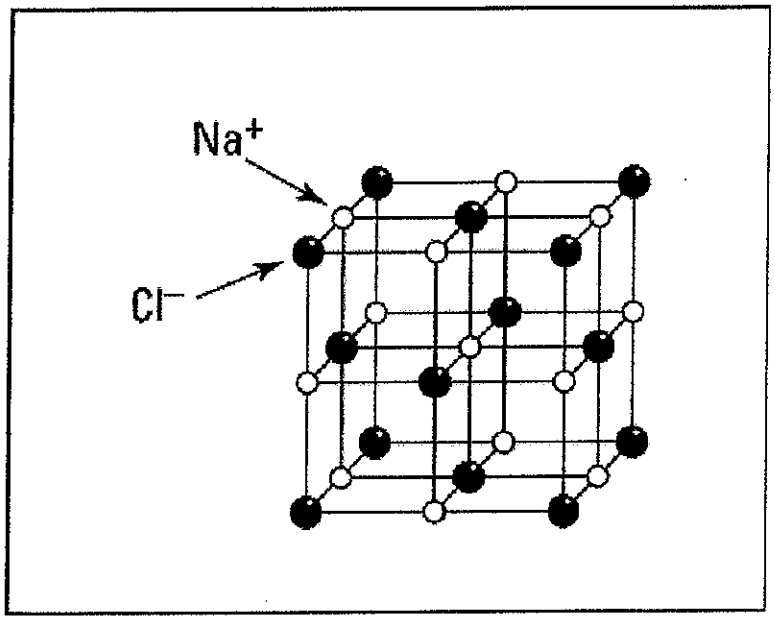
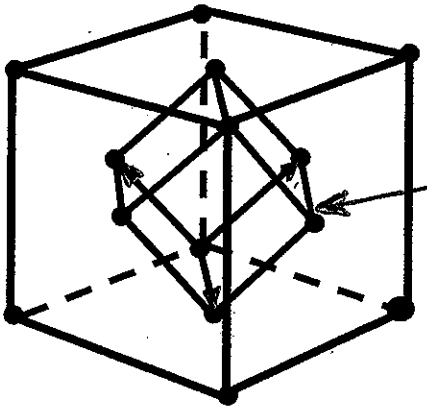
Lecture 3 | Simple Lattices, Symmetry and anisotropy

Na Cl structure



The lattice of NaCl is face-centered cubic

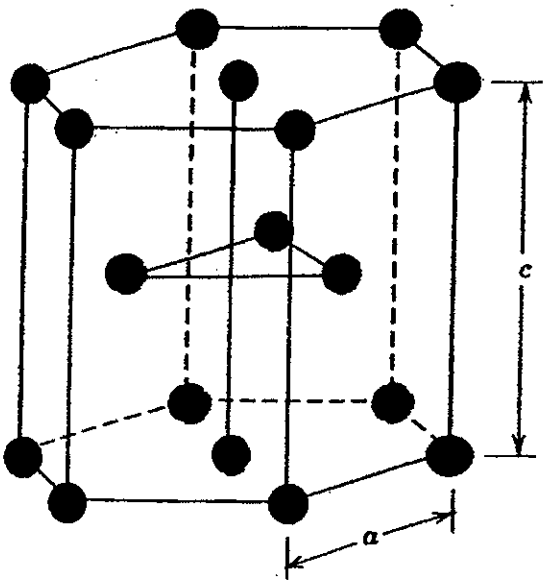
The basis consists of one Na atom and one Cl atom separated by one-half the body diagonal of a unit cube

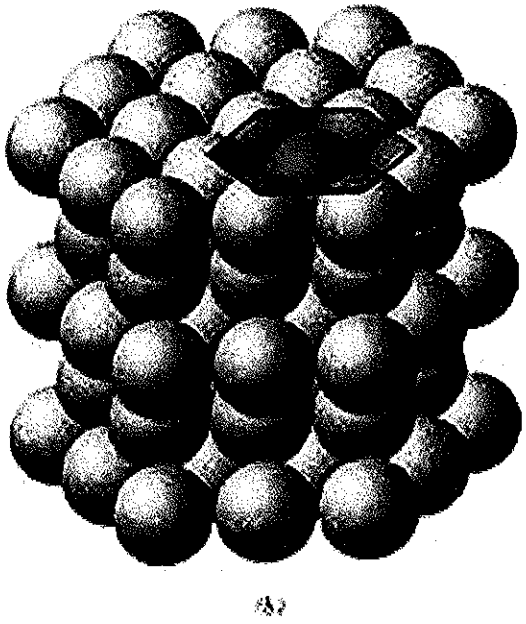


Primitive cell of the fcc lattice

Hexagonal close-packed structure (HCP)

One arranges identical spheres in hexagonal lattice, then put another layer on top of it





HCP

For ideal hcp $c/a = \sqrt{\frac{8}{3}} = 1.633\ldots$

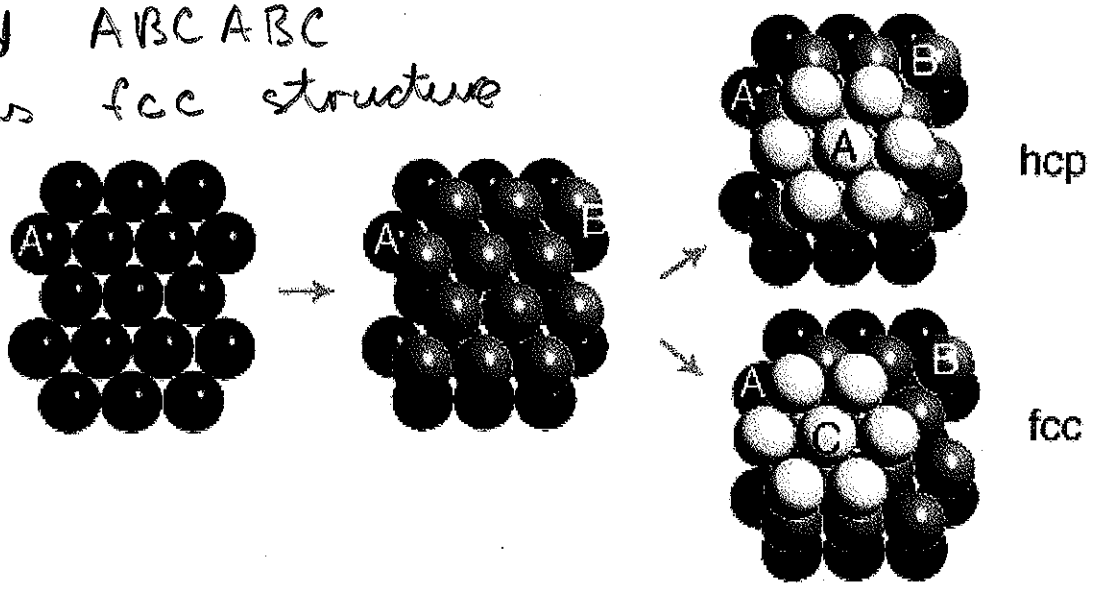
One usually refer to hcp even when $\frac{c}{a}$ is different from this value

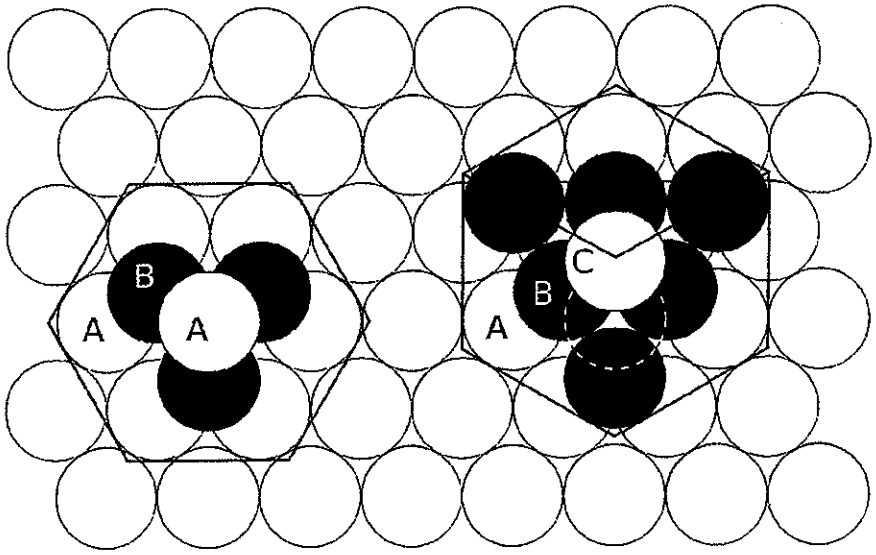
Crystal	c/a
He	1.633
Be	1.581
Mg	1.623
Ti	1.586
Zn	1.861
Co	1.622

Other closed-packed lattices

After we put second layer (B) on the top of the first one (A) there are two options for the third one, just above A : ABABAB... = hcp

or shifted ABCABC
This is fcc structure

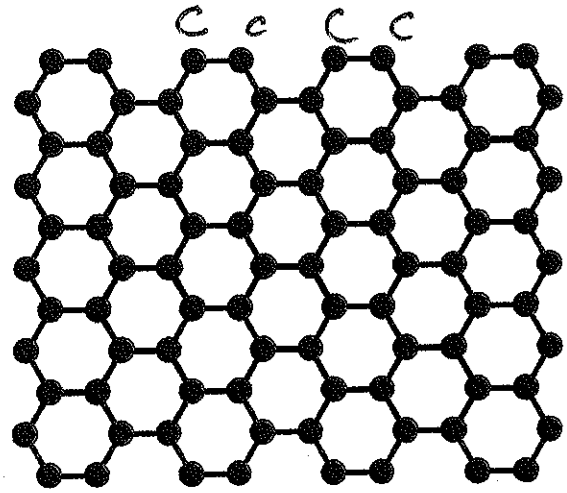




Graphene and Graphite

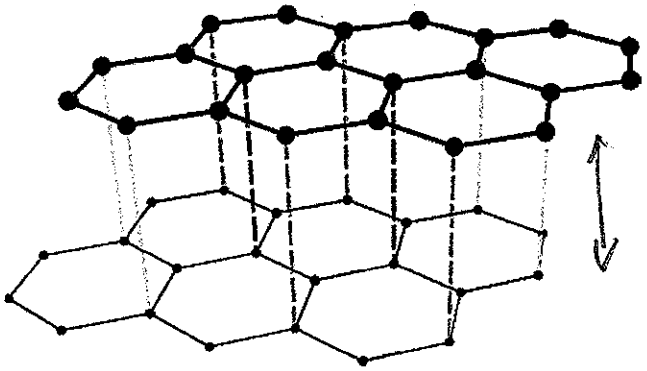
Made from carbon. honeycomb lattice

Graphene

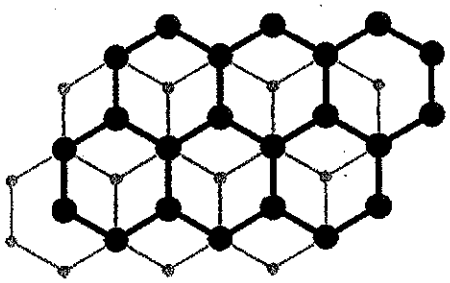


$a = 1.42 \text{ Å}$

Graphite - stacks of Graphene layers

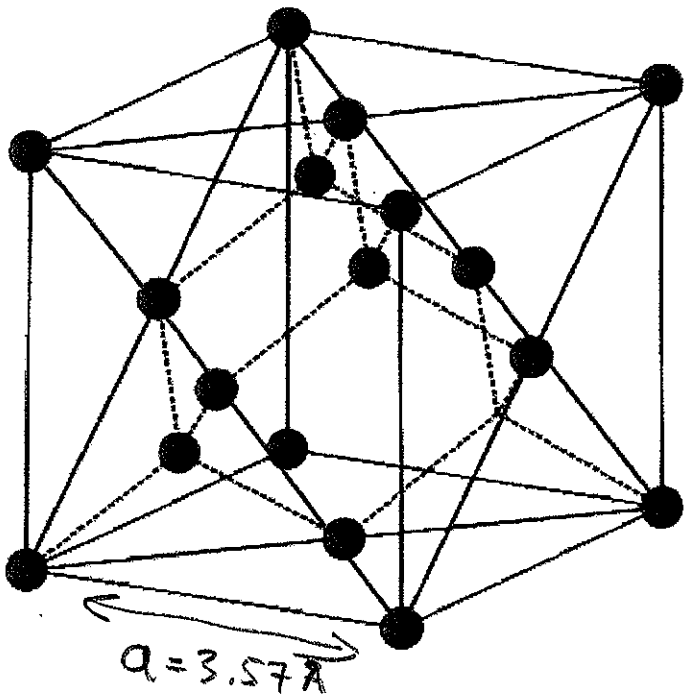


$c = 3.35 \text{ Å}$



Diamond structure

Diamond has the same carbon atoms but in the fcc lattice.



It consist of two interpenetrated fcc lattices displaced along the diagonal of the cubic cell by one quarter of the length of the diagonal

Element with the diamond structure

	a
C (diamond)	3.57 Å
Si	5.43
Ge	5.66

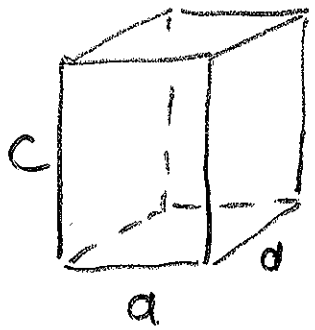
Symmetry and anisotropy of physical properties

In a single crystals dielectric constant or resistivity are not scalar but tensors.

$$D_\alpha = \varepsilon_{\alpha\beta} E_\beta$$

$$E_\alpha = \rho_{\alpha\beta} j_\beta$$

Consider tetragonal crystal system



$\varepsilon_{\alpha\beta}$ and $\rho_{\alpha\beta}$ are symmetric rank 2 tensors, $\varepsilon_{\alpha\beta} = \varepsilon_{\beta\alpha}$, $\rho_{\alpha\beta} = \rho_{\beta\alpha}$

This symmetry has nothing to do with the crystal symmetry. and is valid for any structure. for $\varepsilon_{\alpha\beta}$ it follows from the expression for the free energy

$$F = - \frac{\varepsilon_{\alpha\beta} E_\alpha E_\beta}{8\pi}$$

$$D_\alpha = -4\pi \frac{\partial F}{\partial E_\beta}$$

For resistivity or conductivity it follows from the Onsager relations, that states that heat production (or dissipative fundia)

$$Q = j \cdot E = \rho_{\alpha\beta} j_\alpha j_\beta \Rightarrow$$

$$\rho_{\alpha\beta} = \rho_{\beta\alpha}$$

One can diagonalise symmetric matrix. Then we will have for the tetragonal lattice

$$\rho_{\alpha\beta} = \begin{pmatrix} \rho_{xx} & 0 & 0 \\ 0 & \rho_{yy} & 0 \\ 0 & 0 & \rho_{zz} \end{pmatrix}$$

But for this lattice x and y directions are equivalent $\Rightarrow$

$$\rho_{\alpha\beta} = \begin{pmatrix} \rho_\perp & 0 & 0 \\ 0 & \rho_\perp & 0 \\ 0 & 0 & \rho_z \end{pmatrix}$$ - uniaxial anisotropy

In the same way for cubic crystal resistivity is isotropic $\underline{\rho_{\alpha\beta} = \rho\,\delta_{\alpha\beta}}$!

Not all the properties of the cubic crystal are isotropic. Consider elastic deformations. Since energy of deformed body is not changed by the uniform displacement it should depend on its gradient $\frac{\partial u_\alpha}{\partial x_\beta}$

For isotropic solid one can constructs two quadratic invariants from $\frac{\partial u_\alpha}{\partial x_\beta}$:

$\left(\frac{\partial u_\alpha}{\partial x_\alpha}\right)^2 = (div\ \vec{u})^2$ and

$\sum_{\alpha\beta} \frac{\partial u_\alpha}{\partial x_\beta} \frac{\partial u_\alpha}{\partial x_\beta}$

Infinitesimal rotation by an angle $\delta\vec{\Omega}$

$\vec{u} = \delta\vec{\Omega} \times \vec{r}$ with $\delta\vec{\Omega} = \frac{rot\,\vec{u}}{3}$

Energy should not depend on $\delta\vec{\Omega}$ $\Rightarrow$ from the gradient term we should exclude antisymmetric part and describe deformation by symmetric tensor $u_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right)$

Then the elastic free energy is

$$F = \frac{\lambda}{2} (div\, u)^2 + \mu\, u_{\alpha\beta}^2$$

λ, μ - Lamé coefficients

In general for crystals

$$F = \frac{1}{2} \lambda_{\alpha\beta\gamma\delta} u_{\alpha\beta} u_{\gamma\delta}$$

$\lambda_{\alpha\beta\gamma\delta}$ is elastic moduli tensor

Since $u_{\alpha\beta} = u_{\beta\alpha} \Rightarrow$

$$\lambda_{\alpha\beta\gamma\delta} = \lambda_{\beta\alpha\gamma\delta} = \lambda_{\alpha\beta\delta\gamma} = \lambda_{\delta\gamma\alpha\beta}$$

For cubic symmetry $(x \to -x)$ $(x \to y)$ etc.

we may have 3 independent moduli

$$F = \frac{1}{2} \lambda_{xxxx} (u_{xx}^2 + u_{yy}^2 + u_{zz}^2) +$$

$$+ \lambda_{xxyy} (u_{xx} u_{yy} + u_{xx} u_{zz} + u_{yy} u_{zz}) +$$

$$+ 2 \lambda_{xyxy} (u_{xy}^2 + u_{xz}^2 + u_{yz}^2).$$

The same is true for 2d square lattice

But 2d hexagonal lattice is isotropic:

$$\lambda_{xxxx} = \lambda_{xxyy} !$$