Lecture 13
Ch 10 Rubber Elasticity
+
Ch 6 Defects (vacancy) L1

F 22.08.2025

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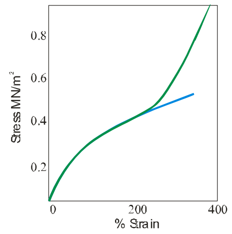
1

Elastomer

Polymers with very extensive elastic deformation



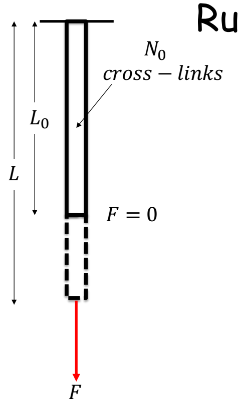
Stress-strain relationship is non-linear

$\boxed{\text{Example: Rubber}}$

2

2

Rubber Elasticity Equation



$$F = \frac{N_0 kT}{L_0}\left[\left(\frac{L}{L_0}\right) - \left(\frac{L_0}{L}\right)^2\right]$$

F applied tensile force
N_0 number of cross-links
k Boltzmann constant
T absolute temperature
L_0 initial length (without F)
L final length (with F)

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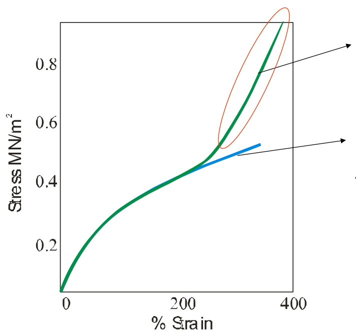
Rubber Elasticity

Bond stretching in straightened out molecules



Experimental: Matches with Theory at low extensions but deviates at high extensions

Theory: Chain uncoiling

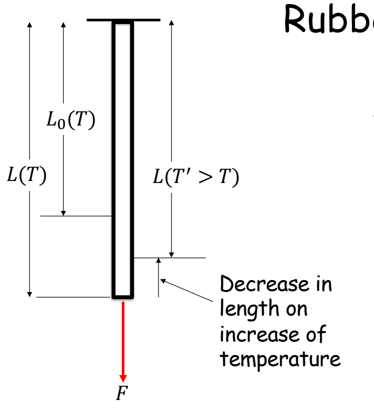
$$F = \frac{N_0 kT}{L_0}\left[\left(\frac{L}{L_0}\right) - \left(\frac{L_0}{L}\right)^2\right]$$

Good at low extensions

4

4

Rubber Elasticity Equation



$$F = \frac{N_0 kT}{L_0}\left[\left(\frac{L}{L_0}\right) - \left(\frac{L_0}{L}\right)^2\right]$$

At constant F

$T \uparrow \Rightarrow L \downarrow$

5

5

Elastomers have -ve thermal expansion coefficient, i.e., they CONTRACT on heating!!

EXPERIMENT 8

Section 10.3 of the textbook

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6

Crystal Defects

Chapter 6

7

Crystal = Lattice + Motif

Is a lattice finite or infinite?

Is a lattice finite or infinite?

Abrupt ending of crystal at free surface

Free surface of a crystal is a defect

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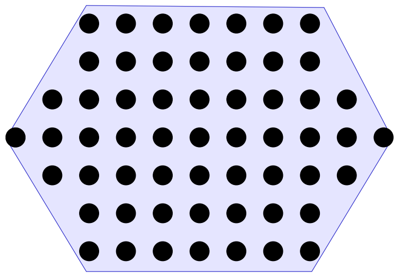
Free surface: a 2D defect



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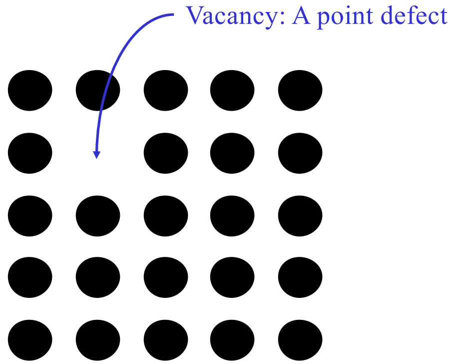

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Defects	*Dimensionality*	*Examples*
Point	0	Vacancy
Line	1	Dislocation
Surface	2	Free surface, Grain boundary Stacking Fault

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Point Defects

Vacancy

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Point Defects: vacancy

A Guess

There *may* be some vacant sites in a crystal

Surprising Fact

There ***must*** be a certain fraction of vacant sites in a crystal in ***equilibrium.***

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Equilibrium?

Equilibrium means Minimum Gibbs free energy G at constant T and P

A crystal with vacancies has a lower free energy G than a perfect crystal

What is the equilibrium concentration of vacancies?

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Gibbs Free Energy G ?

$G = H - T\,S$ — T Absolute temperature

H ?

1. Enthalpy $H = E + PV$ — E internal energy, P pressure, V volume

2. Entropy $S = k \ln W$ — k Boltzmann constant, W number of microstates

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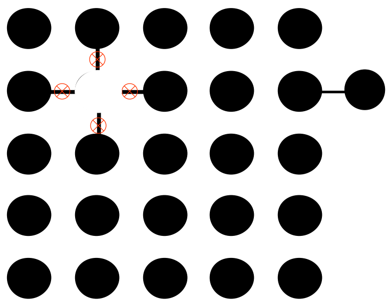
Vacancy increases H of the crystal due to energy required to break bonds



$$\Delta H = n\Delta H_f$$

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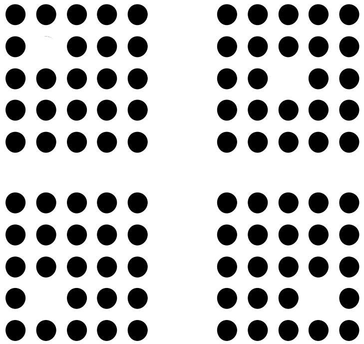
Vacancy increases S of the crystal due to configurational entropy



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Configurational entropy due to vacancy

Number of atoms: N

Number of vacacies: n

Total number of sites: $N+n$

The number of microstates:

$$W = {}^{N+n}C_n = \frac{(N+n)!}{n!\,N!}$$

Increase in entropy S due to vacancies:

$$\Delta S = k \ln W = k \ln \frac{(N+n)!}{n!\,N!}$$
$$= k[\ln(N+n)! - \ln n! - \ln N!]$$

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Stirlings Approximation

$$\ln N! \approx N \ln N - N$$

N	$\ln N!$	$N \ln N - N$
1	0	-1
10	15.10	13.03
100	363.74	360.51

100!=93326215443944152681699238856266700490715968264381621468 5\
92963895217599993229915608941463976156518286253697920 82\
722375825118521091686400000000000000000000000000

19

$$\Delta S = k \ln W = k[\ln(N+n)! - \ln n! - \ln N!]$$

$$\ln N! \approx N \ln N - N$$

$$\Delta S = k[(N+n)\ln(N+n) - n \ln n - N \ln N]$$

$$\Delta H = n\,\Delta H_f$$

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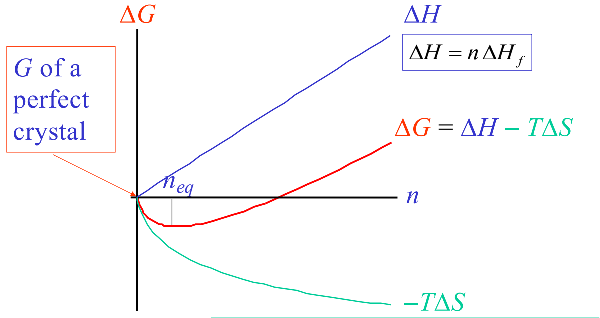
Change in G of a crystal due to vacancy



$$\Delta S = k[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

Fig. 6.4

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Equilibrium concentration of vacancy

$$\Delta S = k[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

$$\Delta H = n\,\Delta H_f$$

$$\Delta G = n\Delta H_f - Tk[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

$$\left.\frac{\partial \Delta G}{\partial n}\right|_{n=n_{eq}} = 0$$

$$\boxed{\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)}$$

With $n_{eq} << N$

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$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$

Al: $\Delta H_f = 0.70$ ev/vacancy
Ni: $\Delta H_f = 1.74$ ev/vacancy

n/N	0 K	300 K	900 K
Al	0	$1.45\text{x}10^{-12}$	$1.12\text{x}10^{-4}$
Ni	0	$5.59\text{x}10^{-30}$	$1.78\text{x}10^{-10}$

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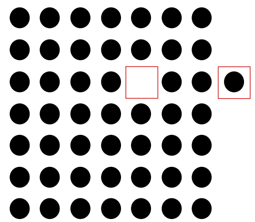
Contribution of vacancy to thermal expansion

Increase in vacancy concentration increases the volume of a crystal



A vacancy adds a volume equal to the volume associated with an atom to the volume of the crystal

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Contribution of vacancy to thermal expansion

Thus vacancy makes a small contribution to the thermal expansion of a crystal

Thermal expansion =

lattice parameter expansion

+

Increase in volume due to vacancy

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Contribution of vacancy to thermal expansion

$V = Nv$

$\Delta V = N\,\Delta v + V\,\Delta N$

V=volume of crystal
v= volume associated with one atom
N=no. of sites (atoms+vacancy)

$$\frac{\Delta V}{V} = \frac{\Delta v}{v} + \frac{\Delta N}{N}$$

Total expansion — Lattice parameter increase — vacancy

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Experimental determination of n/N

$$\frac{\Delta V}{V} = \frac{\Delta v}{v} + \frac{\Delta N}{N}$$

$$\frac{3\Delta L}{L} = \frac{3\Delta a}{a} + \frac{n}{N}$$

$$\frac{n}{N} = 3\left(\frac{\Delta L}{L} - \frac{\Delta a}{a}\right)$$

Problem 6.2

Linear thermal expansion coefficient

Lattice parameter as a function of temperature

XRD

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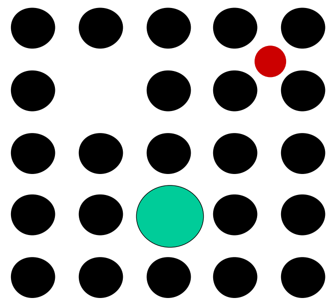
Point Defects



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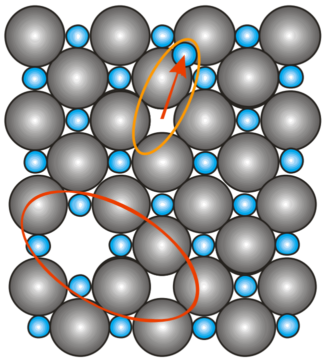
Defects in ionic solids



Frenkel defect

Cation vacancy
+
cation interstitial

Schottky defect

Cation vacancy
+
anion vacancy

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Atomic

or

statistical

interpretation of entropy

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Boltzmann's Tomb

Central Cemetery, Vienna, Austria

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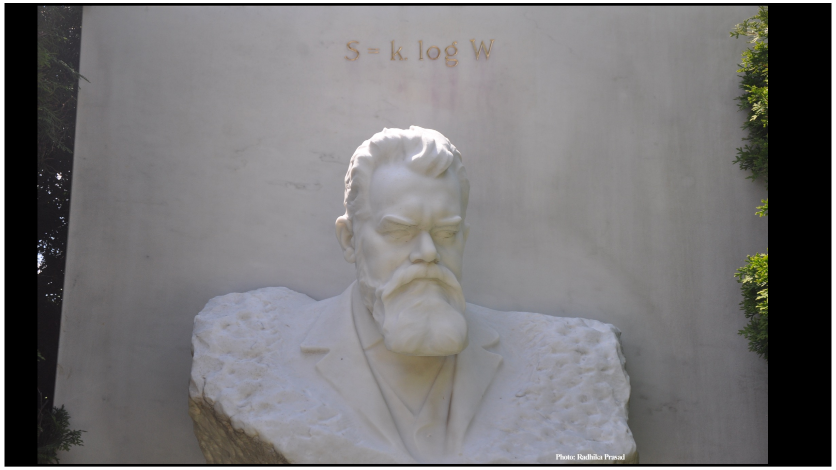

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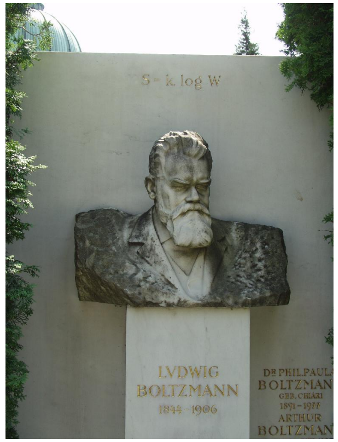
Boltzmann's Epitaph

$$S = k \ln W \quad (2.5)$$

W is the number of microstates corresponding to a given macrostate



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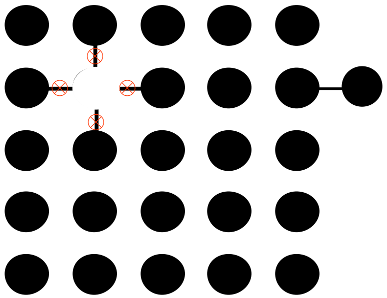
Vacancy increases H of the crystal due to energy required to break bonds



$$\Delta H = n\Delta H_f$$

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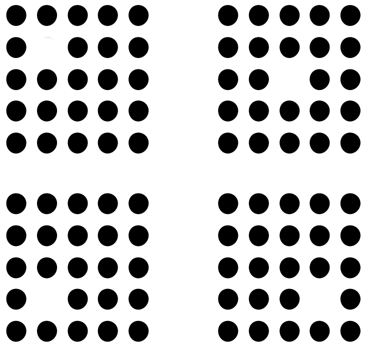
Vacancy increases S of the crystal due to configurational entropy



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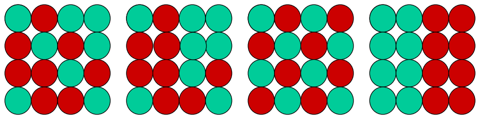
$$W = {}^{N}C_n = \frac{N!}{n!(N-n)!} \qquad (2.9)$$



***N*=16, *n*=8, *W*=12,870**

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Configurational entropy due to vacancy

Number of atoms: N

Number of vacacies: n

Total number of sites: $N+n$

The number of microstates:

$$W = {}^{N+n}C_n = \frac{(N+n)!}{n!N!}$$

Increase in entropy S due to vacancies:

$$\Delta S = k \ln W = k \ln \frac{(N+n)!}{n!N!}$$
$$= k[\ln(N+n)! - \ln n! - \ln N!]$$

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Stirlings Approximation

$$\ln N! \approx N \ln N - N$$

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$$\Delta S = k \ln W = k[\ln(N+n)! - \ln n! - \ln N!]$$

$$\ln N! \approx N \ln N - N$$

$$\Delta S = k[(N+n)\ln(N+n) - n \ln n - N \ln N]$$

$$\Delta H = n \Delta H_f$$

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Change in G of a crystal due to vacancy

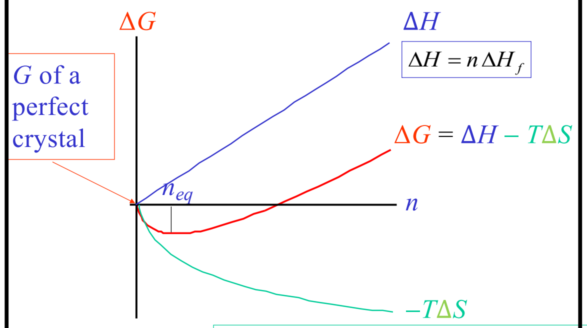

Fig. 6.4

$$\Delta S = k[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

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Equilibrium concentration of vacancy

$$\Delta S = k[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

$$\Delta H = n\,\Delta H_f$$

$$\Delta G = n\Delta H_f - Tk[(N+n)\ln(N+n) - n\ln n - N\ln N]$$

$$\left.\frac{\partial \Delta G}{\partial n}\right|_{n=n_{eq}} = 0$$

$$\boxed{\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)}$$

With $n_{eq} << N$

42

$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$

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Ni: ΔH_f= 1.74 ev/vacancy

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Ni	0	$5.59\text{x}10^{-30}$	$1.78\text{x}10^{-10}$

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$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$ ΔH_f *per vacancy*

$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{RT}\right)$$ ΔH_f *per mole of vacancy*

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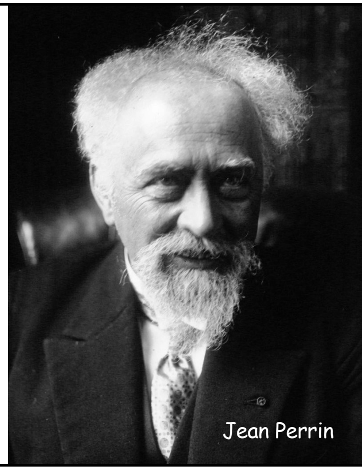

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Lecture 14

+

Ch 6 Defects L2: Dislocations

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Line Defects

Dislocations

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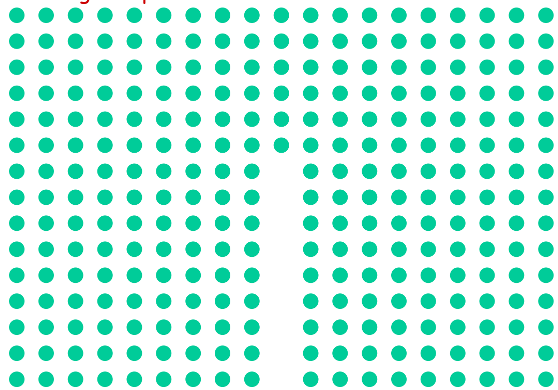
Missing half plane→ A Defect



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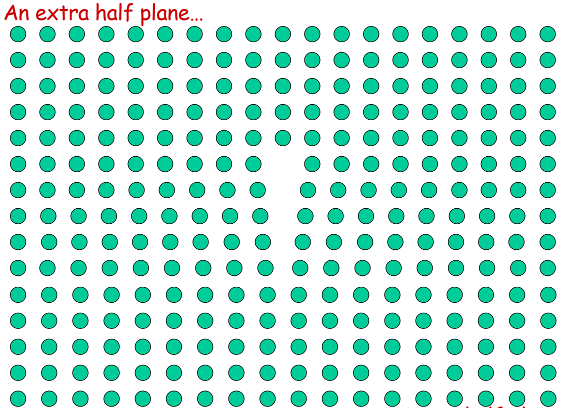
An extra half plane…



…or a missing half plane

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What kind of defect is this?

A line defect?

Or a planar defect?

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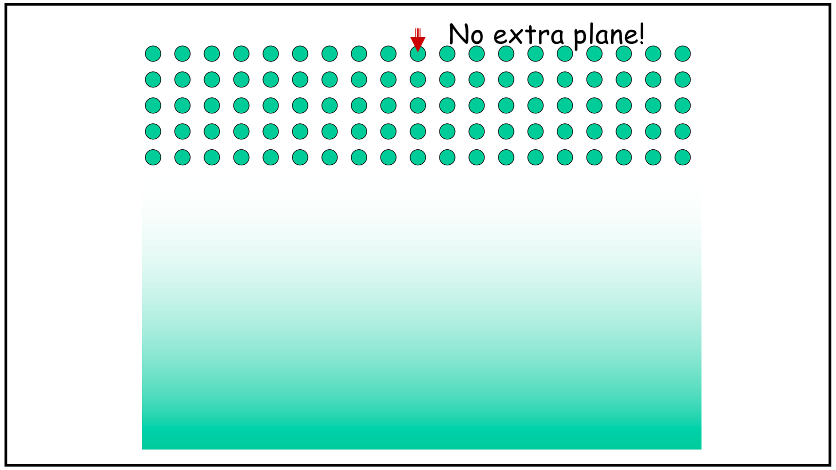
No extra plane!

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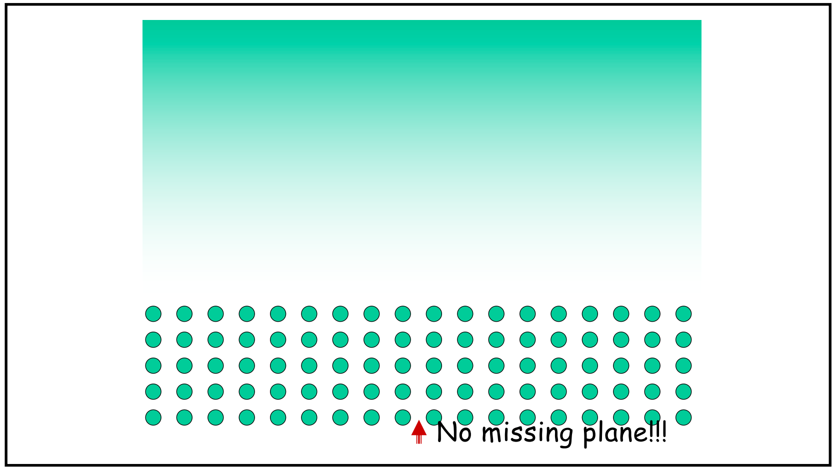
No missing plane!!!

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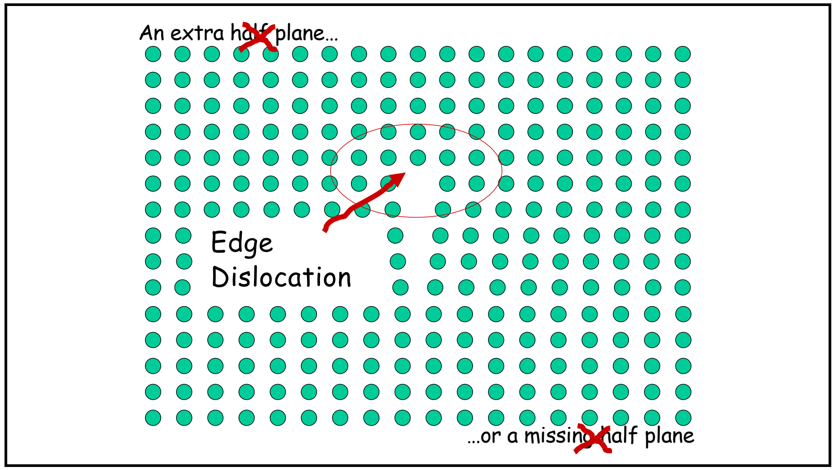
An extra half plane…
Edge
Dislocation
…or a missing half plane

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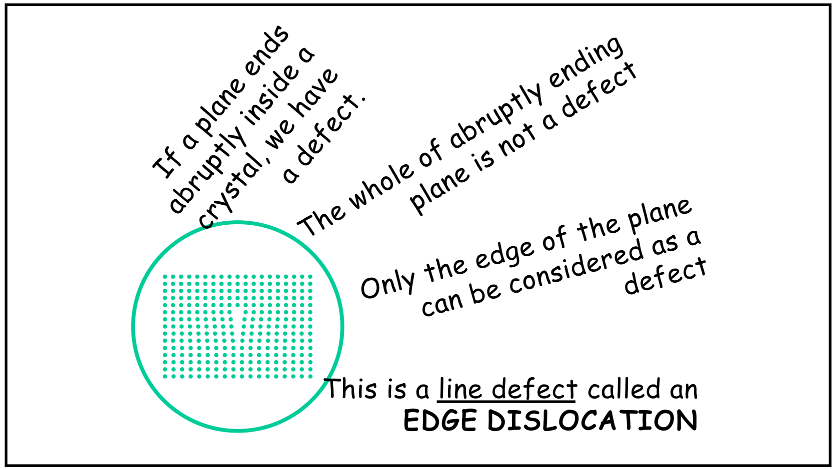
If a plane ends
abruptly inside a
crystal, we have
a defect.
The whole of abruptly ending
plane is not a defect
Only the edge of the plane
can be considered as a
defect
This is a line defect called an
EDGE DISLOCATION

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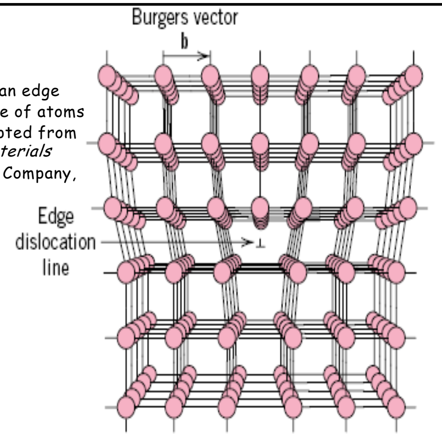
Callister FIGURE 4.3

The atom positions around an edge dislocation; extra half-plane of atoms shown in perspective. (Adapted from A. G. Guy, *Essentials of Materials Science*, McGraw-Hill Book Company, New York, 1976, p. 153.)



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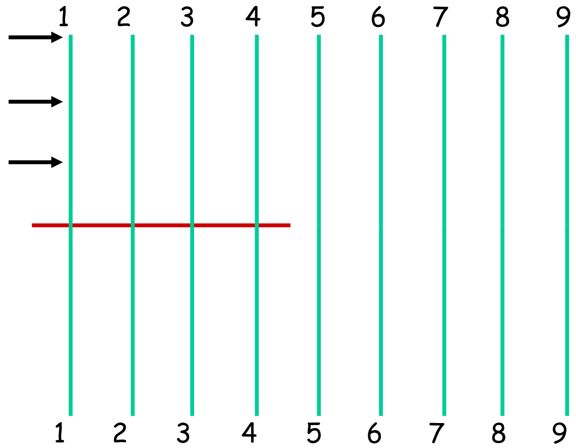

Disloca-tion as boundary between slip and no slip regions of a slip plane

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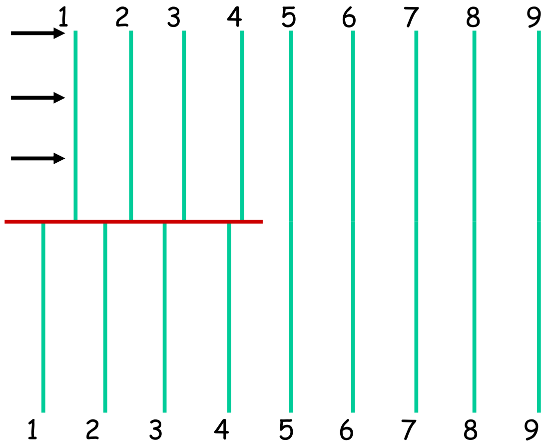

Disloca-tion as boundary between slip and no slip regions of a slip plane

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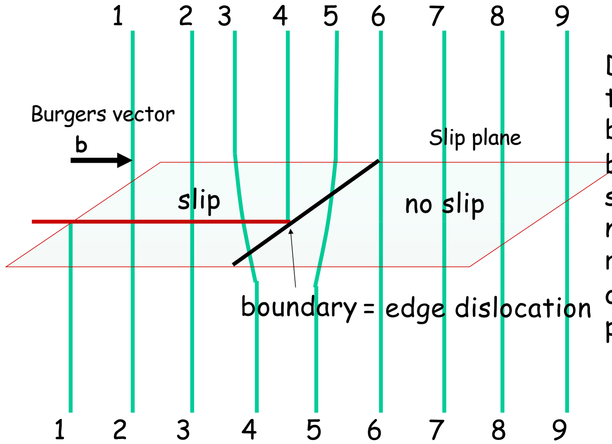
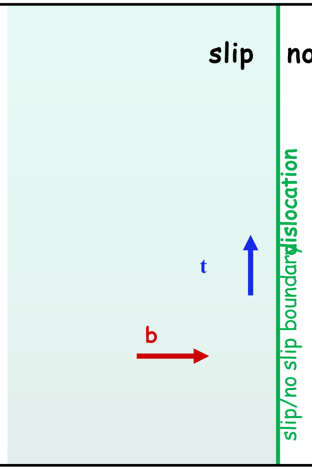


Disloca-tion as boundary between slip and no slip regions of a slip plane

60



Slip plane

Dislocation as boundary between slip and no slip regions of a slip plane

Dislocation: slip/no slip boundary

b: Burgers vector: magnitude and direction of the slip

t: unit vector tangent to the dislocation line

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Dislocation Line:
A dislocation line is the boundary between slip and no slip regions of a crystal

Burgers vector:
The magnitude and the direction of the slip is represented by a vector **b** called the Burgers vector,

Line vector
A unit vector **t** tangent to the dislocation line is called a tangent vector or the line vector.

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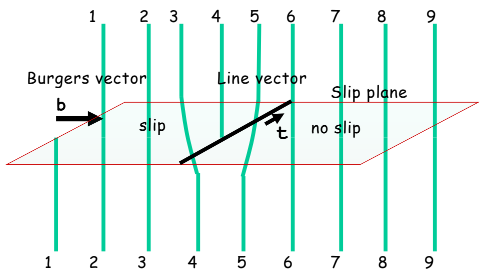
Two ways to describe an EDGE DISLOCATION

1. Bottom edge of an extra half plane
2. Boundary between slip and no-slip regions of a slip plane



What is the relationship between the directions of b and t?

$\boxed{\mathbf{b} \perp \mathbf{t}}$

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Edge Dislocation in the shirt of a careless professor

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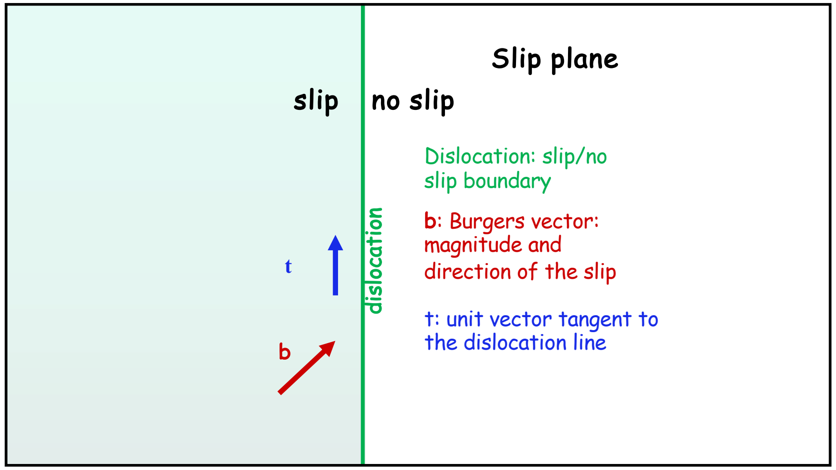

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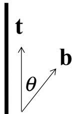

Types of dislocation based on angle between b and t

$\mathbf{b} \perp \mathbf{t}$	$\theta = 90^\circ$	Edge dislocation
$\mathbf{b} \parallel \mathbf{t}$	$\theta = 0^\circ,\ 180^\circ$	Screw dislocation
$\mathbf{b} \not\perp \mathbf{t}$	$\theta \neq 90^\circ$	Mixed dislocation
$\mathbf{b} \nparallel \mathbf{t}$	$\theta \neq 0^\circ,\ 180^\circ$	

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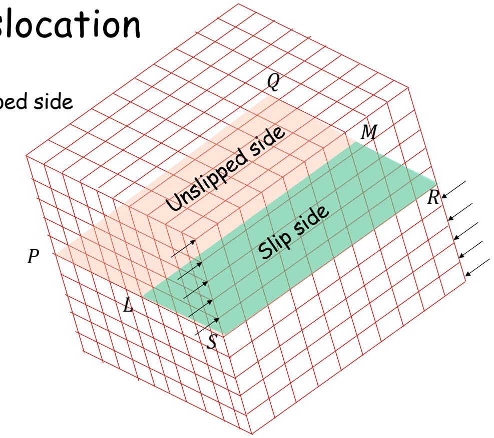
An RH screw dislocation

$PQRS$: Slip plane

$LMRS$: Slip side $LPQM$: Unslipped side



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An RH screw dislocation

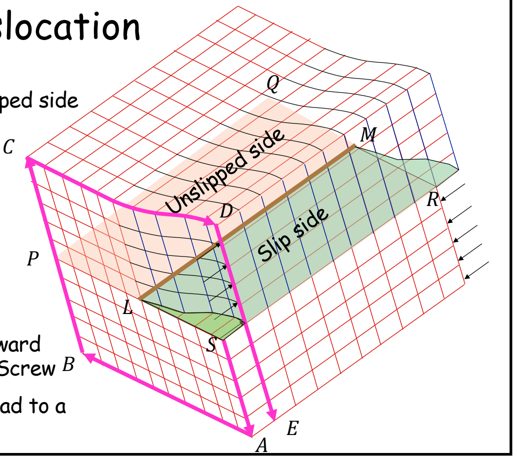
$PQRS$: Slip plane
$LMRS$: Slip side $LPQM$: Unslipped side

LM: Boundary between slipped and unslipped side
$\equiv$ *Dislocation Line*

Distinct ∥ planes ⊥ to the dislocation line have become a single helicoidal surface like that of a screw

Clockwise rotation leads to forward movement: Right-Handed (RH) Screw

Slip in opposite direction will lead to a left-handed screw.



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	Positive	Negative
Edge Dislocation	Extra half plane ***above*** the slip plane ⊥	Extra half plane ***below*** the slip plane T
Screw Dislocation	Left-handed Left-handed screw	Right-handed Right-handed screw

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Lecture 15
+
Ch 6 Defects L3: Dislocations

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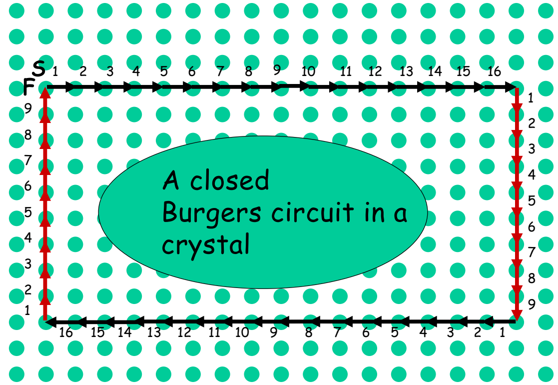
Burgers Circuit



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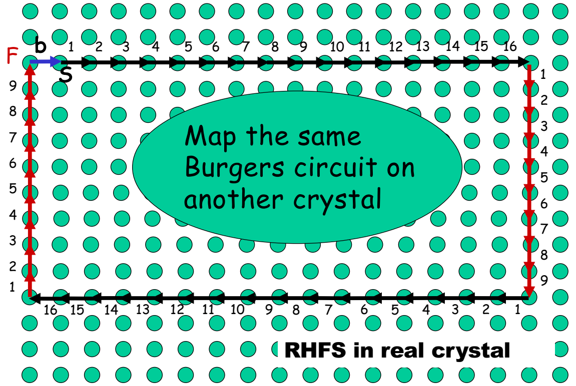
The Burgers circuit fails to close !!



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Two interpretations of Burgers Vector

Magnitude and direction of slip

Closure failure of a Burgers circuit

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Burgers vector

Johannes Martinus BURGERS

Burger's vector

Burgers vector

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Burgers Circuit and Burgers Vector

Circuit closed in an ideal crystal,

Fails to close in a real crystal

Or vice-versa

The closure failure → dislocation

Finish to Start vector → Burgers vector

Or Start to Finish

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Attendance on

https://rollcall.iitd.ac.in

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Conventions for Burgers vector

Closure failure: Real crystal or Ideal crystal

RH or LH

F->S or S->F

MLL100
RHFS Real Crystal

2x2x2=8 conventions

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$\mathbf{b}$ for an RH screw dislocation

$PQRS$: Slip plane

$LMRS$: Slip side $LPQM$: Unslipped side

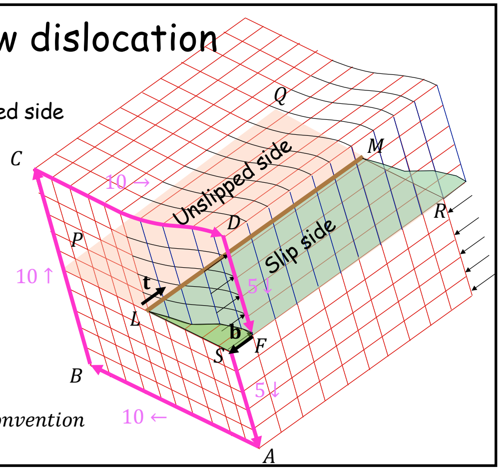
LM: Boundary between slipped and unslipped side
$\equiv$ *Dislocation Line*

$\mathbf{t}$: tangent vector

$SABCDF$: RH Burgers circuit wrt to $\mathbf{t}$

FS: Burgers Vector $\mathbf{b}$

$$\mathbf{b} = -b\mathbf{t}$$ *in our RHFS convention*



79

Two equivalent classes of $\mathbf{b}$ conventions

For RH screw dislocation

$$\mathbf{b} = -b\mathbf{t}$$

$\mathbf{b}$ antiparallel to $\mathbf{t}$

$$\mathbf{b} = b\mathbf{t}$$

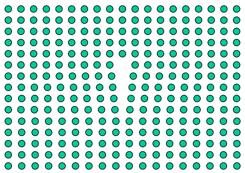
$\mathbf{b}$ parallel to $\mathbf{t}$

RHFS convetion of MLL100

80

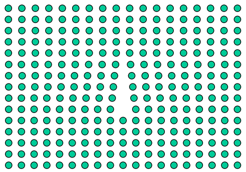
Two types of edge dislocations

$+ve$ ($\perp$) | $-ve$ ($\top$)



180°

You can rotate a $+ve$ edge dislocation to become a $-ve$ edge dislocation

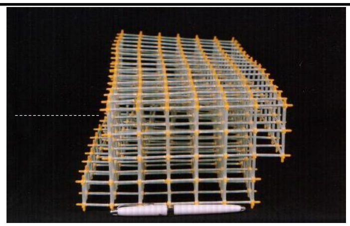


Half plane above the slip plane

Half plane below the slip plane

81

Prof. S. Ranganathan
IISc, Bangalore



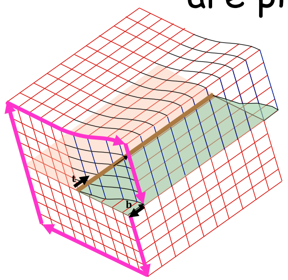
SR: Is this an RH or LH dislocation?

RP: Sir, that depends upon the way you look at it.

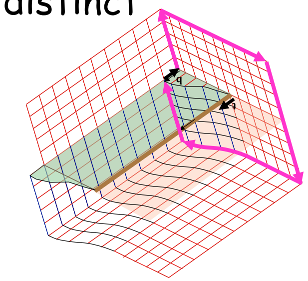
Conference on Perspectives in Physical Metallurgy and Materials Science, Indian Institute of Science, Bangalore, 12-14 July, 2001.
R. Prasad, "*Dislocation Models for Classroom Demonstrations*"

82

RH and LH Screw dislocations are physically distinct



180°



An RH screw dislocation remains RH even after any rotation

83

Positive and negative edge dislocations can be superimposed on each other by 180° rotation about the dislocation line

LH and RH screw dislocations cannot be superimposed on each other by rotation.

They can be superimposed on each other by a reflection. Hence, they are chiral pair.

84

Slip Plane

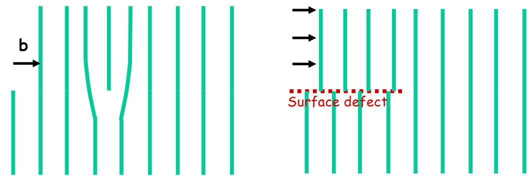
A plane containing b and t is called the slip plane of the dislocation line.

Edge dislocation: $\mathbf{b} \perp \mathbf{t} \Rightarrow$ A unique slip plane

Screw dislocation: $\mathbf{b} \parallel \mathbf{t} \Rightarrow$ Non unique slip planes: Any plane passing through both b and t is possible slip plane

85

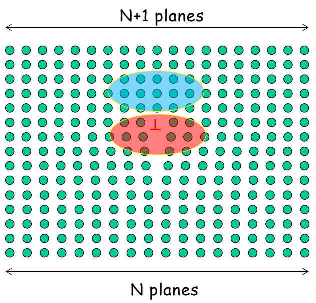
b is a lattice translation



If **b** is not a complete lattice translation then a surface defect (stacking fault) will be associated along with the line defect.

86

Elastic strain field associated with an edge dislocation



Compression

Above the slip plane

Tension

Below the slip plane

87

Line energy of a dislocation

Elastic energy per unit length of a dislocation line

$$E = \frac{1}{2}\mu b^2$$

μ	Shear modulus of the crystal
b	Length of the Burgers vector

Unit: J m^{-1}

88

b is the shortest lattice translation

Energy of a dislocation line is proportional to b^2.

$$E = \frac{1}{2}\mu b^2$$

Thus dislocations with short b are preferred.

b is a lattice translation

b is the shortest lattice translation

89

b is the shortest lattice translation

SC	$\langle 100 \rangle$
BCC	$\frac{1}{2}\langle 111 \rangle$
FCC	$\frac{1}{2}\langle 110 \rangle$
DC	$\frac{1}{2}\langle 110 \rangle$
NaCl	$\frac{1}{2}\langle 110 \rangle$
CsCl	$\langle 100 \rangle$

90

91

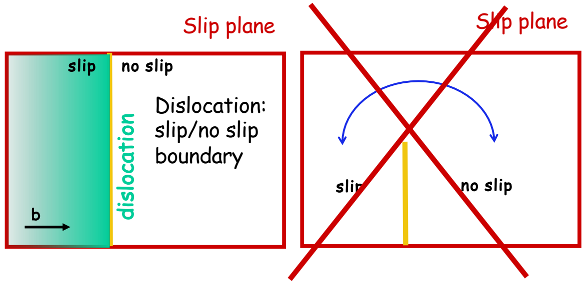
Lecture 16

Ch 6 Defects L4: Dislocations

F 29.08.2025

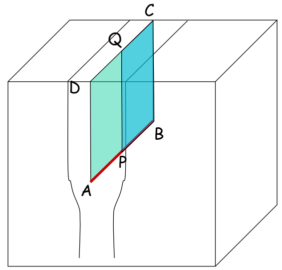
92

A dislocation line cannot end abruptly inside a crystal



93

A dislocation line cannot end abruptly inside a crystal



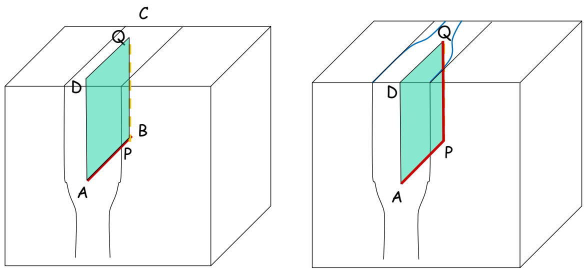
Extra half plane ABCD

Bottom edge AB of the extra half plane is the edge dislocation line

What will happen if we remove the part PBCQ of the extra half plane??

94

A dislocation line cannot end abruptly inside a crystal



Dislocation Line AB

Dislocation Line APQ

It can end on a free surface

95

Do Din me hum kya kya padhen?

Quiz 3 on Wednesday
Syllabus:

L1-L12: Up to structure of solids
Exp 1 to Exp 5

96

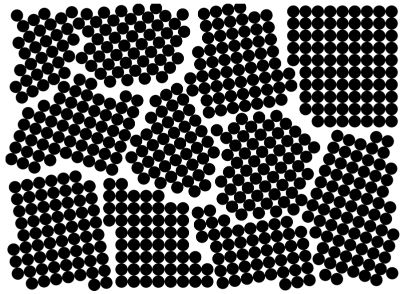
Attendance on rollcall.iitd.ac.in

97

Polycrystals

Differently oriented crystal in the same sample

Individual crystals are called grains

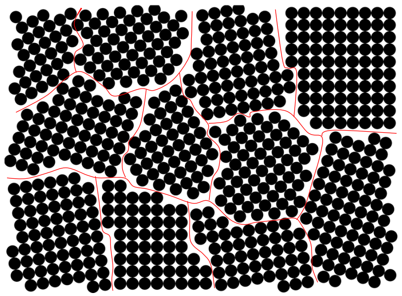


98

Grain boundary

Differently oriented crystal in the same sample

Individual crystals are called grains



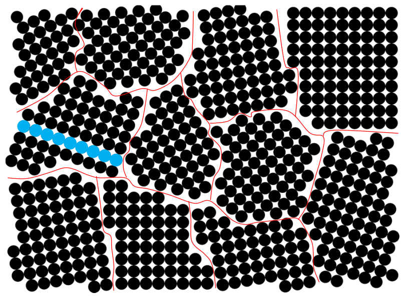
Boundary between two crystals of different orientations (i.e. grains) are called grain boundary

In 3D Grain boundaries are 2D surface defects

99

Dislocation can end on a grain boundary Grain boundary

The blue atoms are the bottom edge of an extra half plane, i.e they are along the dislocation line.

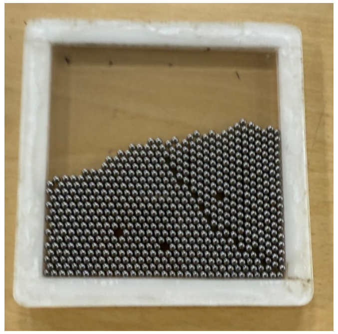


Boundary between two crystals of different orientations (i.e. grains) are called grain boundary

The dislocation line ends abruptly at a grain boundary

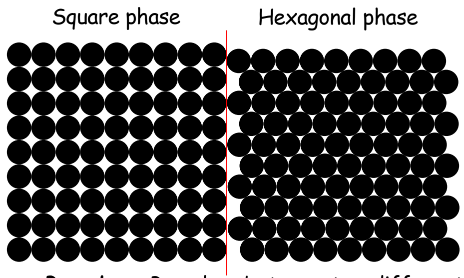
100

Play with the ball bearing models during experiment 6 to observe several defects.



101

Phase Boundary



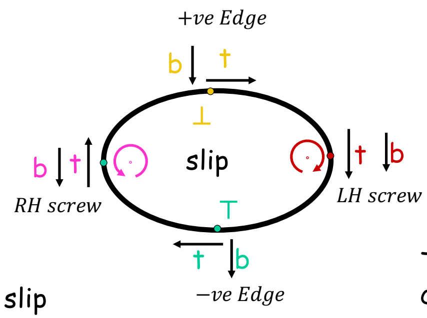
A dislocation line can end on a phase boundary

Phase Boundary: Boundary between two different phases (different crystal structures)

Grain Boundary: Boundary between two different orientations of the same phase (same crystal structure)

102

A dislocation can end on itself forming a loop



The line vector **t** is always tangent to the dislocation line with a consistent sense like a flow

No slip

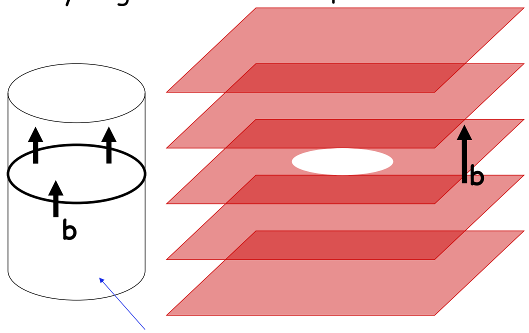
The Burgers vector **b** is constant along a dislocation line; magnitude and direction of the slip

103

Can a loop be entirely edge?

Prismatic dislocation loop

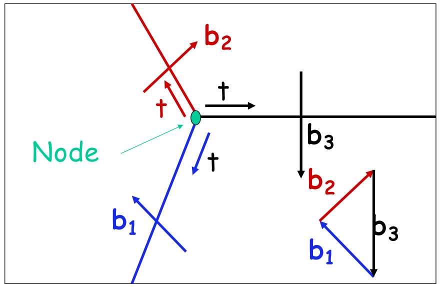
Example 6.2



Cylindrical slip plane (surface)

104

A dislocation can end on another dislocation: Node



All t vectors should either point to the node or away from the node.

$$\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = \mathbf{0}$$ Frank's Rule

105

A dislocation line cannot end abruptly inside a crystal

It can end on

- Free surfaces
- Grain boundaries or phase boundaries
- On itself forming a loop
- On other dislocations at a point called a node

106

107

Lecture 17

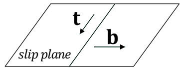
Ch 6 Defects L5: Dislocations

Sat 29.08.2025 (as F)

108

Slip plane

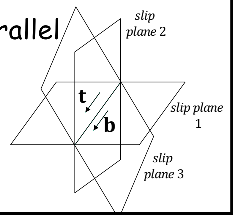
The plane containing the Burgers vector $\mathbf{b}$ and the line vector $\mathbf{t}$ is called the slip plane of a dislocation line.



An edge or a mixed dislocation having non-parallel $\mathbf{b}$ and $\mathbf{t}$ ($\mathbf{b} \neq b\mathbf{t}$) have a unique slip plane.

A screw dislocation having parallel or antiparallel $\mathbf{b}$ and $\mathbf{t}$ ($\mathbf{b} = \pm b\mathbf{t}$) does not have a unique slip plane.

Any plane passing through a screw dislocation is a possible slip plane



109

Dislocation Motion

Glide (for edge, screw or mixed)

Cross-slip (for screw only)

Climb (or edge only)

110

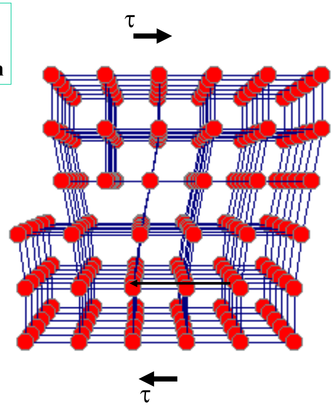
Dislocation Motion: Glide

Glide is a motion of a dislocation in its own slip plane.

All kinds of dislocations, edge, screw and mixed can glide.

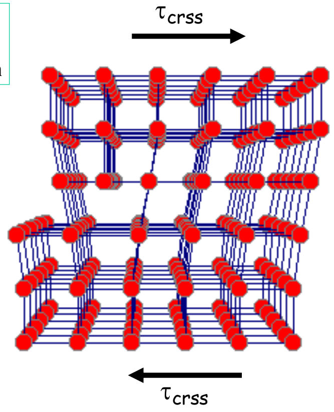
111

Glide of an Edge Dislocation



112

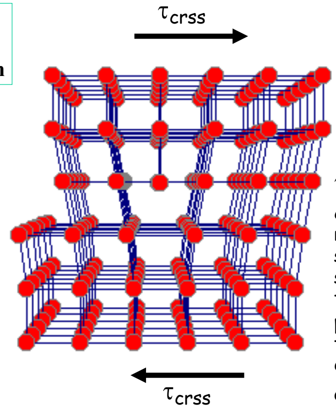
Glide of an Edge Dislocation



τ_{crss} is critical resolved shear stress on the slip plane in the direction of **b**.

113

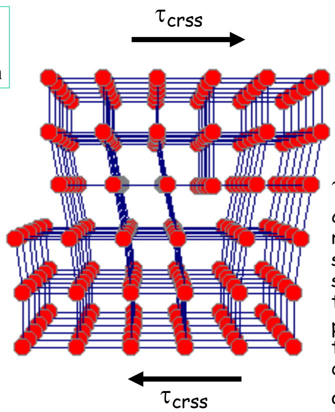
Glide of an Edge Dislocation



τ_{crss} is critical resolved shear stress on the slip plane in the direction of b.

114

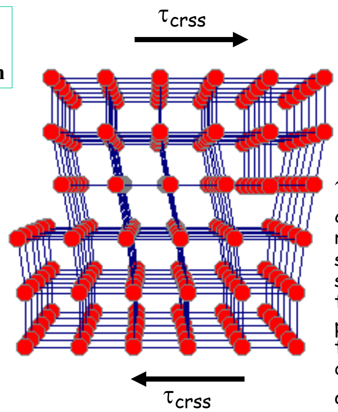
Glide of an Edge Dislocation



τ_{crss} is critical resolved shear stress on the slip plane in the direction of b.

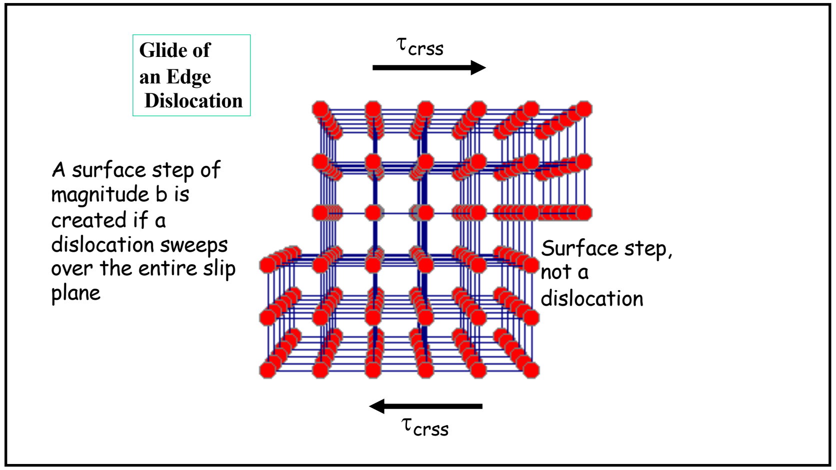
115

Glide of an Edge Dislocation

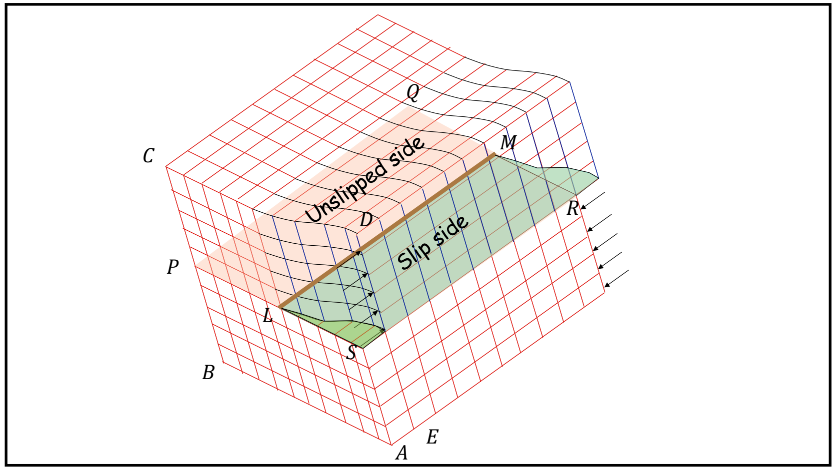


τ_{crss} is critical resolved shear stress on the slip plane in the direction of b.

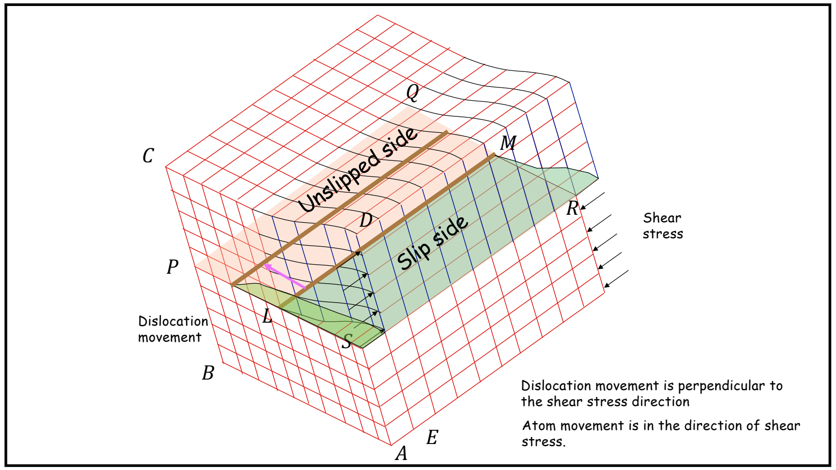
116



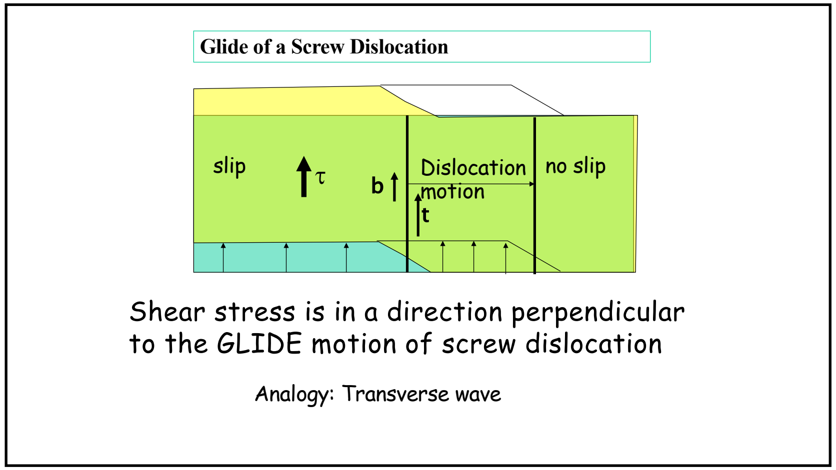
117



118



119



120

Glide Motion and the Shear Stress

For both edge and screw dislocations the glide motion is perpendicular to the dislocation line

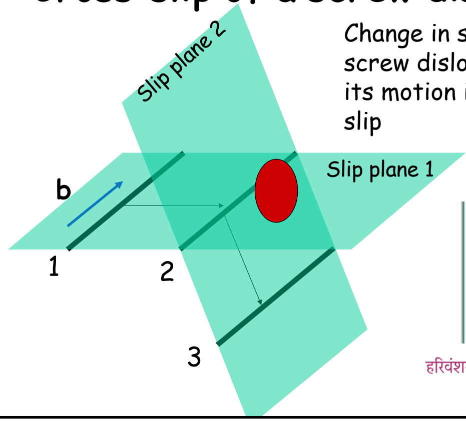
The shear stress causing the motion is in the direction of motion for edge but perpendicular to it for screw dislocation

However, for both edge and screw dislocations the shear stress is in the direction of **b** as this is the direction in which atoms move

121

Cross-slip of a screw dislocation

Change in slip plane of a screw dislocation during its motion is called cross-slip



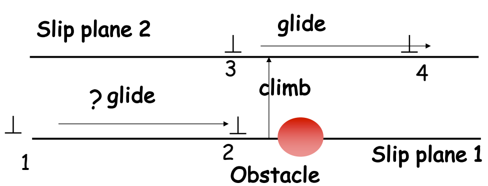
यह बुरा है या कि अच्छा
व्यर्थ दिन इस पर बिताना
अब असंभव छोड़ यह पथ
दूसरे पर पग बढ़ाना

हरिवंशराय बच्चन | पथ की पहचान

122

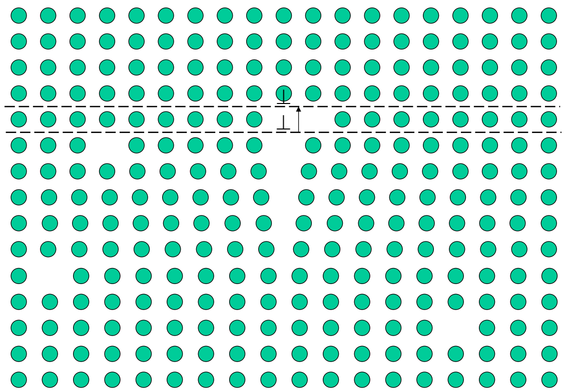
Climb of an edge dislocation

The motion of an edge dislocation from its slip plane to an adjacent parallel slip plane is called **CLIMB**



123

Atomistic mechanism of climb



124

Climb of an edge dislocation

Climb up	Climb down
Half plane shrinks	Half plane stretches
Atoms move away from the edge to nearby vacancies	Atoms move toward the edge from nearby lattice sites
Vacancy concentration goes down	Vacancy concentration goes up

125

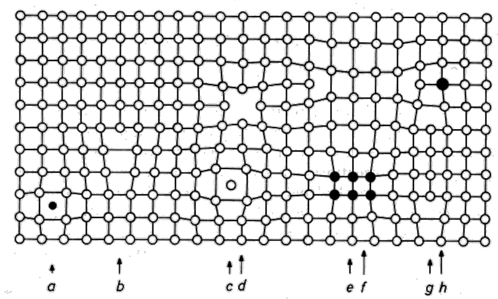
Dislocations in a real crystal can form complex networks

FIGURE 4.6 A transmission electron micrograph of a titanium alloy in which the dark lines are dislocations. 51,450×. (Courtesy of M. R. Plichta, Michigan Technological University.)

From Callister

126

A nice diagram showing a variety of crystal defects



http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html

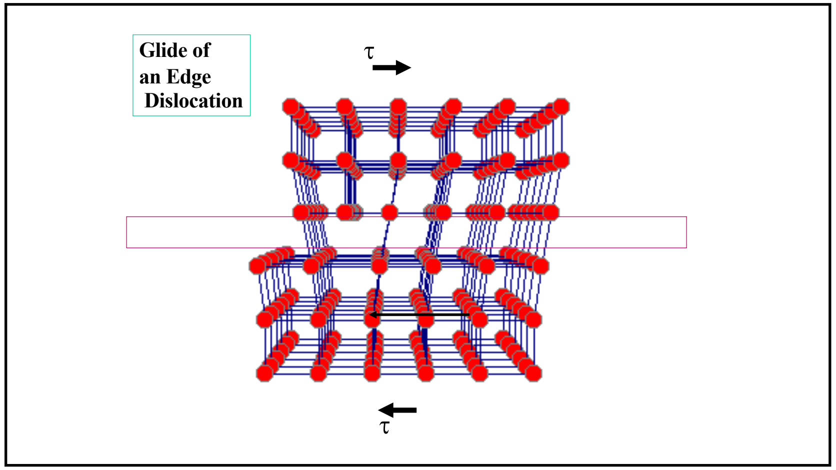
127

Dislocation Motion: Glide

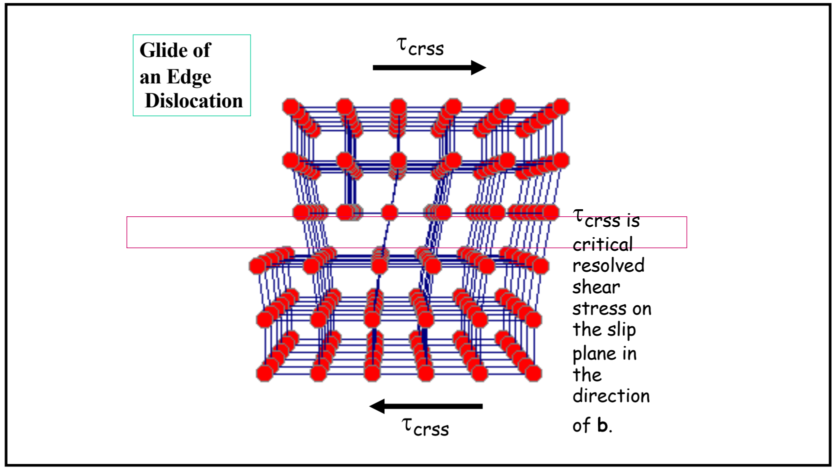
Glide is a motion of a dislocation in its own slip plane.

All kinds of dislocations, edge, screw and mixed can glide.

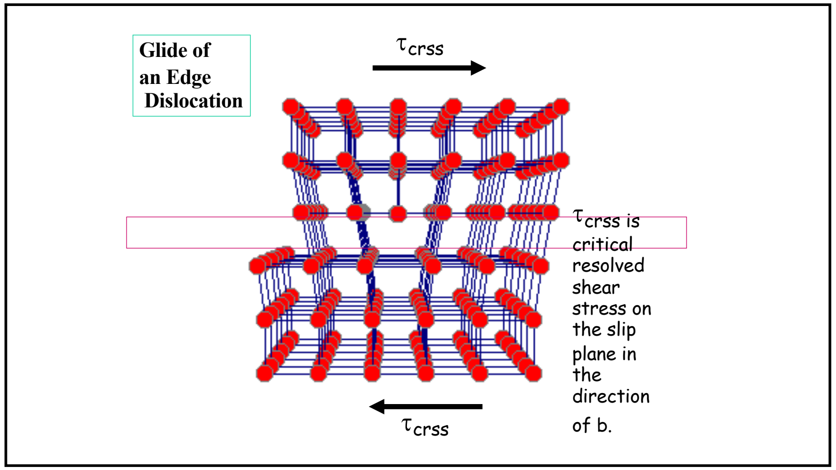
128



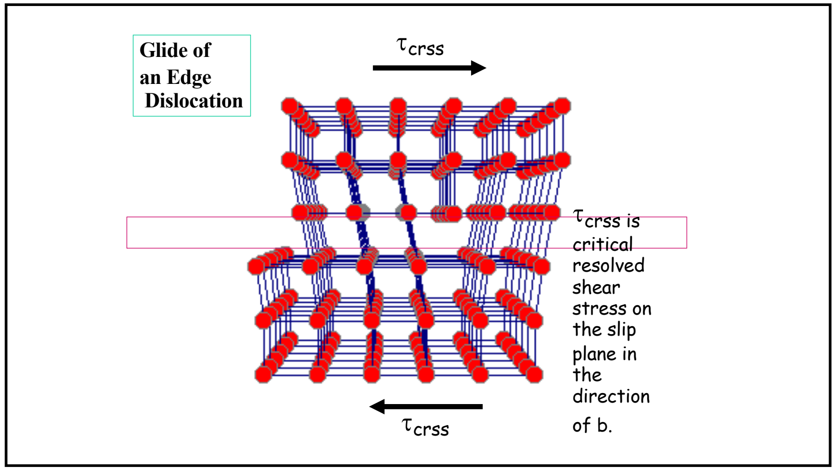
129



130

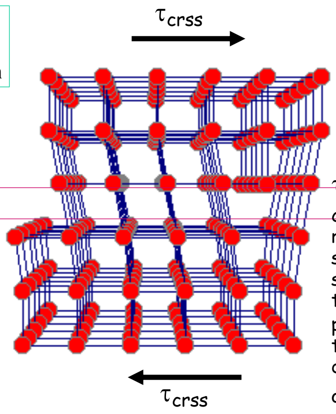


131



132

Glide of an Edge Dislocation

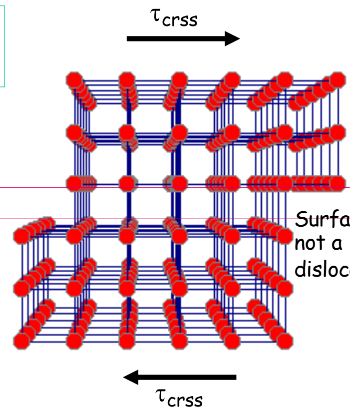


τ_{crss} is critical resolved shear stress on the slip plane in the direction of b.

133

Glide of an Edge Dislocation

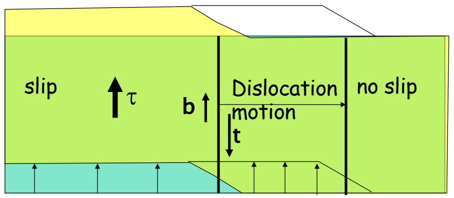
A surface step of magnitude b is created if a dislocation sweeps over the entire slip plane



Surface step, not a dislocation

134

Glide of a Screw Dislocation



Shear stress is in a direction perpendicular to the GLIDE motion of screw dislocation

Analogy: Transverse wave

135

Glide Motion and the Shear Stress

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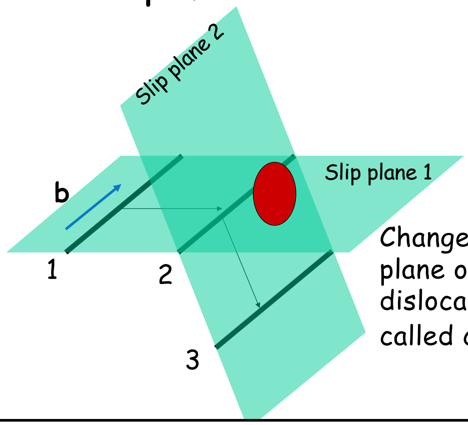
136

Cross-slip of a screw dislocation

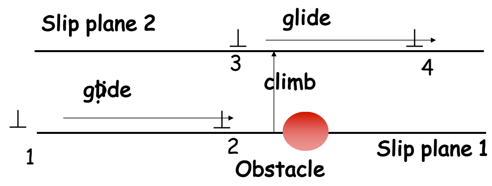


Change in slip plane of a screw dislocation is called cross-slip

137

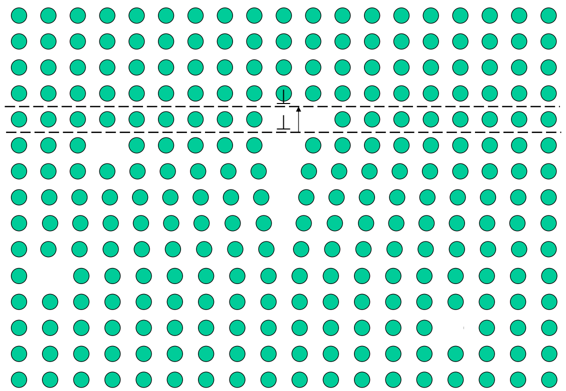
Climb of an edge dislocation

The motion of an edge dislocation from its slip plane to an adjacent parallel slip plane is called **CLIMB**



138

Atomistic mechanism of climb



139

Climb of an edge dislocation

Climb up	Climb down
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140

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FIGURE 4.6 A transmission electron micrograph of a titanium alloy in which the dark lines are dislocations. 51,450×. (Courtesy of M. R. Plichta, Michigan Technological University.)

From Callister

141

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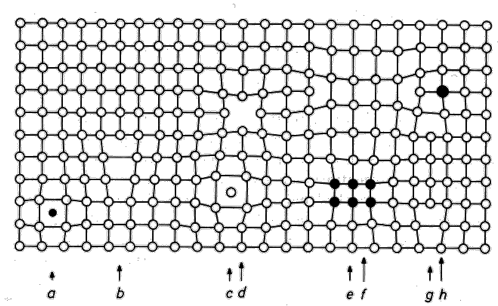

http://www.tf.uni-kiel.de/matwis/amat/def_en/index.html

142

143

Lecture 18

Ch 6 Defects L6: Surface Defects

Tu 02.09.2025

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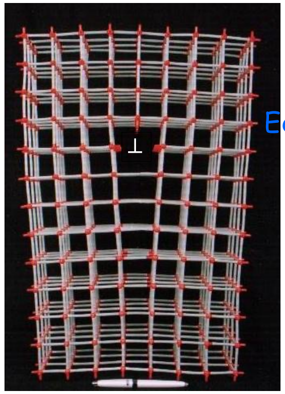
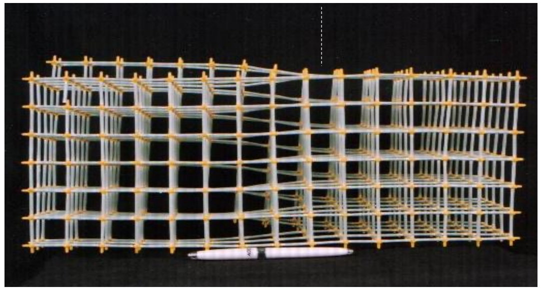


Edge Dislocation

432 atoms
55 x 38 x 15 cm^3

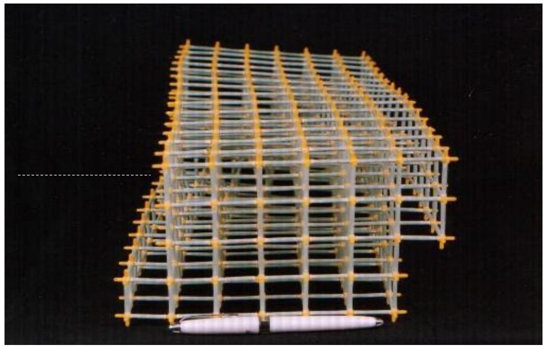
145



Screw Dislocation

525 atoms
45 x 20 x 15 cm^3

146

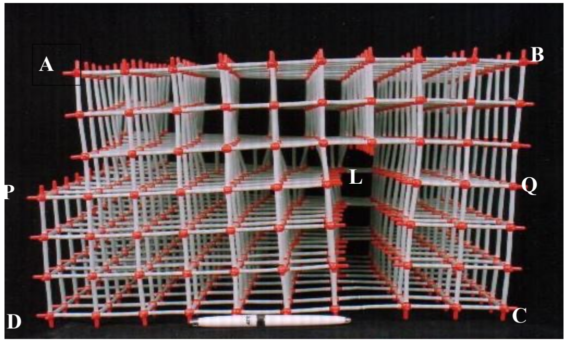


Screw Dislocation (another view)

147

- A dislocation cannot end abruptly inside a crystal
- Burgers vector of a dislocation is constant

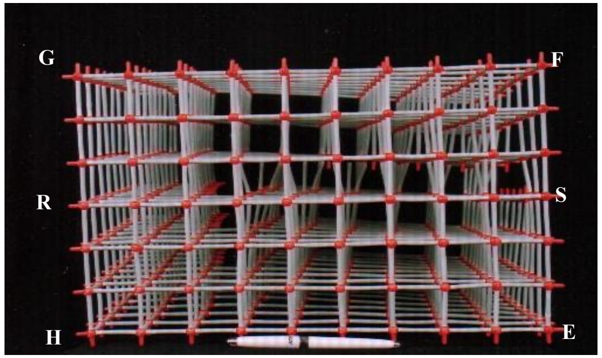
148



Front face: an edge dislocation enters

720 atoms
45 x 39 x 30 cm^3

149



Back face: the edge dislocation does not come out !!

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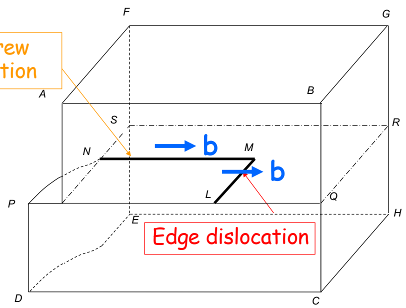
RH Screw dislocation



Edge dislocation

Schematic of the Dislocation Model

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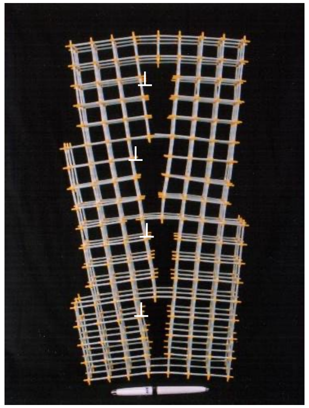

A low-angle Symmetric Tilt Boundary

477 atoms
55 x 30 x 8 cm^3

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MODELS OF DISLOCATIONS FOR CLASSROOM***

R. Prasad

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International Council of Materials Education

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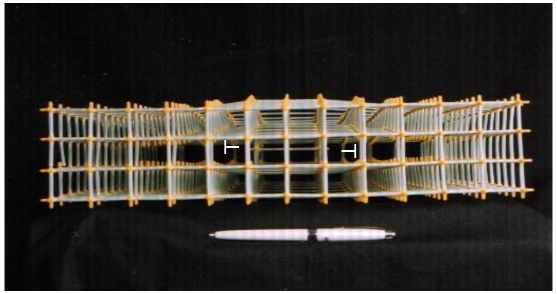

A Prismatic Dislocation Loop

685 atoms
38 x 38 x 12 cm^3

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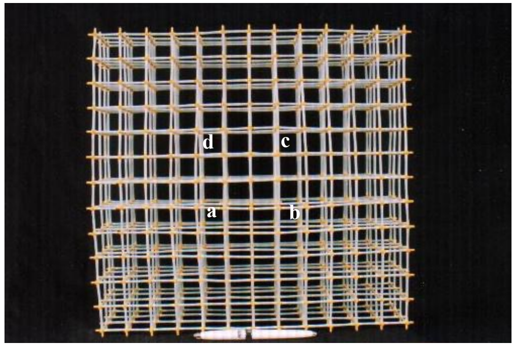

A Prismatic Dislocation Loop
Top View

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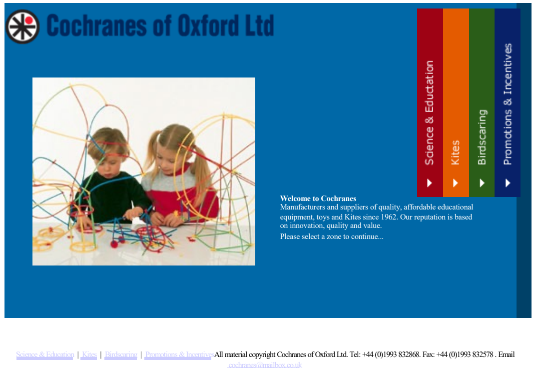

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Cochranes of Oxford Ltd

Resources

The following resources are available:

Crystal Dislocation Models for Teaching
Three-dimensional models for dislocation studies in crystal structures …

Format: **PDF** | Category: **Teaching resources** Click here to open

https://www.cochranes.co.uk/resources/jmepaper.pdf

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Surface Defects

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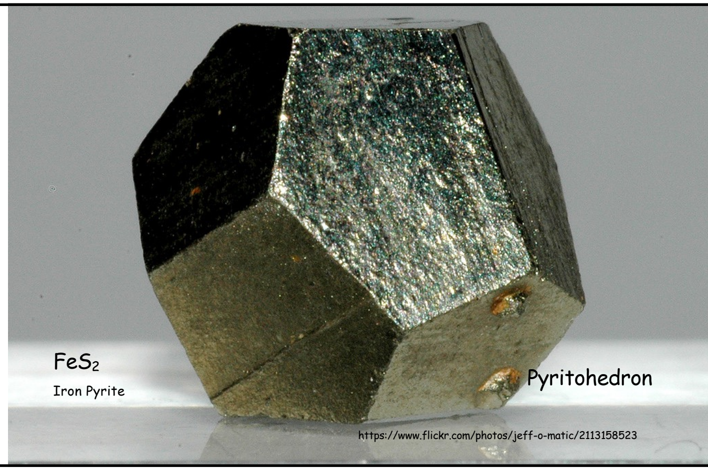

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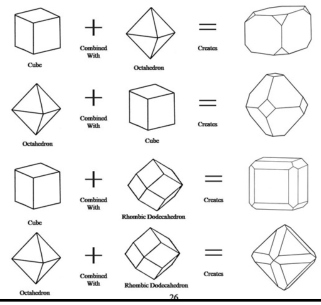
Crystal Combinations
Adding Crystal Forms Together

In nature, a single crystal form can easily be found in a single crystal. You will regularly find pyrite crystals in the form of pyritohedron. Or, you will find a perfectly cubic crystal of galena or fluorite. Also, it is not rare to find a dodecahedral garnet crystal. Beautiful, simple hexagonal prisms are commonly found in beryl crystals like aquamarine.

As you study the crystals you see at mineral museums, as well as crystals in books and in your own collection, you will find that many crystals are actually *combinations* of two or more basic crystal forms.

Here we call it "Crystal Mathematics" where two or more crystal forms are added together.



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Surface Defects

External	Internal	
Free surface	Grain boundary	Same phase
	Stacking fault	
	Twin boundary	
	Interphase boundary	Different phases

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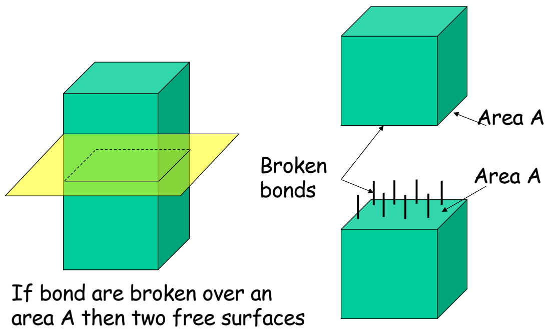
External surface: Free surface



If bond are broken over an area A then two free surfaces of a total area 2A is created

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External surface: Free surface

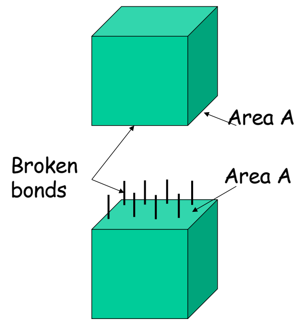
n_A=no. of surface atoms per unit area

n_B=no. of broken bonds per surface atom

ε=bond energy per atom

$$\boxed{\gamma = \frac{1}{2} n_A n_B \varepsilon}$$

Surface energy per unit area



If bond are broken over an area A then two free surfaces of a total area 2A is created

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What is the shape of a naturally grown salt crystal?

Why?

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Surface energy is anisotropic

Surface energy depends on the orientation, i.e., the Miller indices of the free surafce

n_A, n_B are different for different surfaces

Example 6.5 & Problem 6.16

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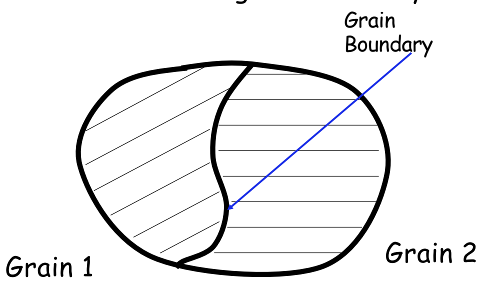
Internal surface: grain boundary



A grain boundary is a boundary between two regions of identical crystal structure but different orientation

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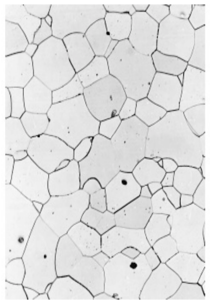
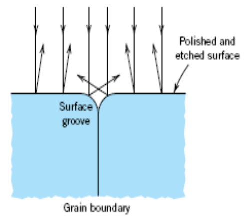
Optical Microscopy, Experiment 8





Photomicrograph an iron chromium alloy. 100X.

Callister, Fig. 4.12

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Grain Boundary: low and high angle

One grain orientation can be obtained by rotation of another grain across the grain boundary about an axis through an **angle**

If the angle of rotation is high, it is called a high angle grain boundary

If the angle of rotation is low it is called a low angle grain boundary

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Grain Boundary: tilt and twist

One grain orientation can be obtained by rotation of another grain about an **axis** through an angle

If the axis of rotation lies in the boundary plane it is called a **tilt boundary**

If the axis of rotation is perpendicular to the boundary plane it is called **a twist boundary**

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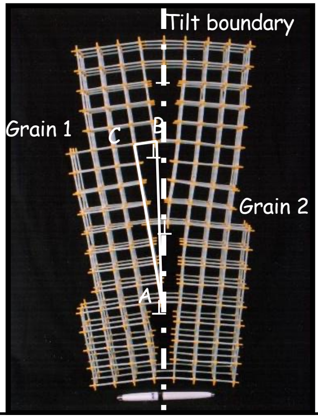
Edge dislocation model of a small angle tilt boundary

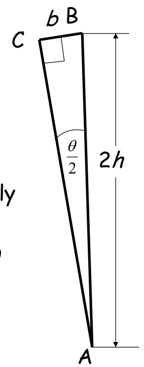


$$\frac{b}{2h} = \sin\frac{\theta}{2}$$

Or approximately

$$\frac{b}{h} = \tan\theta$$

Eqn. 6.7



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Stacking fault

C B A C B A C B A

A missing C plane → Stacking fault

A C B A B A C B A

HCP

A thin region of HCP inserted in CCP

CCP

CCP with a stacking fault

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C	A
B	C
A	B
C	A
B	B
A	A
C	C
B	B
A	A

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A stacking fault is a translation boundary. Crystal on one side of a boundary is translated wrt that on the other side by a non lattice translation.

Q1: Why not a lattice translation?

Q2: Describe the translation vector which will give a stacking fault corresponding to a missing C plane in a CCP crystal (previous slide)

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Twin Plane

C		C
B		A
A		B
C		C
B		A
A		B
C	Twin plane	C
B		B
A		A
C		C
B		B
A		A

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A twin plane is a grain boundary such that crystal on side of the boundary appears to be mirror image of the crystal on the other side of the boundary (although the crystal structure does not change, only the orientation changes)

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