PURDUE
UNIVERSITY

NCN
www.nanohub.org

ECE695A: Reliability Physics of Nano-Transistors
Lecture 4: Structures and Defects in Crystals

Muhammad Ashraful Alam
alam@purdue.edu

Copyright 2013

Outline of lecture 4

1. Background information

2. Defect-free crystal structures

3. Defects in crystals

4. Conclusions

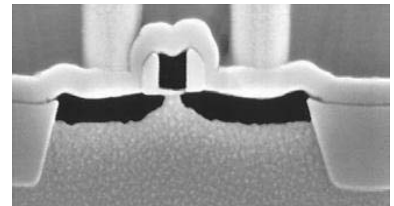
Transistor and interconnect reliability

Transistor reliability issues

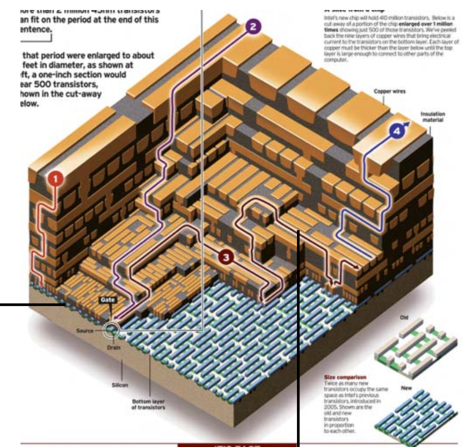
- Gate dielectric breakdown
- Negative bias temperature instability
- Hot carrier degradation
- Radiation induced damage

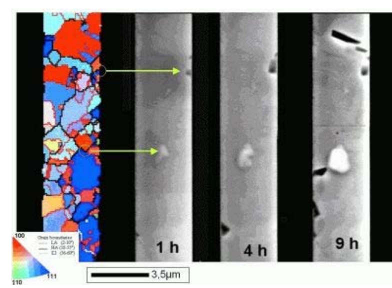
Interconnect reliability issues

- Electro-migration/Stress-migration.
- Inter-level dielectric breakdown

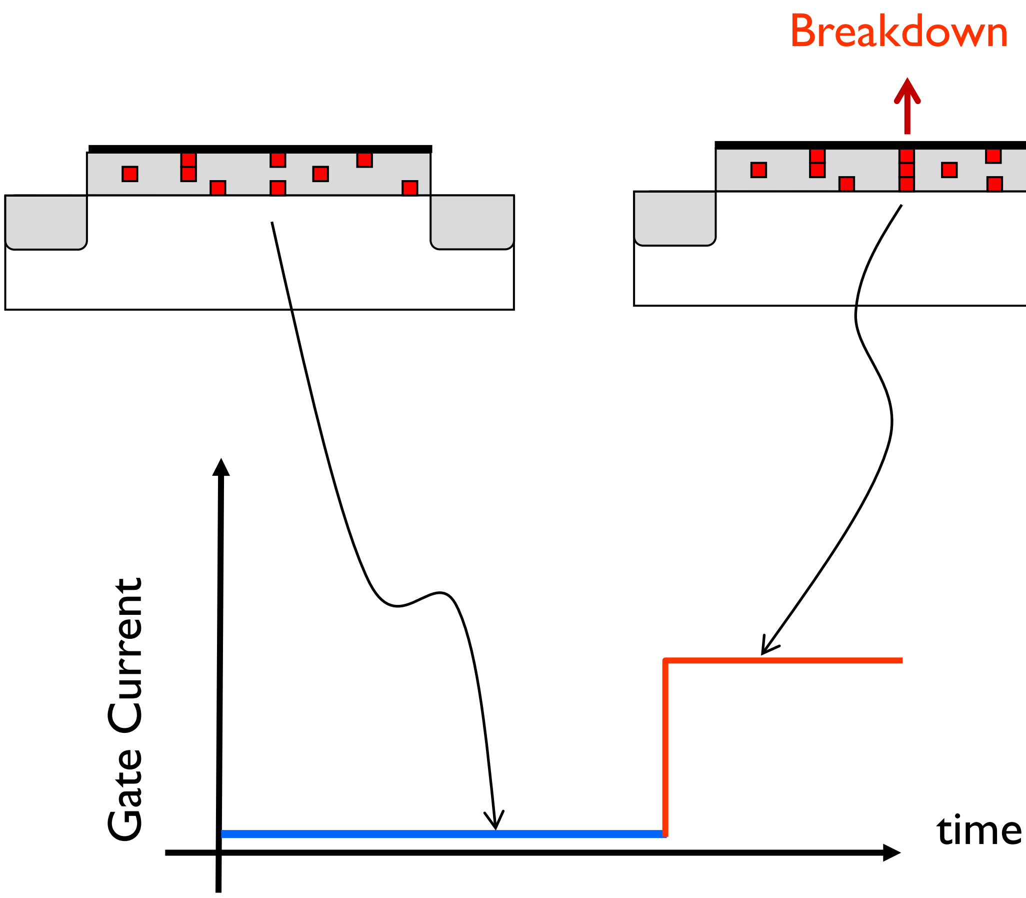


The Oregonian, 2008



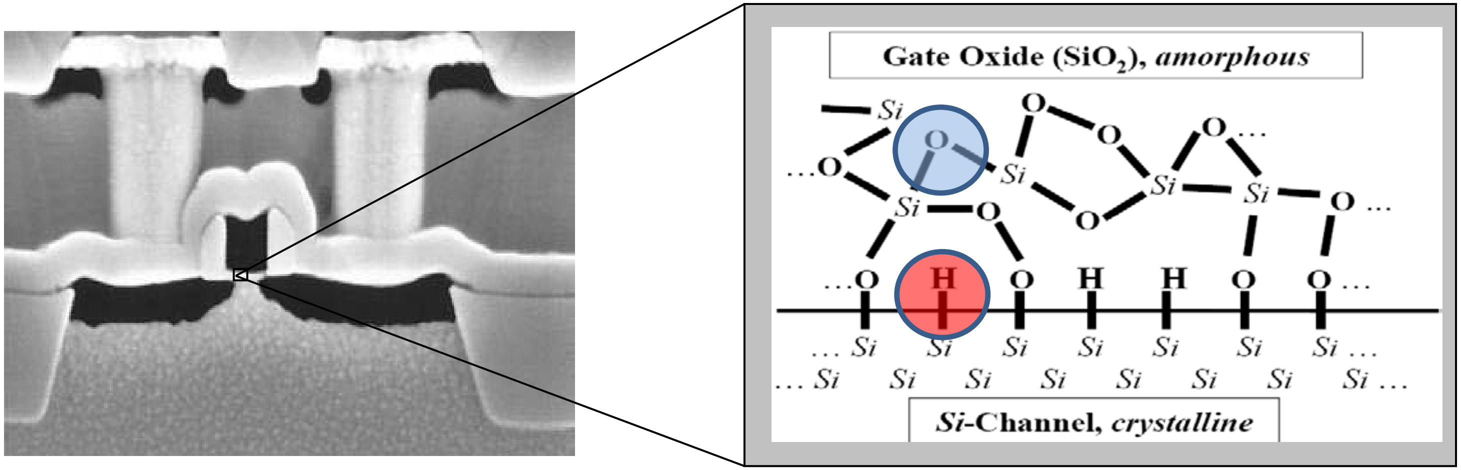


Defects created during oxide breakdown



What do the red boxes represent physically?

Broken SiO and SiH bonds



Broken Si-H bonds

Negative bias temperature instability (NBTI)

Hot carrier degradation (HCI)

Broken Si-O bonds

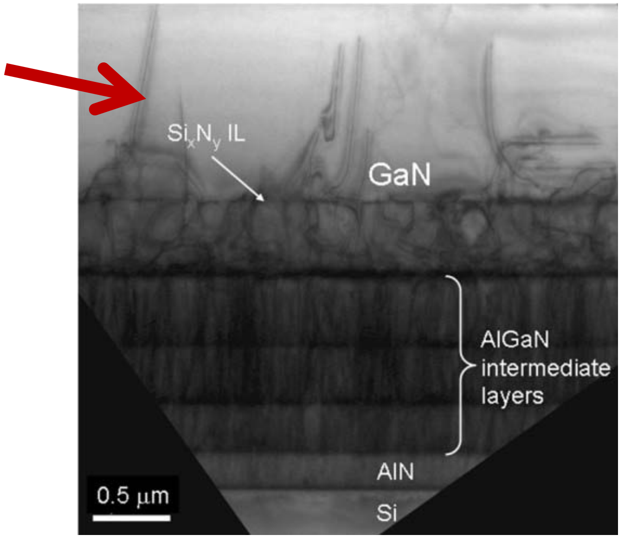
Gate dielectric breakdown (TDDB)

Electrostatic discharge (ESD)

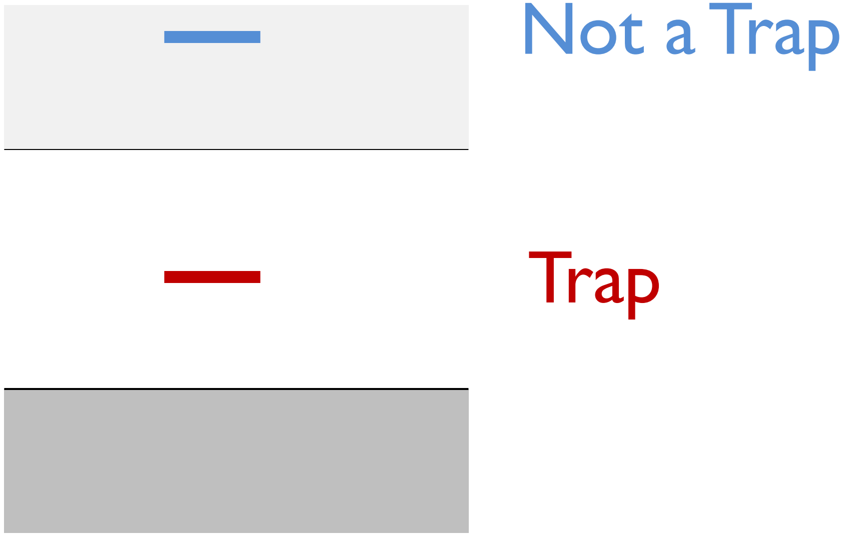
Radiation induced gate rupture (RBD)

Defects vs. traps

Defects

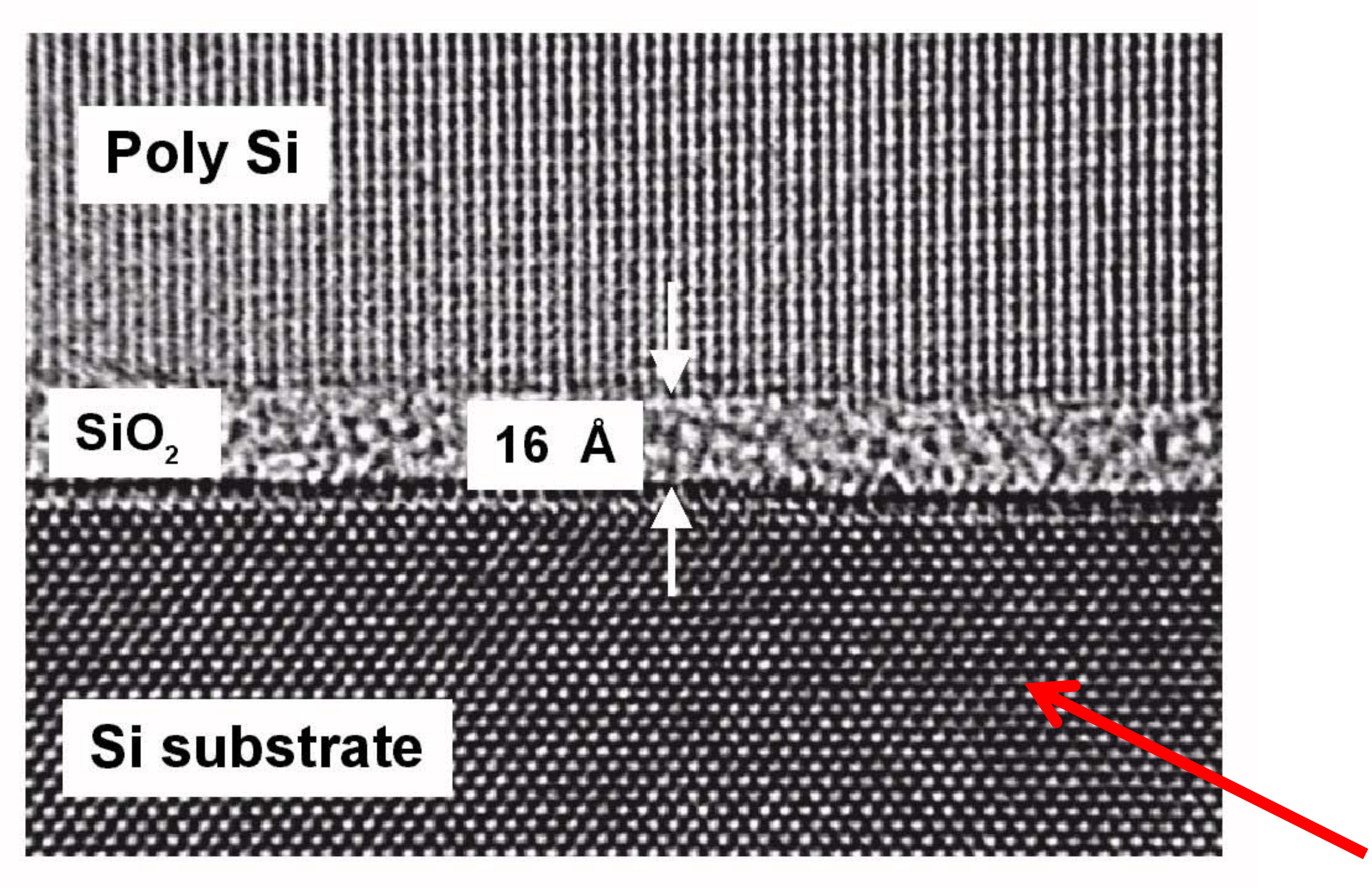


Misplaced atom, incomplete bonds



Defects found in images may not be electrically relevant, e.g. InGaN/GaN blue Light emitting diodes

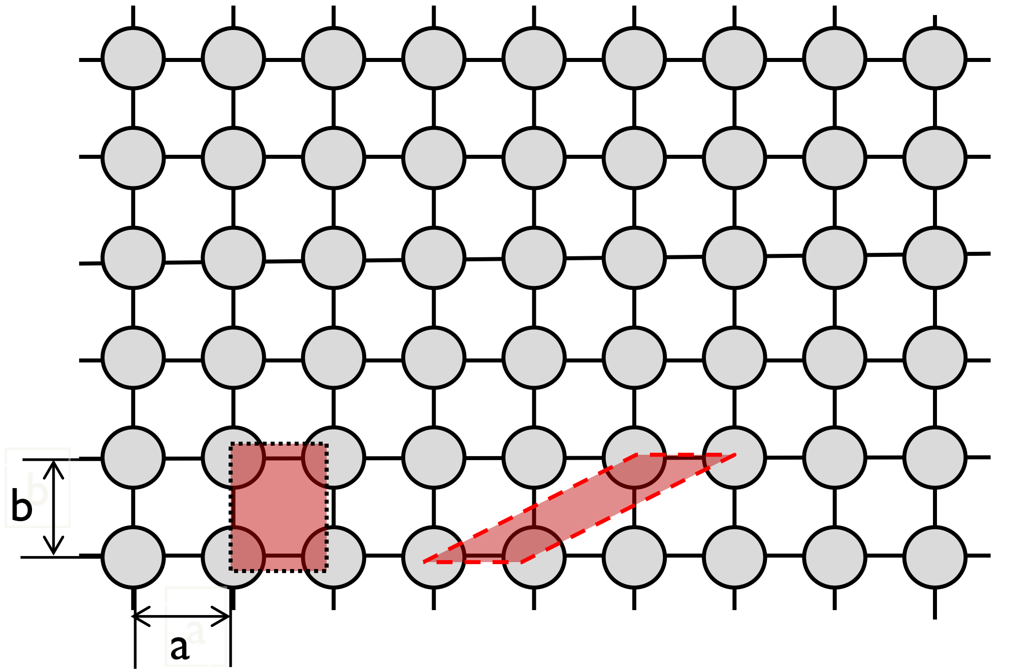
Will begin by defects in crystals



Outline

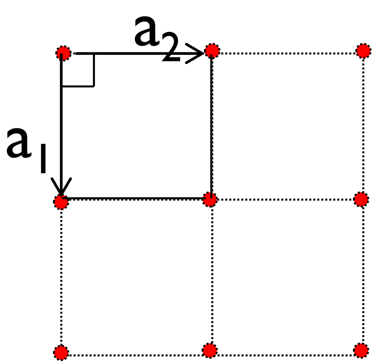
1. Background information
2. Defect-free **crystal** structures
3. Defects in crystals
4. Conclusions

Unit cell of a periodic lattice

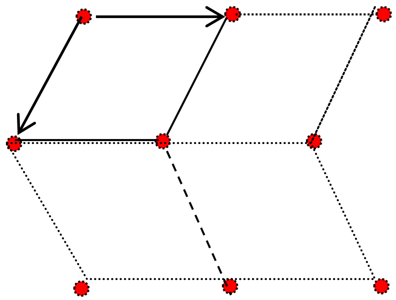


A crystal is represented by unit cells and basis vectors

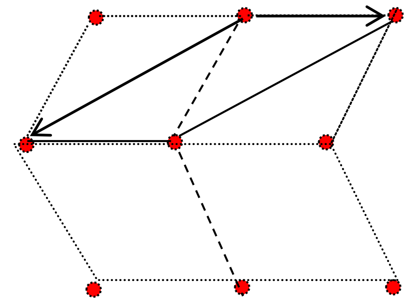
Periodic lattice in 2D (5-types)



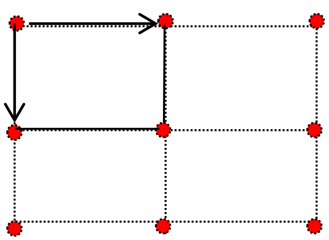
$a_1=a_2$, $\phi=90$



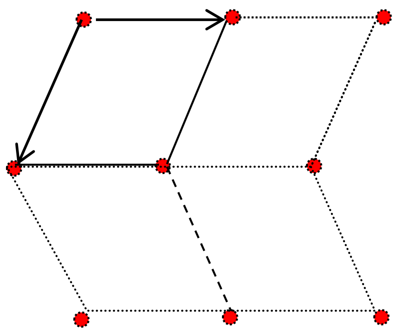
$a_1=a_2$, $\phi>90$



General



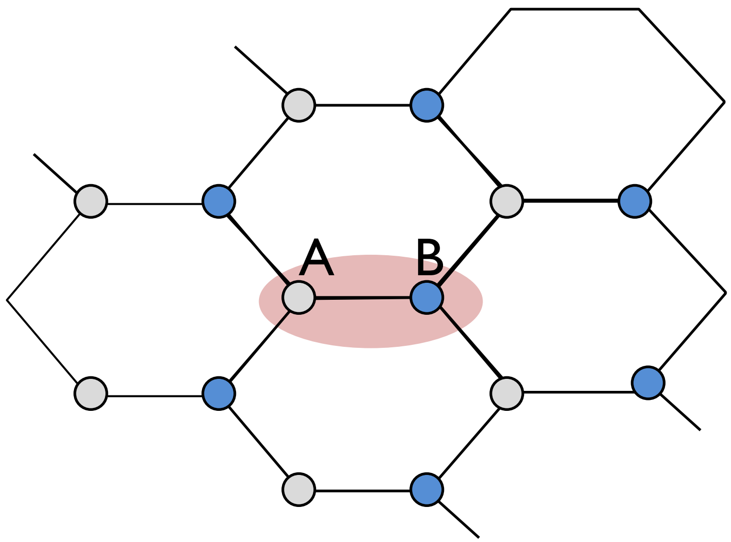
$a_1<a_2$, $\phi=90$



$a_1>a_2$, $\phi>90$

Many systems have 2D lattice (e.g., graphene, Wigner crystals, …)

Not a Bravais lattice …



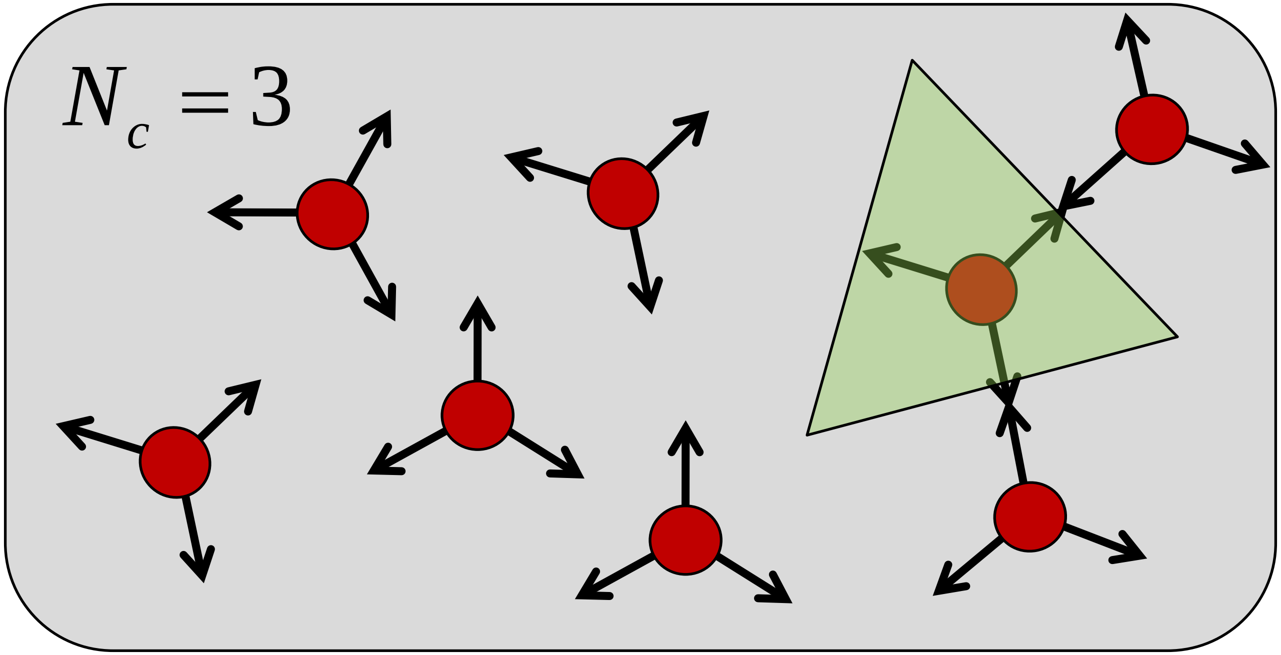
This is graphene sheet which can obtained from graphite by adhesive tape stamping

Ref. Novoselov, Geim, et al. Nature, 438, 197, 2005.

A and B are do not have identical environment

Can be converted to Bravais lattice by creating a new basis

How to crystal arise: Coordination and bonding



Topology of points and Euler formula

Euler relationship in 2D

$$V - E + N = 1$$

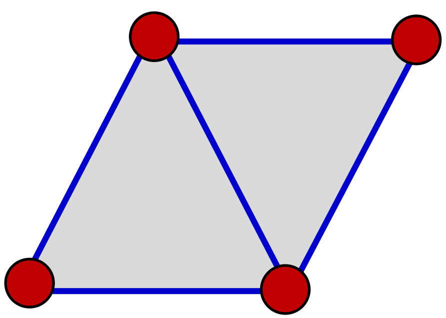
vertices

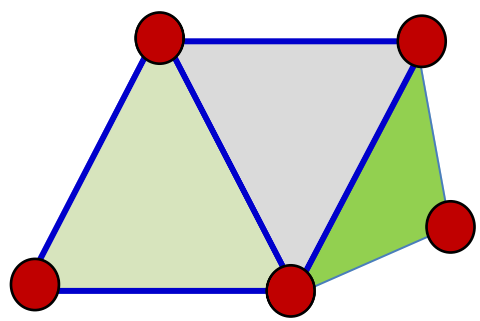
edges

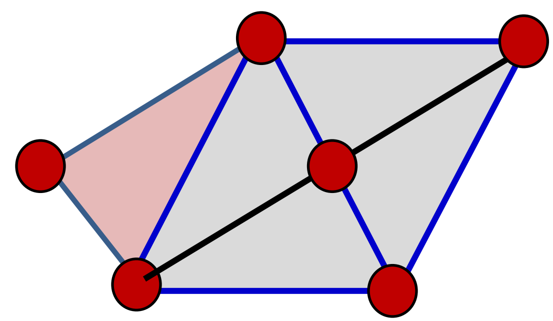
cell number

For large systems ….

$$V - E + N \approx 0$$





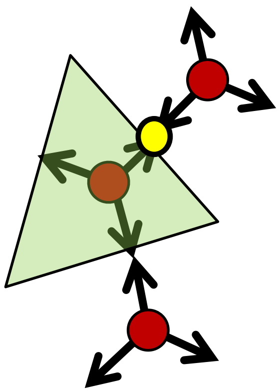


$$\left.\begin{array}{l} V = 4 \\ E = 5 \\ N = 2 \end{array}\right] \Rightarrow 1$$

$$\left.\begin{array}{l} V = 5 \\ E = 7 \\ N = 3 \end{array}\right] \Rightarrow 1$$

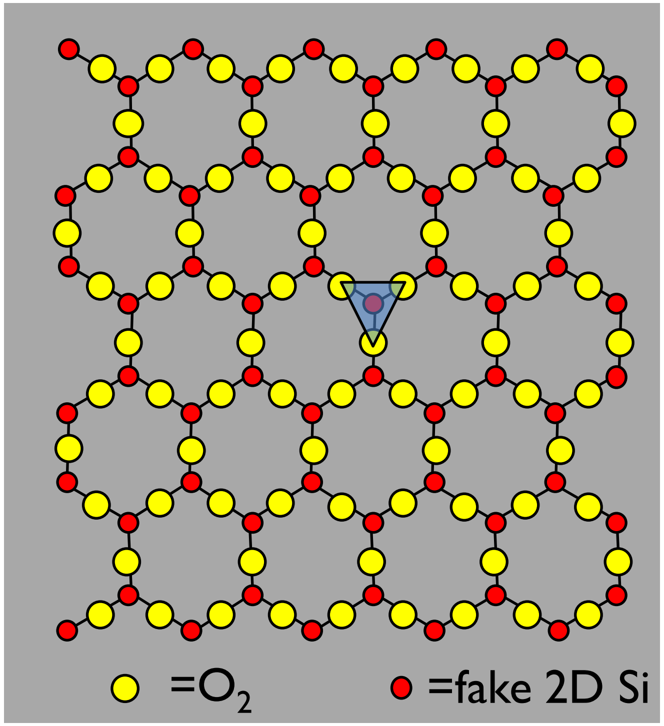
$$\left.\begin{array}{l} V = 6 \\ E = 10 \\ N = 5 \end{array}\right] \Rightarrow 1$$

Euler anticipates 'graphene' lattice

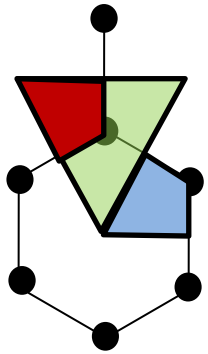


$$\left.\begin{aligned} V &= 1 \\ E &= \frac{3}{2} \end{aligned}\right\} 2E = 3V = N_p N$$

3 bonds/atoms to honeycomb lattice



$$V - E + N = 1$$



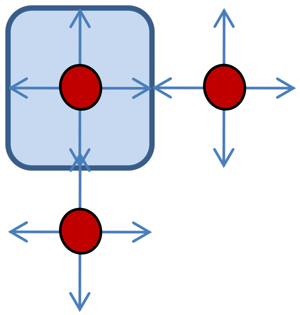
$$\frac{N_p N}{3} - \frac{N_p N}{2} + N \sim 0$$

$$N_p \cong 6 \longleftarrow$$ edges/cell

$$6N = 3V \Rightarrow N = \frac{1}{2}$$

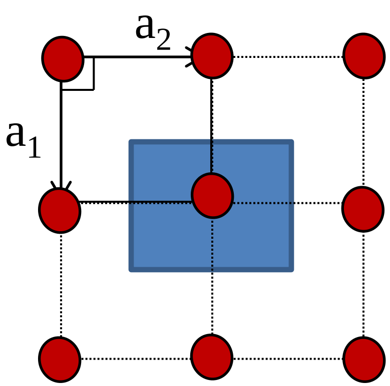
1/2 of a cell; therefore each cell must have **6-sides**!

Exercise: what type of lattice with N_C=4?



$$\left.\begin{array}{l} V = 1 \\ E = \dfrac{4}{2} \end{array}\right\} 2E = 4V = N_p N$$

$$V - E + N = 1 \qquad \frac{N_p N}{4} - \frac{N_p N}{2} + N \sim 0$$



$$\Rightarrow N_p \cong 4$$ Final lattice must have 4 edges/cell

$$4N = 4V \Rightarrow N = 1$$

The volume of each unit must equal the volume of unit lattice

With Euler relationship, you can…..

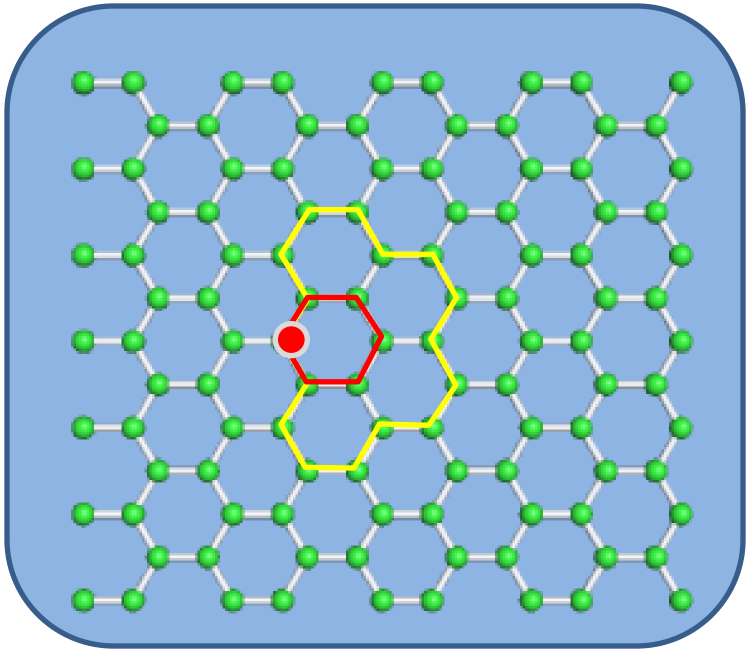
A 6-bond atom leads to triangular lattice

Determine the size of the primitive ring

Show that a five ring lattice is impossible

Calculate Number of rings sharing an atom

Show that odd-number rings are impossible



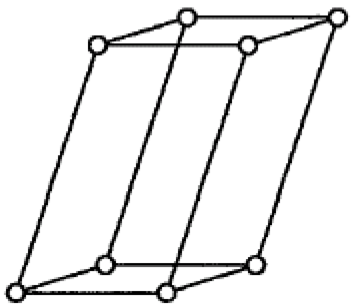
References.

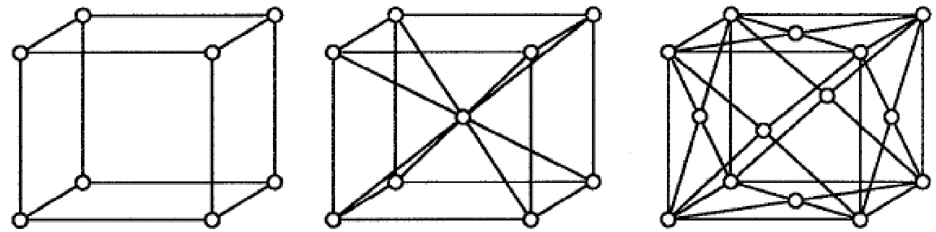
X. Yuan and A. Cormack, Computational Material Science, ***24****, p. 343, 2002.*

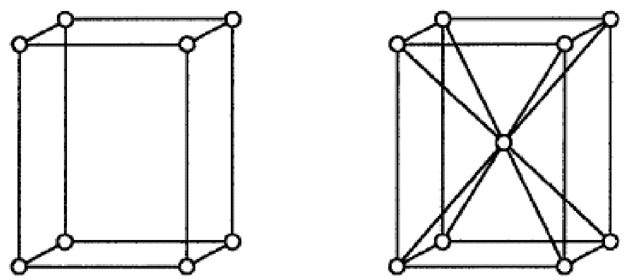
S.V. King Nature ***213*** *(1967), p. 1112. http://rings-code.sourceforge.net/*

3D-Bravais lattices

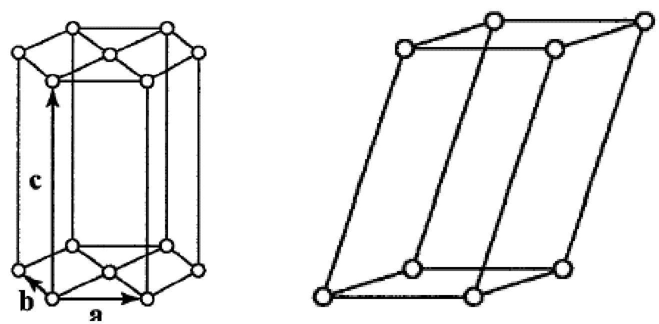
Triclinic





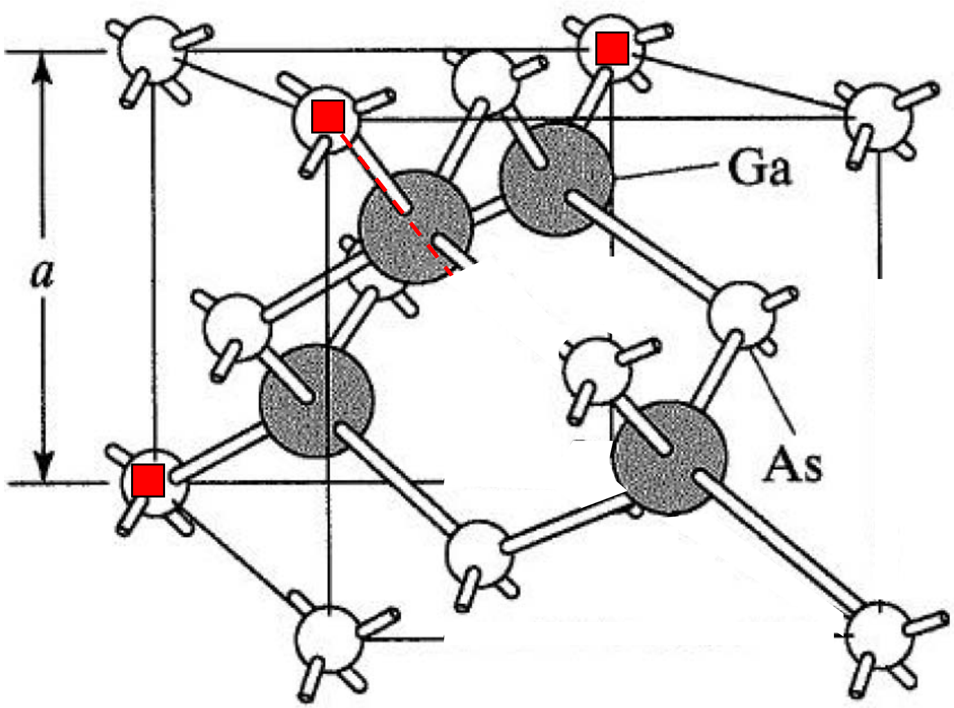


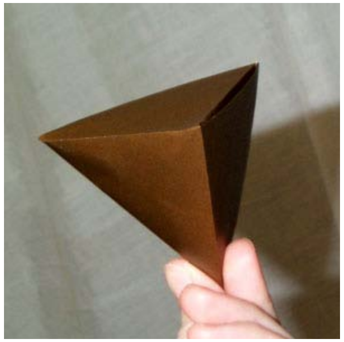
Why not ?



And others …..

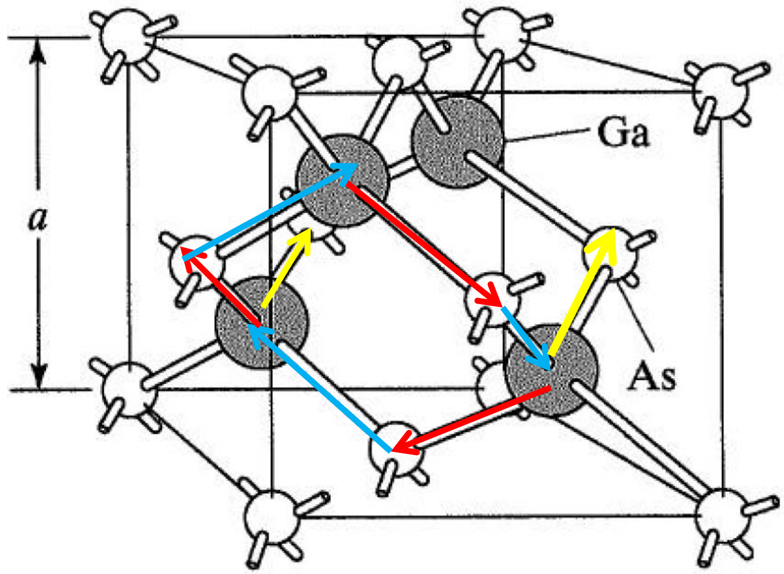
Zinc-Blende lattice for GaAs





Atoms/cell=(1/8)x8 + (1/2)x6 + 4=8
FCC Lattice with a basis
Not a primitive cell
Tetrahedral structure

Homework: ring statistics



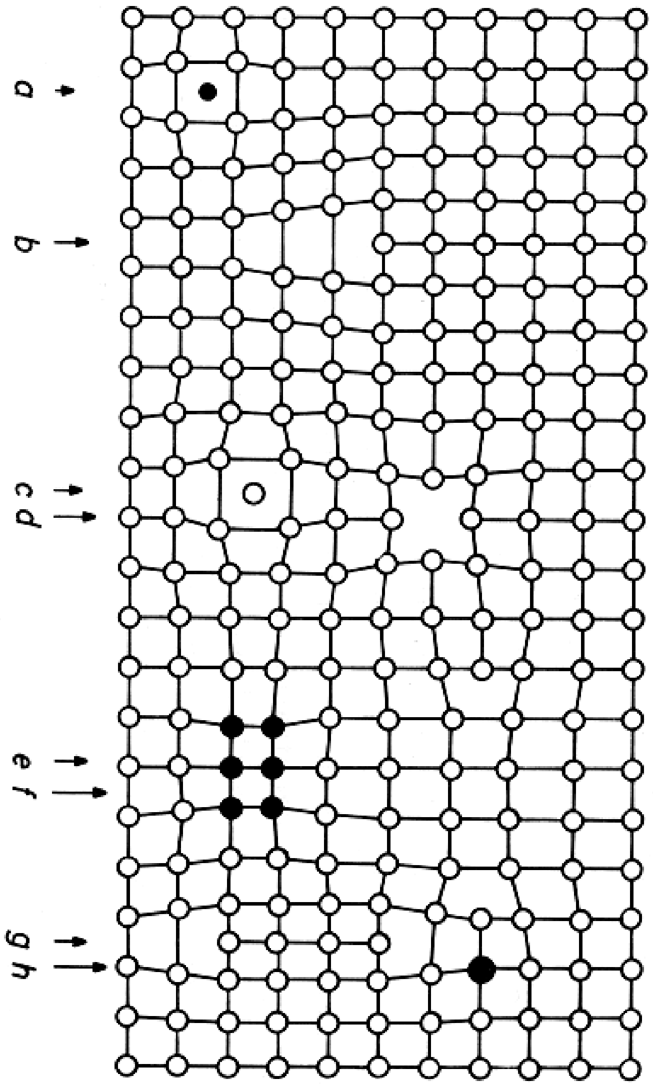
Show that Si has

6-atoms in the primitive (smallest) ring
12 rings through each atoms (4 ways out, 3 ways in)
All rings are even.

Outline

1. Background information
2. Defect-free crystal structures
3. Defects in crystals
4. Conclusions

Types of crystal defects: point & bulk



Now that we know geometry of perfect lattice …

a) **Interstitial atom**

b) Edge dislocation

c) **Self interstitial atom**

d) **Vacancy**

e) Precipitate of impurity atoms

f) vacancy type dislocation loop

g) Interstitial type dislocation loop

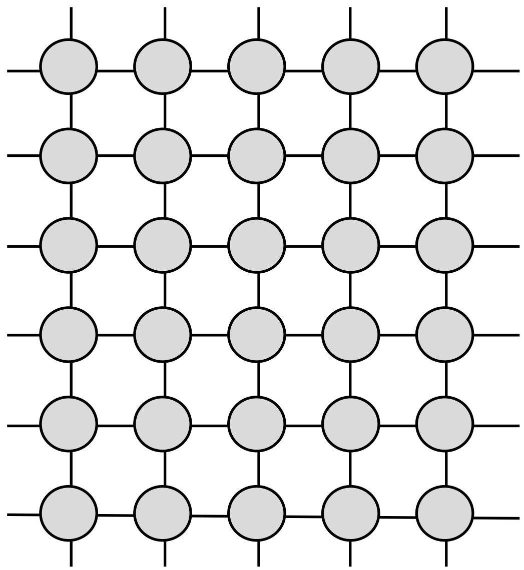
h) **Substitutional impurity atom**

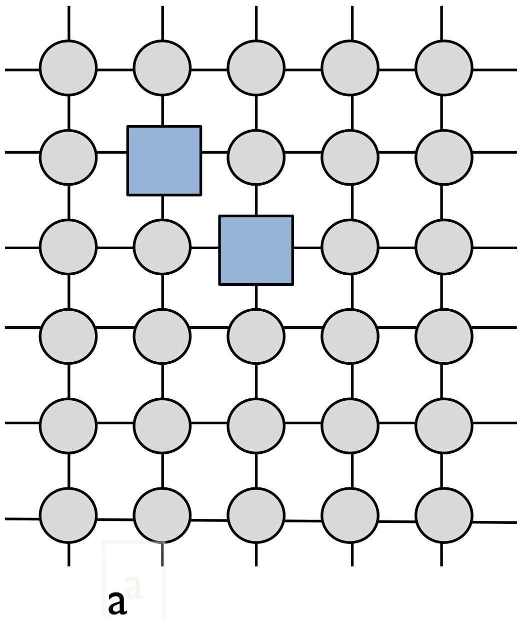
Defects are named formally by Kroger-Vink notation

Concentration of point defects

Energy of the system: $F = E - TS$

Vacancy is created if: $\Delta F = \left(\Delta E - T \cdot \Delta S\right) < 0$





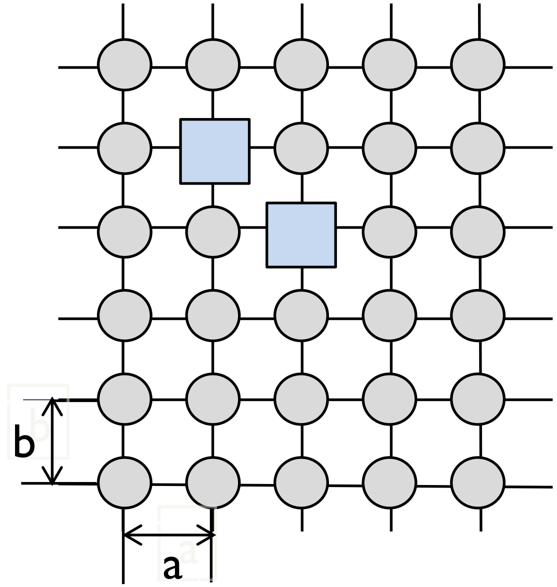
$$\frac{\Delta S}{k_B} = -\ln\frac{N!}{N!0!} + \ln\frac{N!}{\left(N-V\right)!V!}$$

Concentration of point defects

$$\frac{\Delta S}{k_B} \approx N \ln N - (N - V)\ln(N - V) - V \ln V$$

$$\Delta E \approx E_{after} - E_{before} = E_V V - 0$$

$$\Delta F = F_{after} - F_{before} = +VE_V - k_B T \Delta S$$



Minimize F to for equilibrium V
(definition of chemical potential) ….

$$V \sim N \times e^{-\frac{E_V}{k_B T}}$$

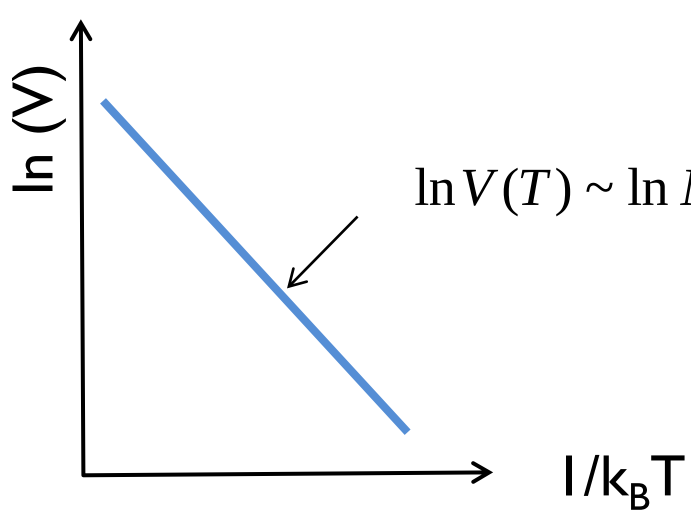
Example: equilibrium defect density

Assume: E_V= 1eV, T=1000C, find V

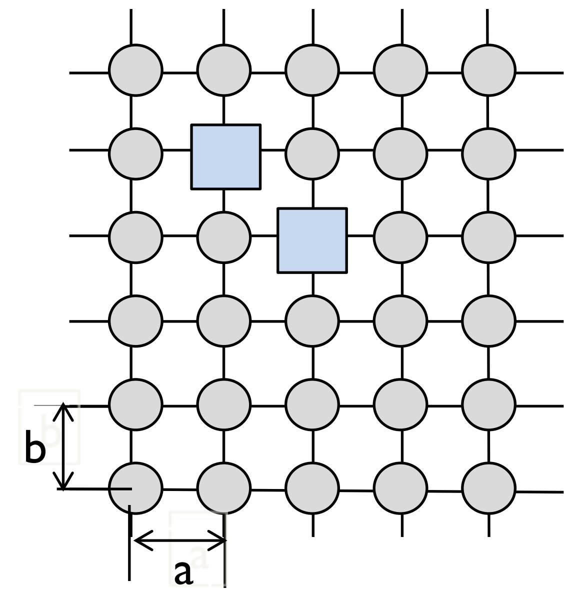
$$V \sim N \times e^{-\frac{E_V}{k_B T}}$$

Answer: 1 part in 10^5 at 1000 C.
In silicon, the number is 10^{17} cm^{-3}!

Activation energy can be obtained from slope of temperature dependent data.



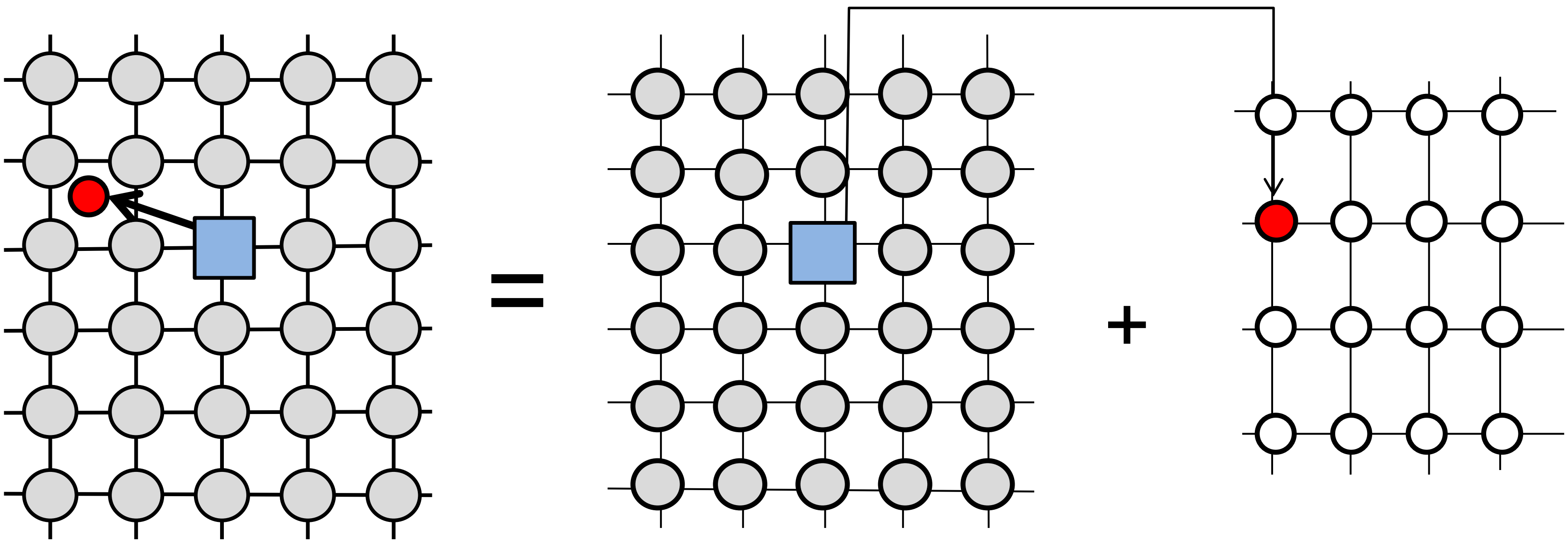
$$\ln V(T) \sim \ln N - \frac{E_V}{k_B T}$$



Homework: Interstitials

Show that the interstitial concentration is

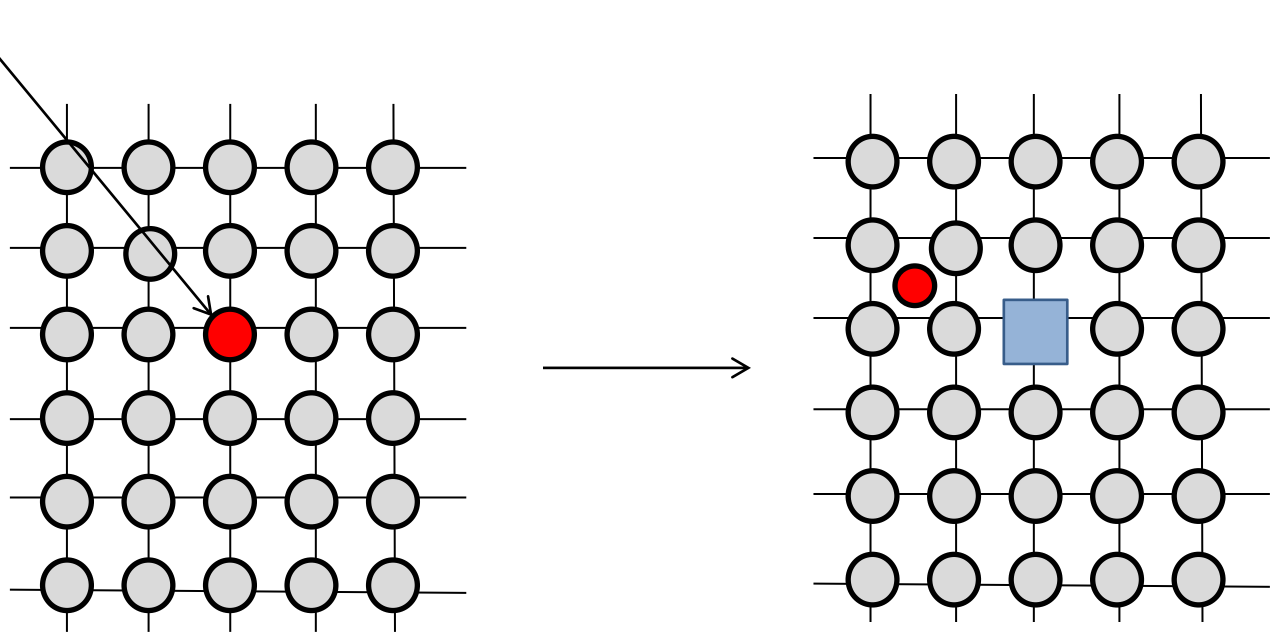
$$I \sim N \times e^{-\frac{(E_V + E_I)}{2k_B T}} \qquad E_I >> E_V$$



Calculate entropy change as a product of two configurations

Dynamics vs. thermodynamics

Radiation induced generation of bulk defects …

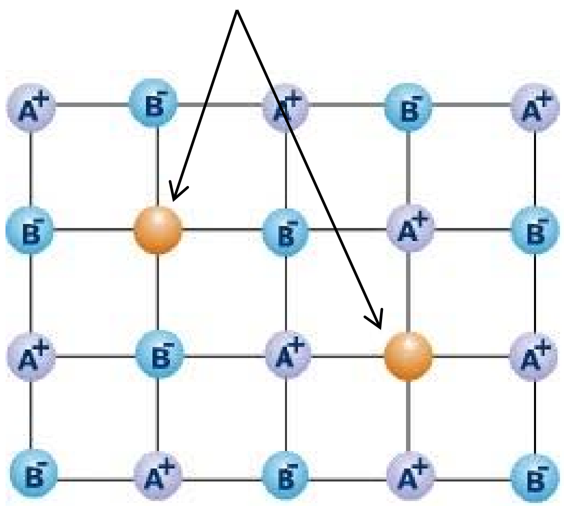


Amorphization by radiation ….

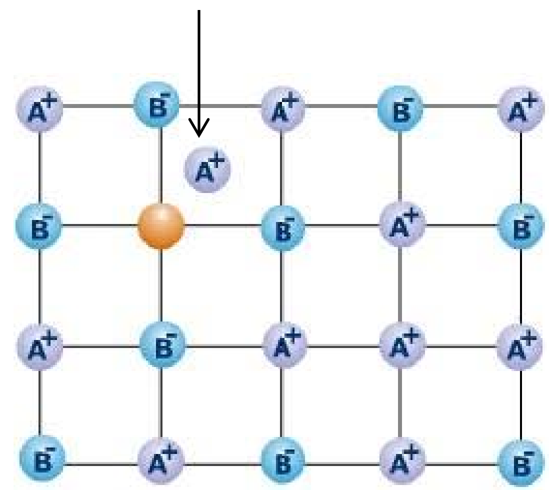
$$I \neq N \times e^{-\frac{E_I}{2k_B T}}$$

Point defects in ionic crystals

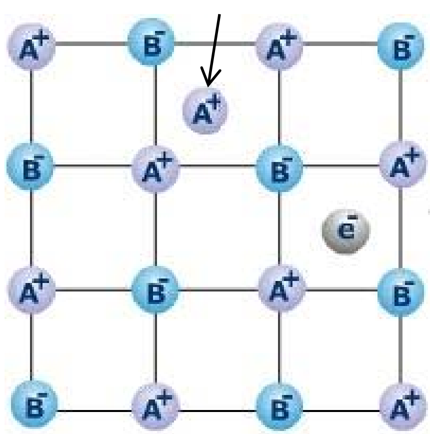
Schottky defect



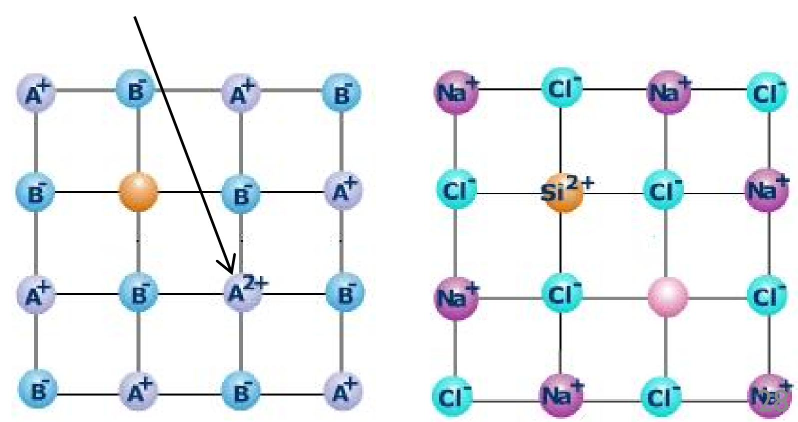
Frenkel defect



Excess metal

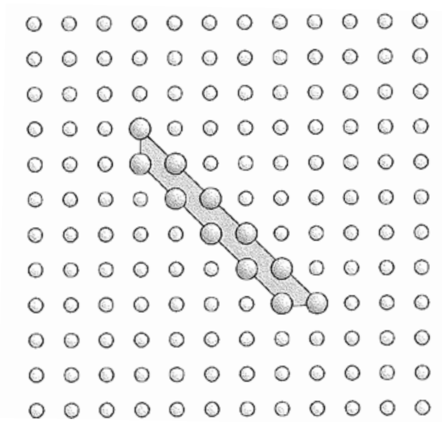


Impurity defect in ionic solids

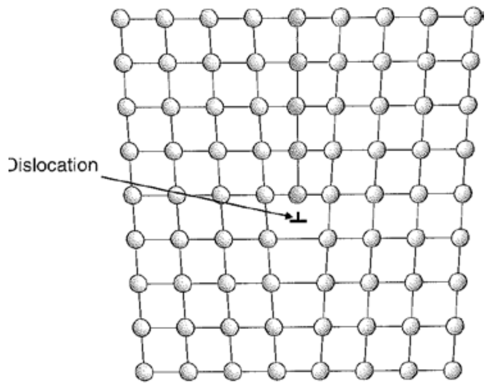


Hierarchical defects in the crystals

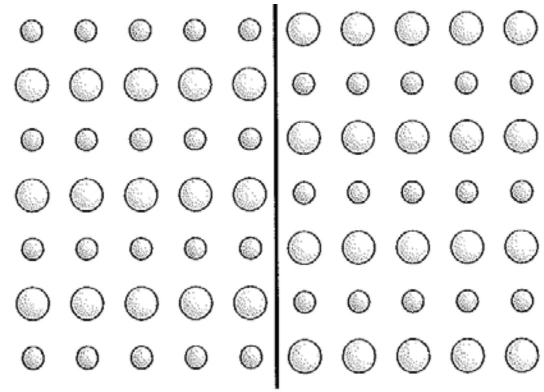
Volume defect

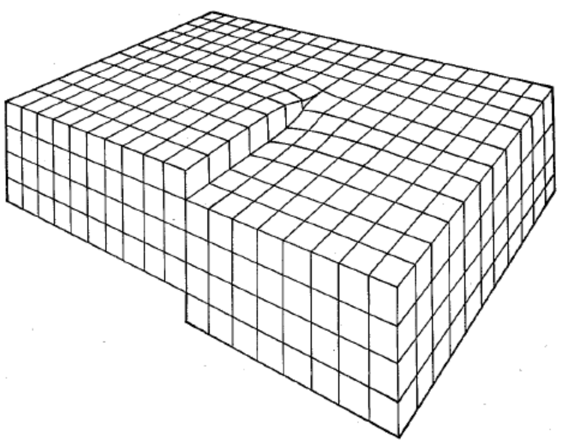


Linear defect

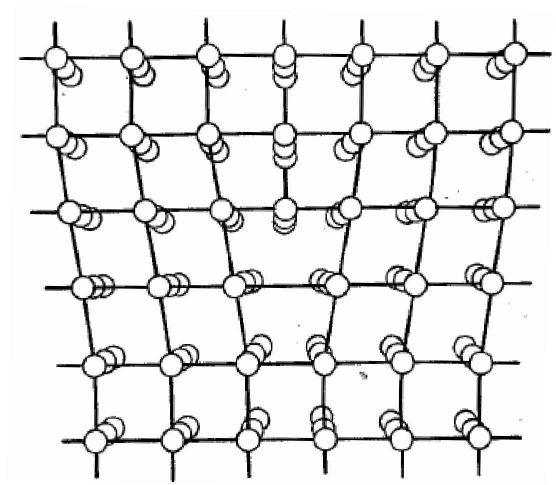


Planar defect





Screw dislocation



Edge dislocation

Defects in Solids, Wiley, 2000.

Conclusions

- Reliability physics deals with pre-existing defects due to processing and newly created defect due to device operation.

- Textbooks on device theory assumes perfect crystal and then the defects sneak in through mobility models and phonon lifetime.

- Standard thermodynamic models predict the creation of defects due to process details. There are hierarchy of these defects.

- Stress and radiation effects generates new defects that must be obtained from kinetic consideration, not thermodynamics.

References

- David E. Richeson, Euler's Gem: The Polyhedron Formula and the Birth of Topology, Princeton University Press,
- Frank Neuman, Euler's Gem and The birth of topolopy, 2010. http://www.tilings.org.uk/T3M2_Euler.pdf
- R. Tilley, Defects in Solids, ISBN: 978-0-470-07794-8, Wiley, 2000
- C. Kittle, Introduction to Solid State Physics, 8th Edition., ISBN 978-0-471-41526-8, 2004.
- Formation energy of vacancy in silicon determined by a new quenching method . *N. Fukata*, , [a], *A. Kasuya*[b] *and M. Suezawa*[a].
- Defects in GaN http://www.imec.be/ScientificReport/SR2008/HTML/1225014.html
- Paul Shewmon Diffusion in solids, ISBN-13: 978-0873391054