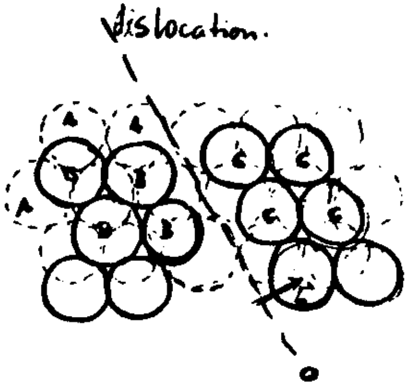
γ stacking fault energy = Cu 40 erg cm^{-2}
Ni 150 erg cm^{-2}

Shockley partial dislocation.



$\Longrightarrow$

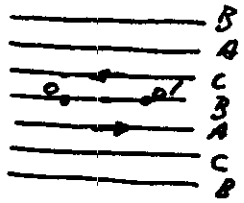
shift all atoms in the upper section relative to those in lower section, parallel to (111) planes in such a direction that the atoms on the lowest plane of the upper section $B \to C$

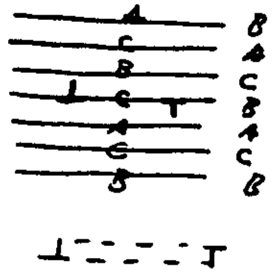


Dislocation line at O lies along $[1\bar{1}0]$ direction. Its Burgers vector points into a $[11\bar{2}]$ direction: $\vec{b} = \frac{1}{6}a[11\bar{2}]$

Shockley partial dislocation.
lying in a (111) plane $\Rightarrow$ mobile !

Between OO' the stacking sequence becomes:
ABCA/CAB
S – Shockley stacking fault.



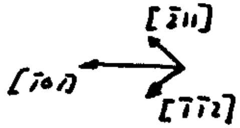


D – Shockley

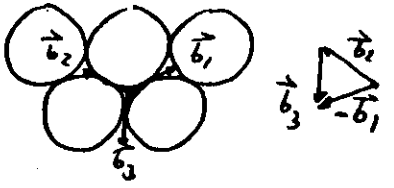
Reactions involving perfect and imperfect dislocations.

$\frac{1}{2}a^2$ $\qquad$ $\frac{1}{3}a^2$

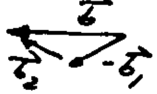
$$\frac{a}{2}[\bar{1}01] \to \frac{a}{6}[\bar{2}11] + \frac{a}{6}[\bar{1}\bar{1}2]$$
on (111)



By Frank's rule this dissociation is favored.



$\vec{b}_2 + \vec{b}_3 = -\vec{b}_1$



The force between the partial dislocations is repulsive. $-\vec{b}_1$ and $\vec{b}_2$ almost in the same direction. Thus qualitatively the two dislocations experience the same mutual force as would two parallel dislocations of the same sign.

$\overset{\vec{b}}{\perp} \longrightarrow \qquad \overset{\vec{b}_2}{\perp} \cdots\cdots \overset{-\vec{b}_1}{\perp}$

Because of the interaction between them the two Shockley dislocations tend to move as far as apart as possible. However, the wider the separation the greater is the total stacking fault energy. An equilibrium spacing is achieved.

A perfect dislocation also can split up into a Frank dislocation and a Shockley dislocation:

$$\frac{a}{2}[01\bar{1}] \rightarrow \frac{a}{6}[\bar{2}1\bar{1}] + \frac{a}{3}[11\bar{1}]$$

This reaction neither increases nor diminishes the self energy of the dislocations.

Stair-rod dislocations

Various combinations between two Shockley dislocations on different slip planes: (111) (11$\bar{1}$) since there are 6 possible $\vec{b}_i$ of each dislocation the Burgers vector of the resultant dislocation may possess any of 36 values. Of the 36 combinations 18 result in a reduction of energy. There are four distinct types of reactions among this favored set:

$$\frac{a}{6}[11\bar{2}] + \frac{a}{6}[112] \rightarrow \frac{a}{3}[110]$$

$$\frac{a}{6}[11\bar{2}] + \frac{a}{6}[\bar{1}21] \rightarrow \frac{a}{6}[03\bar{1}]$$

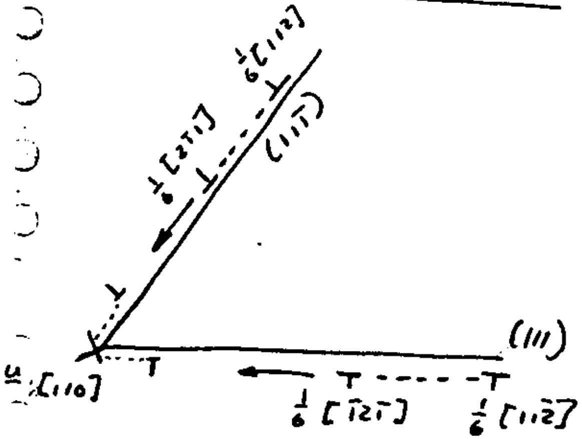
$$\frac{a}{6}[1\bar{2}1] + \frac{a}{6}[\bar{1}21] \rightarrow \frac{a}{3}[001]$$

$$\underset{\uparrow\ (111)}{\frac{a}{6}[1\bar{2}1]} + \underset{\uparrow\ (11\bar{1})}{\frac{a}{6}[\bar{2}1\bar{1}]} \rightarrow \underset{\uparrow\ \text{sessile}}{\frac{a}{6}[\bar{1}\bar{1}0]}$$

(intersection [$\bar{1}$10])

The resultant reactions are called "stair rod dislocations". (A stair-rod is a shaft used to force a rug on a stairway to fit tightly against the intersection of the top of a step and the adjacent riser). A stair rod dislocation can exist only at a bend in a stacking fault

The Cottrell-Lomer Lock



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

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

$\Longrightarrow$ stair-rod:

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

$$E_{tot} = E_{stair\text{-}rod} + 2E_{partial} < E_{Lomer\text{-}lock}$$

1/  → Cottrell-Lomer Lock.

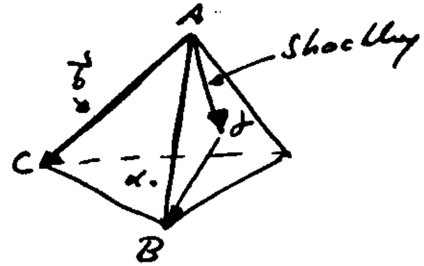
2/ or: Lomer lock created first (two perfect)

$$\frac{a}{2}[110] \rightleftarrows \frac{a}{6}[110] + \frac{a}{6}[112] + \frac{a}{6}[11\bar{2}]$$

Thompson's tetrahedron.

This is a convenient notation for describing all the important dislocations and dislocation reactions in f.c.c. metals.

The 4 different sets of {111} planes lie parallel to the four faces of a regular tetrahedron. The edges of the tetrahedron are parallel to the <110> slip directions. The corners are denoted by A, B, C, D and the mid-points of the opposite faces by $\alpha, \beta, \gamma, \delta$. The Burgers vectors of dislocations are specified by their two end points on the tetrahedron.



$$\vec{AB} = \vec{A\delta} + \vec{\delta B}$$

$$\frac{1}{2}\langle 110\rangle \rightarrow \frac{1}{6}\langle 11\bar{2}\rangle + \frac{a}{6}\langle 112\rangle$$

$$A\alpha = \frac{1}{3}\langle 111\rangle$$

stacking fault tetrahedra

In quenched metals: A platelet of vacancies collapses to form a Frank loop, the stacking fault will be stable if the fault energy is sufficiently low. The Frank partial may dissociate into a stair-rod dislocation and a Shockley partial:

$$\frac{1}{3}[111] \rightarrow \frac{1}{6}[101] + \frac{1}{6}[121]$$

$$b^2 \rightarrow \frac{1}{3} \rightarrow \frac{1}{18} + \frac{1}{6}$$

thompson notation:

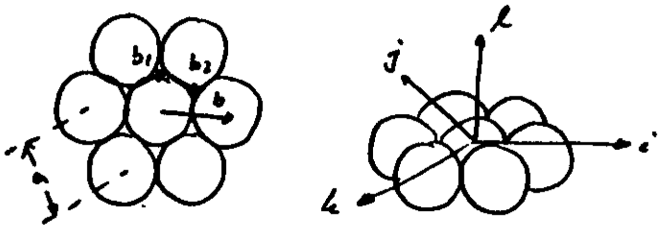
$$\vec{\alpha A} \rightarrow \vec{\alpha\beta} + \vec{\beta A} \quad \text{on } ACD$$
$$\vec{\alpha A} \rightarrow \vec{\alpha\gamma} + \vec{\gamma A} \quad \text{on } ABD$$
$$\vec{\alpha A} \rightarrow \vec{\alpha\delta} + \vec{\delta A} \quad \text{on } ABC$$

The partials $\vec{\beta A}$, $\vec{\gamma A}$, $\vec{\delta A}$ will be repelled by the stair rod dislocations $\vec{\alpha\beta}$, $\vec{\alpha\gamma}$, $\vec{\alpha\delta}$.
Taking into account the dislocation line sense, the partials attract each other in pairs to form stair rods along DA, BA and CA:

$$\vec{\beta A} + \vec{A\gamma} \rightarrow \vec{\beta\gamma} \quad \text{along } DA$$
$$\vec{\gamma A} + \vec{A\delta} \rightarrow \vec{\gamma\delta} \quad \text{along } BA$$
$$\vec{\delta A} + \vec{A\beta} \rightarrow \vec{\delta\beta} \quad \text{along } CA$$

6. Dislocations in other crystal structures

6.1. Hexagonal close-packed lattice

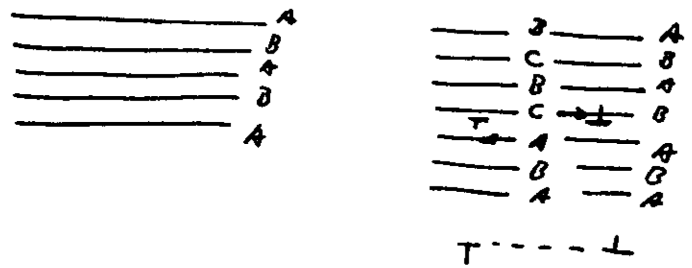


$$\vec{b} = \frac{a}{3}[2\bar{1}\bar{1}0]$$

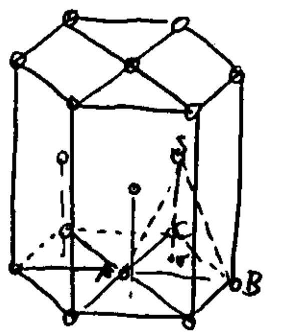
$$\frac{a}{3}[2\bar{1}\bar{1}0] \rightarrow \frac{a}{3}[10\bar{1}0] + \frac{a}{3}[1\bar{1}00]$$

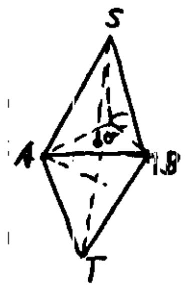
Shockley dislocations.

Only Shockley partial dislocations with S-stacking faults occur in h.c.p. lattices.



Frank dislocation
$$\vec{b} = \frac{a}{2}[0001]$$





$$\vec{AB} \rightarrow \vec{A\sigma} + \vec{\sigma B}$$

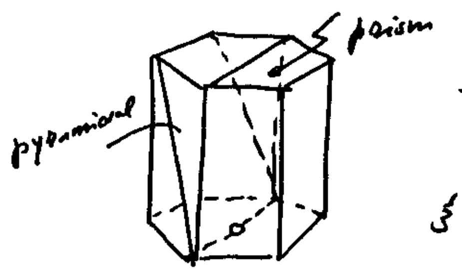
$$\tfrac{1}{3}[11\bar{2}0] \rightarrow \tfrac{1}{3}[10\bar{1}0] + \tfrac{1}{3}[01\bar{1}0]$$

BASAL-slip

$\frac{1}{3}\langle 11\bar{2}0\rangle(0001)$ in Be, Mg, Cd, Zn similar to

$\frac{1}{2}\langle 110\rangle\{111\}$ slip in f.c.c.

PRISM / PYRAMIDAL



$\frac{1}{3}\langle 11\bar{2}0\rangle\{1\bar{1}00\}$ prism slip.

Ti, Zr:

$\frac{1}{3}\langle 11\bar{2}0\rangle \rightarrow \frac{1}{18}[4\,2\,\bar{6}\,3\rangle$ +

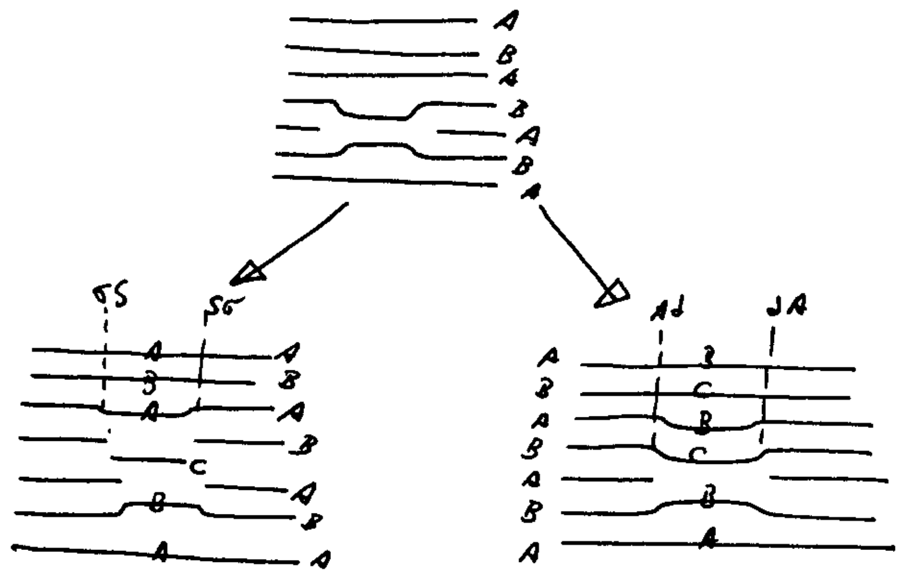
$\frac{1}{18}\langle$ [illegible] $\rangle$

$\frac{1}{3}\langle 11\bar{2}0\rangle \rightarrow \frac{1}{9}\langle 11\bar{2}0\rangle$ +

$\frac{2}{9}\langle 11\bar{2}0\rangle$

condensation of vacancies

results in two similar atomic layers coming into contact. This unstable situation of high energy is avoided in one of two ways.



one layer adjacent to the fault is changed B to C

$\sigma S + \sigma A + A\sigma \Rightarrow \sigma S$

$\frac{1}{2}[0001] + \frac{1}{3}[1\bar{1}00] + \frac{1}{3}[\bar{1}100] \rightarrow \frac{1}{2}[0001]$

two Shockley is required

high energy fault

$A\sigma + \sigma S \rightarrow AS$

$\frac{1}{3}[\bar{1}100] + \frac{1}{2}[0001] \rightarrow \frac{1}{6}[\bar{2}203]$

single Shockley required

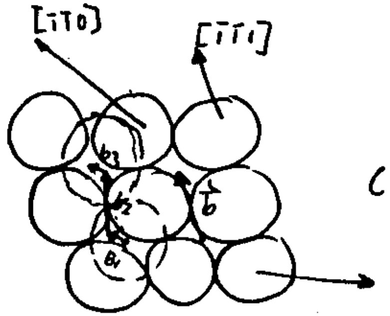
low energy fault

6.2

Body-centered Cubic crystals.

$\vec{b}_{perfect} = \frac{1}{2} a [111]$

slip planes (110)
(112)
(123)



$$\vec{b} = \vec{b}_1 + \vec{b}_2 + \vec{b}_3$$

$$\underset{\frac{3}{4}a^2}{\frac{a}{2}[\bar{1}\bar{1}1]} \rightarrow \underset{\frac{1}{32}a^2}{\frac{a}{8}[\bar{1}\bar{1}0]} + \underset{\frac{3}{8}a^2}{\frac{a}{4}[\bar{1}\bar{1}2]} + \underset{\frac{1}{32}a^2}{\frac{a}{8}[\bar{1}\bar{1}0]} \rightarrow \frac{14}{32}a^2$$

According to Frank's rule it is favored.
Since actual observations by electron microscope of split dislocations are a great rarity in the case of b.c.c. crystals, the stacking fault energy must be high.

Deformation twinning.

Deformation twinning is observed in all b.c.c. transition metals when they are deformed at low temperature and/or high strain rates. Twinning occurs on {112} <111> systems.

The stacking sequence of {112} planes is:
ABCDEFAB....
displacement of $\frac{1}{6}$<111> on every successive {112} plane.

A B C D E F A B ....
$\frac{1}{6}$<111> E layer and above
C D E F A B ....
$\frac{1}{6}$<111>
B C D E F A B ...
$\frac{1}{6}$<111>
A B C D E F ....

A B C D C B A

Twinned crystal

REMARK: $\frac{1}{6}[\bar{1}11]$ displaces E to C, F to D etc
different from $\frac{1}{6}[1\bar{1}\bar{1}]$: E to D.
Untwinned structure

6.3. Ionic crystals.

$\vec{b}$-vector $\frac{1}{2}\langle 110\rangle$

{111} planes contain ions with charges of the same sign. Therefore, although these planes are close packed, glide on these planes seems less favourable. The common glide planes are the electrical neutral {110} planes.

It follows that jogs carry effective charges.

Dissociation on {110} may be considered ($\frac{1}{4}\langle 110\rangle$). Dissociation on the {100} planes does not occur and is small on {111} planes.

6.4. Dislocations in Superlattices.

A_3B (Ni_3Al, Al_3Li etc)

total $\vec{b}$ vector: $\langle 110\rangle$

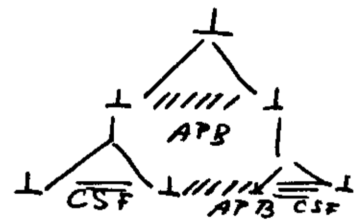
(A) split into two ordinary unit dislocations

$\langle 110\rangle \rightarrow \frac{1}{2}\langle 110\rangle + \frac{1}{2}\langle 110\rangle$

with an APB in between.

$\frac{1}{2}\langle 110\rangle \rightarrow \frac{1}{6}\langle 112\rangle + \frac{1}{6}\langle 112\rangle$

with Complex Stacking fault in between. CSF



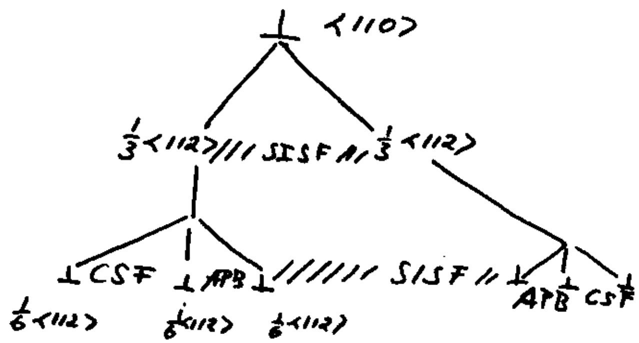
(B)

$\langle 110\rangle \longrightarrow \frac{1}{3}\langle 112\rangle + \frac{1}{3}\langle 112\rangle$

with Superlattice intrinsic stacking fault in between.

$\frac{1}{3}\langle 112\rangle \rightarrow \frac{1}{6}\langle 112\rangle + \frac{1}{6}\langle 112\rangle + \frac{1}{6}\langle 112\rangle$

with APB and CSF in between.



6.5. Dislocations in covalent crystals.

Of the many covalent crystals, the cubic structure of diamond, Si and Ge is one of the simplest and most widely studied. Dislocations in these semiconductors affect both mechanical and electrical properties.

The close-packed {111} planes have a sixfold stacking sequence:

$$A\alpha\, B\beta\, C\gamma\, A\alpha\, B\beta\, C\gamma \ldots$$

By reference to f.c.c. metals, the intrinsic fault has stacking sequence:

$$A\alpha\, B\beta\, A\alpha\, B\beta\, C\gamma$$

and the extrinsic fault:

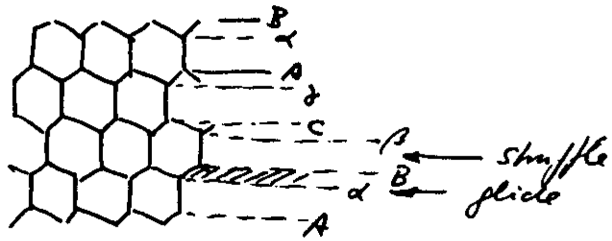
$$A\alpha\, B\beta\, A\alpha\, C\gamma\, A\alpha\, B\beta$$

Faults formed between adjacent layers of the same letter do not restore tetrahedral bonding and have high energy.

Perfect dislocations have $\vec{b} = \frac{1}{2}\langle 110\rangle$ and slip on {111} planes. They usually lie along $\langle 110\rangle$ directions at 0° or 60° to $\vec{b}$ as a result of low core energy.

Two dislocation types may be considered: eg. between αB, or between βB

<u>glide set</u>   <u>shuffle set</u>

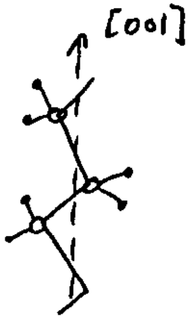


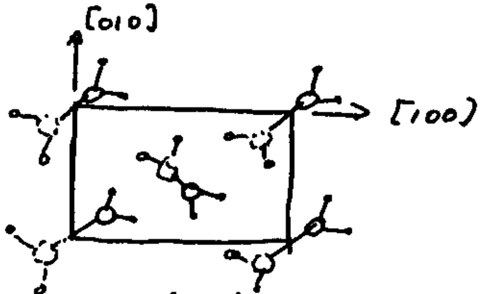
6.6. Dislocations in Polymer Crystals

The plastic deformation of crystalline and semi-crystalline polymers involves the mechanisms well-established for other crystalline solids, dislocation glide, deformation twinning.

consider polyethylene:

strong covalent bonding along [001]
weak van der Waals bonding along [010] [100]





(001) projection
orthorhombic phase

dislocation glide on the {100} {011} planes.