EE669: VLSI Technology

Si crystal and it's growth

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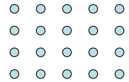
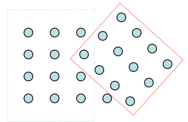
Crystals

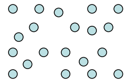
• A material that exhibits perfect periodicity in placement of atoms/groups of atoms/molecules



Crystalline (mono crystalline)



Polycrystalline (multi crystalline)



amorphous

• Crystal can be defined in terms of a symmetric array of <u>points</u> in space called <u>lattice</u>

• The points in the lattice are called the basis. Basis can be atom/group of atoms/molecules.

https://dmishin.github.io/crystals/sodium-chloride.html

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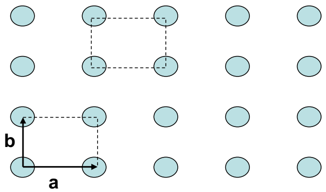
Crystals (2)

• The crystal contains <u>unit cells</u>, which when subjected to integer translation of <u>basis vectors</u>, constructs the crystal lattice



• The crystal is periodic. The unit cell represents a whole crystal!

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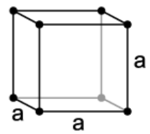
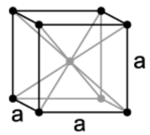
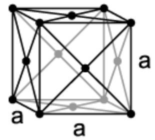
Cubic Lattices



simple



Body centered (bcc)



face centered (fcc)

How many atoms are there in the unit cell?

Hard sphere approximation:
Packing density = 52%

Exercise:
How many atoms are there in these unit cells?

Hard sphere approximation:
What are the packing densities in these two cases?

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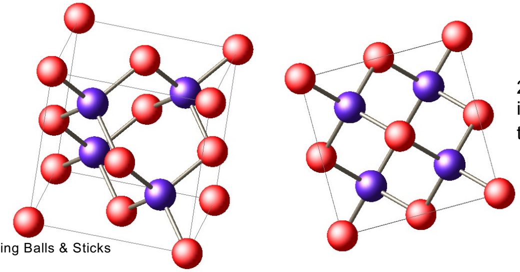
The Silicon Crystal Structure (diamond lattice)

Two interpenetrating face centered cubic lattices displaced by a/4, a/4, a/4



Created using Balls & Sticks

2-D projection in the [100] on the (100) plane

Radius of Si atom: 1.18 Å
Lattice constant: 5.43 Å
Smallest spacing between atoms: 2.35 Å
Hard sphere packing density: 34%

Exercise: play with VESTA
Do the assignment posted in moodle.

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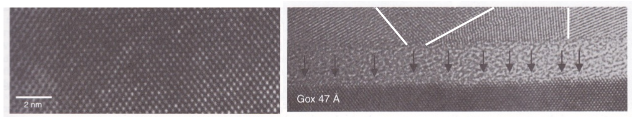
Monocrystalline and poly crystalline Si

Crystalline Polycrystalline amorphous



poly-Si
$a\text{-}SiO_2$
c-Si

C.-H. Tung, G. T. T. Sheng and C.-Y. Lu, ULSI Semiconductor Technology Atlas, Wiley Interscience, 2003

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Crystal Planes

Method:

1. Define a Cartesian coordinate system with the origin at any lattice point and align the axes with the edges of the cubic unit cell
2. Obtain the intercepts of the plane with the crystal axes and express them as integer multiples of basis vectors
3. Take the reciprocals of the three integers and reduce them to the smallest set of integers h, k and l, with the same ratio as the reciprocals
4. The plane is labeled (hkl) and h, k and l are called Miller indices
5. In a lattice there are many equivalent planes. They are collectively called {hkl} planes

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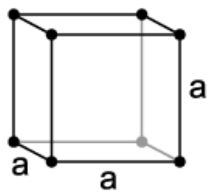
Representation of crystal planes: exercise

Identify the (100), (110) and (111) planes in the cubic lattice.



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Crystal Directions

Method:

1. A direction in a crystal is defined in terms of the components of a vector in that direction
2. The vector components being expressed in the smallest integer multiples of the basis vectors
3. For example, the direction 1a, 1b, 1c in a cubic lattice is represented as [111]
4. The set of equivalent directions are placed in angular brackets <>
5. In a cubic lattice, the direction [hkl] is perpendicular to the plane (hkl)

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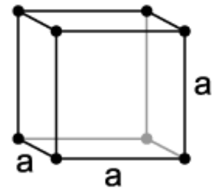
Exercise 2

Identify the [100], [110] and [111] directions in the cubic lattice.



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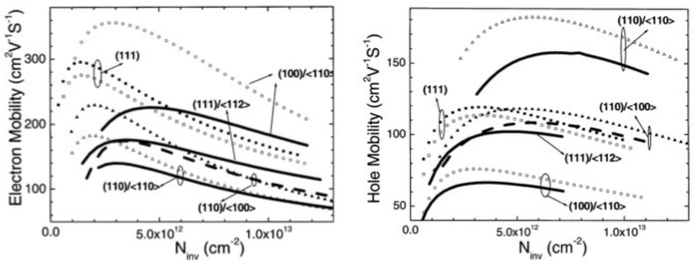
Implications of anisotropy in Si lattice (1): Device Example



M. Yang et al., IEEE Electron Device Letters, vol.24, No. 5, 2003, pp. 339

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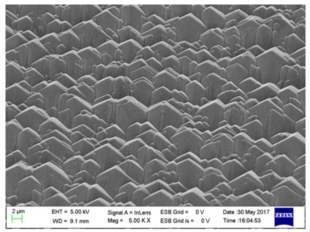
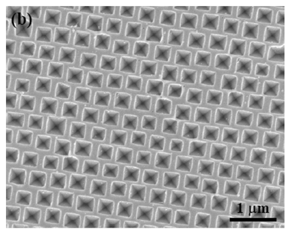
Implications of anisotropy in Si lattice (2): Process Example



Sreejith KP, PhD thesis, IIT Bombay 2022



Sun, et al. " *APL* 91.23 (2007): 23110.

Exercise: Understand anisotropy using VESTA.

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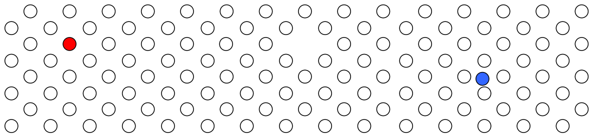
Crystal Defects

Any interruption from the regular arrangement in a crystal is a defect.

- Point defects:

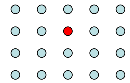


Substitutional   Vacancy   Interstitial

Exercise: How many interstitials sites are there in silicon lattice

Exercise: Write down the coordinates of all interstitial sites in silicon lattice

Crystal Defects: Dopants



Dopant occupying a substitutional or interstitial site is a point defect.

$$\boldsymbol{r_D = r_{Si}(1 \pm \varepsilon)}$$

ε is called the misfit factor.

$\boldsymbol{r_{Si}}$ = 1.18 Å

Dopant	P	As	Sb	B	Al	Ga	In
Radius (Å)	1.10	1.18	1.36	0.88	1.26	1.26	1.44
Misfit factor	0.068	0	0.153	0.254	0.068	0.068	0.22
	N-type			P-type			

Vacancies and interstitials

V		I	
$E_C - E_{V-}$	0.57 eV	$E_C - E_{I-}$	0.3 eV
$E_C - E_{V--}$	0.11 eV	$E_C - E_{I--}$	??
$E_{V+} - E_V$	0.05 eV	$E_{I+} - E_V$	0.4 eV
$E_{V++} - E_V$	0.13 eV	$E_{I++} - E_V$	??

- A vacancy interstitial pair is called a Frenkel defect
- Such defects can act as efficient recombination centres
- Can be created in Si by neutron radiation or <u>during high temperature processing</u>

Vacancies and interstitials

$$C_{I^0} = 10^{27} e^{-3.8/kT}$$

$$C_{V^0} = 9 \times 10^{23} e^{-2.6/kT}$$

C_{V0} and C_{I0} are concentration of vacancies under equilibrium conditions in Si in numbers per cm^3. kT is the thermal energy in eV.

Exercise: Calculate the vacancy and interstitial concentrations at 1000C and compare it to the intrinsic carrier concentration in Si.

$$n_i(T) = 5.29 \times 10^{19} (T/300)^{2.54} e^{(-6726/T)}$$

K. Misiakos and Tsamakis, D., "Accurate measurements of the silicon intrinsic carrier density from 78 to 340 K", Journal of Applied Physics, vol. 74, no. 5, p. 3293, 1993.

Higher order defects: formation

Stress: Internal forces within a material in response to external forces and is expressed in force per unit area (N/m^2)
Strain: measure of the deformation of the material in response to stress

Elastic limit/yield strength: stress at which the material starts to deform plastically.
Plastic deformation: irreversible deformation of the material

Discussion: What happens if you pour boiling water into a glass bottle?

Higher order defects relaxes the stress.

Higher order defects: formation example

Examples from Si processing:

Thermal stresses: Rapid Thermal Processing, crystal growth

$$\sigma = \alpha Y \Delta T$$

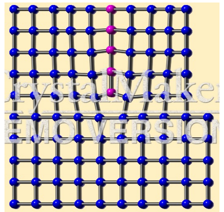
σ is the thermal stress, α is the thermal expansion coefficient, Y is the Young's modulus and ΔT the temperature difference.

When thermal stress exceeds yield strength, plastic deformation can happen leading to defects.

For Si:
Y_{111} = 1.9 x 10^7 N/cm^2, Yield strength ~ 0.5 x 10^4 N/cm^2, α = 2.6 x 10^{-6} /^{o}C

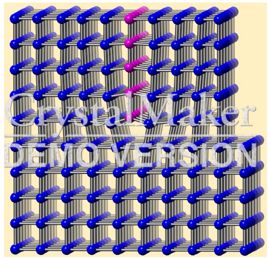
What value of ΔT could lead to defect formation?

Dislocations



- dislocation is a 1D defect
- for example, insertion of an extra line of atoms or vacancies into an otherwise perfect lattice
- the inserted line is typically the same kind as the host material, i.e. Si in Si

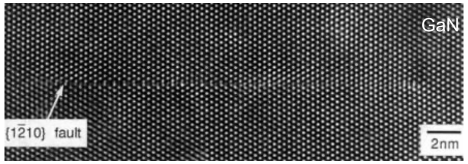
Stacking faults



Example from Crystal Maker software package

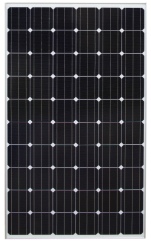
- A stacking fault can be considered as a 2D version of a dislocation
- A missing crystal plane is called an intrinsic stacking fault
- An extra plane is called an extrinsic stacking fault
- A stacking fault terminates in a dislocation

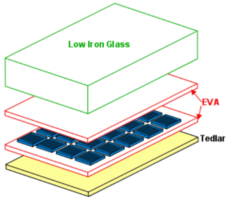
Stacking faults

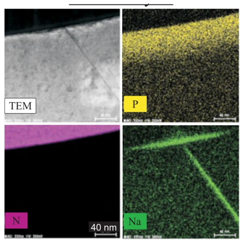


Electron microscopy group, Department of Materials Science and Metallurgy, University of Cambridge. http://www-hrem.msm.cam.ac.uk/gallery/pics/ganlarge.jpg

A practical example of degradation of solar cells due to stacking faults







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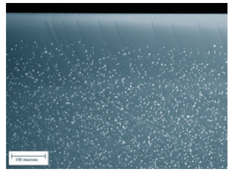
Precipitates and voids

- Precipitates are 3D defects. Agglomeration of point, line and 2D defects. Typically of foreign atoms or molecules in an otherwise crystalline material.
  - Can be of large size ~ micro meters
  - Local order of the precipitated species, can be different from the crystal of interest => bounded by lower order defects
  - Precipitation of unwanted impurities is a technique to keep them away from device regions
- Voids are usually not present in grown crystals. But we would see examples in SOI wafers later on.

Image of oxygen precipitates in Si wafer from G. K. Su (MEMC), Controlling dislocations and bulk microdefects on fabricated wafers to prevent device leakage, http://www.micromagazine.com/archive/03/07/su.html



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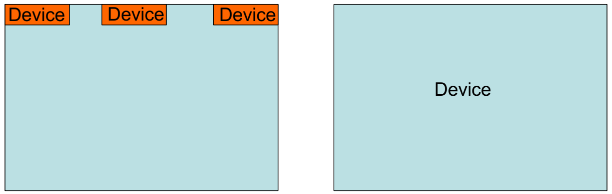
Defects and device regions in a wafer



Example: VLSI

Examples: some of the power devices, photovoltaics

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Properties of planes and directions in *cubic crystals*

- A plane and the direction normal to the plane have the same indices
- The separation between two adjacent planes is given by

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

- The angle between directions [$h_1k_1l_1$] and [$h_2k_2l_2$] is given by

$$\cos(\theta) = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2+k_1^2+l_1^2)(h_2^2+k_2^2+l_2^2)}}$$

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