Advanced Topics in Condensed Matter

Lecture 2: Crystal lattices and structures

Dr. Ivan Zaluzhnyy Prof. Dr. Frank Schreiber

EBERHARD KARLS UNIVERSITÄT TÜBINGEN



Periodicity



M. C. Escher, Regular Division of the Plane #25 (1939)

Periodicity



Translation symmetry

M. C. Escher, Regular Division of the Plane #25 (1939)

Periodicity M. C. Escher, Regular Division of the Plane #25 (1939) WiSe 2024/25 J PHY-VFATCM 4

Crystal lattice



 $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

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Crystal lattice

Lattice - an infinite array of discrete points, generated by a set of discrete translation operations: $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

Rotational symmetry



Only rotational axes of orders n = 1, 2, 3, 4, 6 are possible

Rotational symmetry



 $ka = a - 2a\cos\beta$ $\cos\beta = \frac{1-k}{2}$ k = -1, 0, 1, 2, 3 $\beta = 0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$

Only rotational axes of orders n = 1, 2, 3, 4, 6 are possible

Crystal lattice



<u>Lattice</u> – an infinite array of discrete points, generated by a set of discrete translation operations: $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$



<u>Unit cell</u> – a volume, a repetitive arrangement of which (pure translations, i.e. $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$) can fill the whole space without overlaps and gaps.

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Primitive unit cell – one lattice cite per cell

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Conventional unit cell – contains the full symmetry of the lattice and include more than one lattice point

Crystal systems in 2D



5 Bravais lattices are possible in 2D.

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Crystal systems in 3D



Orthorhombic

b

1/

α

b

Triclinic

a

a

Blc

Tetragonal

Cubic

С

Bravais lattices in 3D

14 Bravais lattices are possible in 3D.

Crystal Family	Lattice System	Schönflies	14 Bravais Lattices						
			Primitive (P)	Base-centered (C)	Body-centered (I)	Face-centered (F)			
Triclinic		Ci	$ \begin{array}{c} $						
Monoclinic		C _{2h}	$\beta \neq 90^{\circ}$ $a \neq c$ $a \neq c$ b	$\beta \neq 90^{\circ}$ $a \neq c$ $a \neq c$ b					
Orthorhombic		D _{2h}	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$			
Tetragonal		D _{4h}	$a \neq c$		$a \neq c$				
Hexagonal	Rhombohedral	D _{3d}	$\begin{array}{c} \alpha \neq 90^{\circ} \\ & & \\ \alpha \\ a \\ a \\ a \\ a \\ a \end{array} a$						
	Hexagonal	D _{6h}	$\gamma = 120^{\circ}$						
Cubic		O _h			a				

Primitive unit cells for cubic lattices



Face Centered Cubic (FCC)





Primitive unit cells for cubic lattices



Face Centered Cubic (FCC)



rhombic dodecahedron



Body Centered Cubic (BCC)



truncated octahedron

Primitive unit cells for cubic lattices

Face Centered Cubic (FCC)

Body Centered Cubic (BCC)





1. Unit cell parameters

cubic unit cell: a = b = c = 4.15 Å $\alpha = \beta = \gamma = 90^{\circ}$





2. Locating atoms within the unit cell

La:





2. Locating atoms within the unit cell

La:

$$\vec{r} = 0 \cdot \vec{a}_1 + 0 \cdot \vec{a}_2 + 0 \cdot \vec{a}_3 = (0,0,0)$$

B:

$$\vec{r}_1 = \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{5} \cdot \vec{a}_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{5})$$





2. Locating atoms within the unit cell

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$$\vec{r}_1 = \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{5} \cdot \vec{a}_3 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{5})$$

$$\vec{r}_2 = \frac{1}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = (\frac{1}{5}, \frac{1}{2}, \frac{1}{2})$$





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$$\vec{r}_2 = \frac{1}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = (\frac{1}{5}, \frac{1}{2}, \frac{1}{2})$$

$$\vec{r}_3 = \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{5} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = (\frac{1}{2}, \frac{1}{5}, \frac{1}{2})$$





2. Locating atoms within the unit cell

La:

$$\vec{r}_{1} = \frac{1}{2} \cdot \vec{a}_{1} + \frac{1}{2} \cdot \vec{a}_{2} + \frac{1}{5} \cdot \vec{a}_{3} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{5})$$

$$\vec{r}_{2} = \frac{1}{5} \cdot \vec{a}_{1} + \frac{1}{2} \cdot \vec{a}_{2} + \frac{1}{2} \cdot \vec{a}_{3} = (\frac{1}{5}, \frac{1}{2}, \frac{1}{2})$$

$$\vec{r}_{3} = \frac{1}{2} \cdot \vec{a}_{1} + \frac{1}{5} \cdot \vec{a}_{2} + \frac{1}{2} \cdot \vec{a}_{3} = (\frac{1}{2}, \frac{1}{5}, \frac{1}{2})$$

$$\vec{r}_{4} = \frac{4}{5} \cdot \vec{a}_{1} + \frac{1}{2} \cdot \vec{a}_{2} + \frac{1}{2} \cdot \vec{a}_{3} = (\frac{4}{5}, \frac{1}{2}, \frac{1}{2})$$





2. Locating atoms within the unit cell

La:

$$\begin{aligned} \vec{r}_1 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{5} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{5}\right) \\ \vec{r}_2 &= \frac{1}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{5}, \frac{1}{2}, \frac{1}{2}\right) \\ \vec{r}_3 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{5} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{1}{5}, \frac{1}{2}\right) \\ \vec{r}_4 &= \frac{4}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{4}{5}, \frac{1}{2}, \frac{1}{2}\right) \\ \vec{r}_5 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{4}{5} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{4}{5}, \frac{1}{2}\right) \end{aligned}$$





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$$\begin{aligned} \vec{r}_1 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{5} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{5}\right) \\ \vec{r}_2 &= \frac{1}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{5}, \frac{1}{2}, \frac{1}{2}\right) \\ \vec{r}_3 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{5} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{1}{5}, \frac{1}{2}\right) \\ \vec{r}_4 &= \frac{4}{5} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{4}{5}, \frac{1}{2}, \frac{1}{2}\right) \\ \vec{r}_5 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{4}{5} \cdot \vec{a}_2 + \frac{1}{2} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{4}{5}, \frac{1}{2}\right) \\ \vec{r}_6 &= \frac{1}{2} \cdot \vec{a}_1 + \frac{1}{2} \cdot \vec{a}_2 + \frac{4}{5} \cdot \vec{a}_3 = \left(\frac{1}{2}, \frac{4}{5}, \frac{1}{2}\right) \end{aligned}$$





230 crystal families

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#221 *Pm*-3*m* Example – ZIF-71-RHO



More information at crystalsymmetry.wordpress.com

Crystal structures drawn v K. Momma and F. Izumi, J. Appl. Crystollogr. 2011, 44, 1

Point symmetry of LaB₆



3. Applying translational symmetry





3. Applying translational symmetry



Crystal structure

Crystal structure = lattice + basis

Lattice describes periodicity of the structure. It is determined by the unit cell (3 lengths and 3 angles)

Basis describes arrangement of atoms within a unit cell

Position of any atom inside a crystal:

$$\vec{r} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 + x \vec{a}_1 + y \vec{a}_2 + z \vec{a}_3$$
$$\vec{R}_n \qquad \vec{r}_j$$







Crystallographic directions

In a lattice, each translation vector $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ determines a direction

Directions are described with three integer Miller indices as [uvw], where u,v,w- are three smallest integer numbers, proportional to the components of \vec{R}_n .

[uvw] - direction

 $\langle uvw \rangle$ - set of equivalent directions



Crystallographic planes

Lattice plane is defined by 3 non-collinear lattice points.

- Lattice planes are described with three integer Miller indices as (hkl), where h,k,l are three smallest integer numbers, proportional to $\frac{1}{u}, \frac{1}{v}, \frac{1}{w}$.
- (*hkl*) lattice plane
- $\{hkl\}$ set of equivalent planes





Crystallographic planes

Lattice plane is defined by 3 non-collinear lattice points.

Lattice planes are described with three integer Miller indices as (hkl), where h,k,l are three smallest integer numbers, proportional to $\frac{1}{u}, \frac{1}{v}, \frac{1}{w}$.



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Crystallographic planes

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- (*hkl*) lattice plane



Why do we need lattice planes?



A.K. Bentley, S.E. Skrabalak. J. Chem. Educ. 100, 3425 (2023)

Equivalent planes for tetragonal lattice

 $\{100\} \rightarrow (100), (010), (\overline{1}00), (0\overline{1}0)$



Miller indices of equivalent planes can be obtained as permutations

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 $\{100\} \rightarrow (100), (010), (\overline{1}00), (0\overline{1}0), (\overline{1}10), (1\overline{1}0)$



Miller indices of equivalent planes cannot be obtained as permutations

 x_1, x_2, x_3 - equivalent axis for the hexagonal symmetry



 $\{1\overline{1}00\} \rightarrow (10\overline{1}0), (01\overline{1}0), (\overline{1}100), (\overline{1}010), (0\overline{1}10), (1\overline{1}00)$



Miller-Bravais indices of equivalent planes can be obtained as permutations

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Transformation from Miller indices to
Miller-Bravais indices for directions

$$[uvw] \Longrightarrow [u'v't'w']$$

$$u\vec{a}_1 + v\vec{a}_2 + w\vec{c} = u'\vec{a}_1 + v'\vec{a}_2 + t'\vec{a}_3 + w'\vec{c}$$

$$\vec{a}_3 = -(\vec{a}_1 + \vec{a}_2)$$

$$\begin{cases}
u = u' - t' \\
v = v' - t' \\
w = w' \\
t' = -(u' + v')
\end{cases}$$

$$u' = \frac{1}{3}(2u - v)$$

$$v' = \frac{1}{3}(2v - u)$$

$$t' = -\frac{1}{3}(u + v)$$

$$w' = w$$

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Fourier series

In Fourier space (reciprocal space), description is done in terms of waves.

$$f(x) = \sum_{n=-\infty}^{+\infty} c_n \cdot exp(ik_n x)$$

sum of waves with wavevectors
$$k_n = \frac{2\pi}{L}n$$

and complex amplitudes

$$c_n = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} f(x) \cdot exp(-ik_n x) dx$$



periodic function with period *L*

Fourier transform

In Fourier space (reciprocal space), description is done in terms of waves.



almost any function (not necessarily periodic)

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k

Dirac comb



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Fourier transform of a lattice







Reciprocal space J. Als-Nielsen, D. McMorrow, Elements of Modern X-ray Scattering (2011)

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Fourier transform of a lattice



Reciprocal space

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