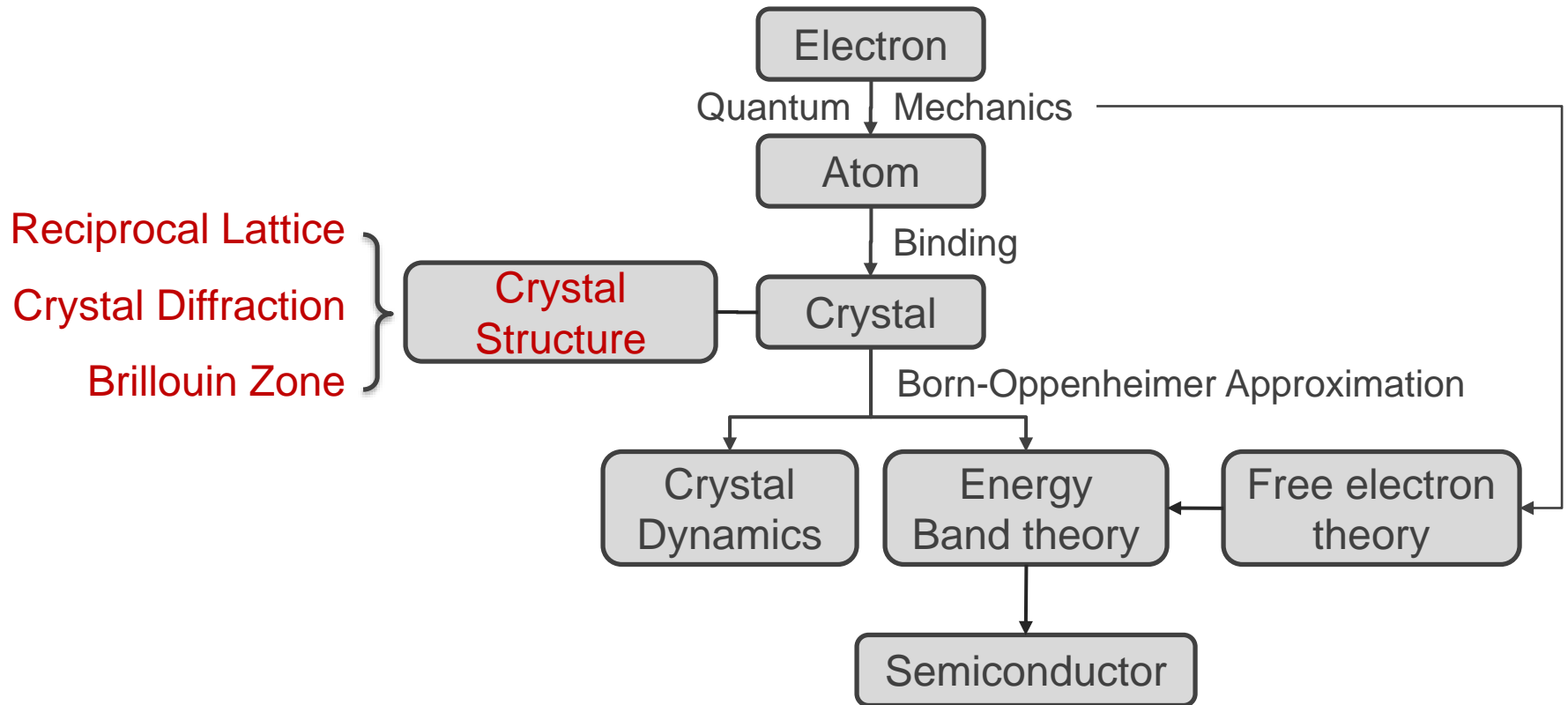


# Chapter 1

## Formation of Crystal

Profile



# Chapter 1 Formation of Crystal

1.1 Quantum Mechanics and atomic structure

1.2 Interatomic bonding in solids

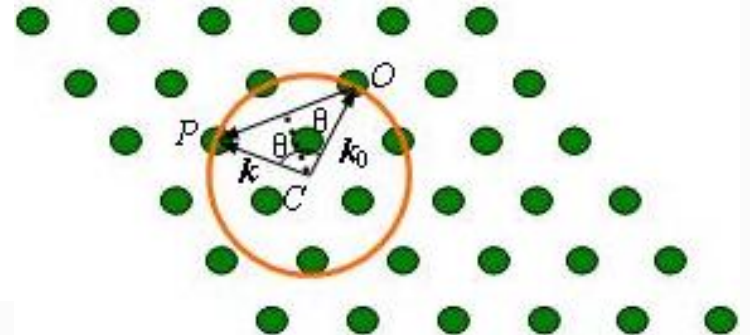
1.3 Crystal structure and typical crystals

1.4 Reciprocal Lattice and Brillouin Zone

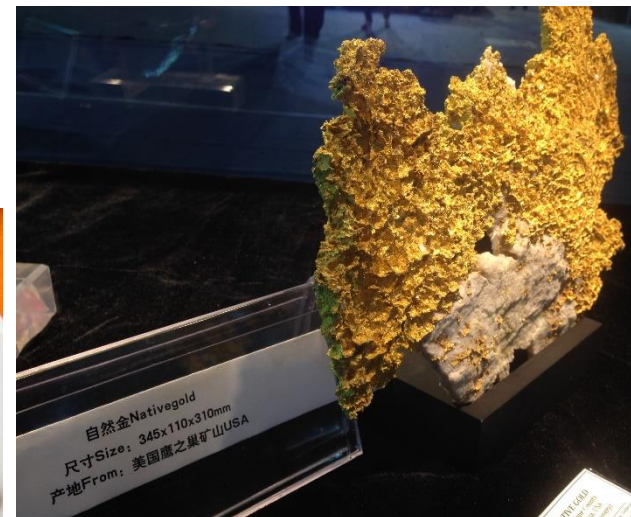
1.4.1 Reciprocal Lattice

1.4.2 Crystal Diffraction

1.4.3 Brillouin Zone



·Fourier series ·Reciprocal lattice (space) ·Reciprocal space & wave-vector space (k-space)



·Fourier series ·Reciprocal lattice (space) ·Reciprocal space & wave-vector space (k-space)

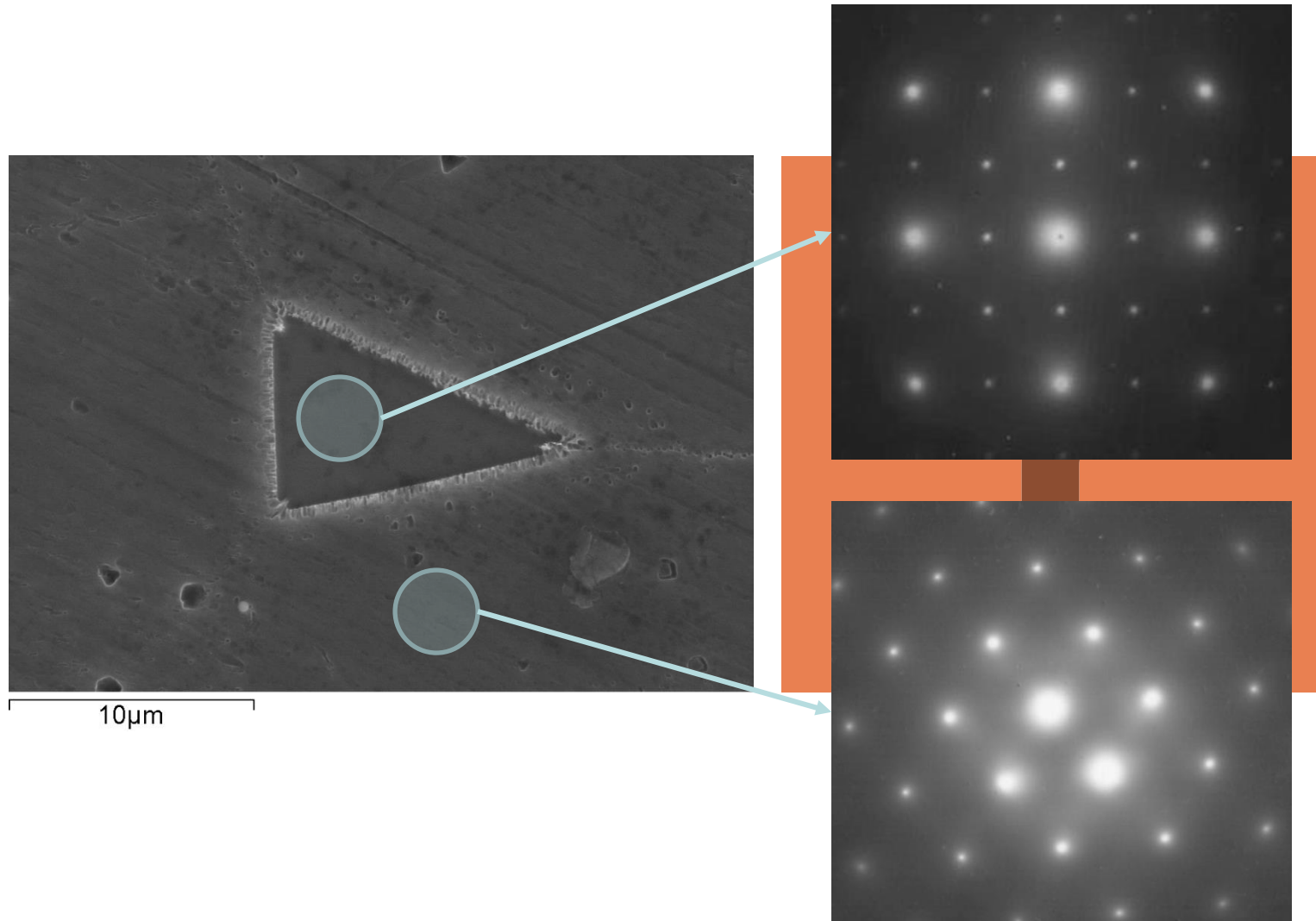
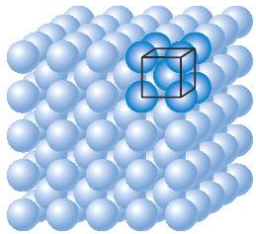
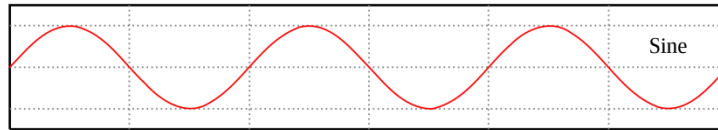


Image of Reciprocal lattice

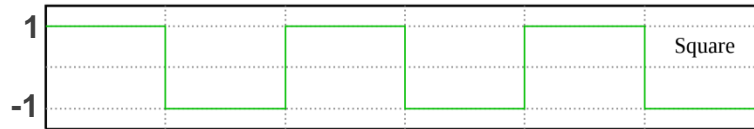
• **Fourier series** • Reciprocal lattice (space) • Reciprocal space & wave-vector space (k-space)



$$n(\mathbf{r} + \mathbf{T}) = n(\mathbf{r})$$

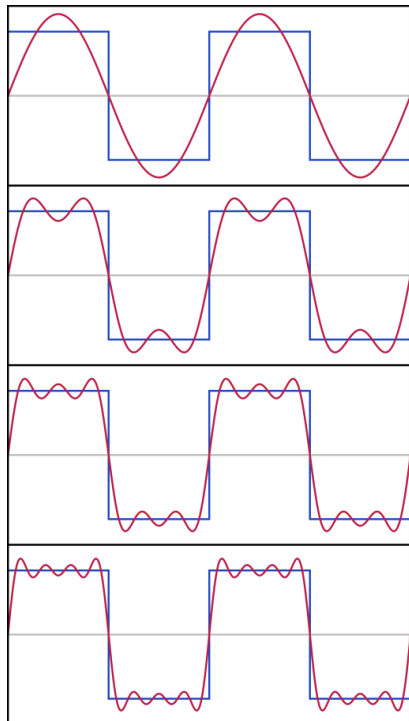


$$f(x) = \sin x$$

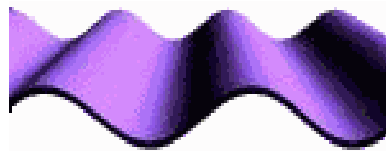


$$f(x) = \begin{cases} -1 & (2k-1)\pi \leq x < 2k\pi \\ 1 & 2k\pi \leq x < (2k+1)\pi \end{cases}$$

$$f(x) \sim \frac{4}{\pi} \sin x + \frac{4}{3\pi} \sin 3x + \frac{4}{5\pi} \sin 5x + \frac{4}{7\pi} \sin 7x + \dots$$



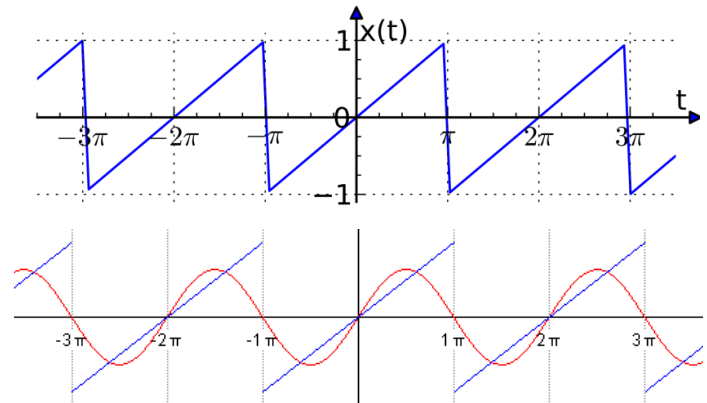
$$n = 1 \quad = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin(2n-1)x}{2n-1}$$



**First four Fourier approximations for a square wave**

$$f(x + 2\pi) = f(x)$$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx)$$



• **Fourier series** • Reciprocal lattice (space) • Reciprocal space & wave-vector space (k-space)

$$f(x + 2\pi) = f(x)$$

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx)$$

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx$$

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx dx$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx dx$$

$$e^{\pm ix} = \cos x \pm i \sin x$$

$$e^{i\pi} + 1 = 0$$

$$\cos nx = \frac{1}{2} (e^{inx} + e^{-inx})$$

$$\sin nx = -\frac{i}{2} (e^{inx} - e^{-inx})$$

$$f(x) = \sum_n c_n e^{inx}$$

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx} dx$$

• **Fourier series** • Reciprocal lattice (space) • Reciprocal space & wave-vector space (k-space)

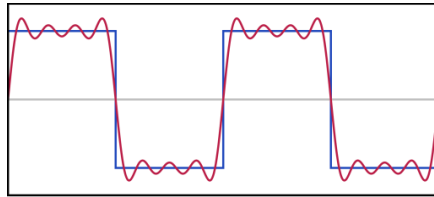
$$n(x + a) = n(x)$$

$$n(x) = \sum_p n_p e^{i \frac{2\pi p}{a} x}$$



• Fourier series • **Reciprocal lattice (space)** • Reciprocal space & wave-vector space (k-space)

1  $n(x+a) = n(x)$



$$n(x) = \sum_p n_p e^{i \frac{2\pi p}{a} x}$$

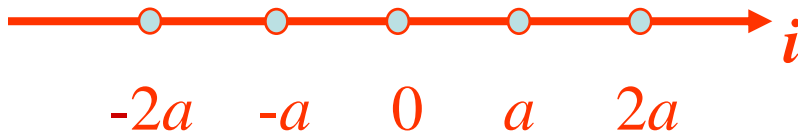
3

$$\begin{aligned} \vec{\mathbf{x}} &= x \hat{i} \\ \vec{\mathbf{G}} &= \frac{2\pi p}{a} \hat{i} \end{aligned}$$

$$n(x) = \sum_p n_p e^{i \mathbf{G} \cdot \mathbf{x}}$$

$$= \sum_G n_G e^{i \mathbf{G} \cdot \mathbf{x}}$$

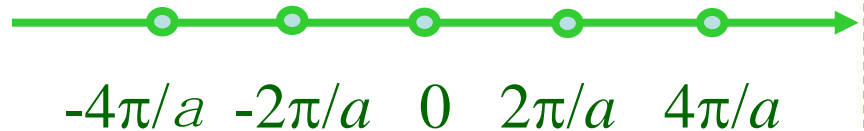
2



$$\mathbf{a} = a \hat{i}$$

$$\mathbf{R} = m a \hat{i} = m \mathbf{a}$$

4



$$\mathbf{b} = \frac{2\pi}{a} \hat{i}$$

$$\mathbf{G} = \frac{2\pi p}{a} \hat{i} = p \mathbf{b}$$

倒易点阵  
倒易空间  
波矢空间

• Fourier series • **Reciprocal lattice (space)** • Reciprocal space & wave-vector space (k-space)

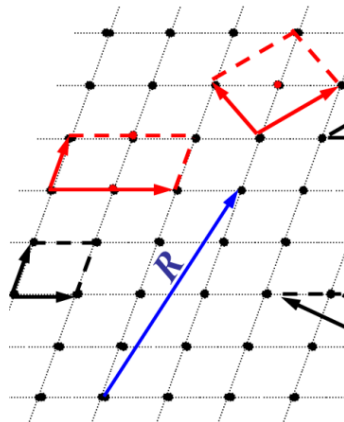
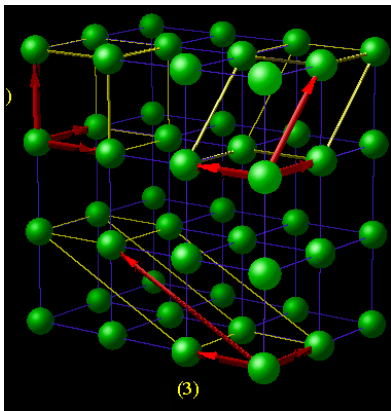
1 **1D**  $n(\mathbf{x} + \mathbf{a}) = n(\mathbf{x})$

$$n(\mathbf{x}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{x}}$$

$$\mathbf{a} = a\hat{i} \quad \mathbf{R} = ma\hat{i} = m\mathbf{a}$$

$$\mathbf{b} = \frac{2\pi}{a}\hat{i} \quad \mathbf{G} = \frac{2\pi p}{a}\hat{i} = p\mathbf{b}$$

2



$$\mathbf{R} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$$

3 **3D**  $n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r})$

$$n(\mathbf{r}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{r}}$$

4  $n(\mathbf{r} + \mathbf{R}) = \sum_G n_G e^{i\mathbf{G} \cdot (\mathbf{r} + \mathbf{R})} = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{r}} e^{i\mathbf{G} \cdot \mathbf{R}}$

=

$$n(\mathbf{r}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{r}}$$

$$e^{\pm ix} = \cos x \pm i \sin x$$

$$e^{i\mathbf{G} \cdot \mathbf{R}} = 1$$

$$\mathbf{G} \cdot \mathbf{R} = 2\pi m, \quad m - \text{integers}$$

5

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$$

$$\mathbf{R} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \quad (i, j = 1, 2, 3)$$

$$\mathbf{G} \cdot \mathbf{R} = (u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3) \cdot (v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3) = (u_1 v_1 \mathbf{a}_1 \cdot \mathbf{b}_1 + u_2 v_2 \mathbf{a}_2 \cdot \mathbf{b}_2 + u_3 v_3 \mathbf{a}_3 \cdot \mathbf{b}_3) = 2\pi m$$

•Fourier series •**Reciprocal lattice (space)** •Reciprocal space & wave-vector space (k-space)

$$0 \quad \mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} (i, j = 1, 2, 3)$$

$$1 \quad \mathbf{b}_1 \perp (\mathbf{a}_2, \mathbf{a}_3)$$

$$\mathbf{b}_1 = (\mathbf{a}_2 \times \mathbf{a}_3)$$

$$\mathbf{b}_1 = c \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

2

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = c \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

$$2\pi = cv$$

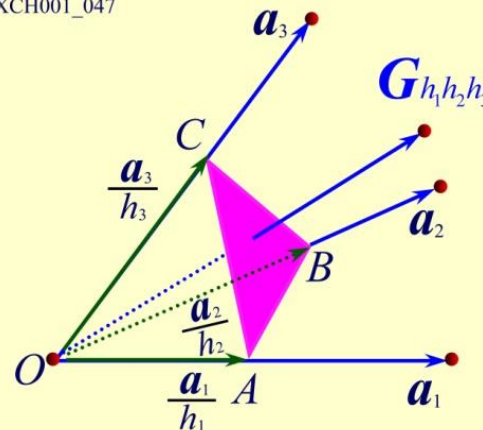
$$c = 2\pi / v$$

$$3 \quad = \frac{2\pi}{v} \mathbf{a}_2 \times \mathbf{a}_3$$

$$\mathbf{b}_2 = \frac{2\pi}{v} \mathbf{a}_3 \times \mathbf{a}_1$$

$$\mathbf{b}_3 = \frac{2\pi}{v} \mathbf{a}_1 \times \mathbf{a}_2$$

XCH001\_047



$$n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

1

$$v_a = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \quad v_a = \frac{(2\pi)^3}{v_b}$$

2

$$\mathbf{G}_{h_1 h_2 h_3} \perp (h_1 h_2 h_3)$$

$$|\mathbf{G}_{h_1 h_2 h_3}| = \frac{2\pi}{d_{h_1 h_2 h_3}}$$

$$d_{h_1 h_2 h_3} = \mathbf{OA} \cdot \frac{\bar{\mathbf{G}}_{h_1 h_2 h_3}}{G_{h_1 h_2 h_3}} = \frac{\mathbf{a}_1 \cdot (h_1 \mathbf{b}_1 + h_2 \mathbf{b}_2 + h_3 \mathbf{b}_3)}{h_1 G_{h_1 h_2 h_3}} = \frac{2\pi}{G_{h_1 h_2 h_3}}$$

3

SC-SC FCC-BCC BCC-FCC

·Fourier series ·**Reciprocal lattice (space)** ·Reciprocal space & wave-vector space (k-space)

**1D**  $n(\mathbf{x} + \mathbf{a}) = n(\mathbf{x})$

$$n(\mathbf{x}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{x}}$$

$$\mathbf{b} = \frac{2\pi}{a} \hat{i}$$

$$\mathbf{G} = \frac{2\pi p}{a} \hat{i} = p\mathbf{b}$$

·Fourier series ·**Reciprocal lattice (space)** ·Reciprocal space & wave-vector space (k-space)

$$\mathbf{1D} \quad n(\mathbf{x} + \mathbf{a}) = n(\mathbf{x})$$

$$n(\mathbf{x}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{x}}$$

$$\mathbf{b} = \frac{2\pi}{a} \hat{i}$$

$$\mathbf{G} = \frac{2\pi p}{a} \hat{i} = p\mathbf{b}$$

$$\mathbf{3D} \quad n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{r}}$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} (i, j = 1, 2, 3)$$

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$$

• Fourier series • **Reciprocal lattice (space)** • Reciprocal space & wave-vector space (k-space)

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \quad (i, j = 1, 2, 3)$$

### Real lattice

**SC**

$$\begin{cases} \mathbf{a}_1 = a\hat{x} \\ \mathbf{a}_2 = a\hat{y} \\ \mathbf{a}_3 = a\hat{z} \end{cases}$$

**FCC**

$$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\hat{y} + \hat{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(\hat{z} + \hat{x}) \\ \mathbf{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y}) \end{cases}$$

**BCC**

$$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z}) \end{cases}$$

### Reciprocal lattice

**SC**

$$\begin{cases} \mathbf{b}_1 = (2\pi/a)\hat{x} \\ \mathbf{b}_2 = (2\pi/a)\hat{y} \\ \mathbf{b}_3 = (2\pi/a)\hat{z} \end{cases}$$

**BCC**

$$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z}) \end{cases}$$

**FCC**

$$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(\hat{y} + \hat{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\hat{x} + \hat{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y}) \end{cases}$$

### Volume

$$(2\pi/a)^3$$

$$4(2\pi/a)^3$$

$$2(2\pi/a)^3$$

•Fourier series •**Reciprocal lattice (space)** •Reciprocal space & wave-vector space (k-space)

$$\text{1D} \quad n(\mathbf{x} + \mathbf{a}) = n(\mathbf{x})$$

$$n(\mathbf{x}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{x}}$$

$$\mathbf{b} = \frac{2\pi}{a} \hat{i}$$

$$\mathbf{G} = \frac{2\pi p}{a} \hat{i} = p\mathbf{b}$$

3D

$$n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_G n_G e^{i\mathbf{G} \cdot \mathbf{r}}$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} (i, j = 1, 2, 3)$$

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$$

$$\mathbf{b}_1 = \frac{2\pi}{v} \mathbf{a}_2 \times \mathbf{a}_3$$

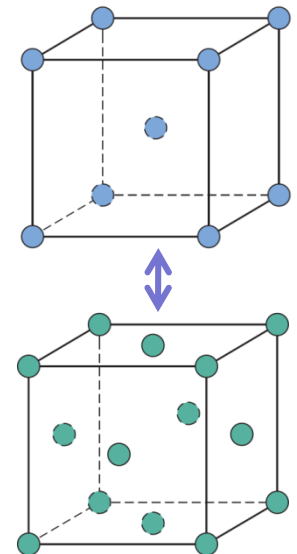
$$\mathbf{b}_2 = \frac{2\pi}{v} \mathbf{a}_3 \times \mathbf{a}_1$$

$$\mathbf{b}_3 = \frac{2\pi}{v} \mathbf{a}_1 \times \mathbf{a}_2$$

$$v_b = \frac{(2\pi)^3}{v_a}$$

$$\mathbf{G}_{v_1 v_2 v_3} \perp (v_1 v_2 v_3)$$

$$|\mathbf{G}_{v_1 v_2 v_3}| = \frac{2\pi}{d_{v_1 v_2 v_3}}$$



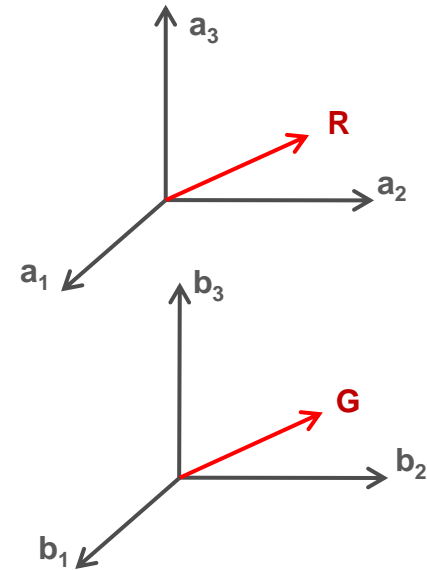
•Fourier series •**Reciprocal lattice (space)** •Reciprocal space & wave-vector space (k-space)

$$\mathbf{R} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3$$

$$n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r}) \quad n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \quad (i, j = 1, 2, 3)$$

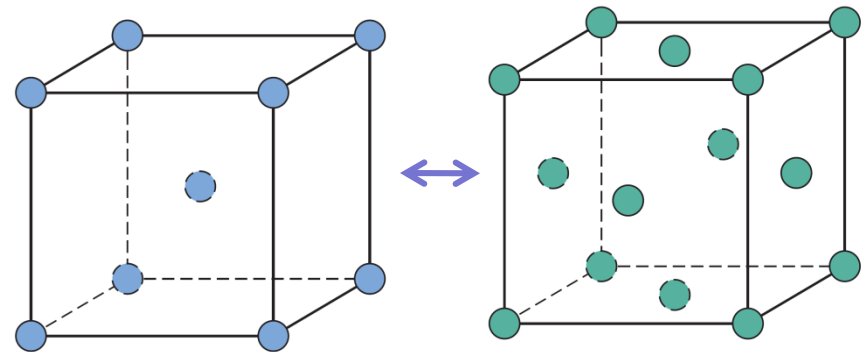
$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3$$



$$v_b = \frac{(2\pi)^3}{v_a}$$

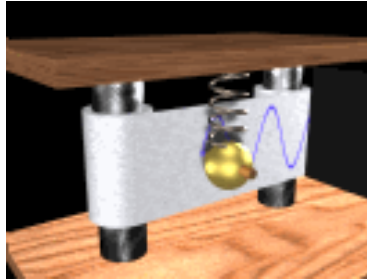
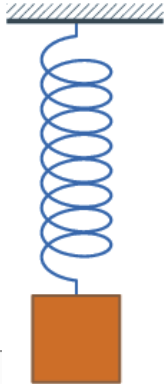
$$\mathbf{G}_{v_1 v_2 v_3} \perp (v_1 v_2 v_3)$$

$$|\mathbf{G}_{v_1 v_2 v_3}| = \frac{2\pi}{d_{v_1 v_2 v_3}}$$

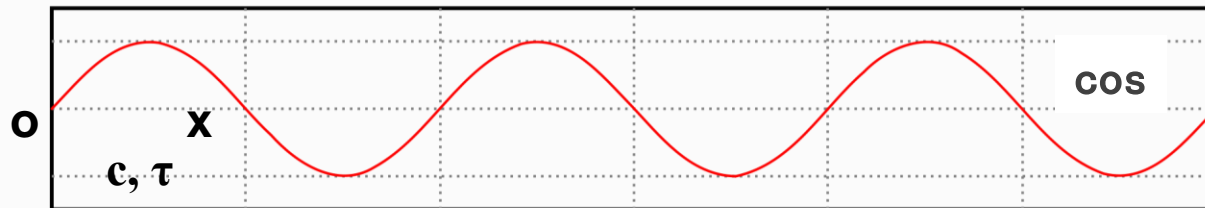




•Fourier series •Reciprocal lattice (space) •Reciprocal space & wave-vector space (k-space)



$$u(x=0, t) = A \cos(\omega t + \varphi_0)$$



$$\begin{aligned} u(x, t) &= A \cos[\omega(t - \tau) + \varphi_0] = A \cos[\omega(t - \frac{x}{c}) + \varphi_0] \\ &= A \cos(\omega t - \frac{2\pi}{T} \frac{x}{c} + \varphi_0) = A \cos(\omega t - \frac{2\pi}{\lambda} x + \varphi_0) = A \cos(\omega t - kx + \varphi_0) \end{aligned}$$

•Fourier series •Reciprocal lattice (space) •Reciprocal space & wave-vector space (k-space)

$$u(x, t) = A \cos(\omega t - \frac{2\pi}{\lambda} x + \varphi_0)$$

$$= A \cos(\omega t - \mathbf{k}x + \varphi_0)$$

$$\tilde{u}(x, t) = \tilde{A} e^{i(\omega t - \mathbf{k}x)}$$

$$v = \frac{1}{T}$$

$$\lambda = cT = \frac{c}{v}$$

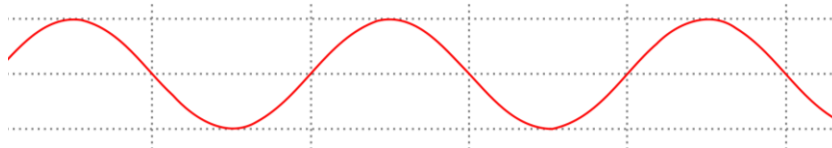
$$T = \frac{2\pi}{\omega}$$

$$\omega = \frac{2\pi}{T} = 2\pi v$$

$$c = \frac{\lambda}{T} = \frac{\omega}{2\pi} \lambda = \frac{\omega}{k}$$

$$k = \frac{2\pi}{\lambda}$$

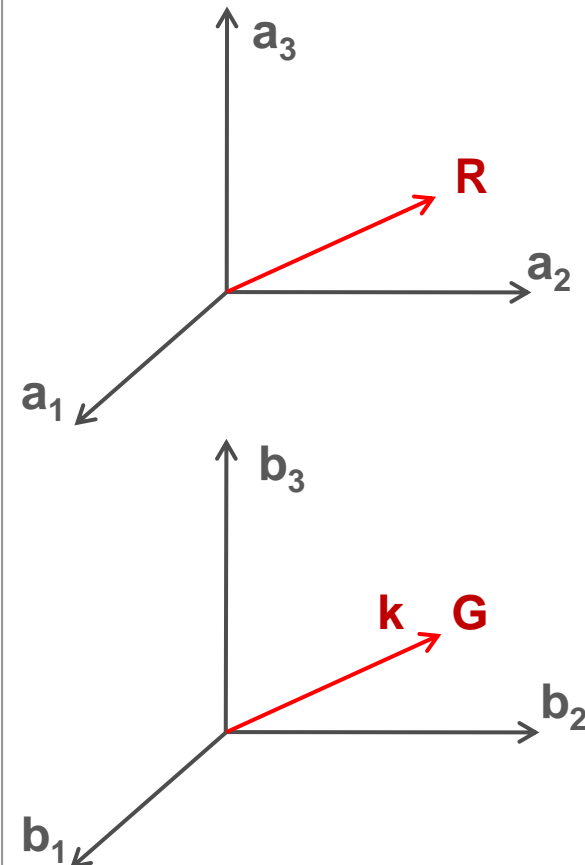
$$\mathbf{k} = \frac{2\pi}{\lambda} \hat{\mathbf{n}}$$



$$\mathbf{p} = \hbar \mathbf{k}$$

$$E_k = \frac{(\hbar k)^2}{2m}$$

$$\mathbf{k} = \frac{2\pi}{\lambda} \hat{\mathbf{n}} \quad \mathbf{b} = \frac{2\pi}{a} \hat{\mathbf{i}} \quad \mathbf{G} = \frac{2\pi p}{a} \hat{\mathbf{i}}$$



## How to learn?

1

## Basic Concept

Periodic function

Fourier series

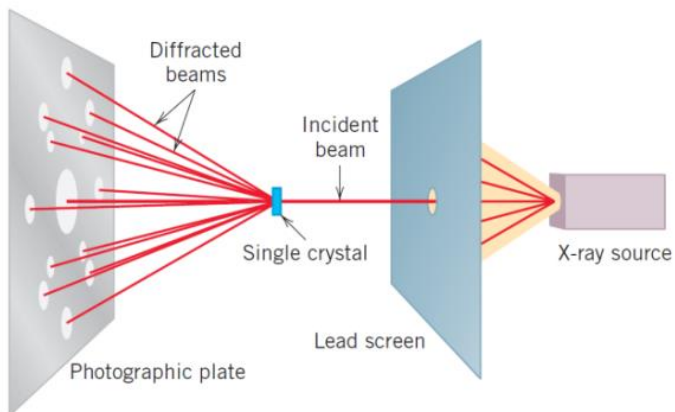
Reciprocal vector

Reciprocal lattice

Wave-vector space

2

## Train of Thought



# Chapter 1 Formation of Crystal

1.1 Quantum Mechanics and atomic structure

1.2 Interatomic bonding in solids

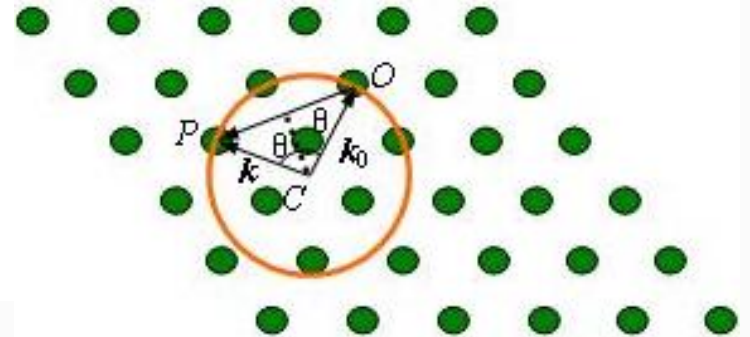
1.3 Crystal structure and typical crystals

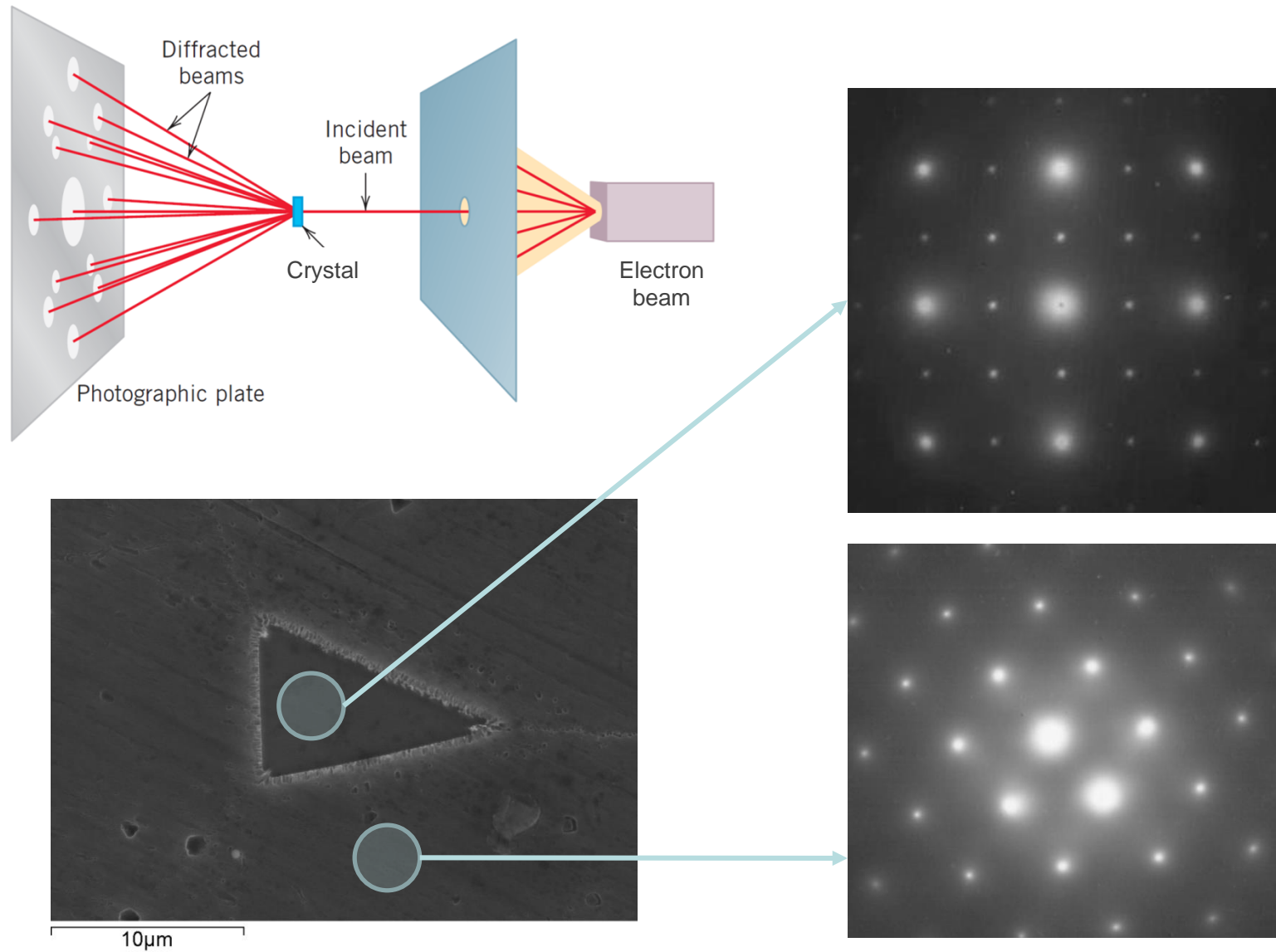
1.4 Reciprocal Lattice and Brillouin Zone

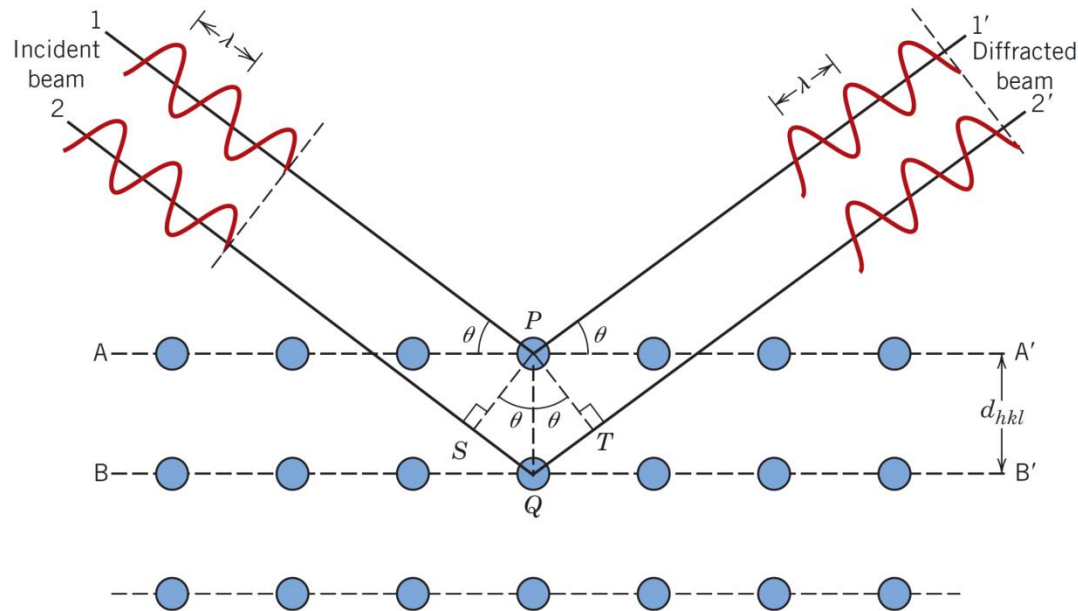
1.4.1 Reciprocal Lattice

1.4.2 Crystal Diffraction

1.4.3 Brillouin Zone

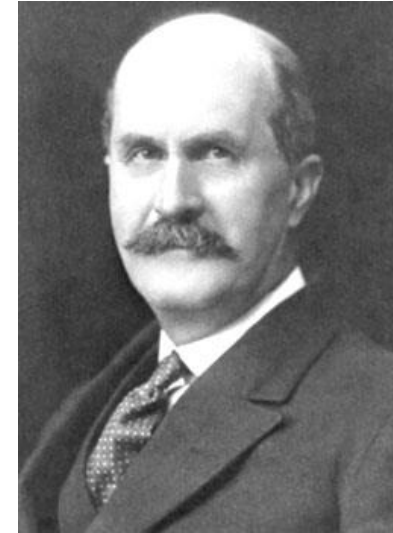


**-The Bragg law** -Laue equation -Ewald structure

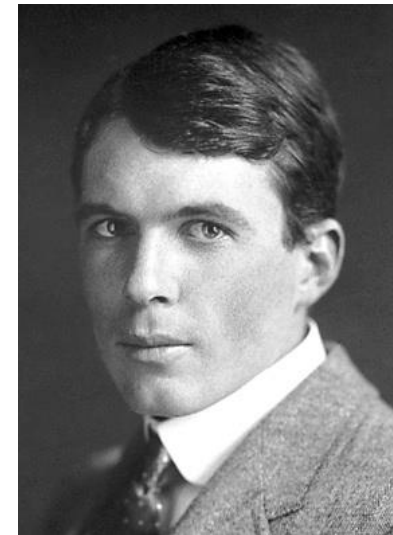
**•The Bragg law •Laue equation •Ewald structure**

$$2d\sin\theta = n\lambda$$

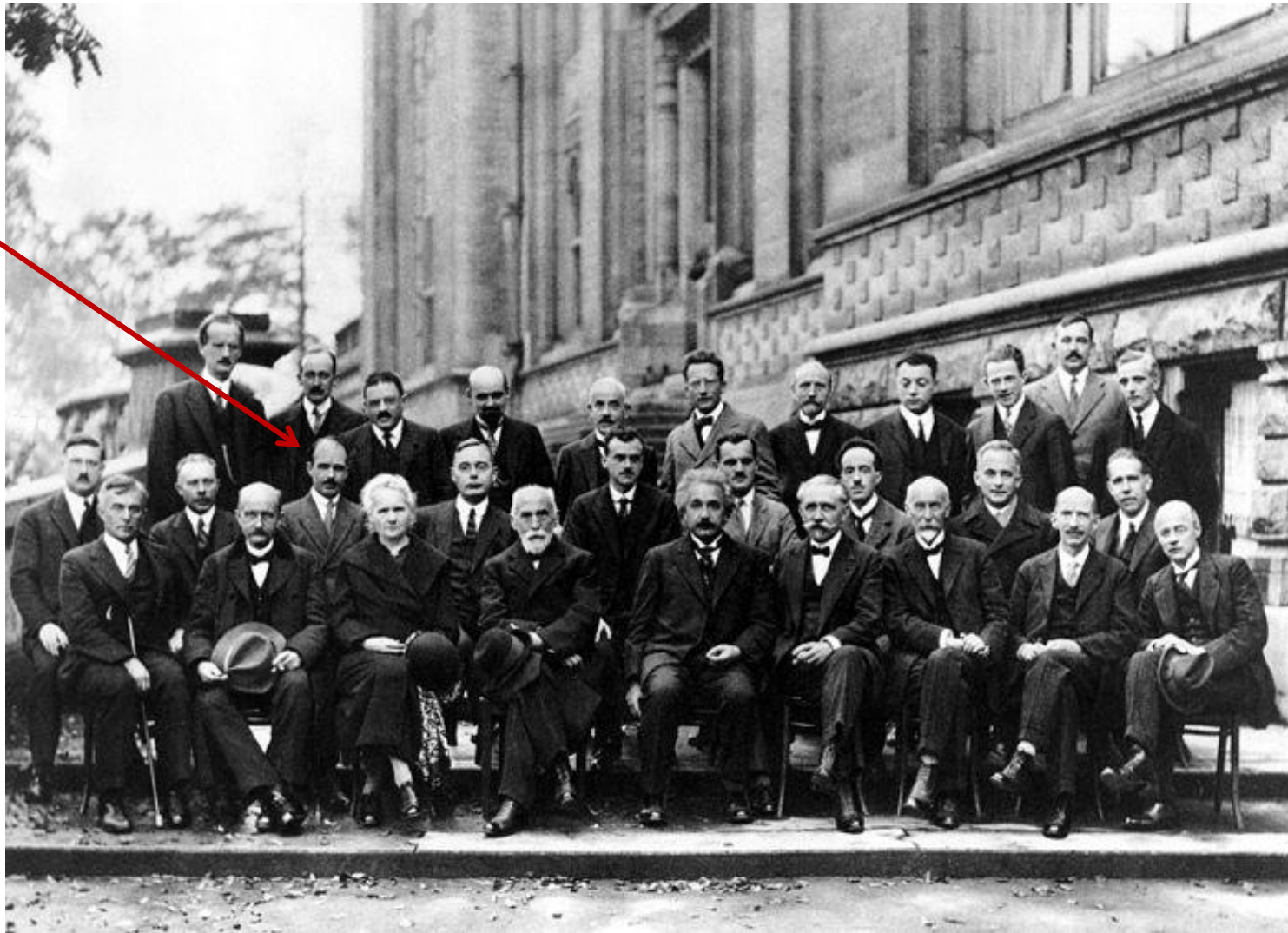
**Nobel Prize 1915**



**Sir William Henry Bragg (1862-1942)**

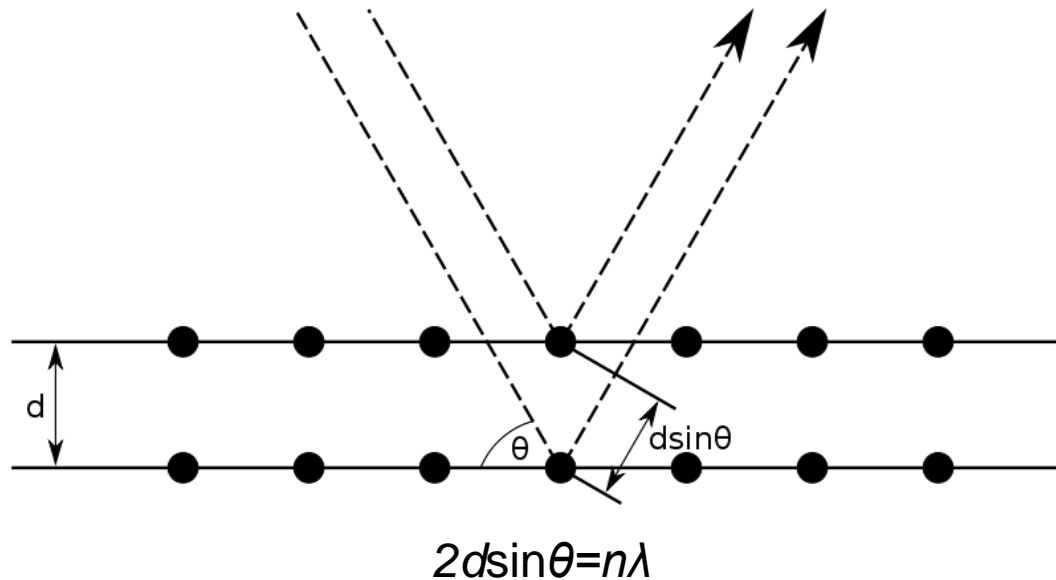
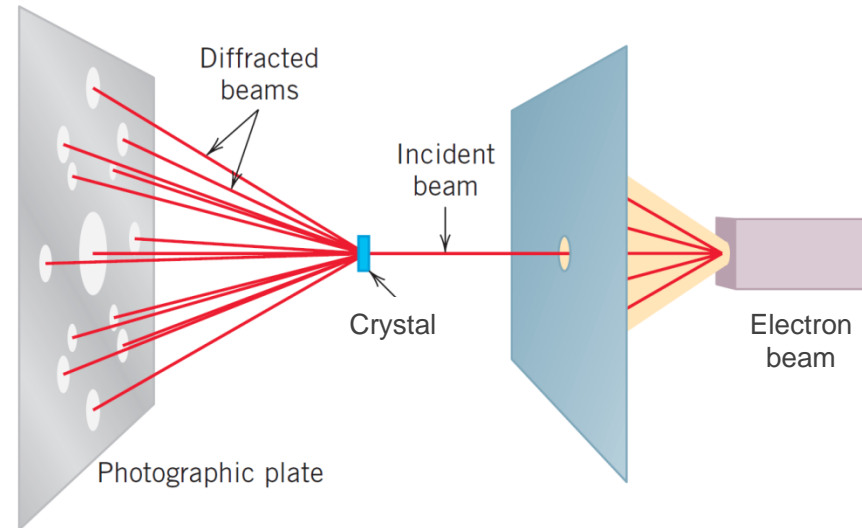
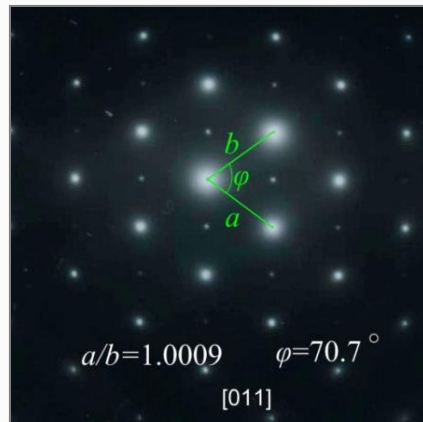


**William Lawrence Bragg (1890-1971)**

**•The Bragg law** •Laue equation •Ewald structure

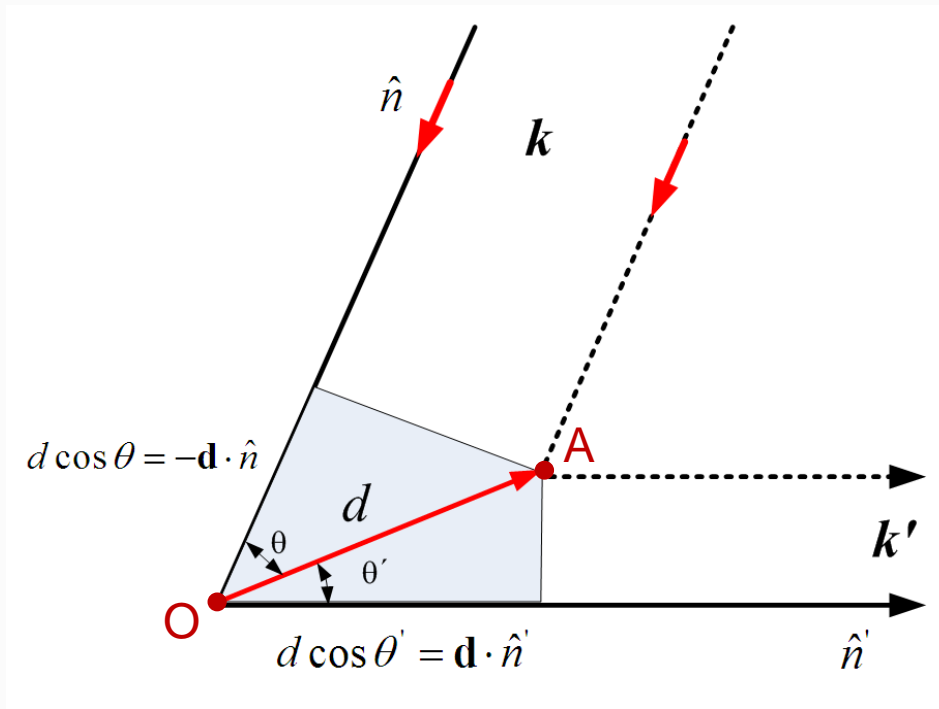
A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. De Donder, E. Schrödinger, J.E. Verschaffelt, W. Pauli, W. Heisenberg, R.H. Fowler, L. Brillouin;  
A. P. Debye, M. Knudsen, **W.L. Bragg**, H.A. Kramers, P.A.M. Dirac, A.H. Compton, L. de Broglie, M. Born, N. Bohr;  
I. Langmuir, M. Planck, M. Skłodowska-Curie, H.A. Lorentz, A. Einstein, P. Langevin, Ch. E. Guye, C.T.R. Wilson, O.W. Richardson



**-The Bragg law** -Laue equation -Ewald structure



• The Bragg law • **Laue equation** • Ewald structure



$$\mathbf{k} = \frac{2\pi}{\lambda} \hat{n}$$

$$\mathbf{k}' = \frac{2\pi}{\lambda} \hat{n}'$$

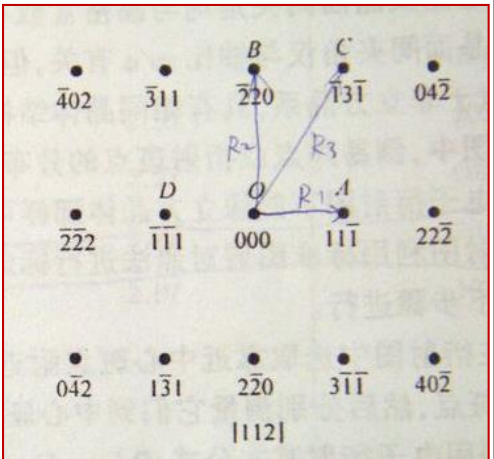
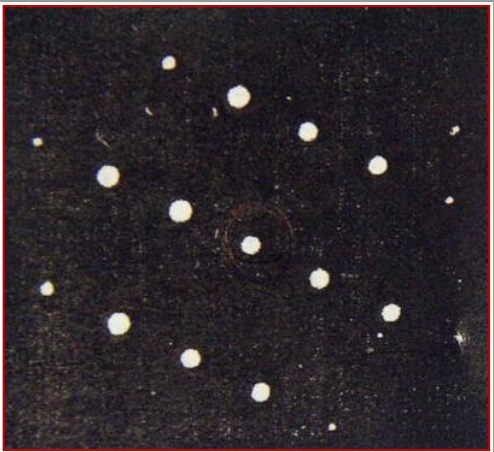
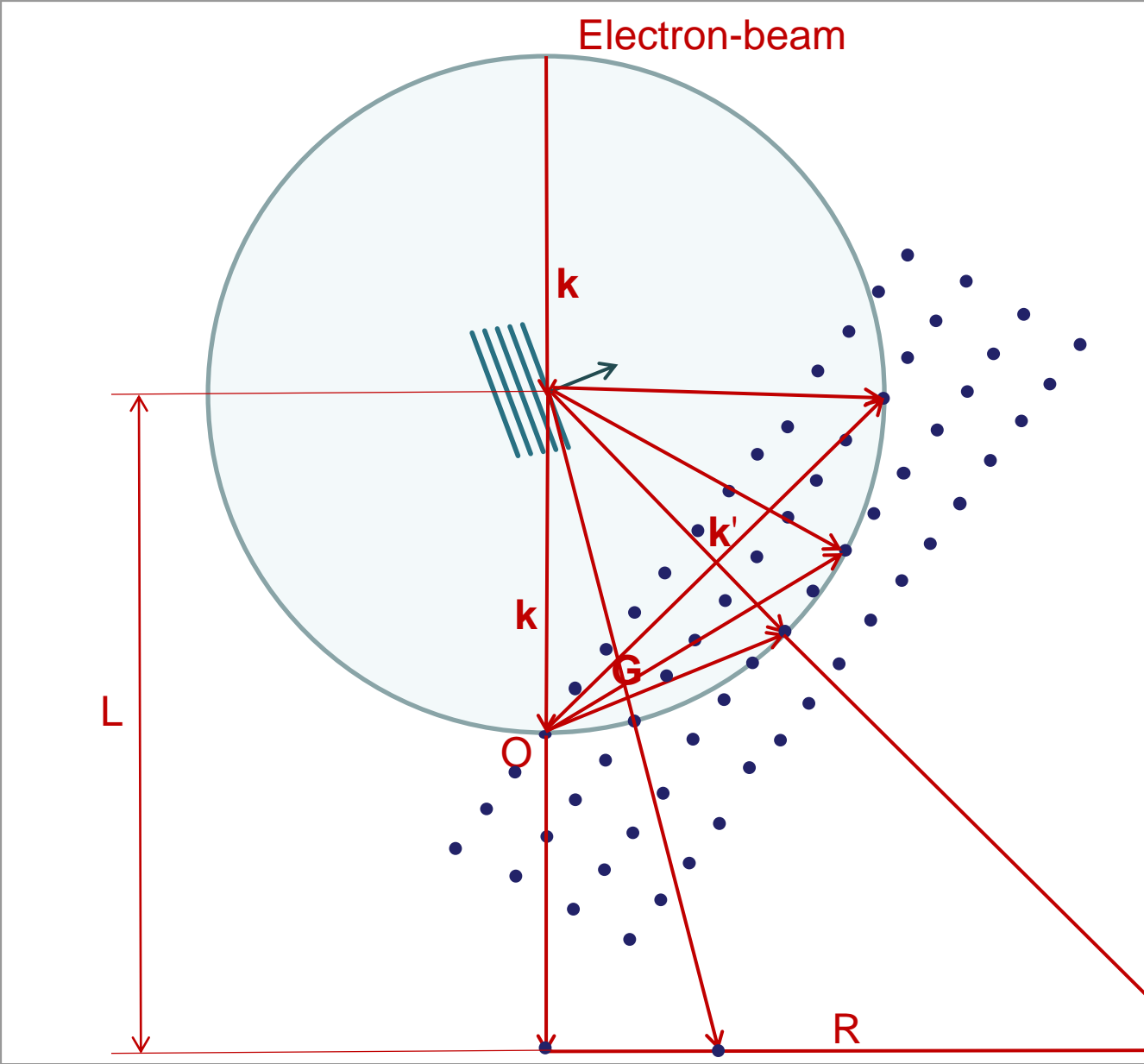
$$d \cos \theta + d \cos \theta' = \mathbf{d} \cdot (\hat{n}' - \hat{n}) = m\lambda$$

$$\mathbf{d} \cdot (\mathbf{k}' - \mathbf{k}) = 2\pi m$$

$$\mathbf{d} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{k}' - \mathbf{k} = \mathbf{G} \quad \Delta \mathbf{k} = \mathbf{G}$$

- The Bragg law •Laue equation •Ewald structure

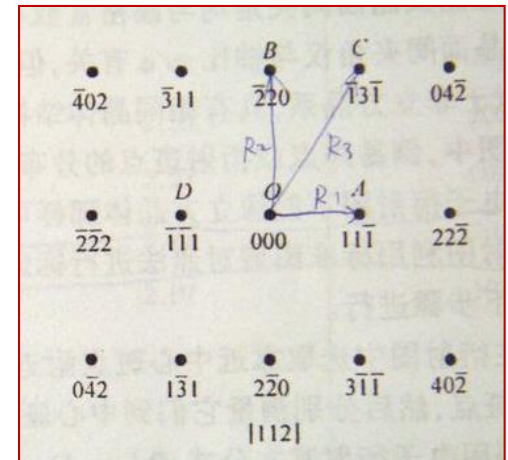
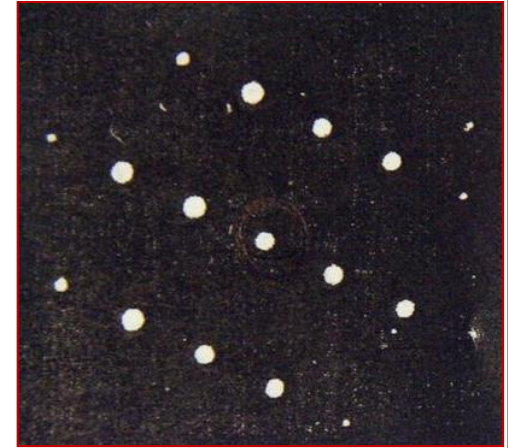
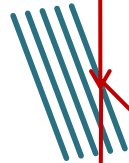


$$\mathbf{k}' - \mathbf{k} = \mathbf{G}$$

$$R_d = L\lambda$$

• The Bragg law • Laue equation • **Ewald structure**

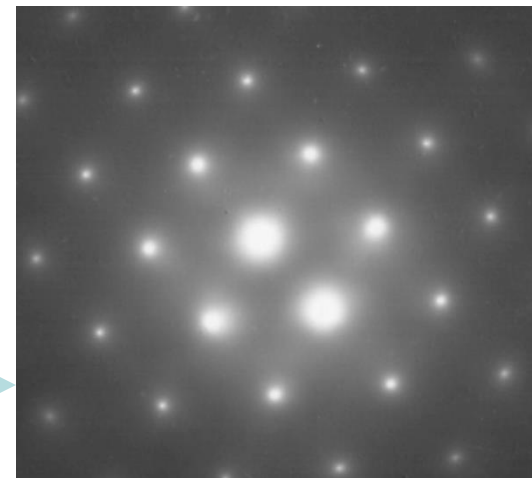
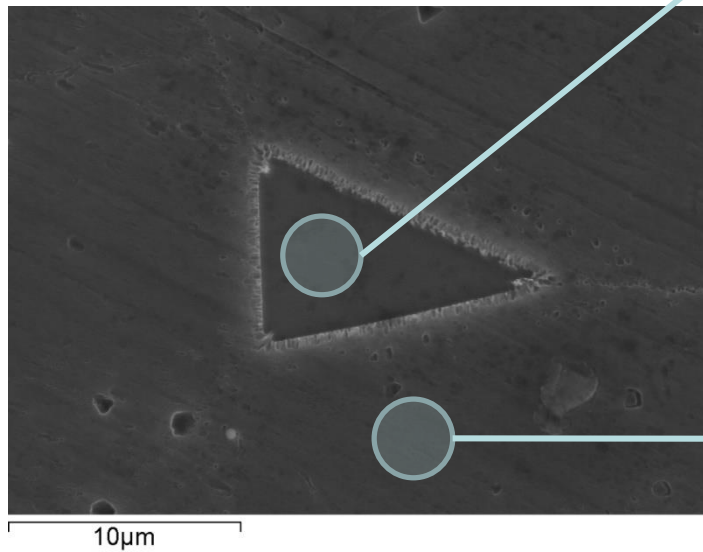
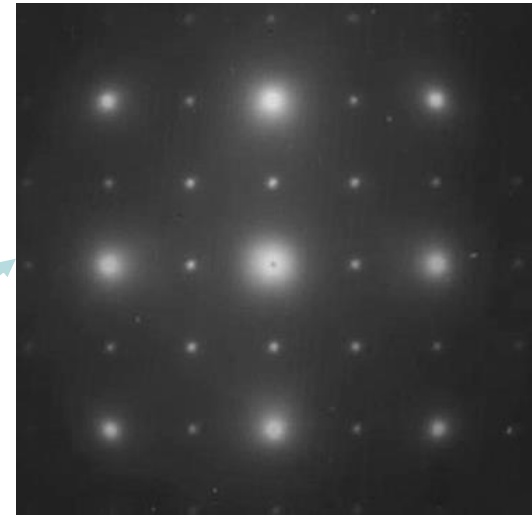
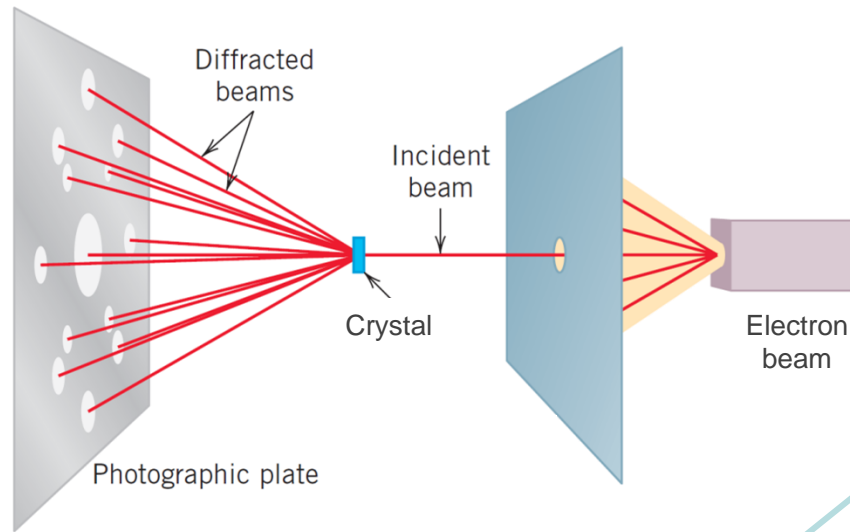
Electron-beam



$$\mathbf{k}' - \mathbf{k} = \mathbf{G}$$

$$Rd = L\lambda$$

•The Bragg law •Laue equation •Ewald structure



## How to learn?

1

## Basic Concept

Periodic function

Fourier series

Reciprocal vector

Reciprocal lattice

Wave-vector space

The Bragg law

Laue equation

Ewald structure

Brillouin Zone

2

## Train of Thought

# Chapter 1 Formation of Crystal

1.1 Quantum Mechanics and atomic structure

1.2 Interatomic bonding in solids

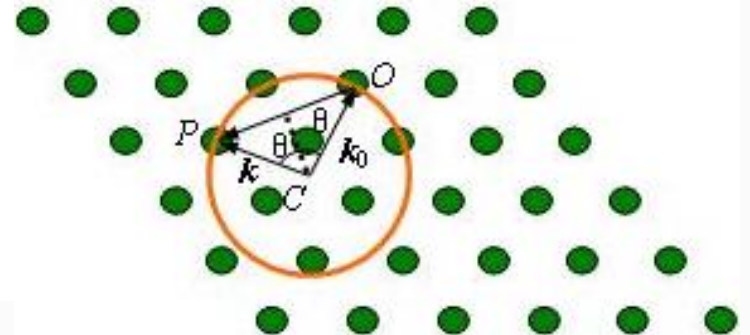
1.3 Crystal structure and typical crystals

1.4 Reciprocal Lattice and Brillouin Zone

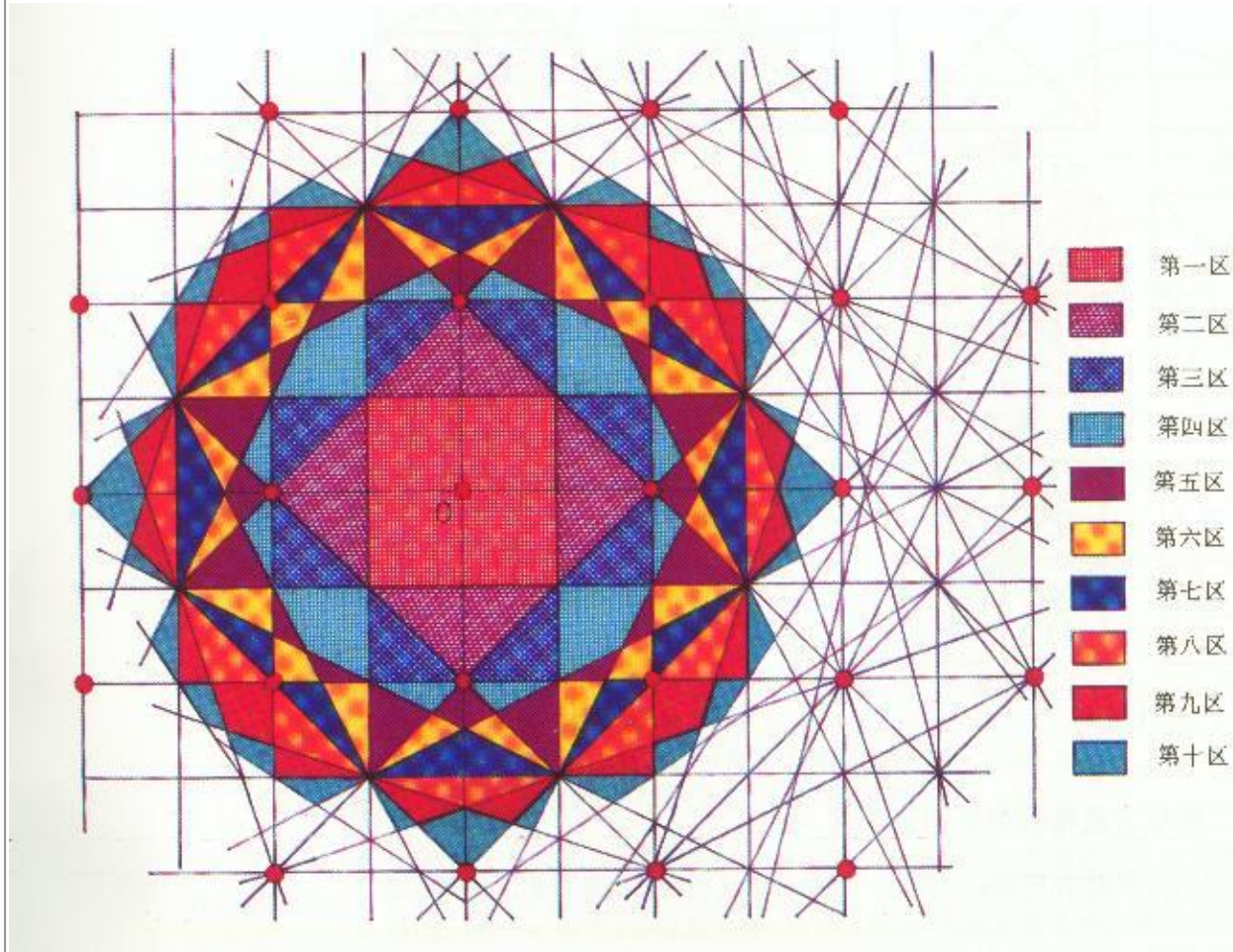
1.4.1 Reciprocal Lattice

1.4.2 Crystal Diffraction

1.4.3 Brillouin Zone

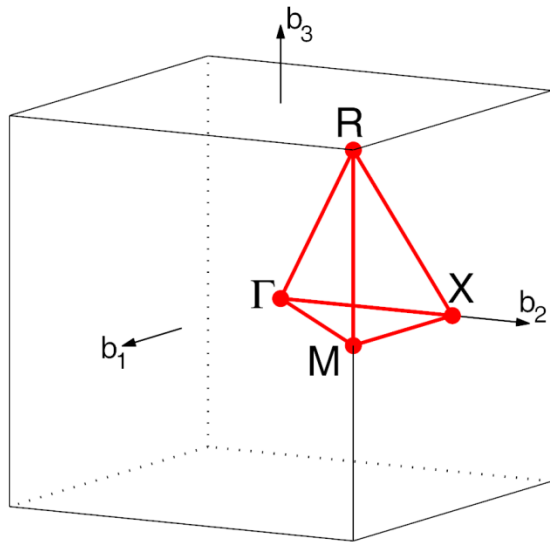




**• Brillouin Zone 2D • Brillouin Zone 3D • Brillouin Zone Interface & Crystal diffraction**

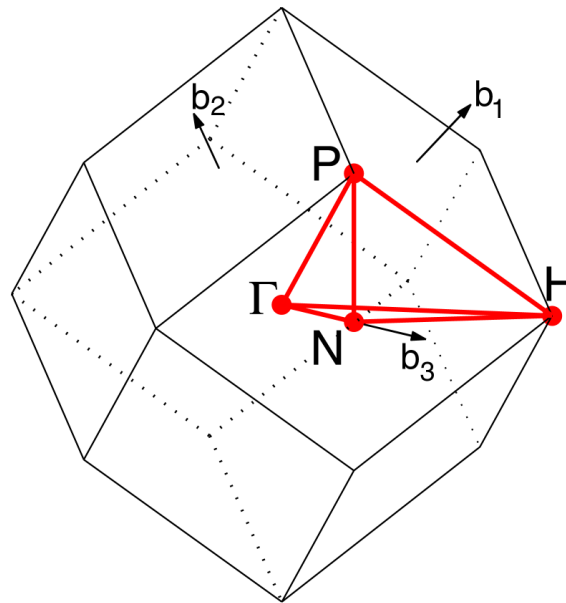
- ❖ The reciprocal lattice point is in the middle of its first BZ.
- ❖ All BZs have the same volume.
- ❖ Every BZ just contains one lattice point.

• Brillouin Zone 2D • **Brillouin Zone 3D** • Brillouin Zone Interface & Crystal diffraction



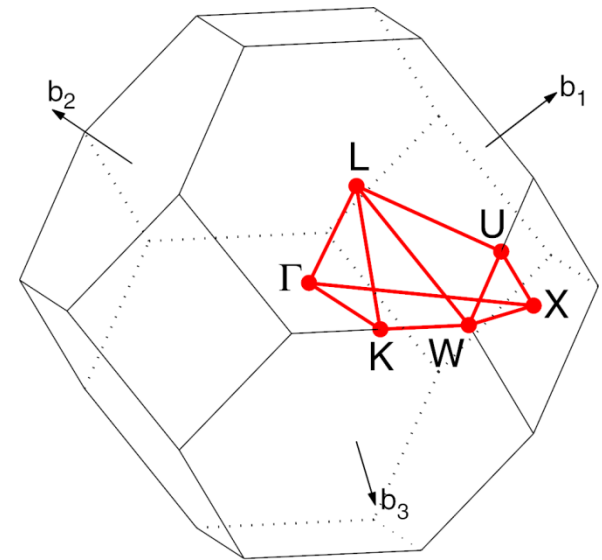
CUB path:  $\Gamma$ -X-M- $\Gamma$ -R-X|M-R

[Setyawan & Curtarolo, DOI: 10.1016/j.commat.2010.05.010]



BCC path:  $\Gamma$ -H-N- $\Gamma$ -P-H|P-N

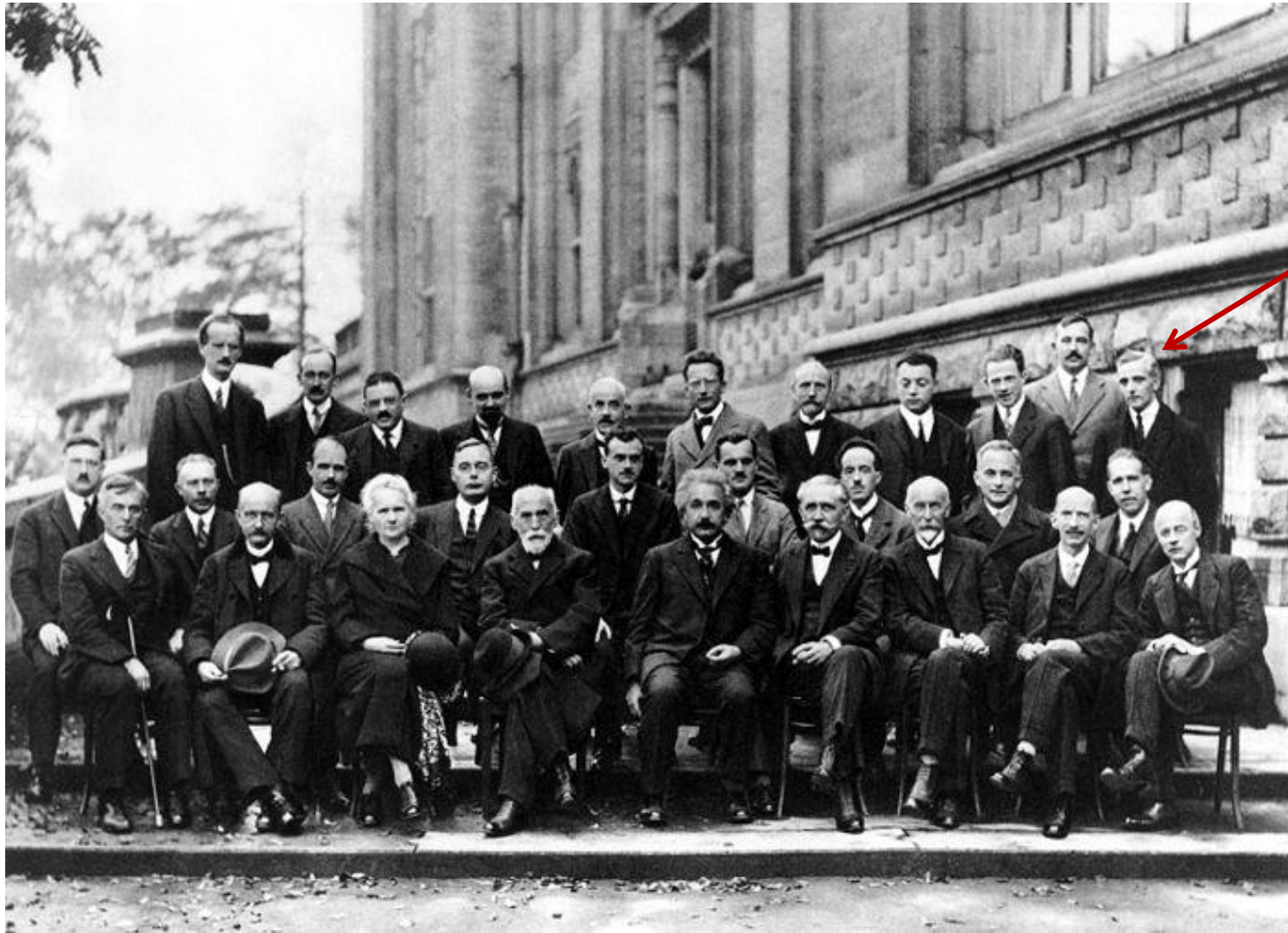
[Setyawan & Curtarolo, DOI: 10.1016/j.commat.2010.05.010]



FCC path:  $\Gamma$ -X-W-K- $\Gamma$ -L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commat.2010.05.010]



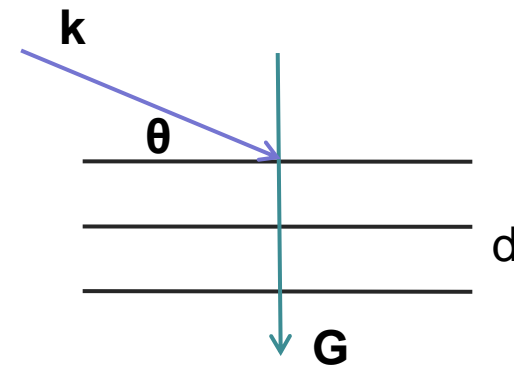
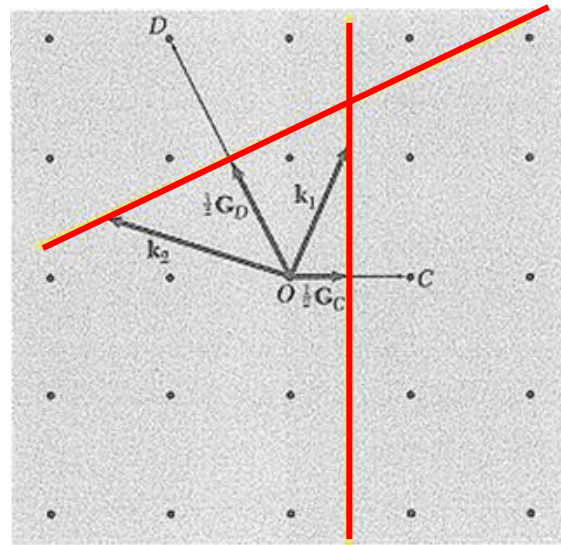
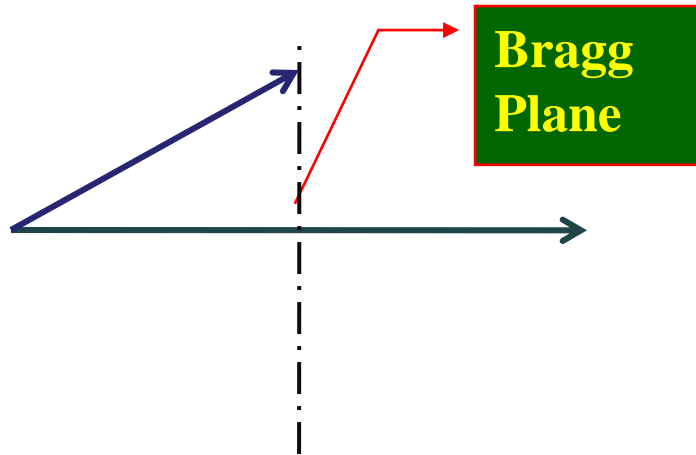
**-Brillouin Zone 2D -Brillouin Zone 3D -Brillouin Zone Interface & Crystal diffraction**

A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. De Donder, E. Schrödinger, J.E. Verschaffelt, W. Pauli, W. Heisenberg, R.H. Fowler, **L. Brillouin**;  
B. P. Debye, M. Knudsen, W.L. Bragg, H.A. Kramers, P.A.M. Dirac, A.H. Compton, L. de Broglie, M. Born, N. Bohr;  
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-Brillouin Zone 2D -**Brillouin Zone 3D** -Brillouin Zone Interface & Crystal diffraction

Photograph of the first conference in 1911 at the Hotel Metropole. Seated (L-R): [W. Nernst](#), [M. Brillouin](#), E. Solvay, [H. Lorentz](#), E. Warburg, J. Perrin, W. Wien, M. Skłodowska-Curie, and [H. Poincaré](#). Standing (L-R): [R. Goldschmidt](#), [M. Planck](#), H. Rubens, [A. Sommerfeld](#), F. Lindemann, [M. de Broglie](#), M. Knudsen, F. Hasenöhl, G. Hostelet, E. Herzen, [J.H. Jeans](#), [E. Rutherford](#), H. Kamerlingh Onnes, [A. Einstein](#) and [P. Langevin](#).

• Brillouin Zone 2D • Brillouin Zone 3D • **Brillouin Zone Interface & Crystal diffraction**



$$\mathbf{k} \cdot \frac{\mathbf{G}}{G} = \frac{1}{2} G$$

$$2\mathbf{k} \cdot \mathbf{G} = G^2$$

$$2kG \sin \theta = G^2$$

$$2 \frac{2\pi}{\lambda} \sin \theta = \frac{2\pi}{d}$$

$$2d \sin \theta = \lambda$$

All wave vectors  $\mathbf{k}$  which tips are on the boundary of BZ can be Bragg reflected.  
Only waves whose wave vector drawn from the origin of  $\mathbf{k}$ -space terminates on the boundary of BZ will satisfy the condition for diffraction.



## How to learn?



1

Train of Thought

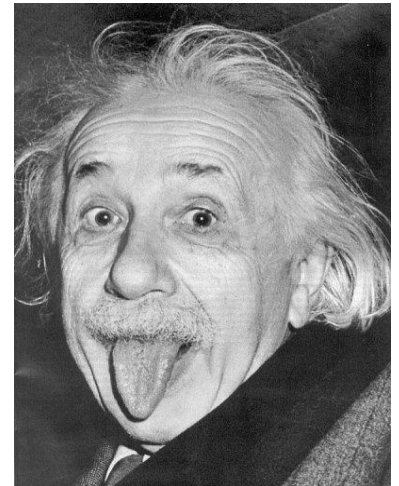
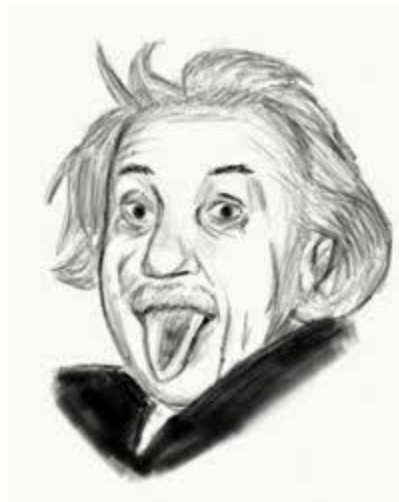
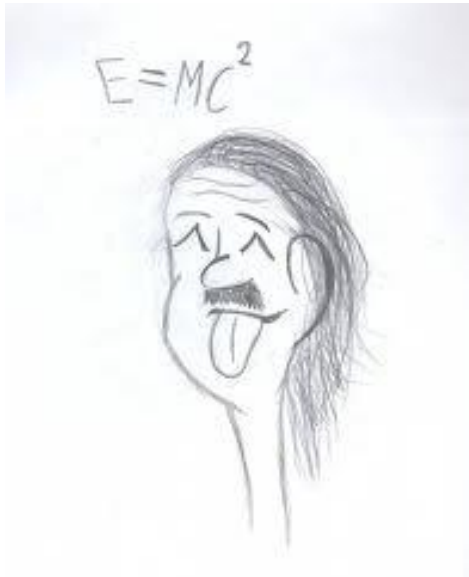
2

Conclusions

3

Basic Concept

4

Math and  
physical Details

## Summary &amp; Basic Concepts

1

## Basic Concept

Periodic function

Fourier series

Reciprocal vector

Reciprocal lattice

Wave-vector space

The Bragg law

Laue equation

Ewald structure

Brillouin Zone

2

## Train of Thought

Fourier series

3

## Conclusions

We know  
and  
we see.

**Summary**

Thank you for  
your attention!

