Lecture1: Basic physics of semiconductors

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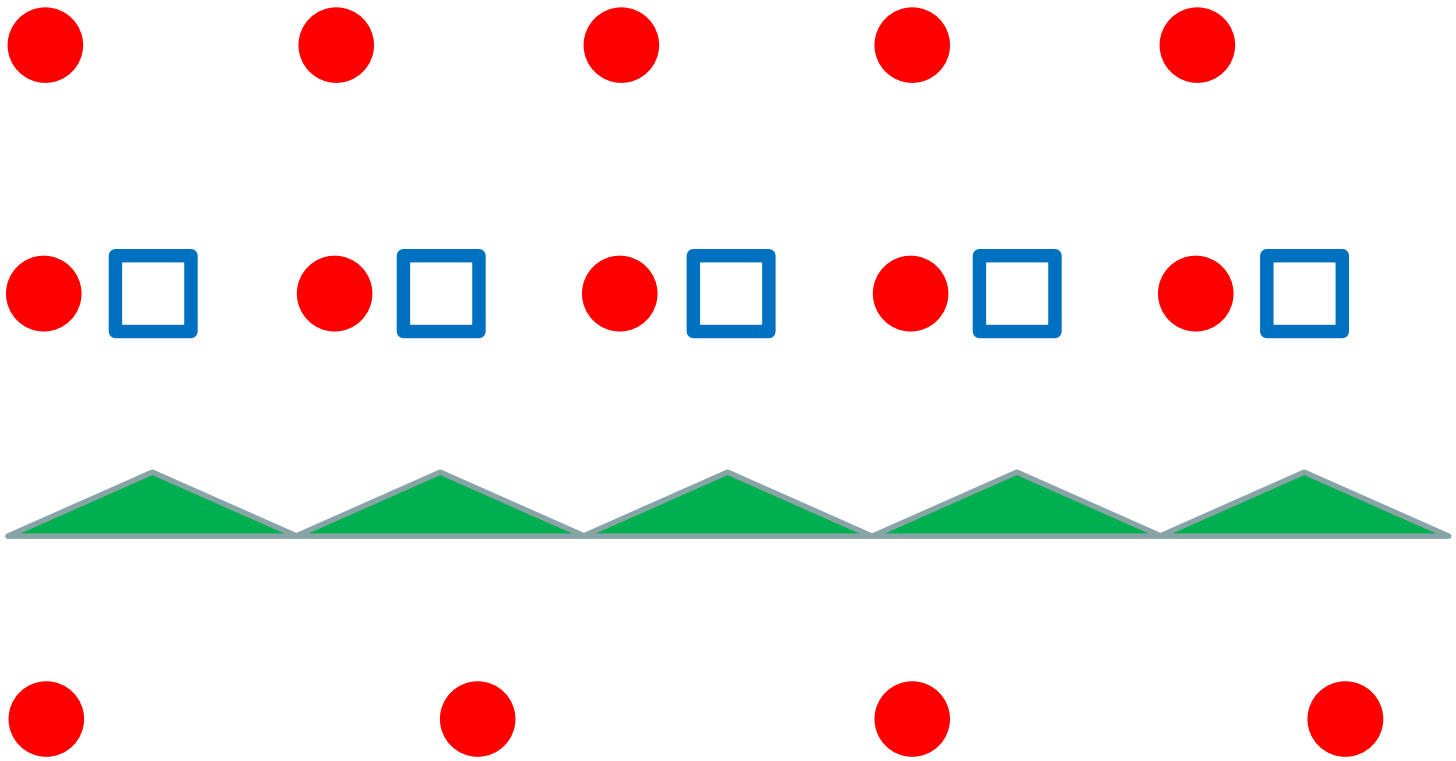
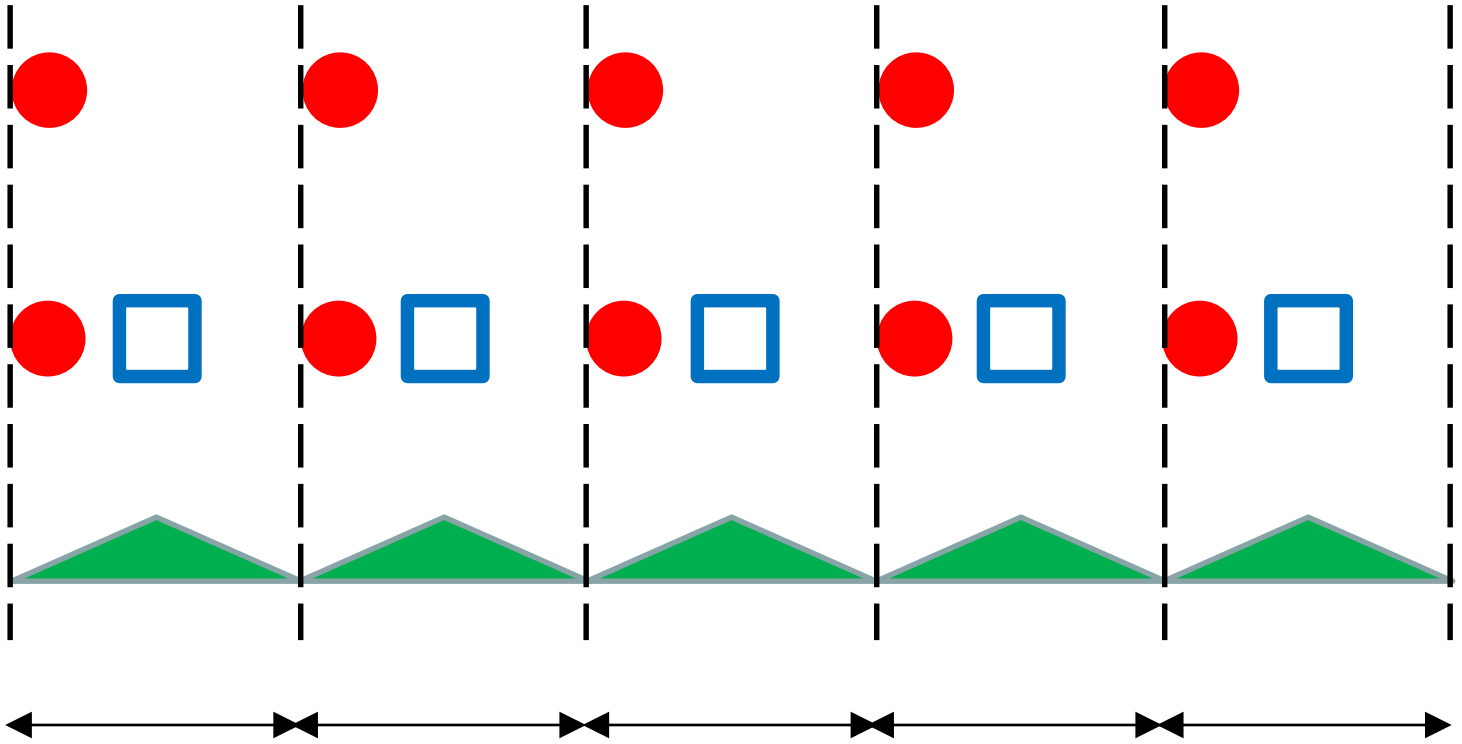
Periodicity

- Find one with a different period. (They are 1D patterns.)
  - 1)
  - 2)
  - 3)
  - 4)



Why did I ask it?

- You can easily find the correct solution!
  - 1)
  - 2)
  - 3)

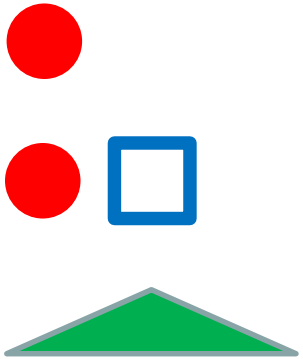


  - They DO share the period. However, they look different.

Now you understand that

- We have to distinguish two different quantities.
  - Periodic array of points (“Lattice” in our terminology)

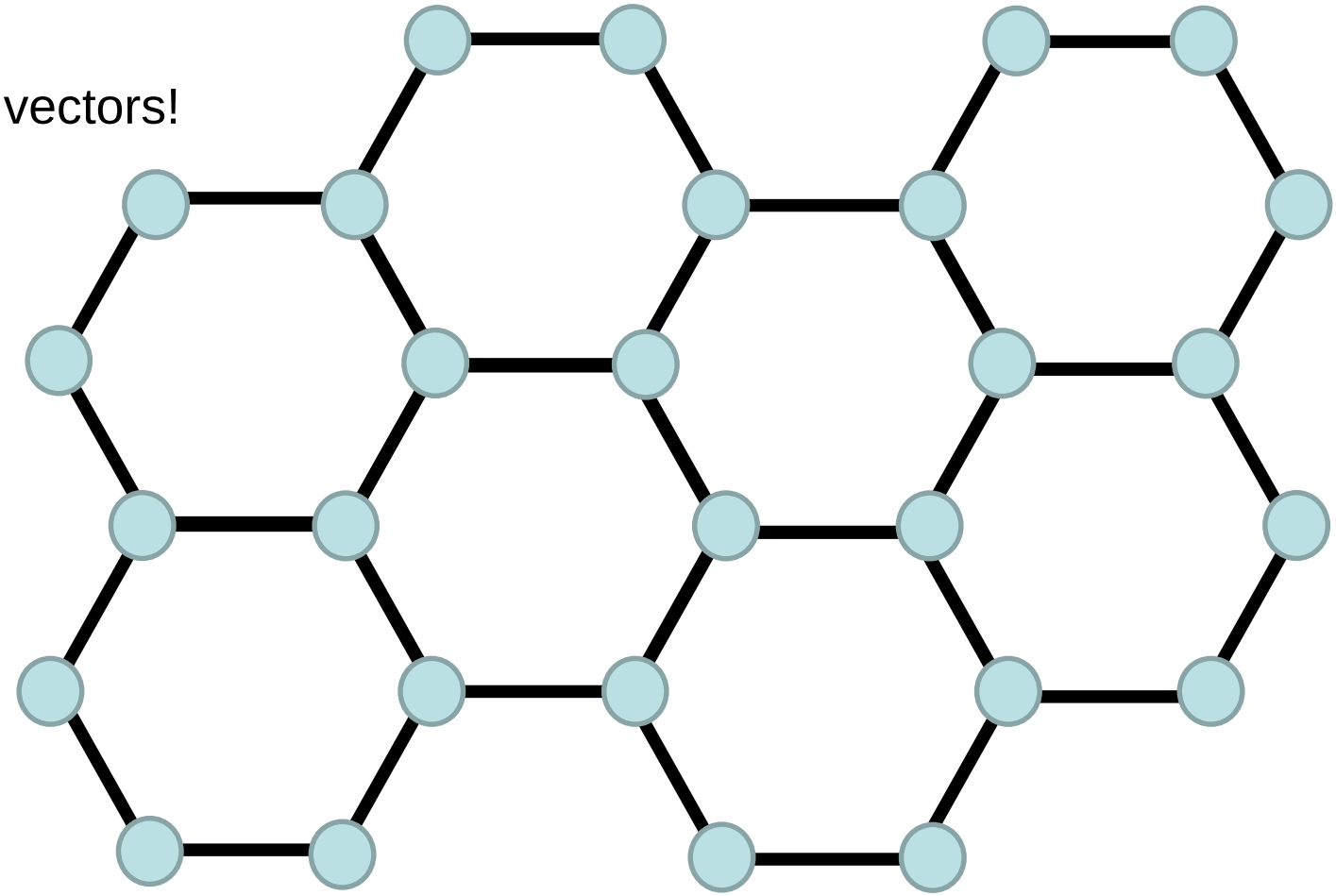
  - Pattern to be repeated (“Basis” in our terminology)



- Non-trivial 2D example?

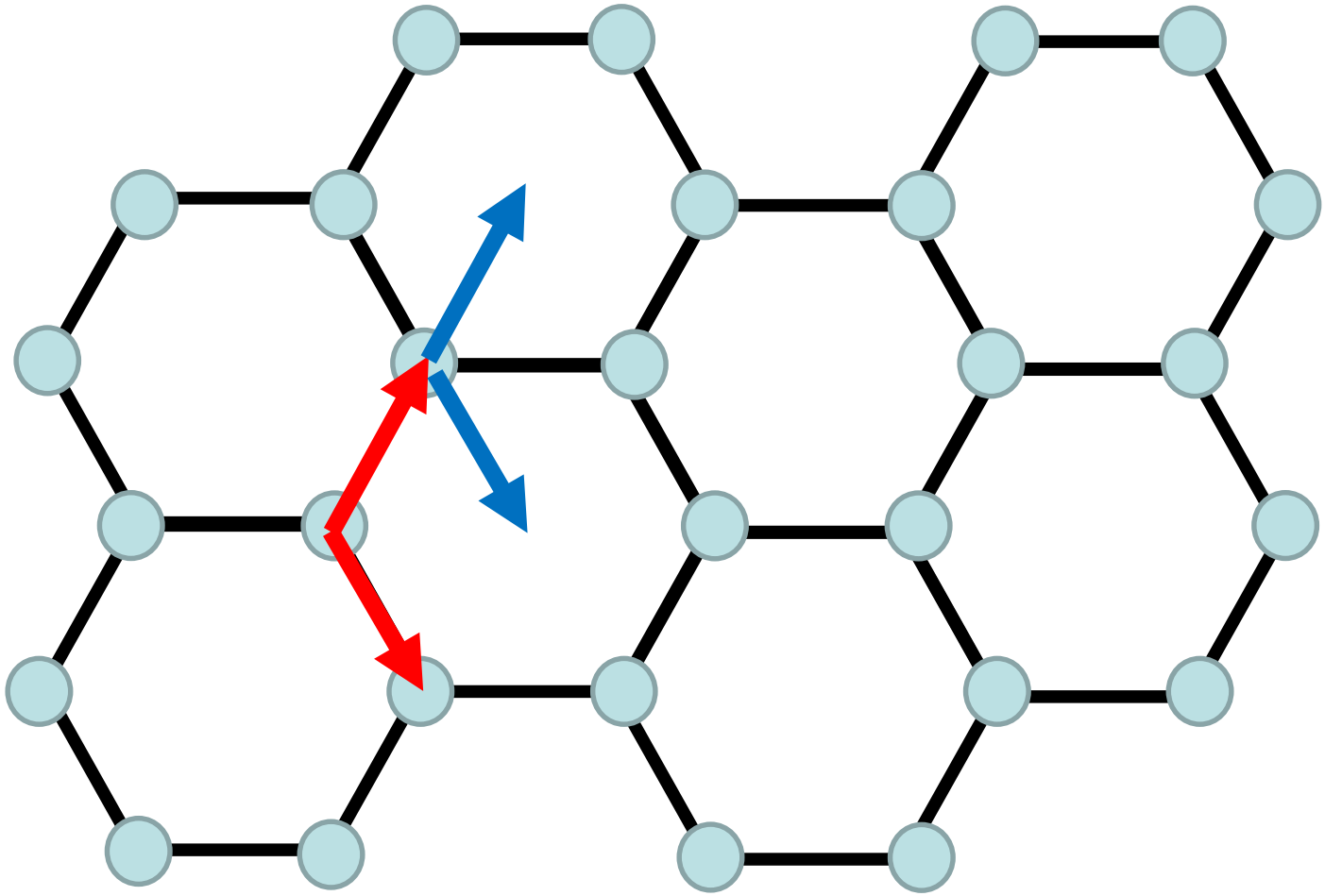
Graphene

- Single layer of carbon atoms in a 2D hexagonal lattice.
  - Find two vectors!



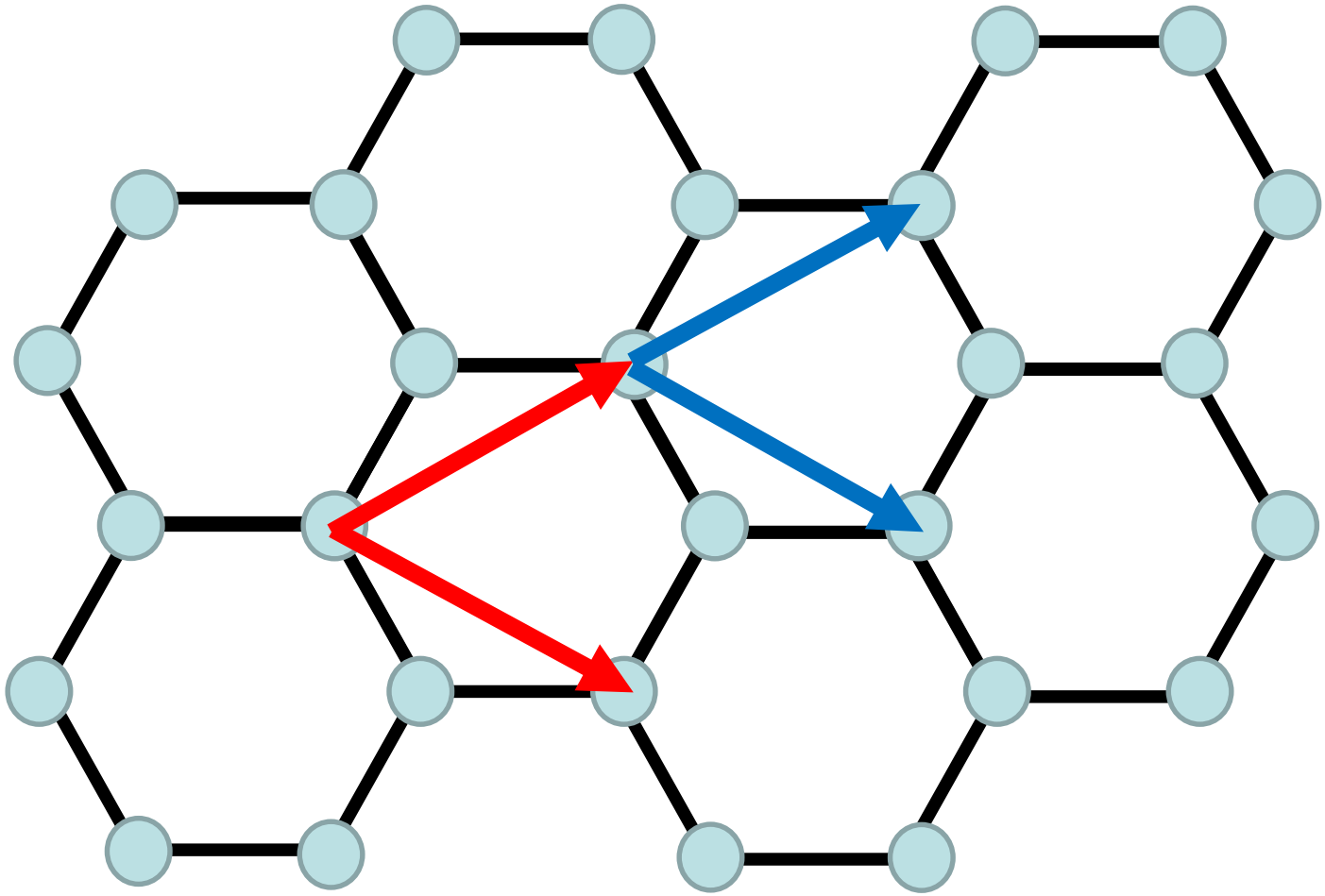
First trial

- A wrong answer!



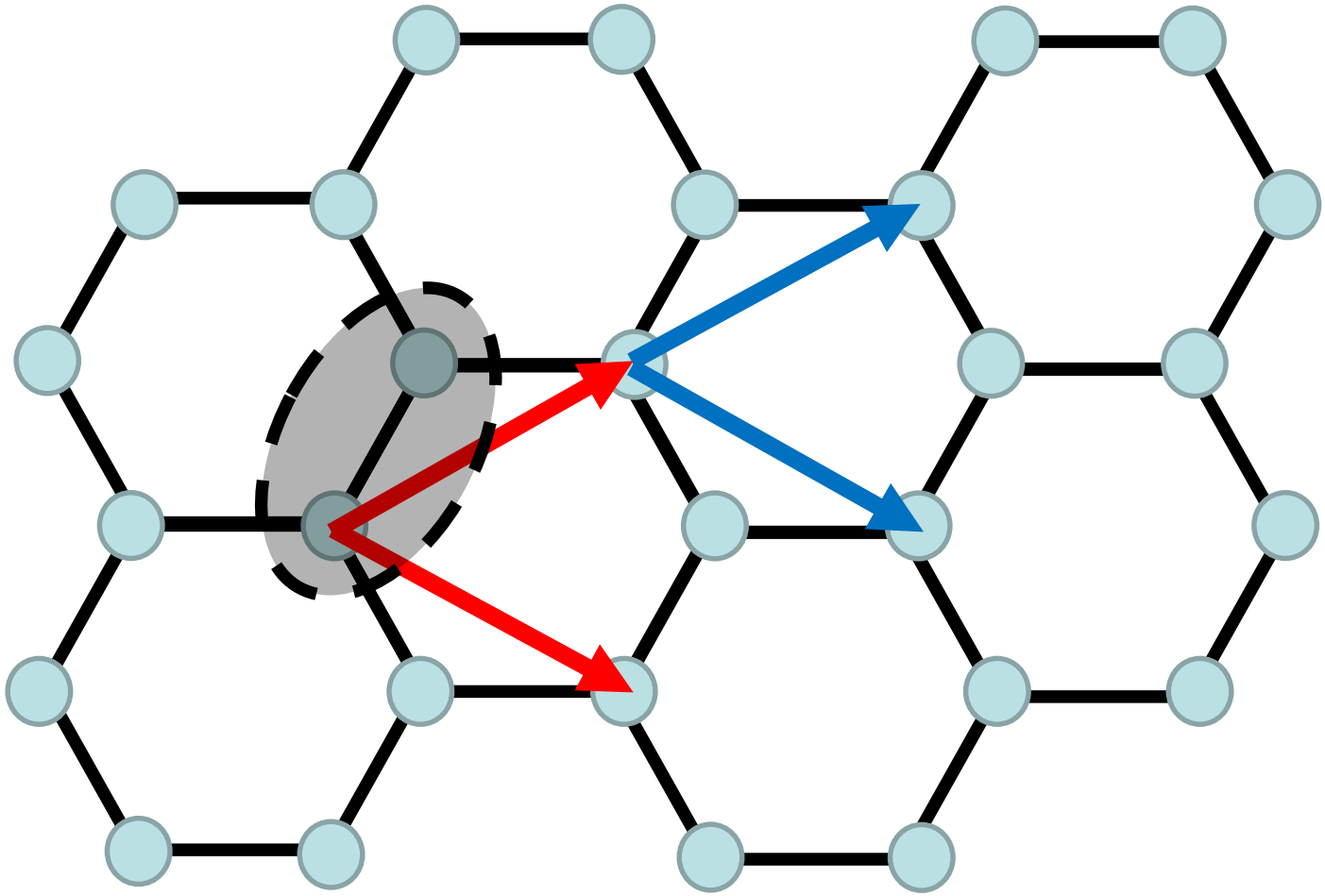
Lattice vectors

- Vectors connecting the second nearest neighbors.



Basis

- Two neighboring atoms consist of the basis.



Basis

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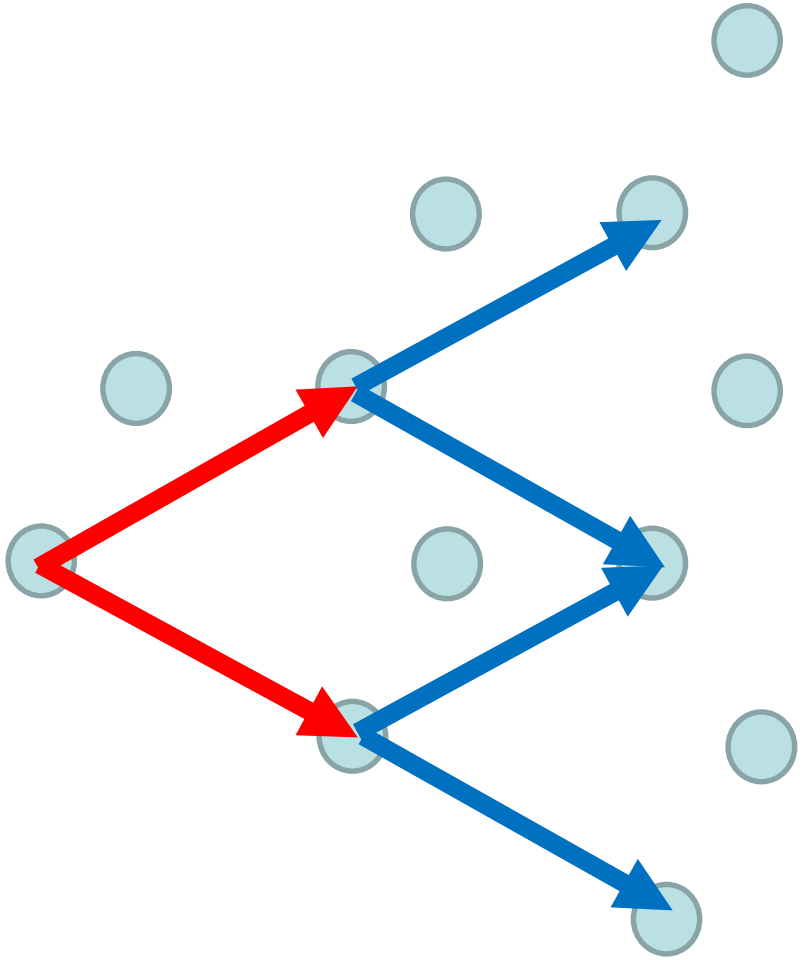
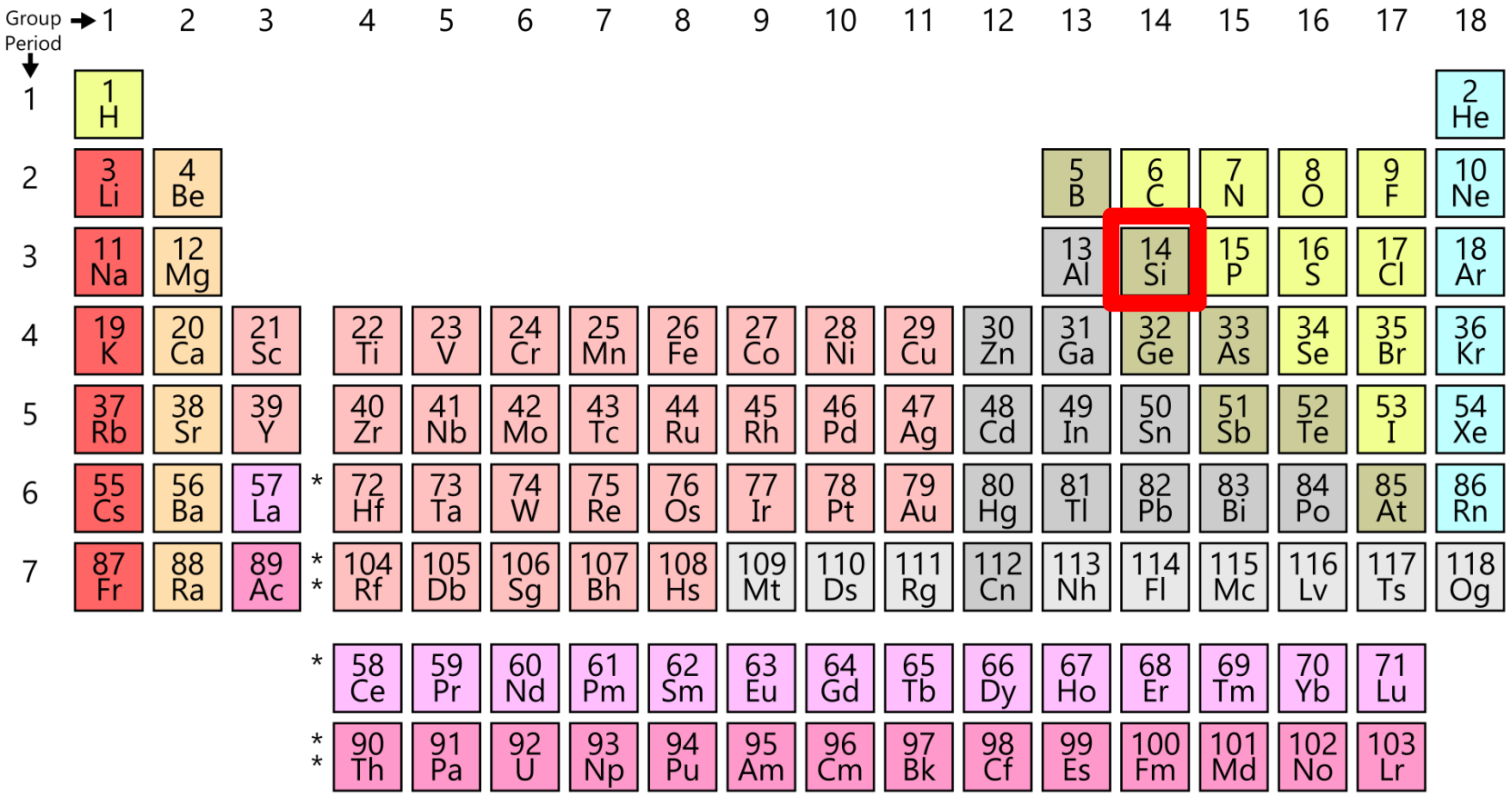


Silicon

- Atomic number: 14



Periodic table (Wikipedia)

Face-centered cubic (fcc)

- Lattice points of the simple cubic lattice
  - For example, (assuming the edge length of 1)

  (0, 0, 0)

  (1, 0, 0) (0, 1, 0) (0, 0, 1)

  (1, 1, 0) (1, 0, 1) (0, 1, 1)

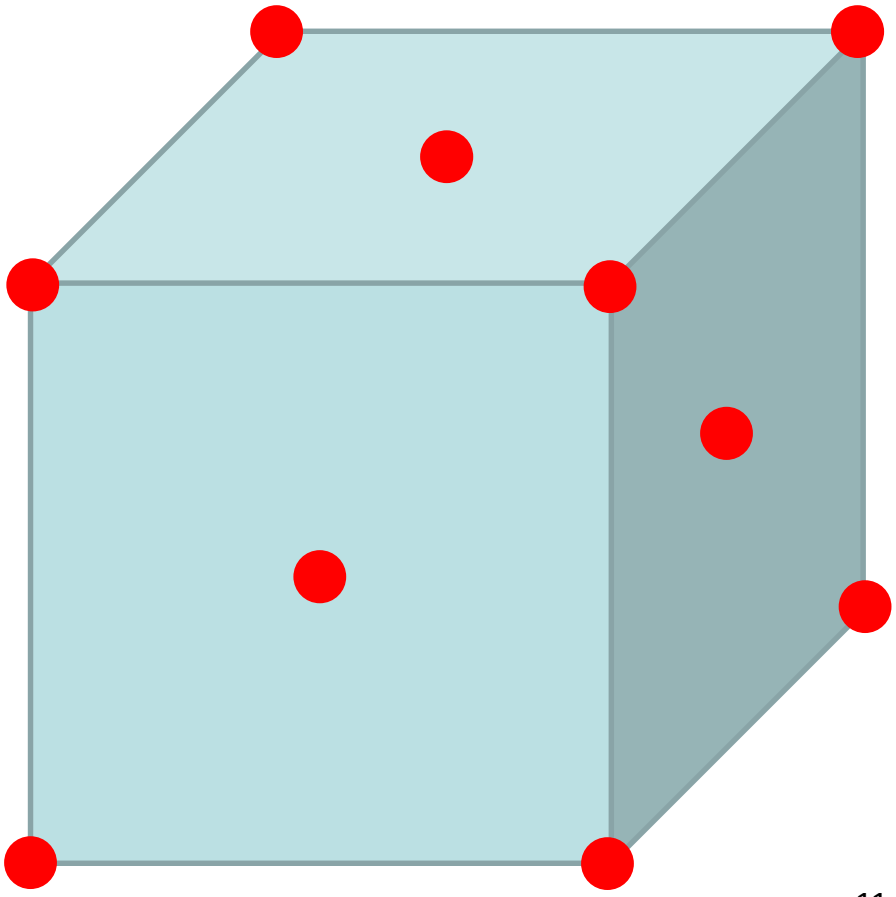
  (1, 1, 1)

- Lattice points at all faces
  - For example,

  (0.5, 0.5, 0)

  (0.5, 0, 0.5)

  (0, 0.5, 0.5)



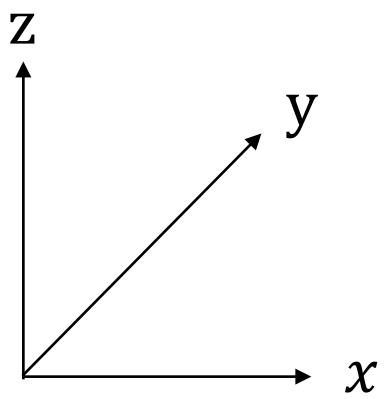
Lattice vectors

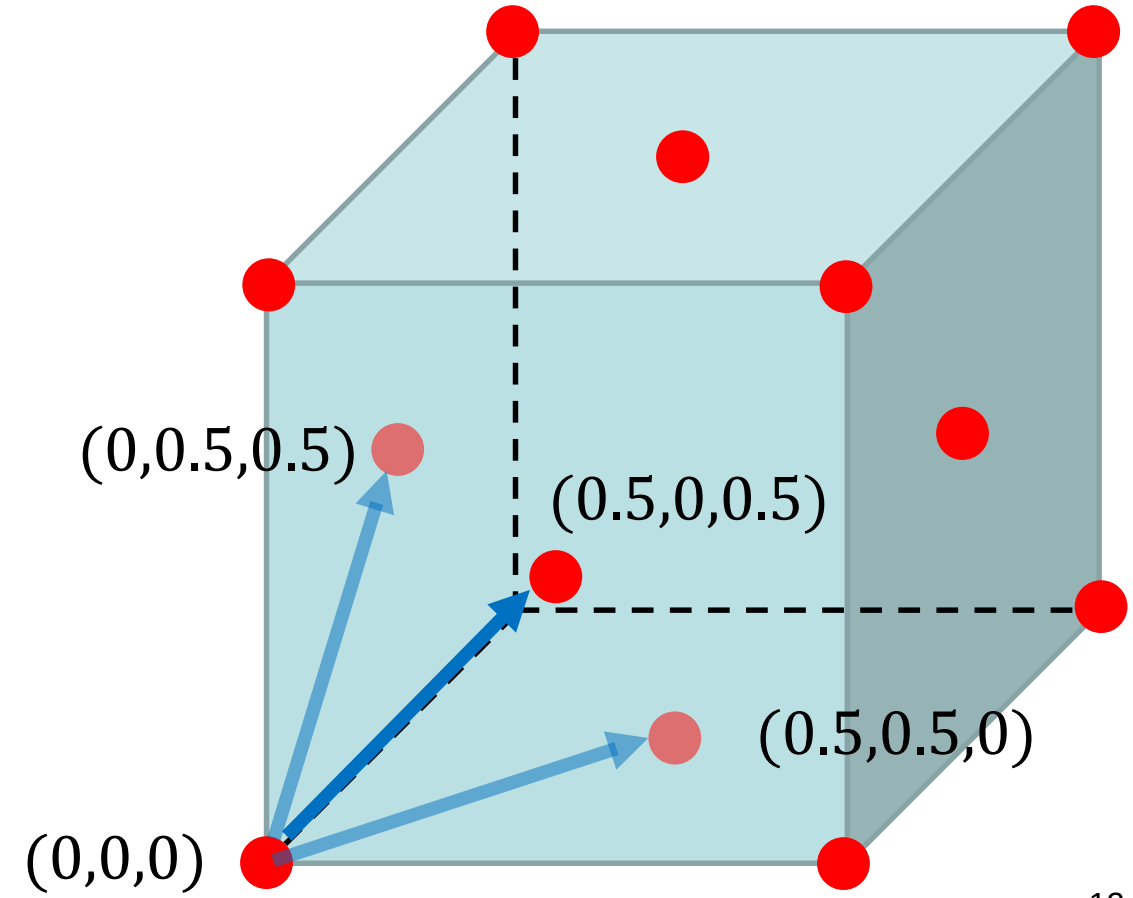
- Three vectors connecting the nearest neighbors.
  - They are

(0.5, 0.5, 0)

(0.5, 0, 0.5)

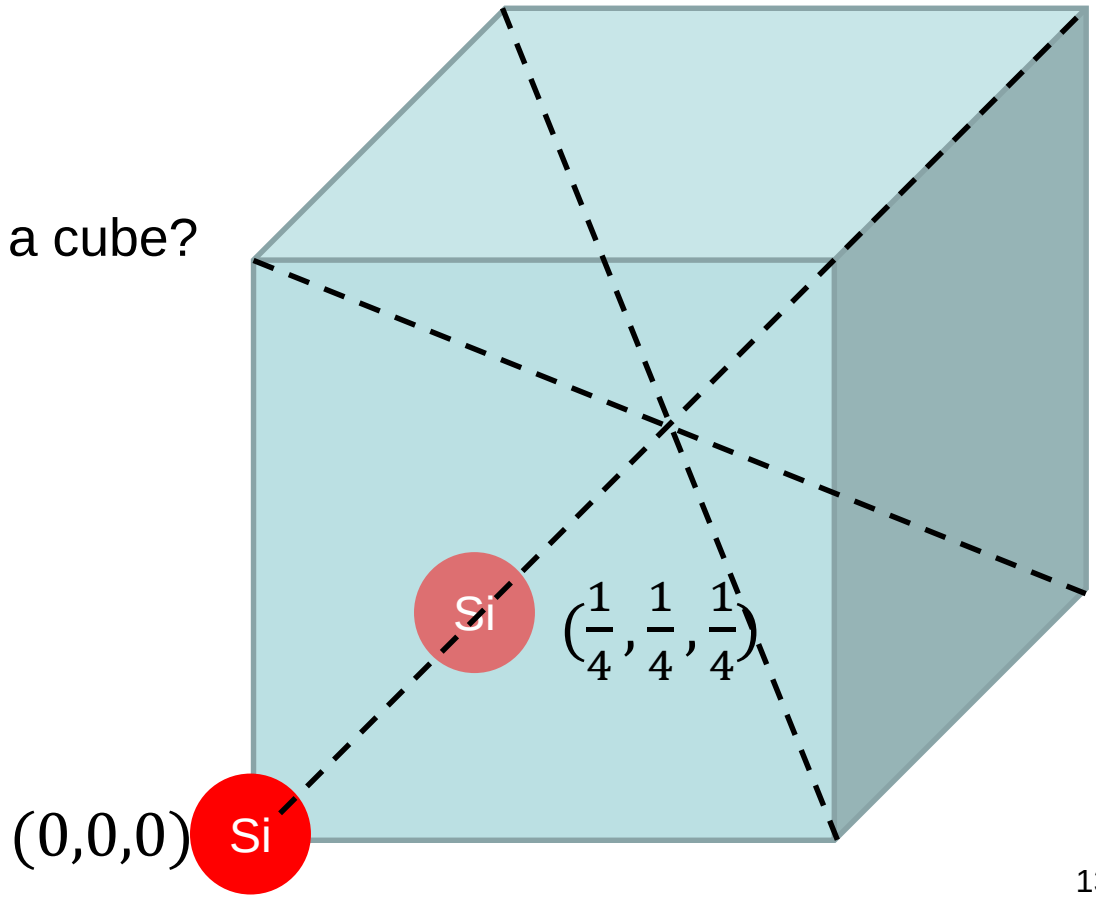
(0, 0.5, 0.5)





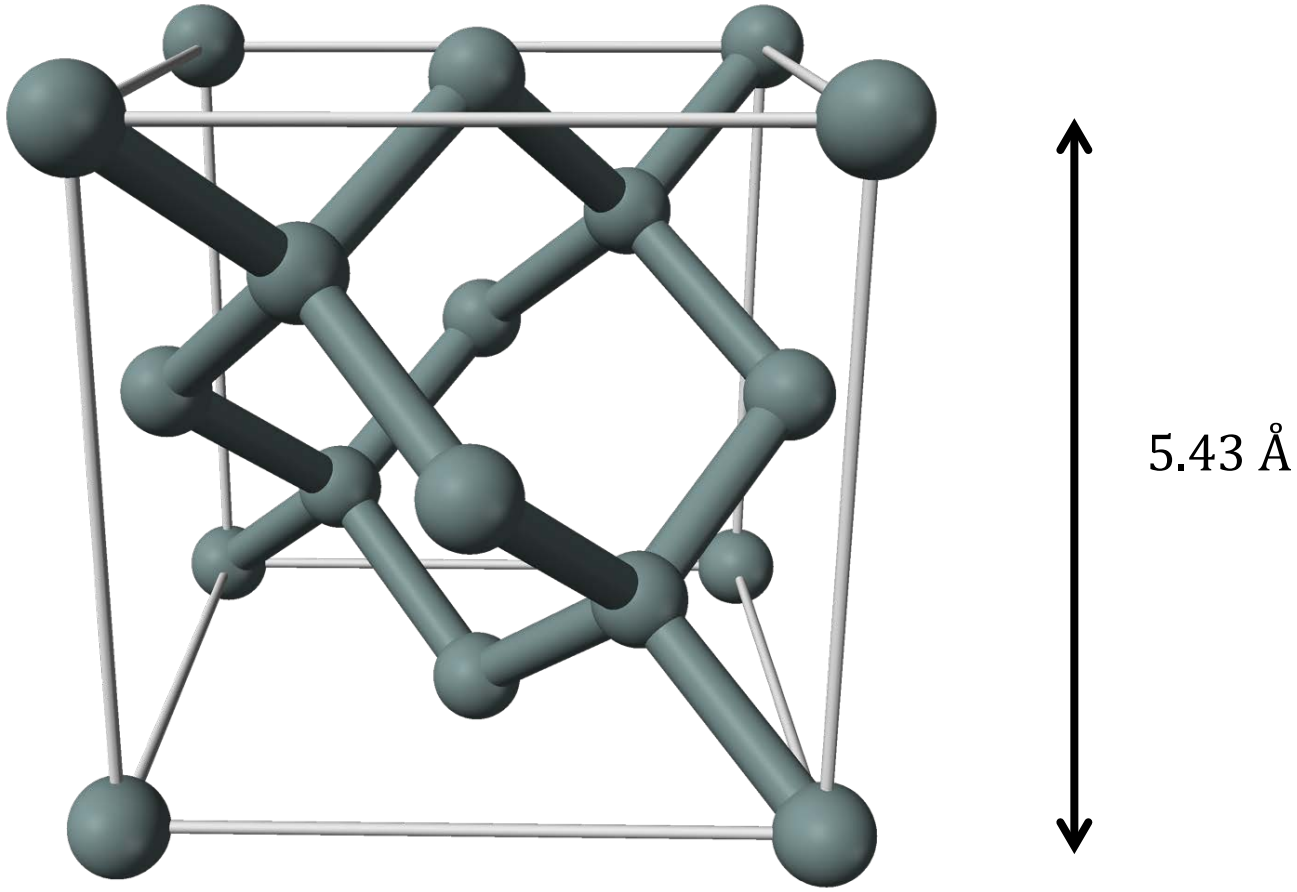
Basis

- Two silicon atoms
  - When an atom is placed at (0, 0, 0), position of the other one is (0.25, 0.25, 0.25).
- Question
  - How many atoms in a cube?



Crystal structure of Si

- Diamond cubic crystal structure



Diamond cubic crystal structure (Wikipedia)

Free electron

- Wavefunction, ψ
  - We want to know $\psi(\mathbf{r}, t)$.
  - When the potential is constant, we simply have

$$\psi(\mathbf{r}, \mathrm{t}) \propto \exp\left(i\left(\mathbf{k}\cdot\mathbf{r} - \frac{E}{\hbar}t\right)\right)$$

  - A wave propagating along the direction of $\mathbf{k}$
  - Question) When time is increased by δt, where can we find a point with the same phase?

$$\text{At } t = t_0 + \Delta t,\ \mathbf{r} = \mathbf{r}_0 + ?$$

$$\text{At } t = t_0,\ \mathbf{r} = \mathbf{r}_0.$$

Velocity

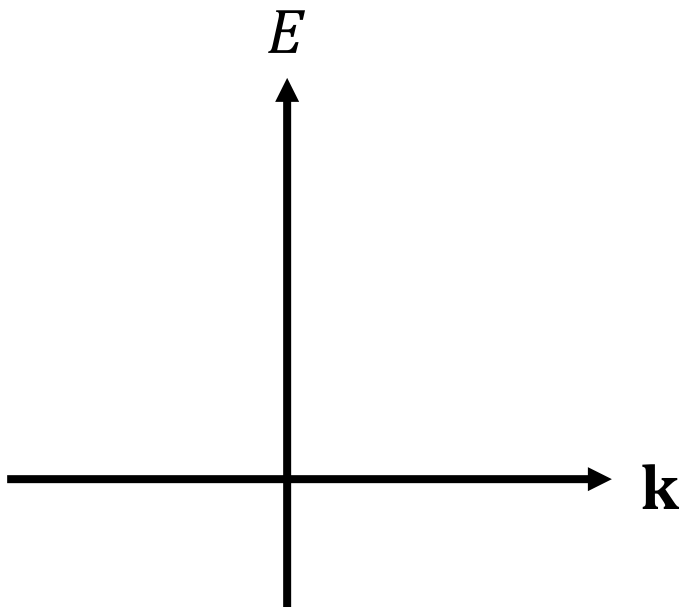
- When the displacement is $\Delta\mathbf{r}$,

$$\mathbf{k}\cdot\Delta\mathbf{r}-\frac{E}{\hbar}\Delta t=0$$

  - Direction: The direction of $\mathbf{k}$
  - Distance during Δt:

$$\frac{|\Delta\mathbf{r}|}{\Delta t}=\frac{1}{\hbar}\frac{E}{|\mathbf{k}|}$$

- Velocity of a free electron
  - Energy, E
  - Wave vector, $\mathbf{k}$

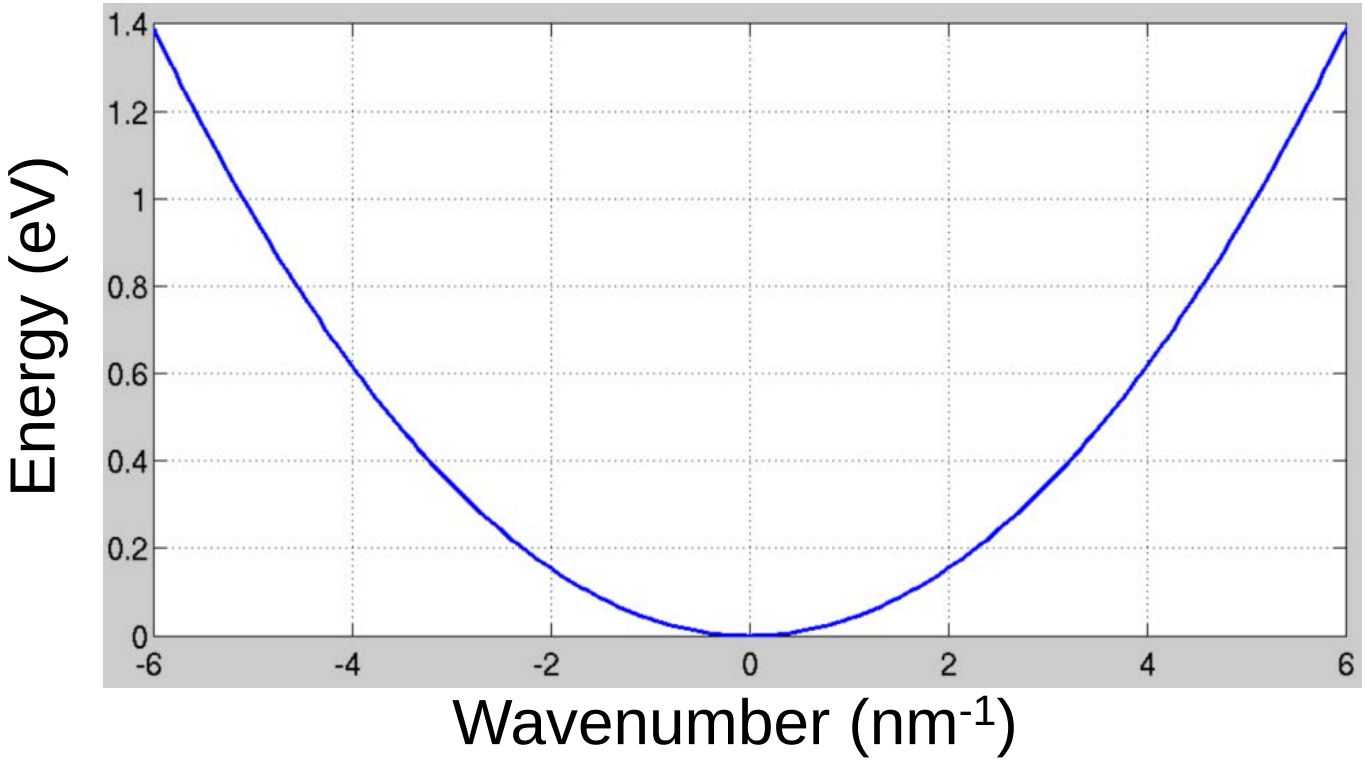


$E - \mathbf{k}$ relation

- Parabolic relation

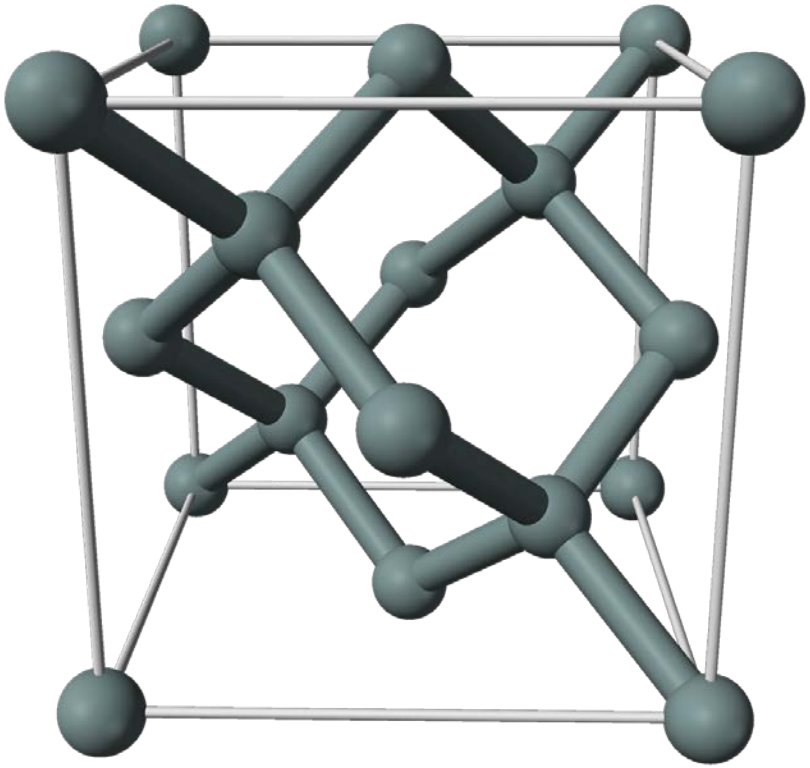
$$E = \frac{\hbar^2}{2m}|\mathbf{k}|^2$$

  - Can you see the gap?

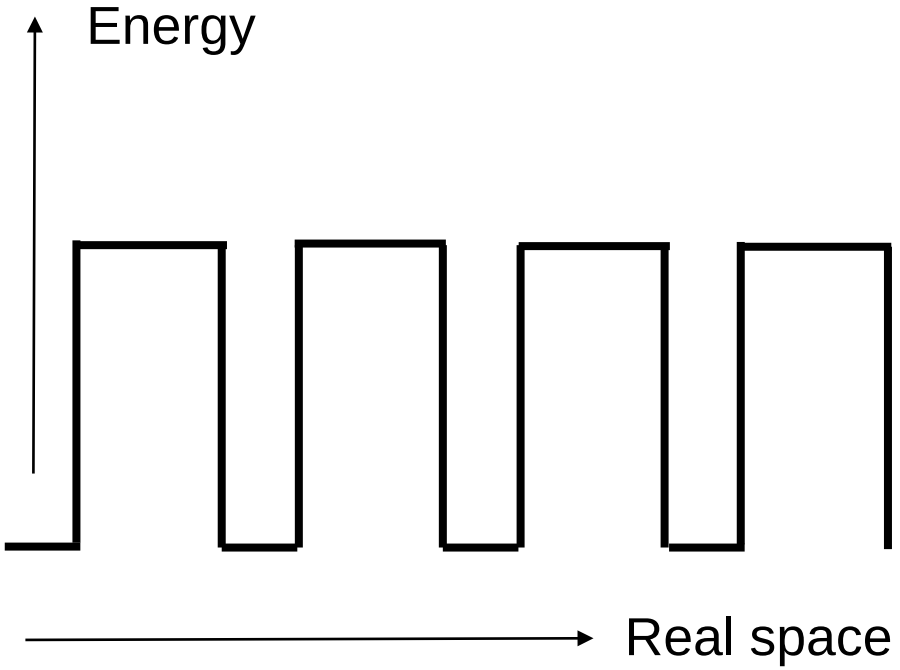


Periodic potential

- Atomic cores are positively charged.
  - Electrons are attracted by them.
  - Potential energy is PERIODICALLY modulated.



Diamond cubic crystal structure (Wikipedia)

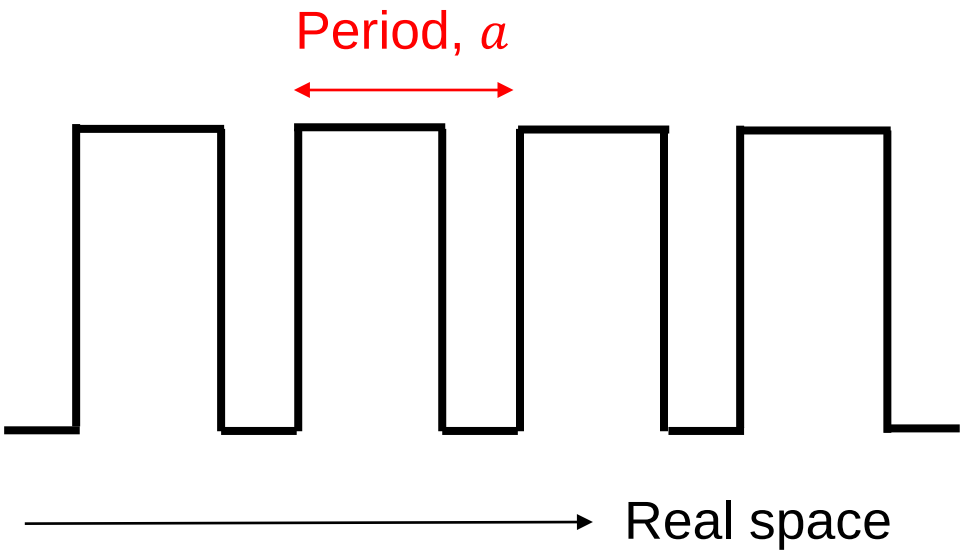


Expansion

- Periodic function can be expanded.
  - With a period of a, the potential energy can be expressed as

$$V(x) = V_0 + \sum_{n=1}^{\infty} V_{c,n} \cos\left(n\frac{2\pi}{a}x\right) + V_{s,n} \sin\left(n\frac{2\pi}{a}x\right)$$

  - Simplest example) $V(x) = V_{c,1} \cos\left(\frac{2\pi}{a}x\right)$



Coupling

- Now, the potential contains $\exp\left(i\frac{2\pi}{a}x\right)$ and $\exp\left(-i\frac{2\pi}{a}x\right)$.
  - Therefore, an operation of $V\psi$ on a free electron, $\exp(ikx)$, yields

$$\exp\left(i\left(k+\frac{2\pi}{a}\right)x\right)$$

and

$$\exp\left(i\left(k-\frac{2\pi}{a}\right)x\right)$$

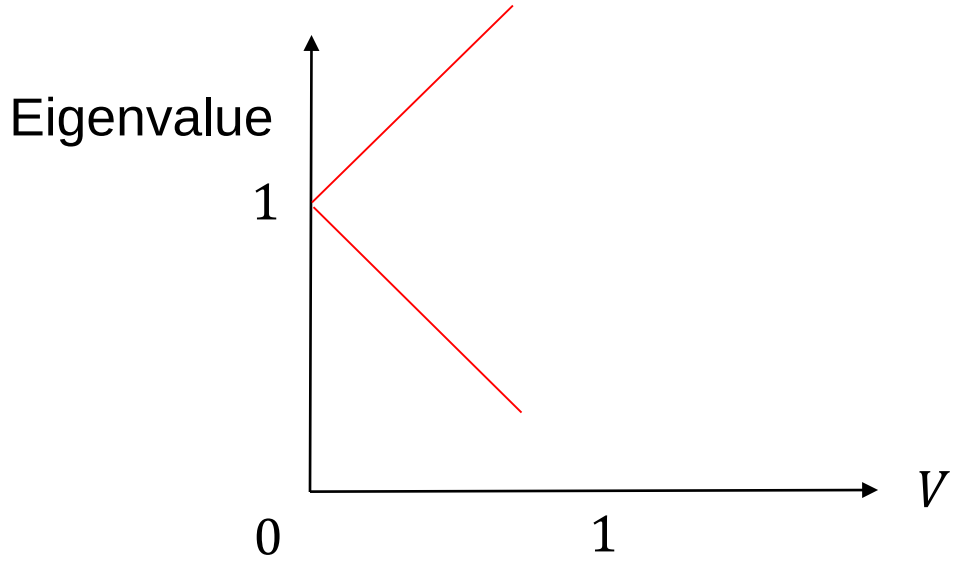
  - When $k=\frac{\pi}{a}$, we have the coupling between $\exp\left(i\frac{\pi}{a}x\right)$ and $\exp\left(-i\frac{\pi}{a}x\right)$.
  - And they have the same energy!

A simple eigenvalue problem

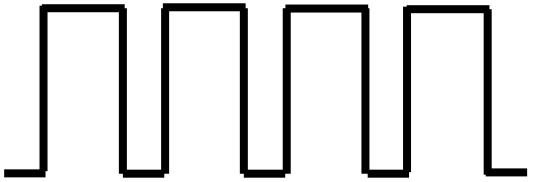
- Solve a simple eigenvalue problem.

$$\begin{bmatrix} 1 & V \\ V & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

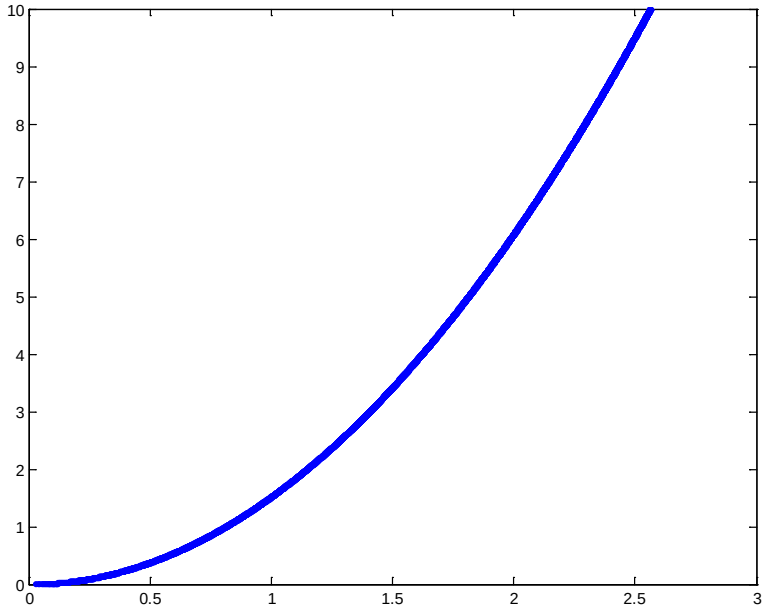
  - Of course, when $V = 0$, two eigenvalues are 1.
  - When $V \neq 0$, two eigenvalues are $1 + V$ and $1 - V$.
  - Two eigenvectors are $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$.

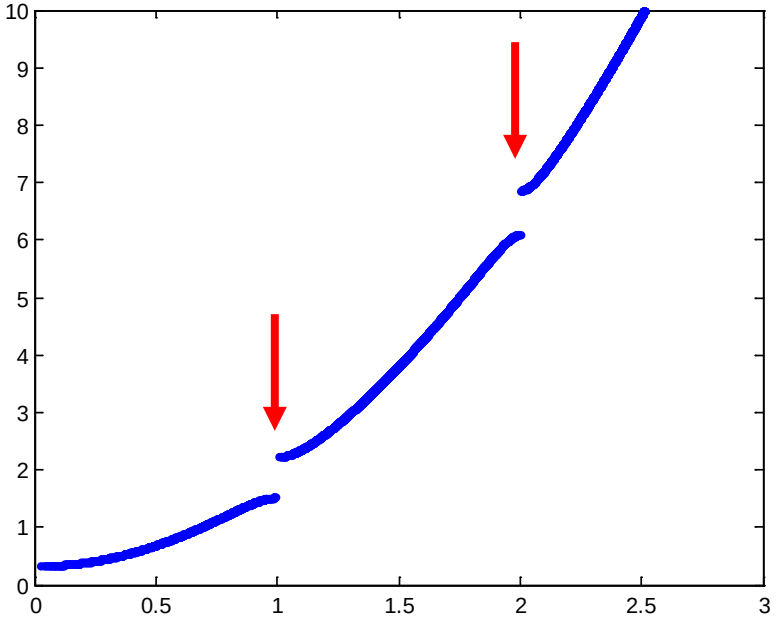


Kronig-Penny model



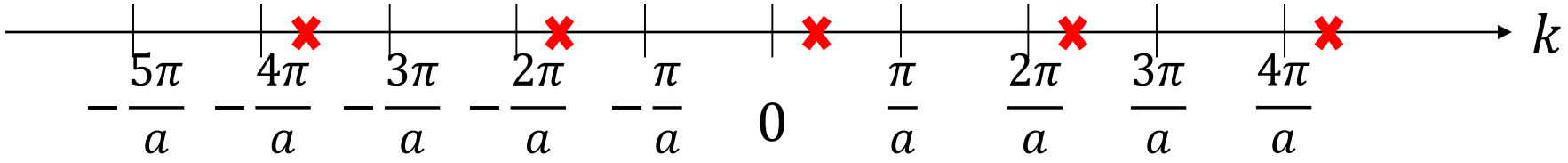
- Square potential
  - (Left) When $V = 0$, it is just a free electron.
  - (Right) When $V \neq 0$, the energy discontinuity is clearly shown.
  - Discontinuity occurs at points such as $\frac{\pi}{a}$, $\frac{2\pi}{a}$, …





1st Brillouin zone

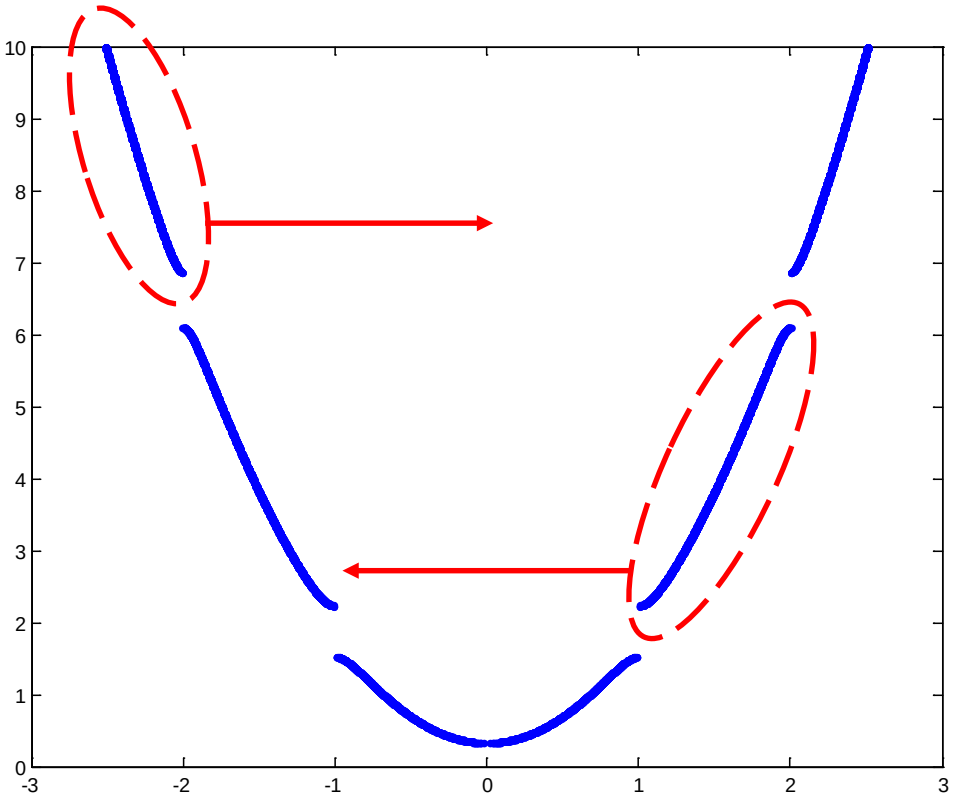
- Shifting the wave number by $\pm\frac{2\pi}{a}$,
  - Following states (Red crosses) are all coupled.

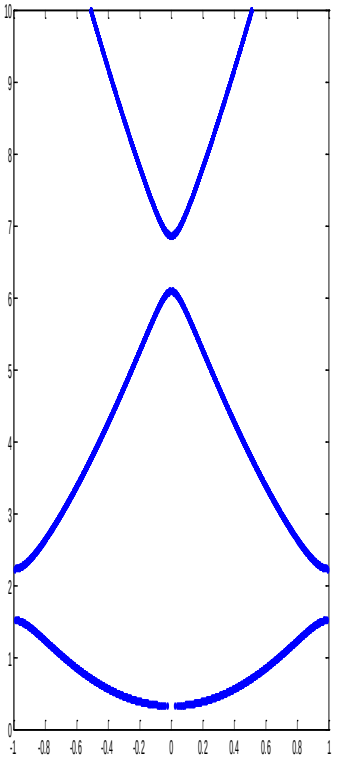


  - Then, instead of $(-\infty,\infty)$, a range of $\left[-\frac{\pi}{a},\frac{\pi}{a}\right]$ is used to represent the wave number axis.
  - Such range is called the "1st Brillouin zone."

1D case

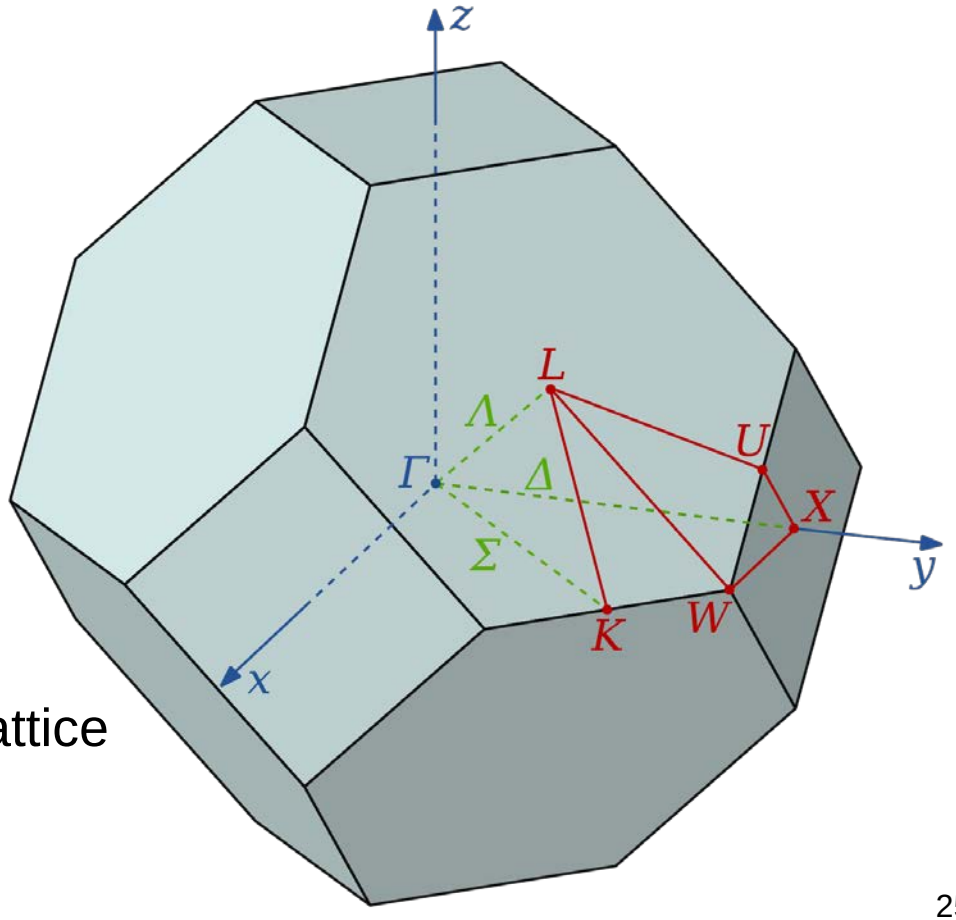
- Consider the Kronig-Penney model.
  - Bands are clearly identified.





3D case

- The 1st Brillouin zone is a volume.
  - How does the Brillouin zone of silicon look like?
  - Silicon has the fcc lattice.



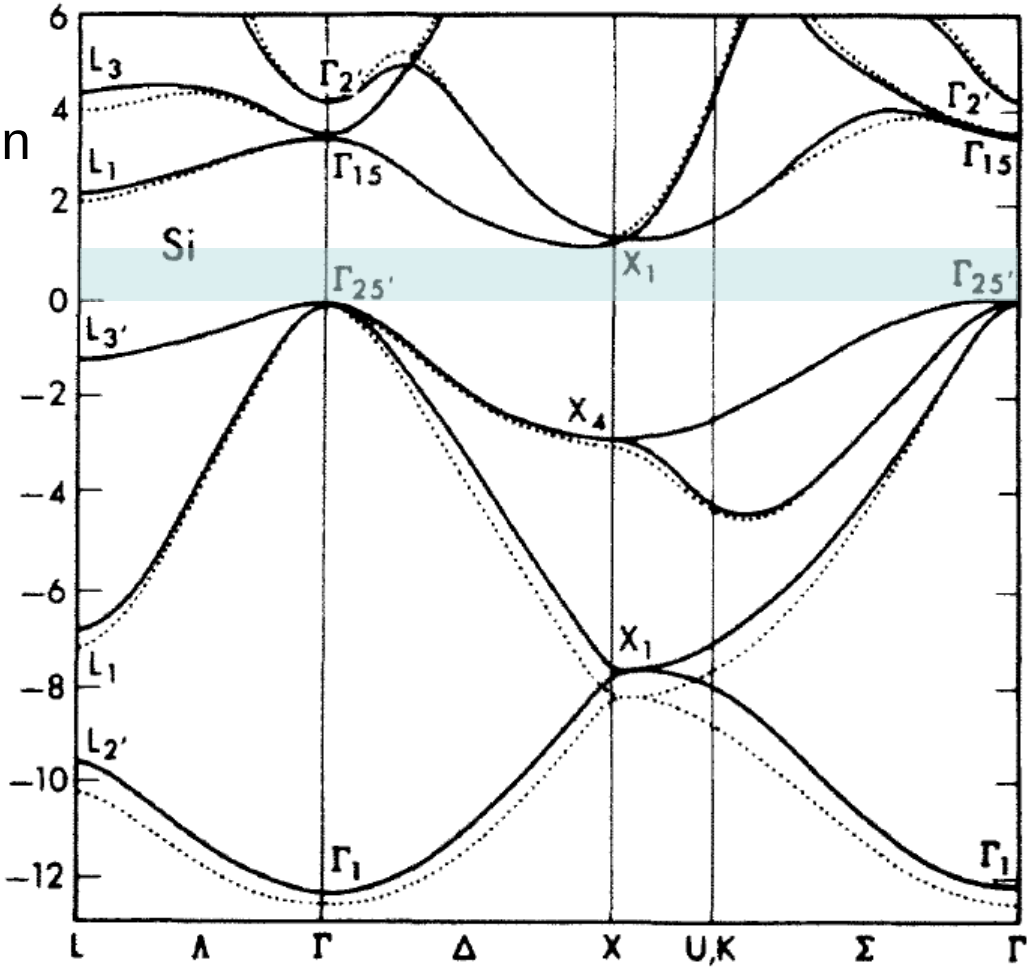
First Brillouin zone of the fcc lattice (Wikipedia)

Band structure

- Band structure of silicon (Band gap ~ 1.12 eV)

Conduction bands

Valence bands



(J. R. Chelikowsky and M. L. Cohen, PRB, vol. 14, p. 556, 1976)

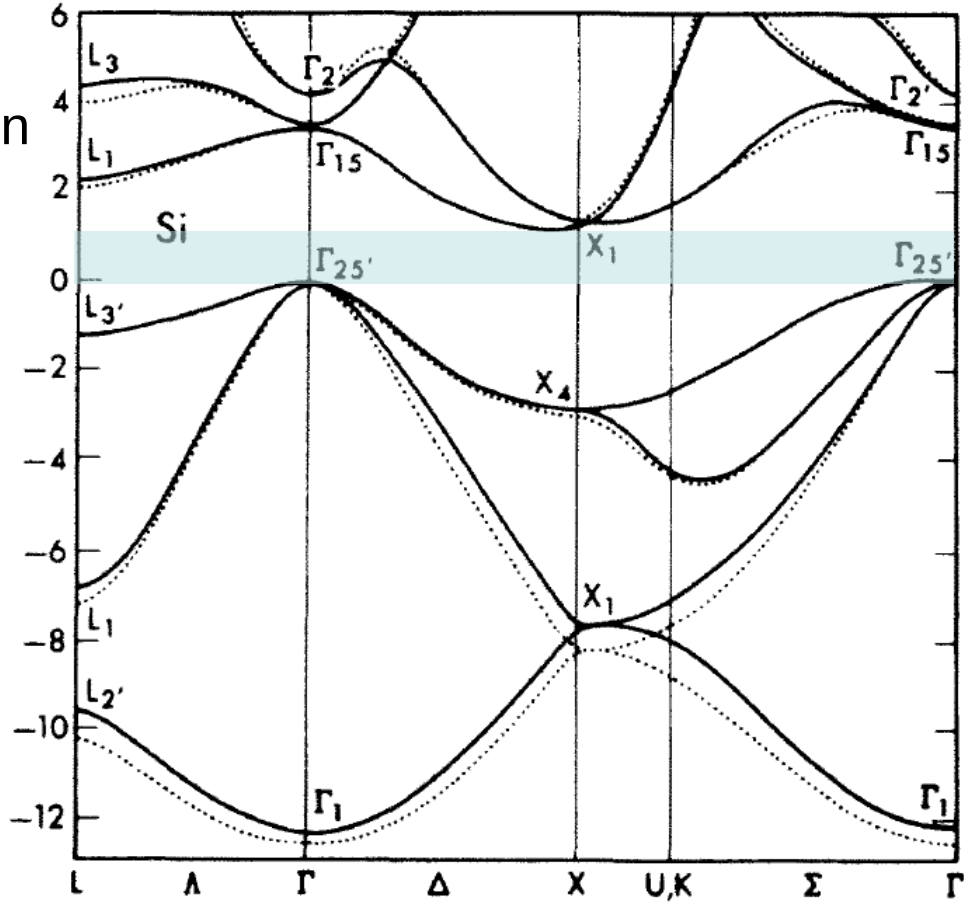
Wavevector

At 0 K

- Valence bands are fully filled by electrons.
- Conduction bands are completely empty.

Conduction bands

Valence bands

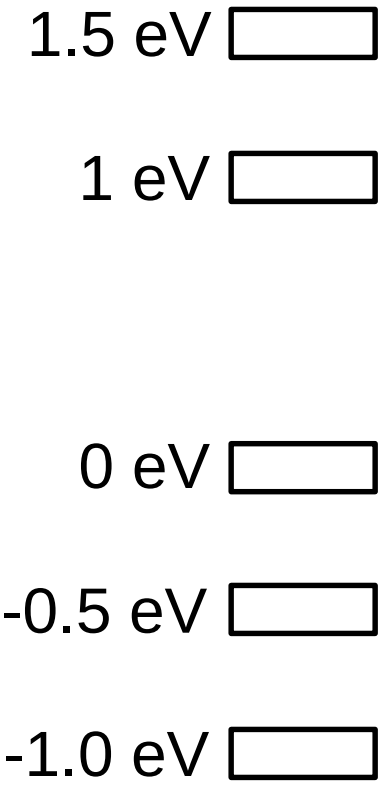


Fully *un*occupied

Fully occupied

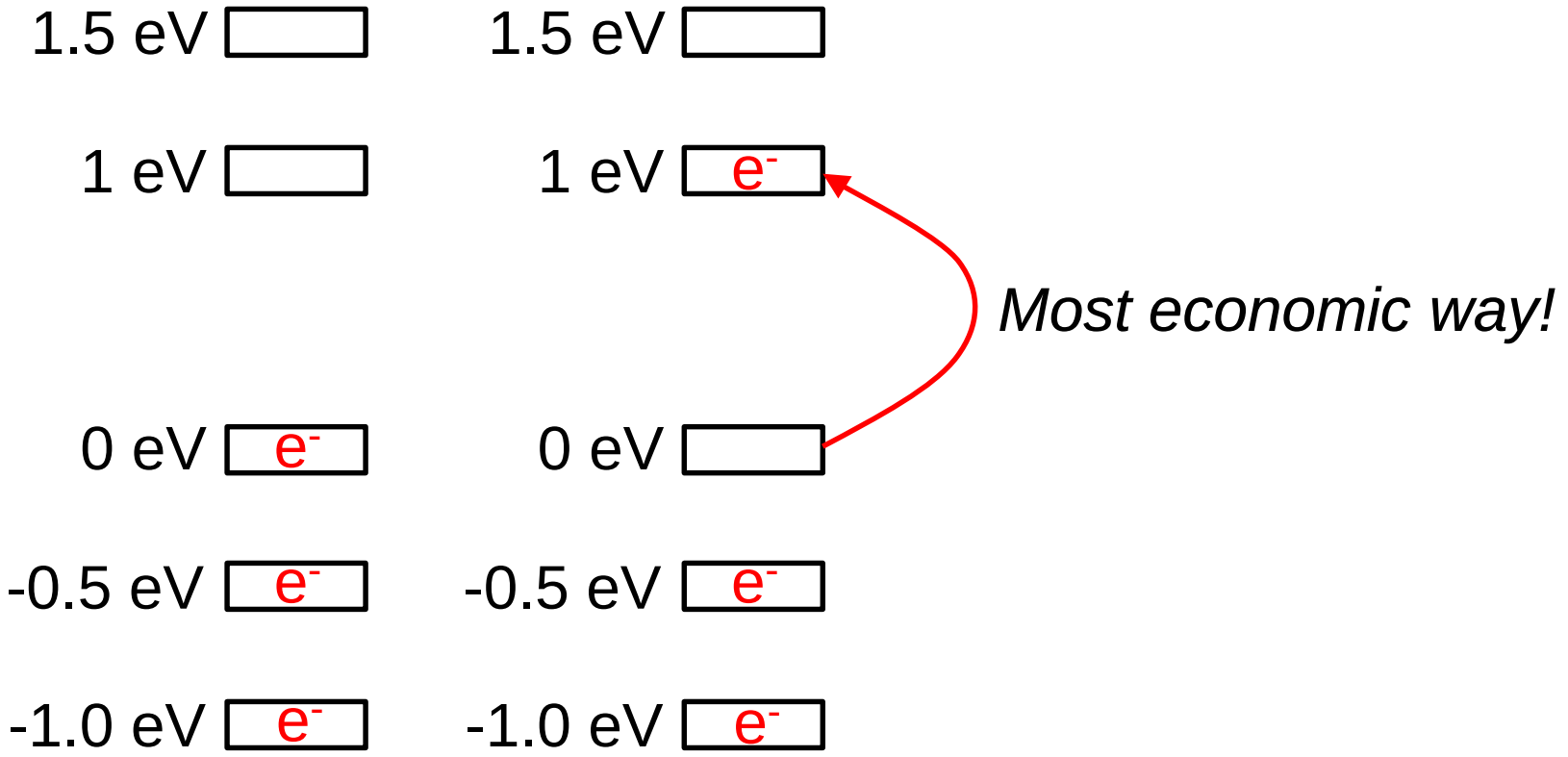
At a non-zero temperature

- Electrons gain thermal energies.
  - A small number of electrons can occupy states in the conduction bands.
  - Example) 5 states in a system. 3 electrons.
  - What is the ground energy?
  - What is the second lowest energy?



Answers

- Minimizing an additional energy
  - Occupying the lowest energy state in the conduction bands
  - Leaving a “hole” in the valence bands.



Higher temperature

- Electrons gain even larger thermal energies.
  - More electrons in the conduction bands
  - More holes in the valence bands
- How many electrons are in the conduction bands?
  - The answer is the intrinsic carrier density, n_i, at a given temperature.
  - Expression of n_i (Silicon)

$$n_i = 5.2 \times 10^{15}\, T^{1.5} \exp\left(-\frac{E_g}{2k_B T}\right) \quad \text{(electrons/cm}^3\text{)}$$

  - Note that k_B is the Boltzmann constant.

Razavi, Example 2.1

- Intrinsic carrier densities at different temperatures
  - At 300 K, 1.08 X 10^{10} electrons/cm^3
  - At 600 K, 1.54 X 10^{15} electrons/cm^3

- What is the meaning?
  - When we have a pure silicon (without any impurities) ➔ Intrinsic
  - The density of both electrons and holes ➔ Carrier density
  - Therefore, for the intrinsic material,

$$n = p = n_i$$

At equilibrium,

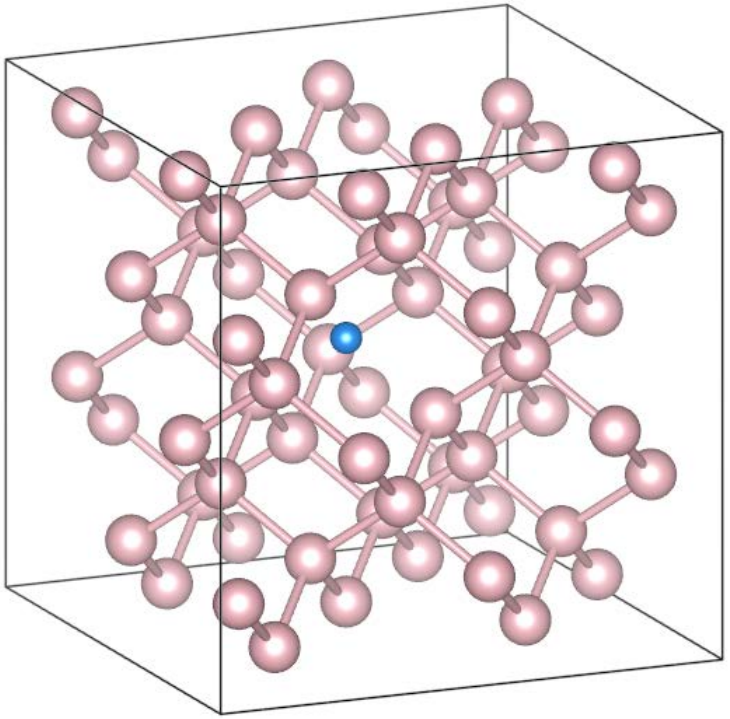
- We have a useful relation.
  - The product between the electron density (n) and the hole density (p) is constant.

$$np = n_i^2$$

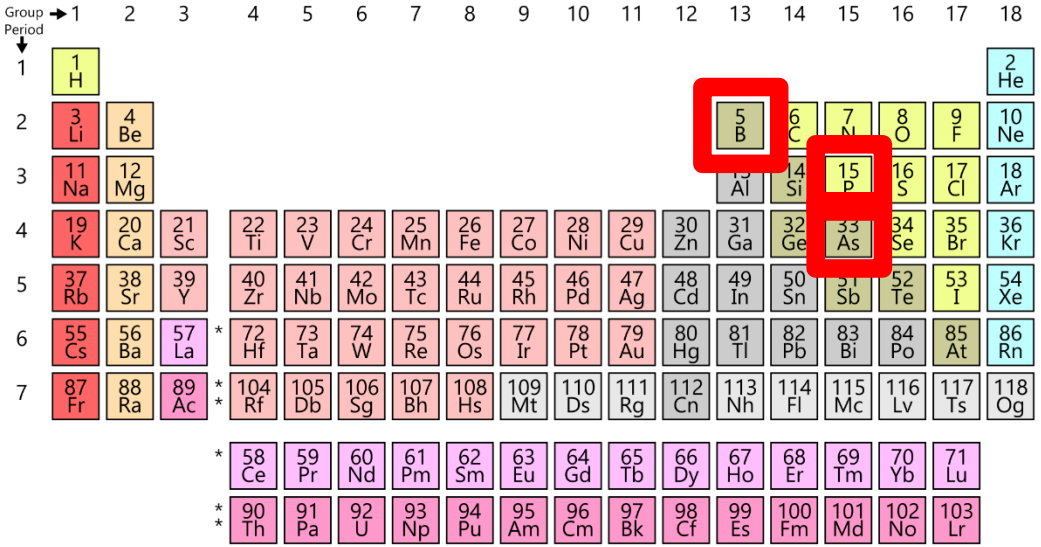
  - For an intrinsic material, it is immediately verified.
  - How about the EXTRINSIC case?

Typical impurity atoms

- The phosphorus (P) atom has 5 valence electrons.
- The arsenic (As) atom, too.
- The boron (B) atom has 3 valence electrons.



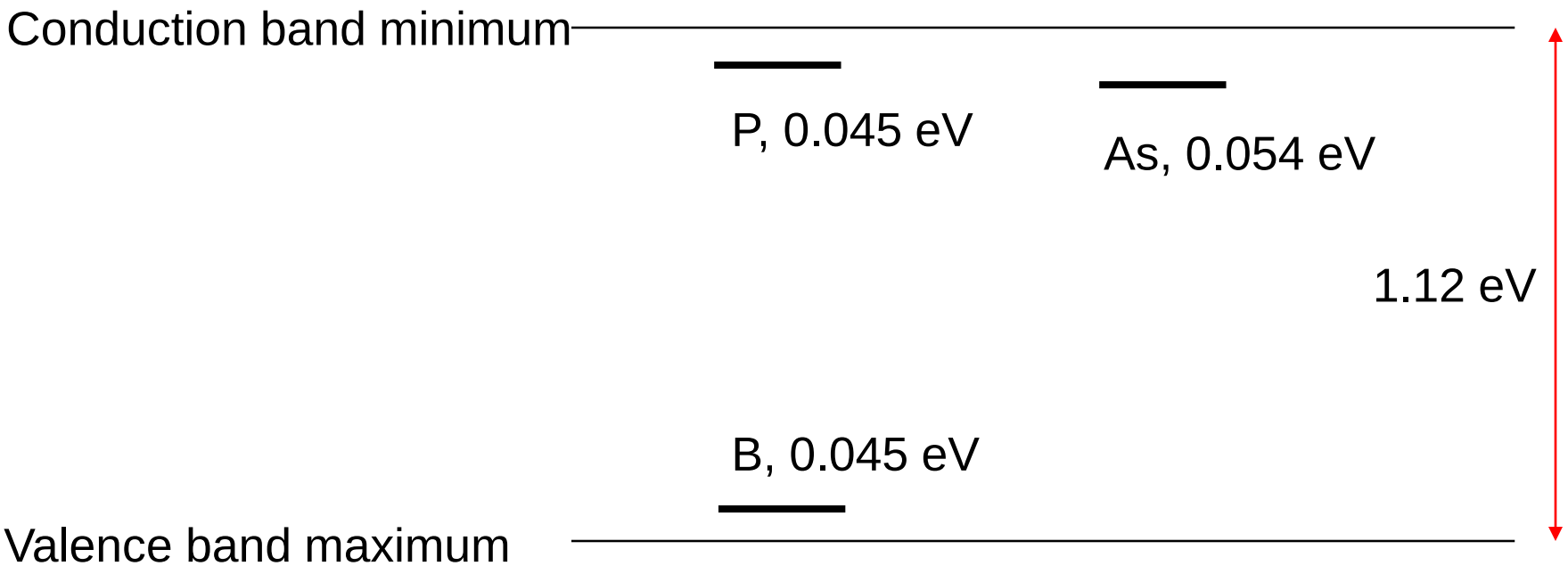
An impurity atom in the silicon crystal



Periodic table (Wikipedia)

Energy states

- Donor (Phosphorus and arsenic)
  - Close to the conduction band minimum
- Acceptor (Boron)
  - Close to the valence band maximum



Results of ionization

- Donor (Phosphorus and arsenic)
  - Positively charged
  - An ionized donor contributes an electron in the conduction bands.
- Acceptor (Boron)
  - Negatively charged
  - An ionized acceptor contributes a hole in the valence bands.
- N_D (/cm^3) donors? N_D electrons in the conduction bands.
- N_A (/cm^3) acceptors? N_A holes in the valence bands.

Numbers

- First of all, the volume density of silicon atoms is 5 X 10^{22} cm^{-3}.
  - The impurity density is limited to ~ 2 X10^{20} cm^{-3}.
- Various impurity densities
  - 10^{15} cm^{-3}: Almost no impurity
  - 10^{17} cm^{-3}: Low (or moderate) impurity density
  - 10^{19} cm^{-3}: High impurity density (Not extremely high)
  - 2 X 10^{20} cm^{-3}: High impurity density (Approximately, the maximum limit)

N-type? P-type?

- Semiconductor doped with donors
  - N-type
  - In the n-type semiconductor, we have

$$n \approx N_D > n_i$$

- Semiconductor doped with acceptors
  - P-type
  - In the p-type semiconductor, we have

$$p \approx N_A > n_i$$

- Majority carriers
  - Electrons in the n-type
  - Holes in the p-type
- Minority carriers

Remember $np = n_i^2$.

- (It is valid only at equilibrium.)
- N-type
  - The electron density is almost equal to N_D.
  - The hole density is

$$p \approx \frac{n_i^2}{N_D}$$

- For the p-type material, $n \approx \frac{n_i^2}{N_A}$.
- Razavi, Example 2.3
  - When the donor density is 10^{16} cm^{-3}, the hole density is about 10^4 cm^{-3}.