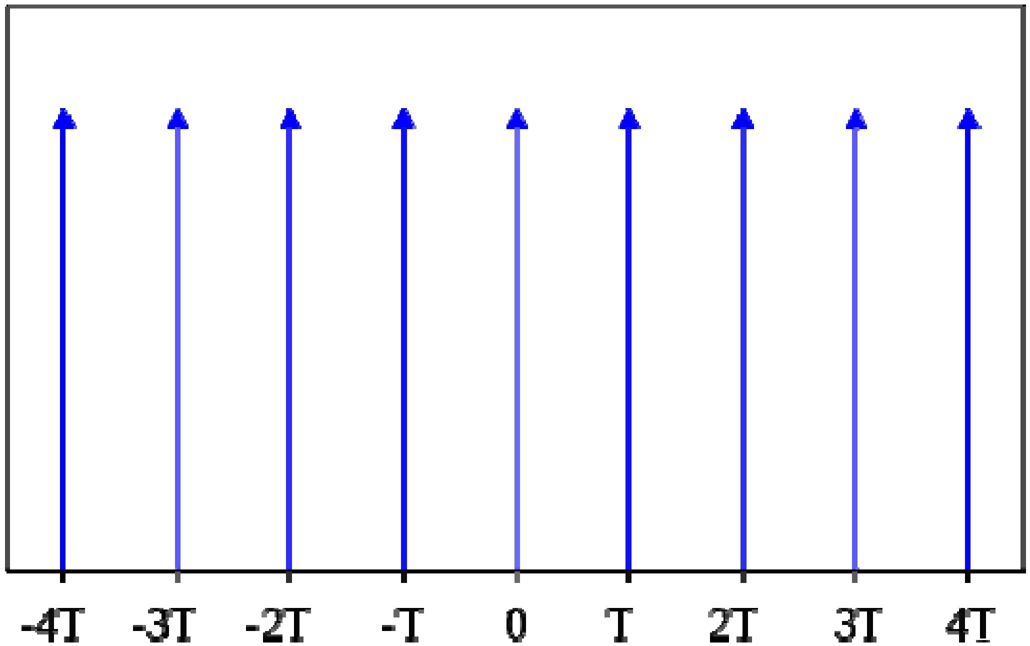
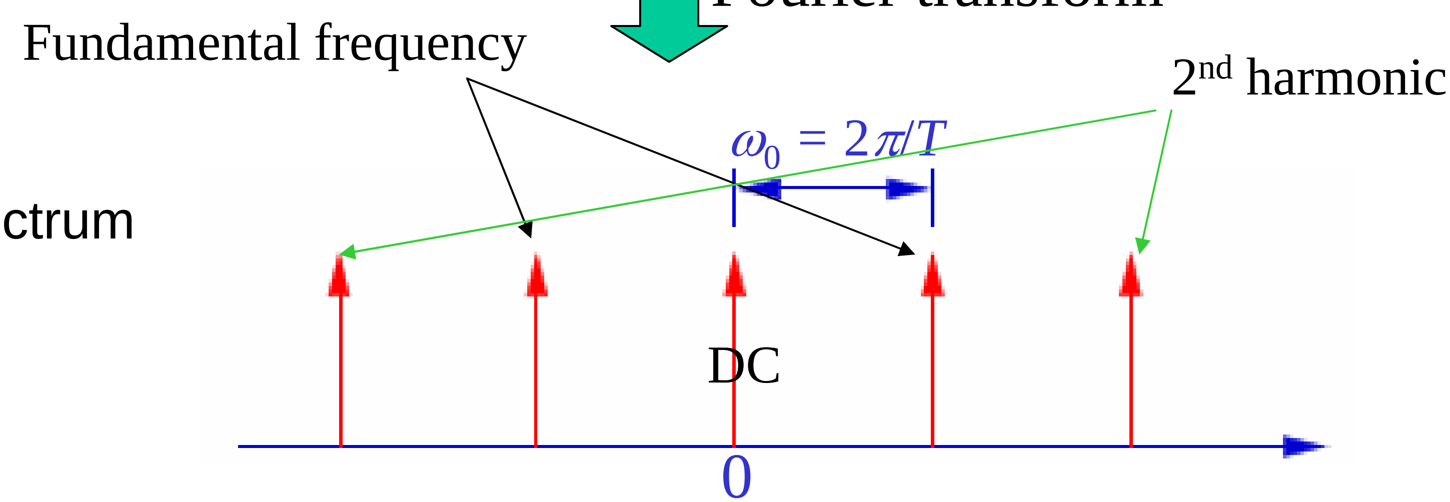
Let's talk about periodic things

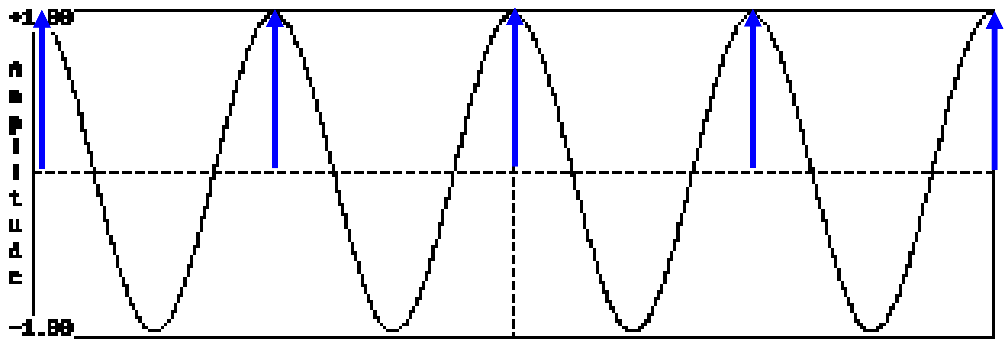
Time-domain signal



Fourier transform

Spectrum



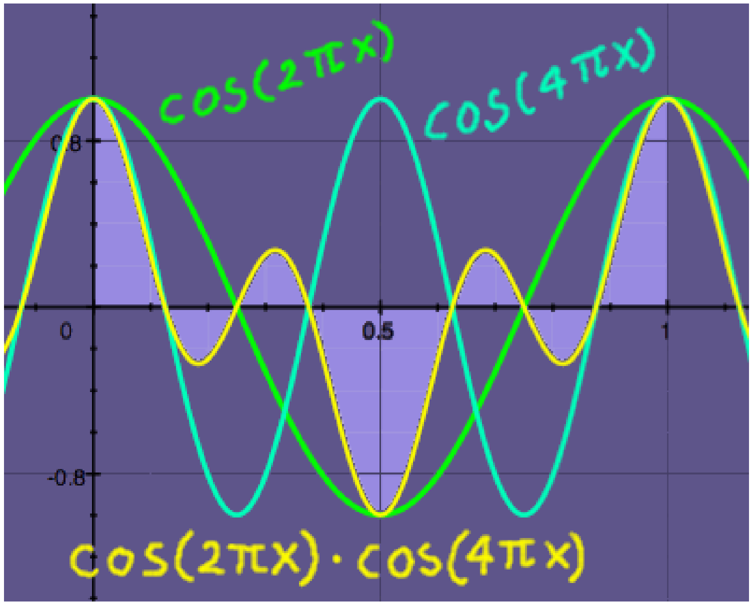


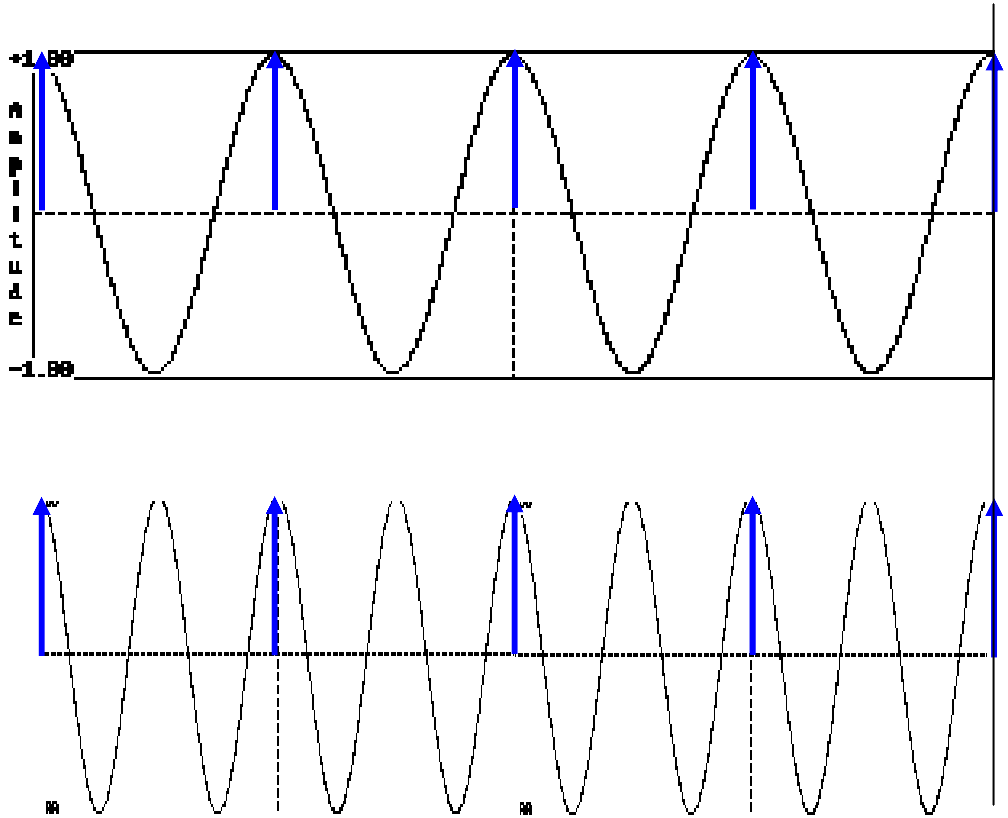
To find the fundamental frequency component: $$\int_{-\infty}^{+\infty} \delta(t-nT)\cos\omega_0 t\,dt$$

In contrast,

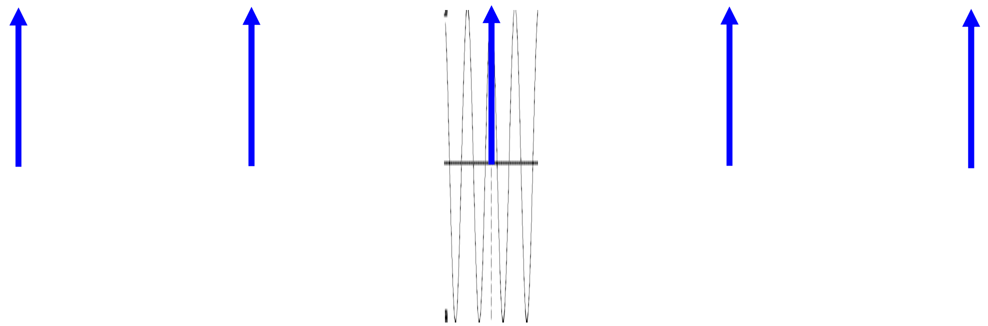
$$\int_{-\infty}^{+\infty} \cos 2\omega_0 t \cos\omega_0 t\,dt = 0$$

The 2nd harmonic is orthogonal to the fundamental.





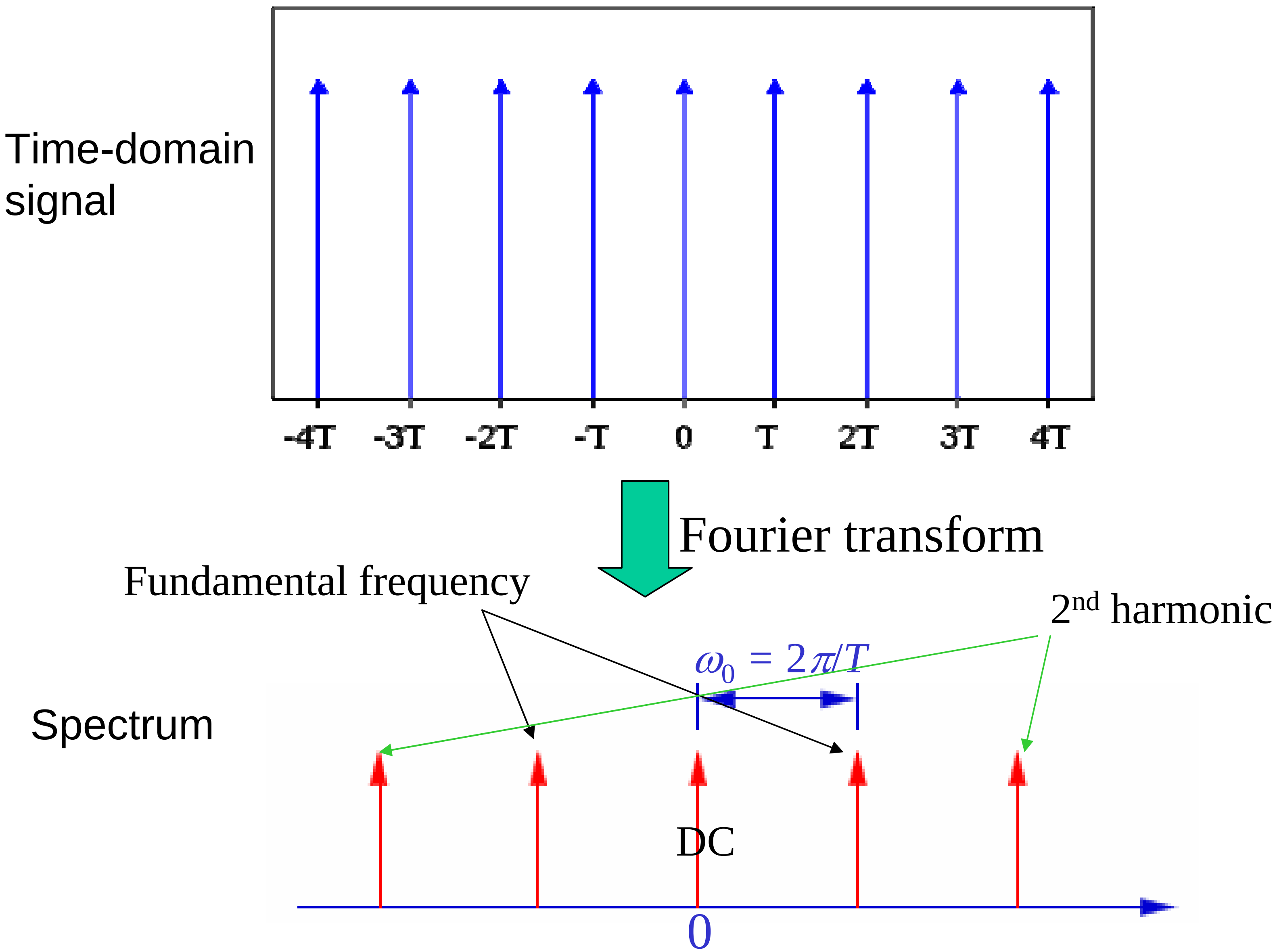
To find the 2nd harmonic: $$\int_{-\infty}^{+\infty}\delta(t-nT)\cos 2\omega_0 t dt$$



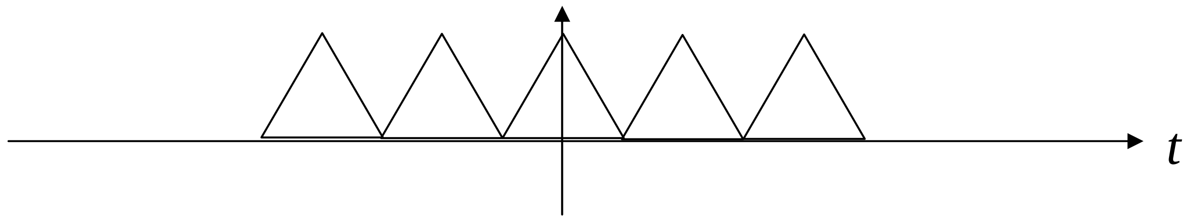
Since the spike is infinitely sharp, we have the *n*th harmonic as a spike in the frequency domain, no matter how big *n* is.

$$\int_{-\infty}^{+\infty} \delta(t - nT)\cos n\omega_0 t\,dt$$

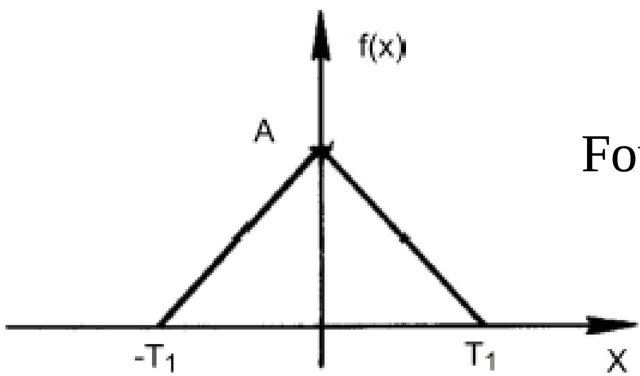
Therefore,


Time-domain signal
-4T
-3T
-2T
-T
0
T
2T
3T
4T
Fourier transform
Fundamental frequency
2nd harmonic
$\omega_0 = 2\pi/T$
Spectrum
DC
0

How do we find the spectrum of a periodic signal like this one



if we know

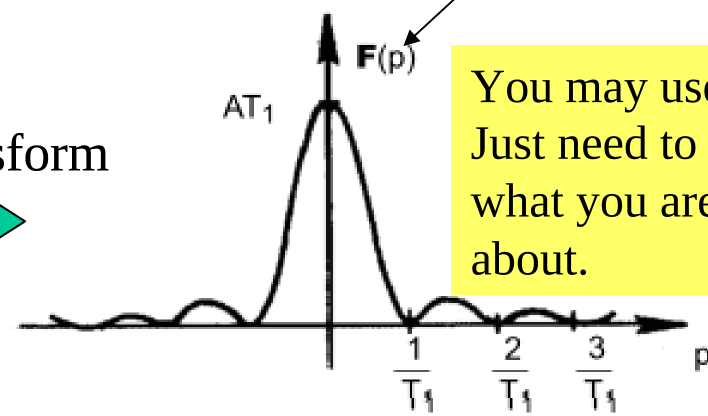


$$f(x) = -\frac{A}{T_1}|x| + A$$

$f(x)=0 \quad |x| < T_1 \quad$ and $\quad |x| > T_1$

Fourier Transform

p is frequency



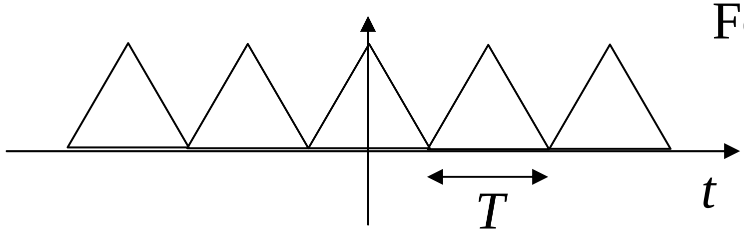
You may use *f* or *ω*. Just need to know what you are talking about.

$$F(p) = AT_1\left[\frac{\sin(\pi T_1 p)}{\pi T_1 p}\right]^2 = AT_1 \operatorname{sinc}^2(\pi T_1 p)$$

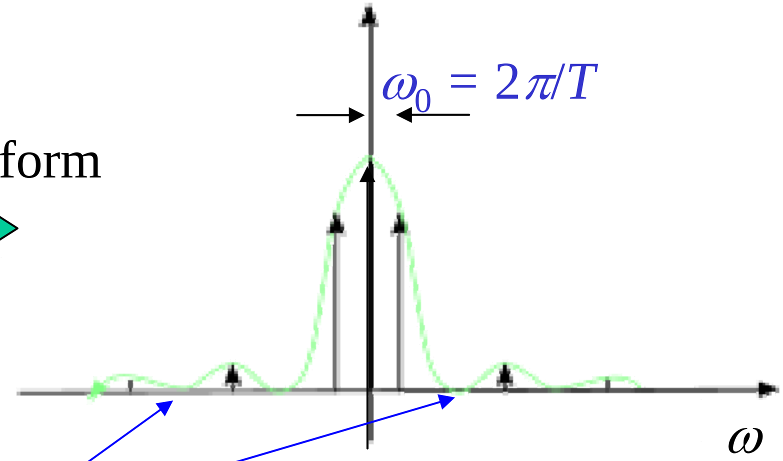
(Figures taken from http://www.roymech.co.uk/Useful_Tables/Maths/fourier/Maths_Fourier_transforms.html)

Images taken from Web. Function of *x*, but the math is the same; actually that's what we really will talk about.

It turns out

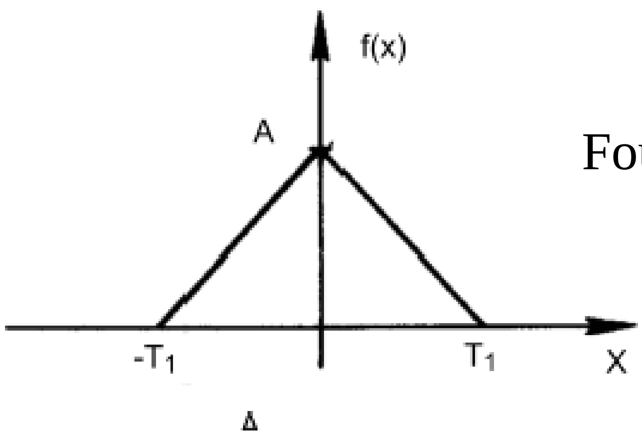


Fourier Transform

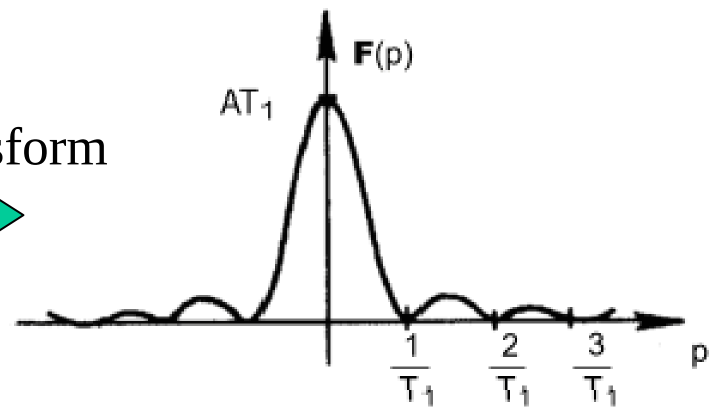


Spikes disappear. We'll revisit this when we talk about diffraction patterns.

because

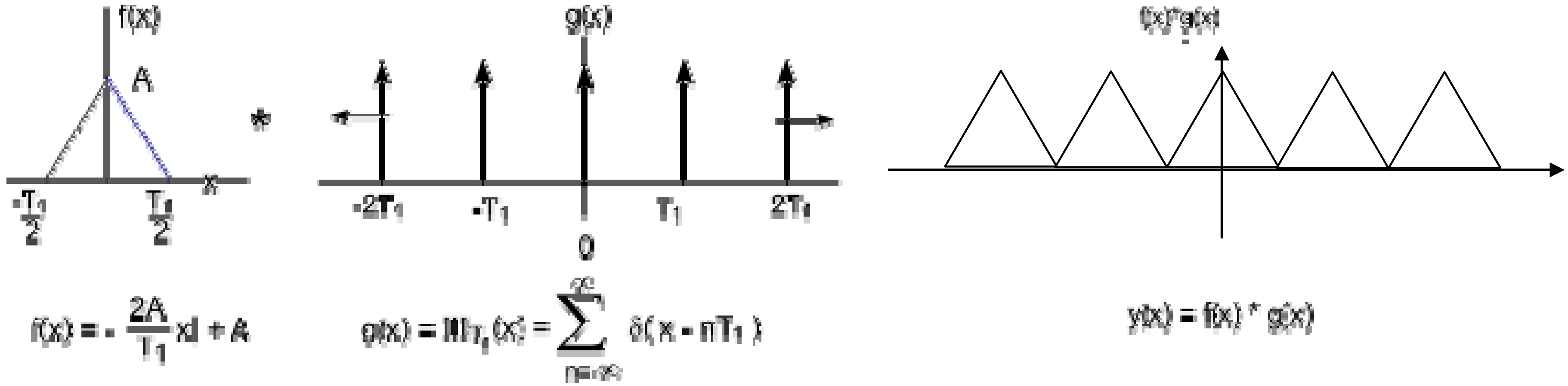


Fourier Transform



A bit more math if you were into signals and systems:

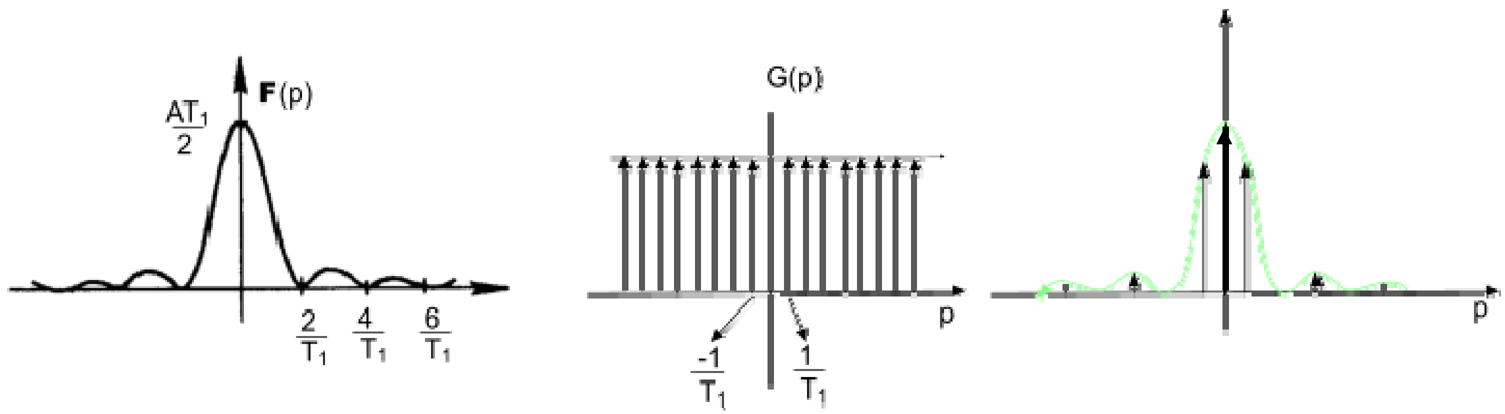
In the time (or space) domain:



Convolution: $f(t) * \delta(t) = f(t)$

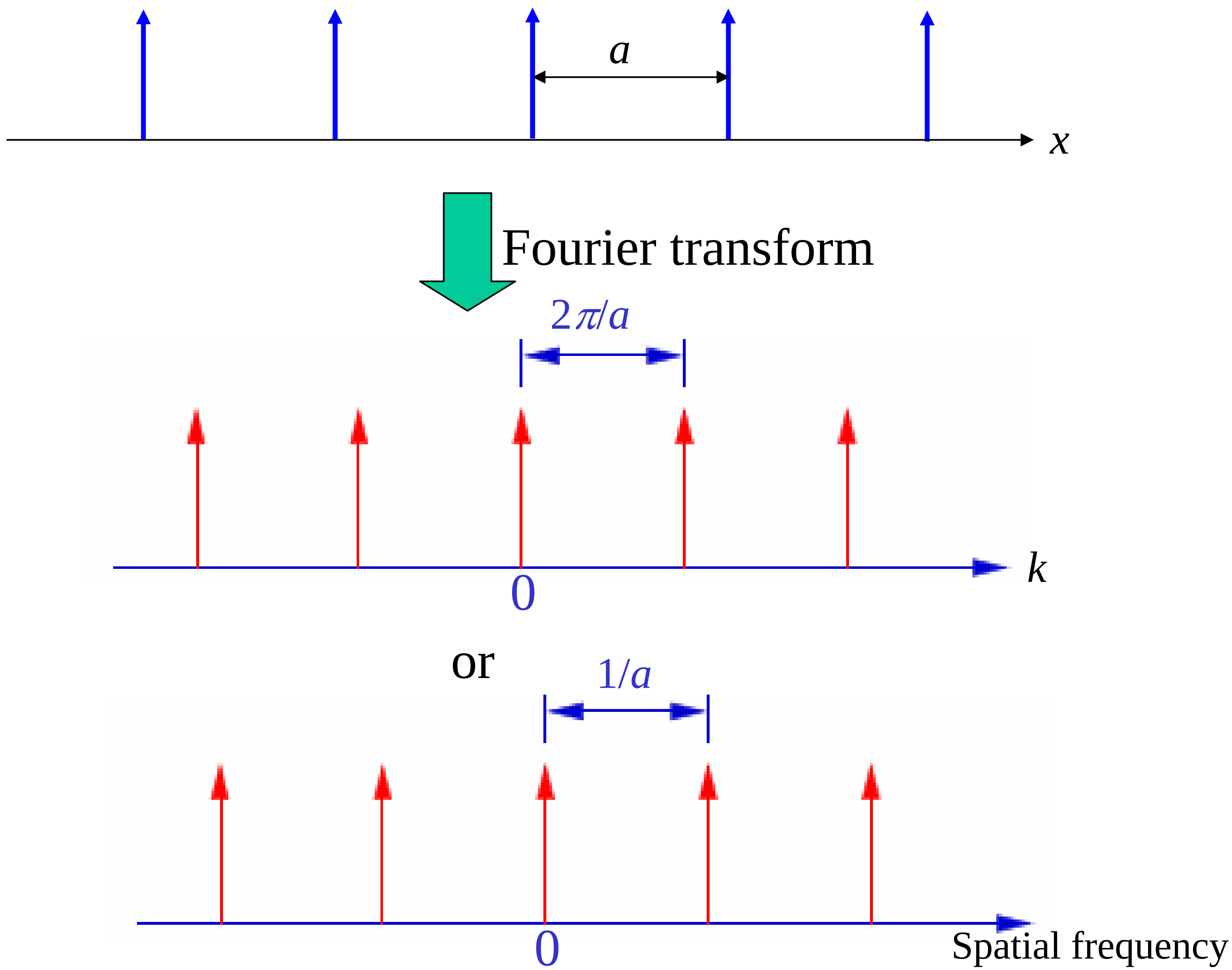
Shift: $f(t) * \delta(t - nT) = f(t - nT)$

Construct the pulse train: $f(t) * \sum_n \delta(t - nT) = \sum_n f(t - nT)$



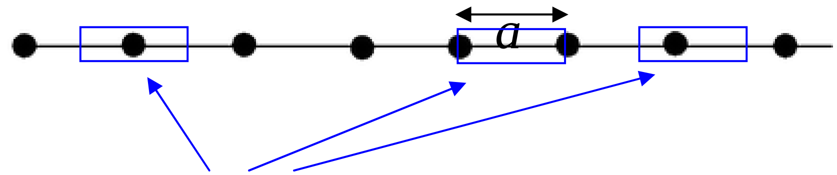
$f_1(t) * f_2(t)$ Fourier Transform $F_1(\omega)F_2(\omega)$

The math is the same for space (as for time)



You may replace the spikes with points

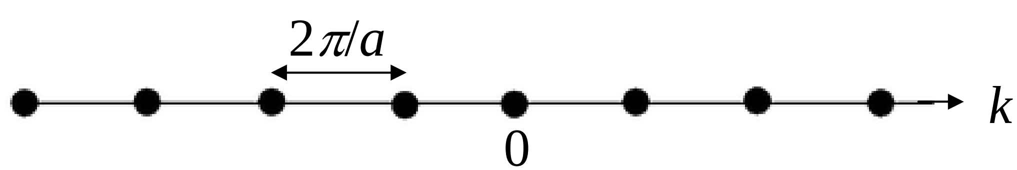
In real space:



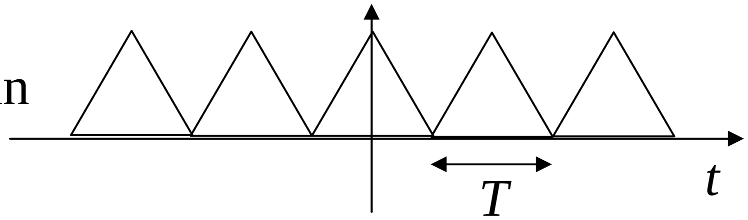
We call a period a “unit cell.” Infinite choices for the unit cell.

Fourier transform

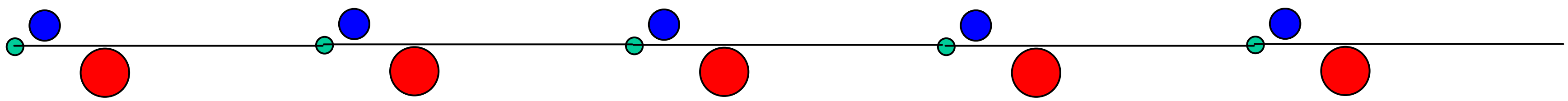
In reciprocal (or k-) space:

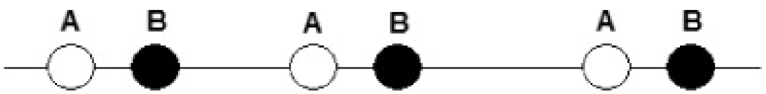


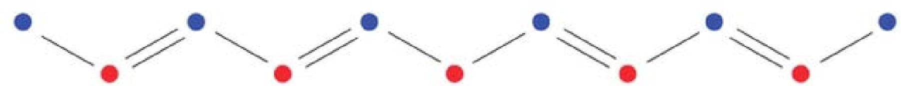
Just like you can have a pulse train in time domain



the unit cell can have an internal structure



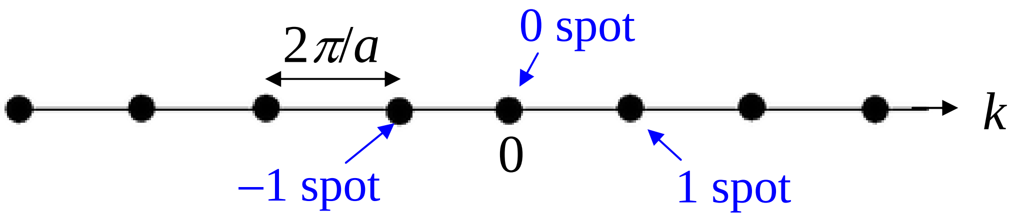




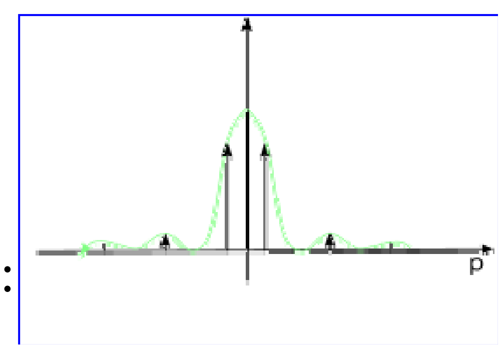
Again, you have infinite choices defining the unit cell.

Fourier transform

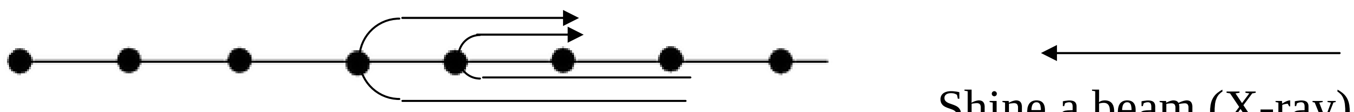
(A computer can do FFT)



The intensities of the spots vary due to the unit cell internal structure, just like in the spectrum of a time-domain pulse train:



Nature's way of doing Fourier transform: Diffraction



Shine a beam (X-ray) with many wavelengths (broadband)

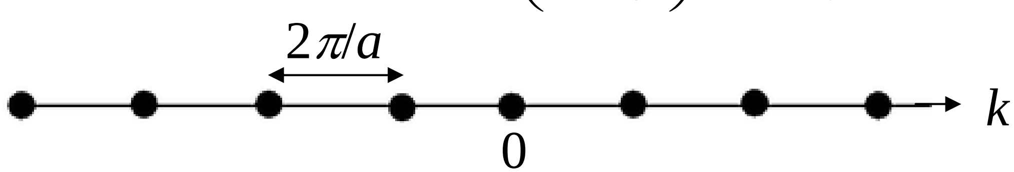
To have constructive interference between reflections by all atoms/unit cells:

$$a = \frac{\lambda}{2} n \quad \Longrightarrow \quad \frac{2\pi}{k} = \lambda = \frac{2a}{n} \quad \Longrightarrow \quad \boxed{k = n\frac{2\pi}{2a}}$$

The k of the photon

The $\boldsymbol{k}$ (vector, proportional to its momentum) of the photon is changed upon reflection by

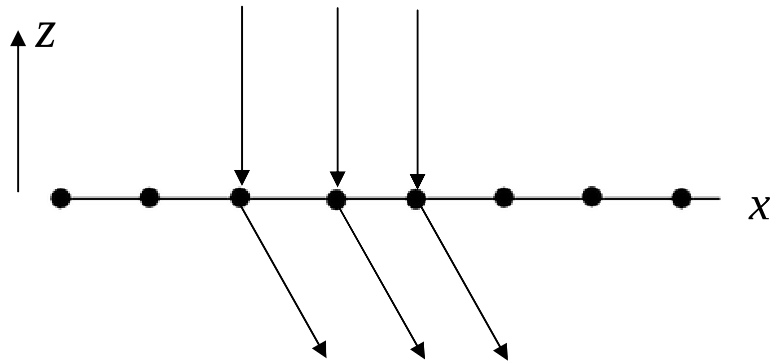
$$|\Delta \boldsymbol{k}| = |\boldsymbol{k}_f - \boldsymbol{k}_i| = 2\left(n\frac{2\pi}{2a}\right) = n\frac{2\pi}{a}$$

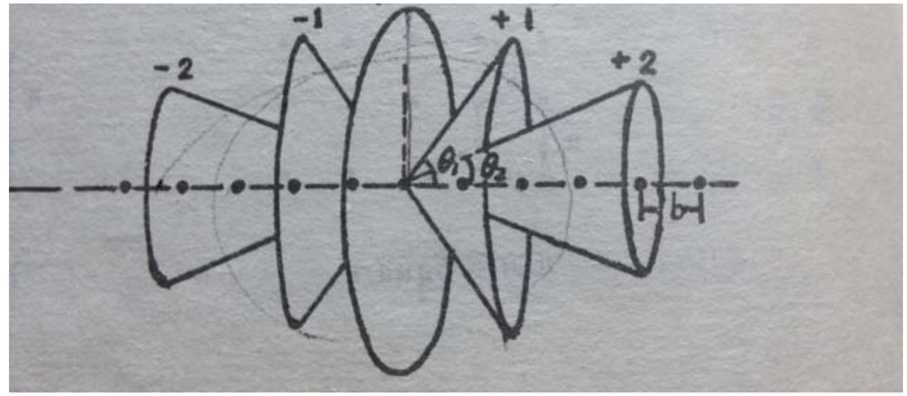


You see, the Fourier transform is just a "spectrum" of $\Delta\boldsymbol{k}$.

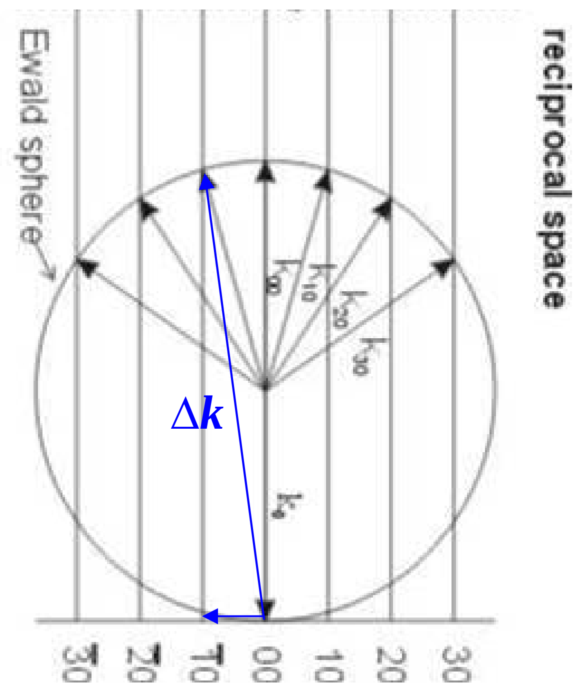
It feels like the lattice gives the photons momenta $n(2\pi/a)$. You have a kind of "momentum conservation."

You can shine a monochrome beam in a second dimension (more like the way that's actually practiced)

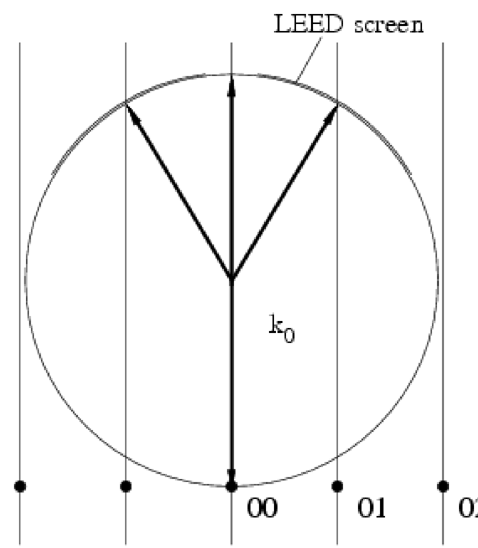




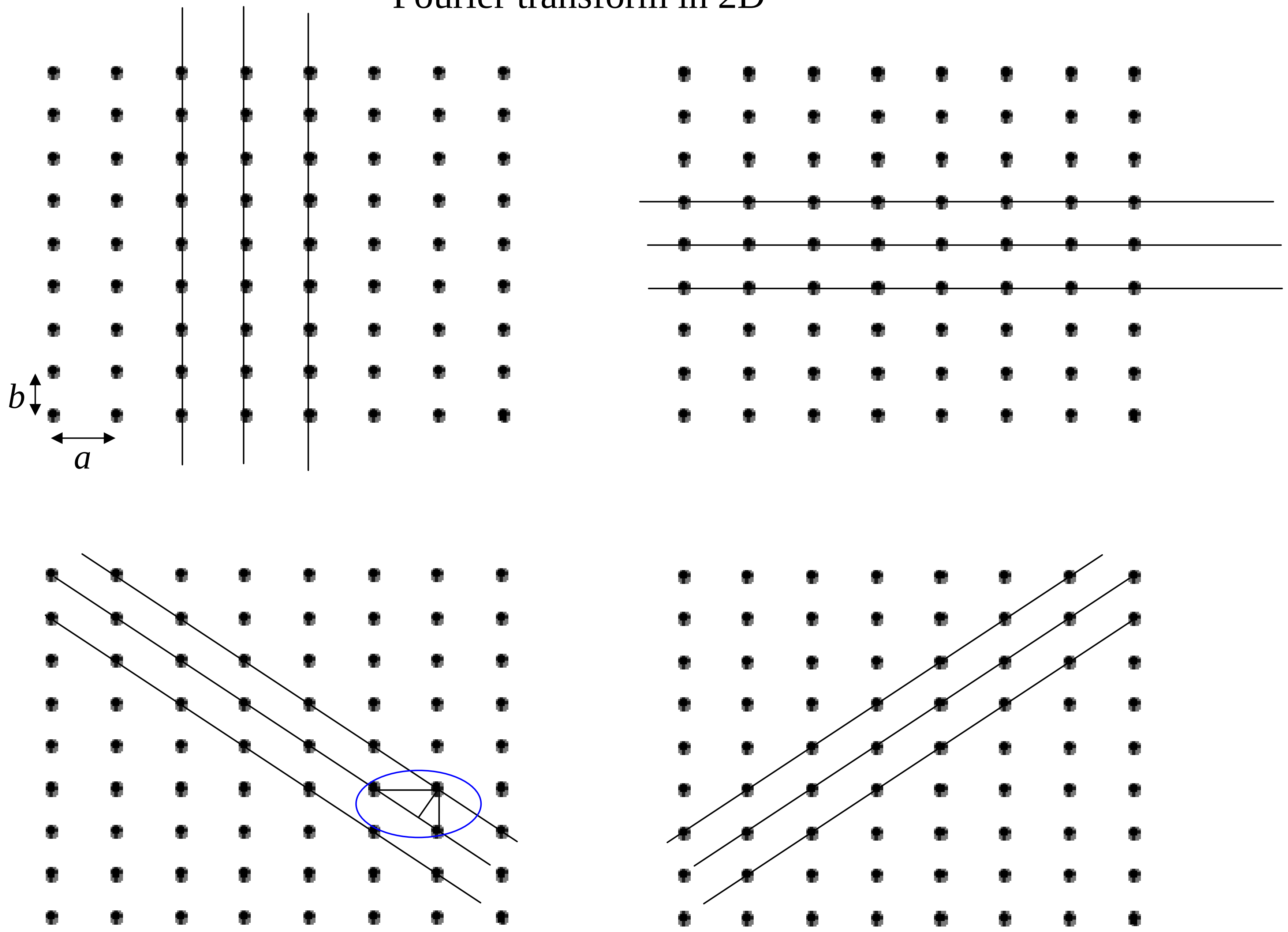
In some directions, you have the right $\Delta \boldsymbol{k}$ for constructive diffraction.

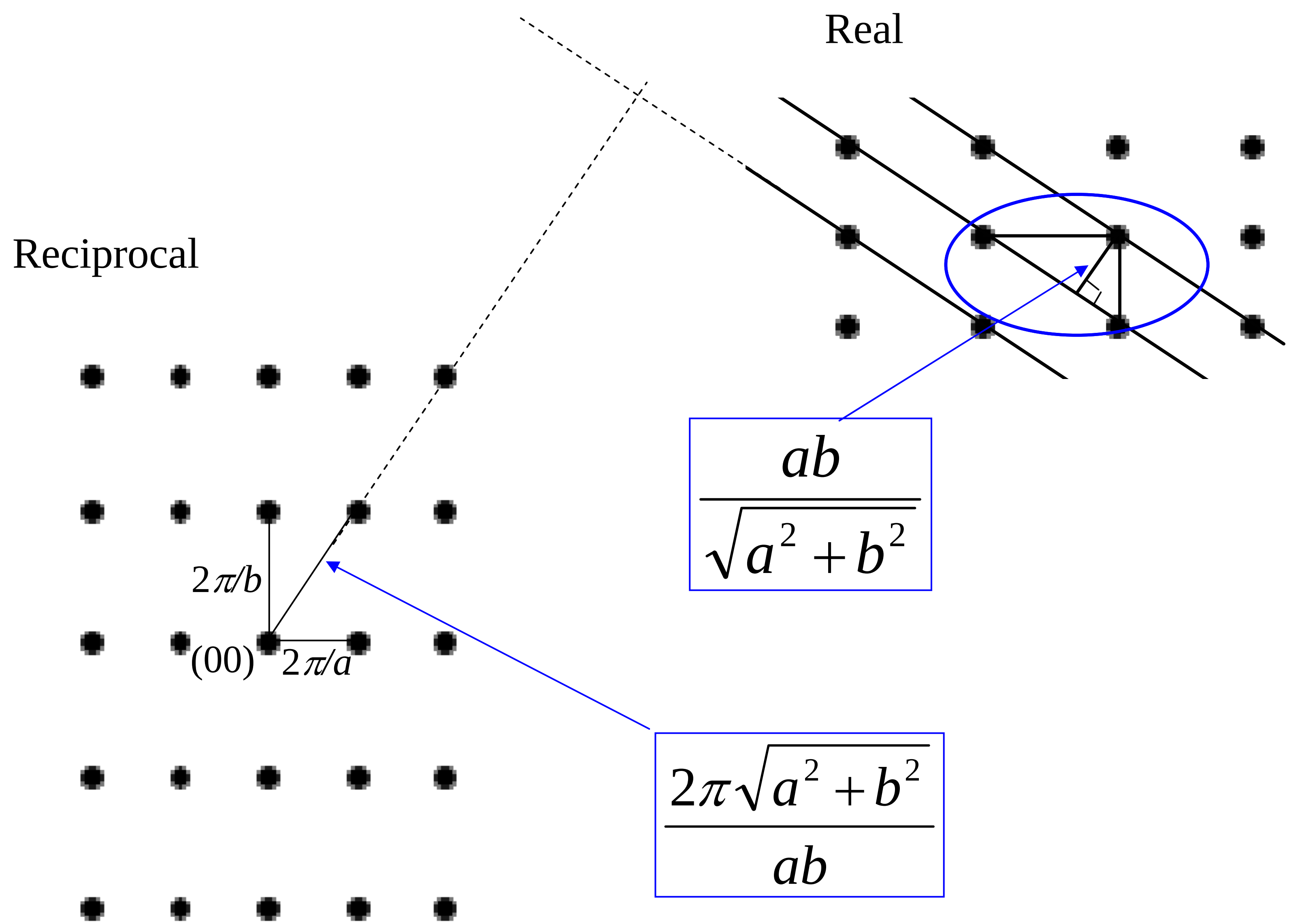


- Momentum conserves only in the *x* direction.
- k_z is free to keep $k_f = k_i$.
- The pattern is a bunch of parallel lines,
- Each standing for a Δk_x,
- Set by the lattice.
- The pattern is a spectrum of Δk_x,
- Representing the spatial frequencies (momenta) of the lattice.

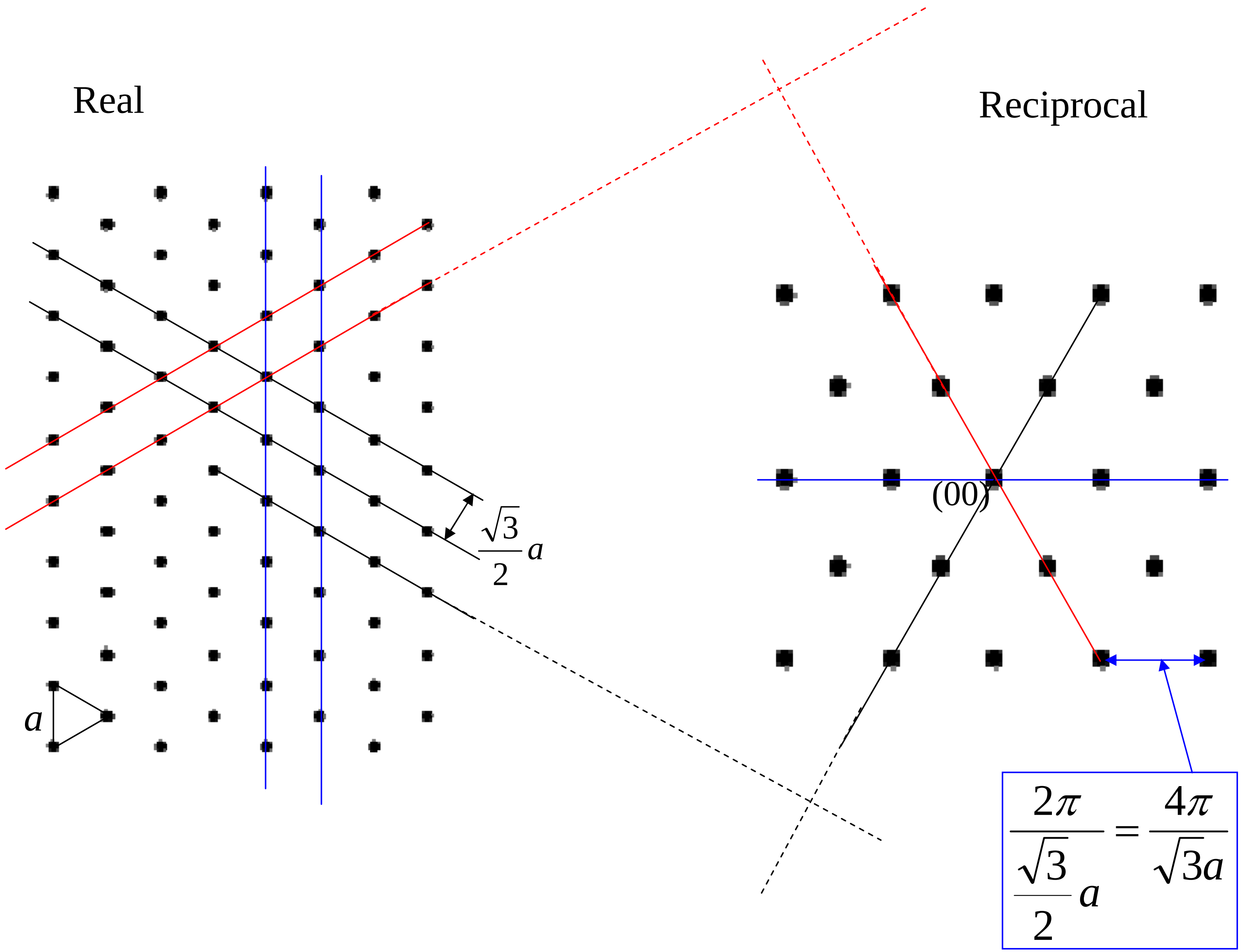


Fourier transform in 2D



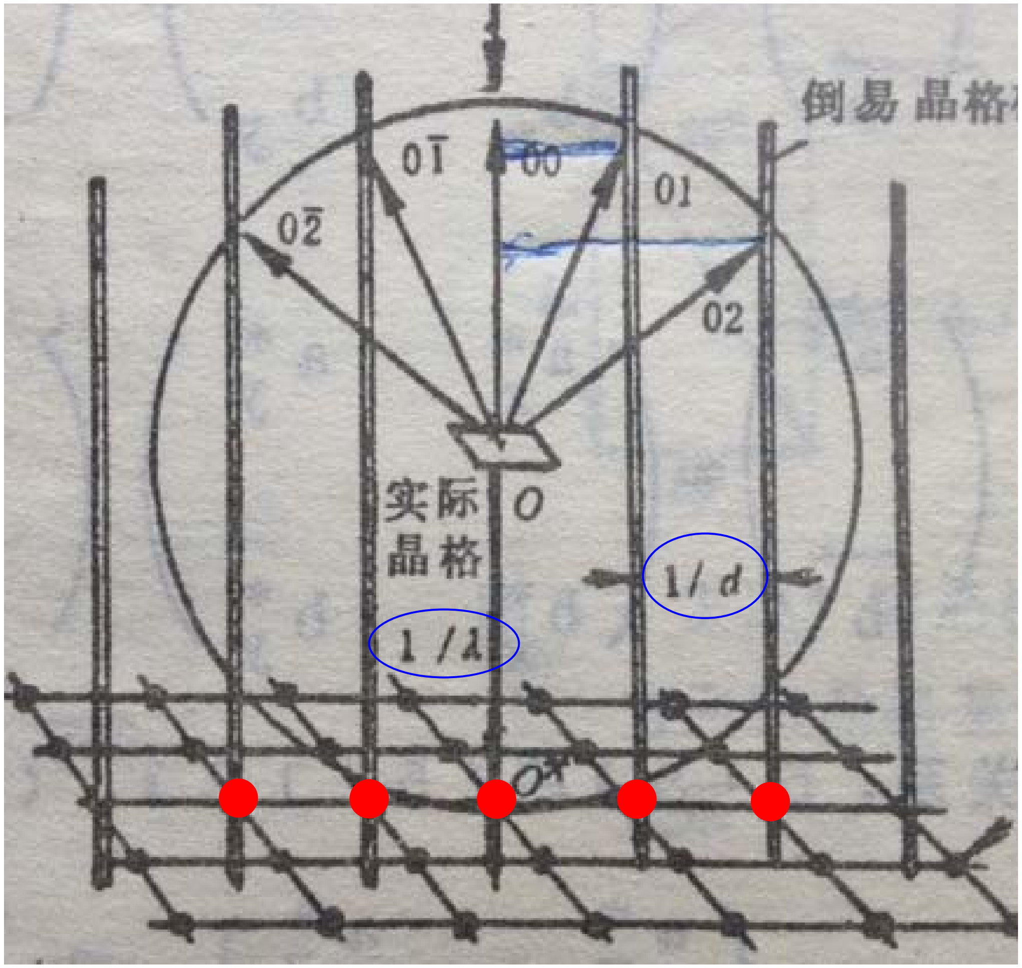


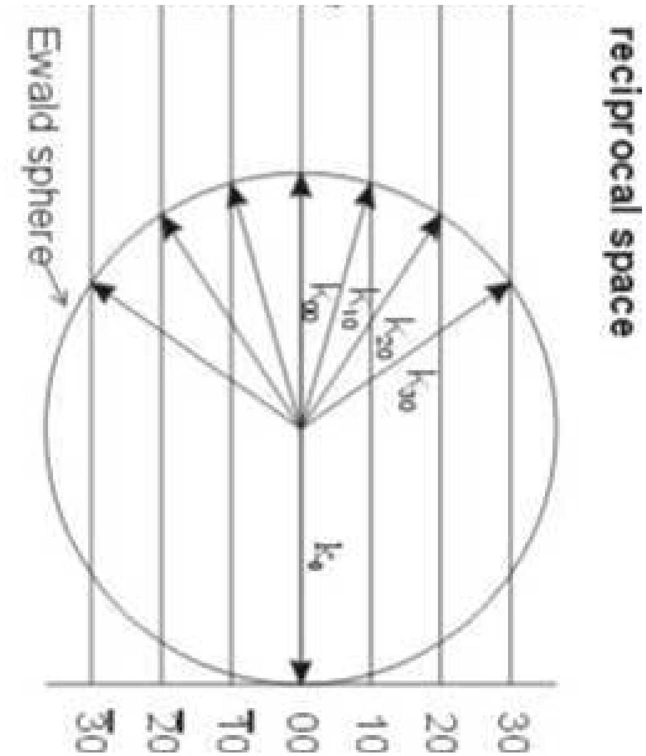
A reciprocal lattice represents a family of parallel real lattice planes.



Real
Reciprocal
$\frac{\sqrt{3}}{2}a$
a
(00)
$\frac{2\pi}{\frac{\sqrt{3}}{2}a} = \frac{4\pi}{\sqrt{3}a}$

Diffraction by 2D Lattice

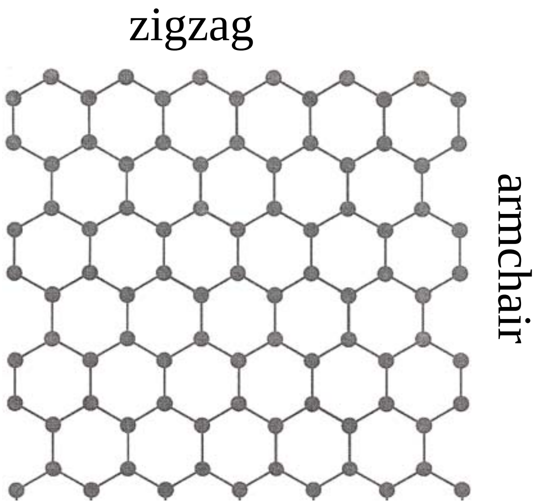


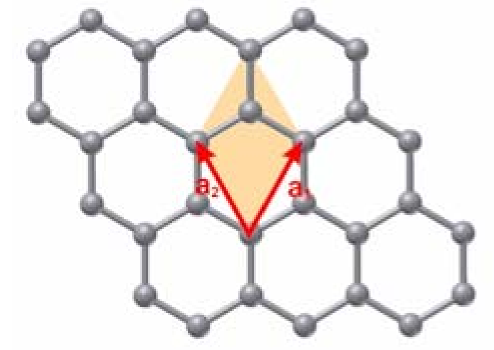


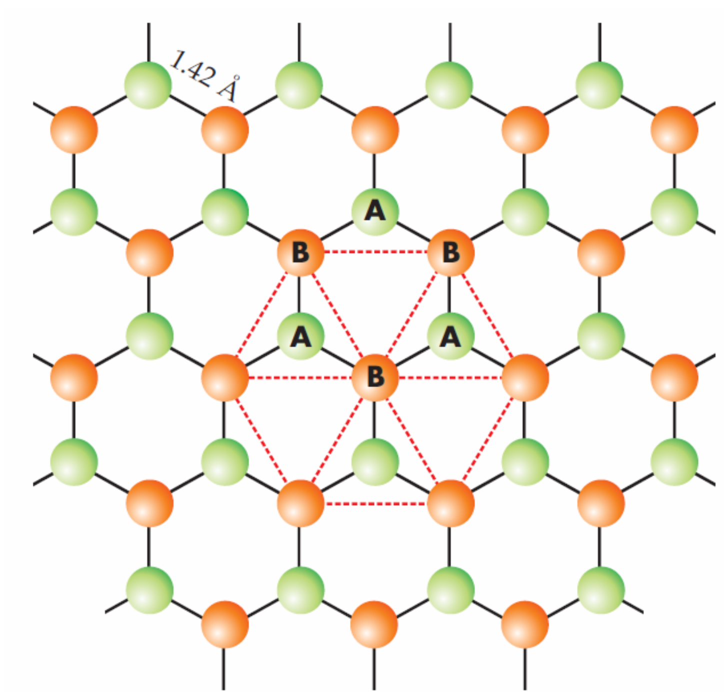
The wave may be an electron beam.
We have talked about the very basics. Now it should be easy for you to read about the details of LEED and SAED.

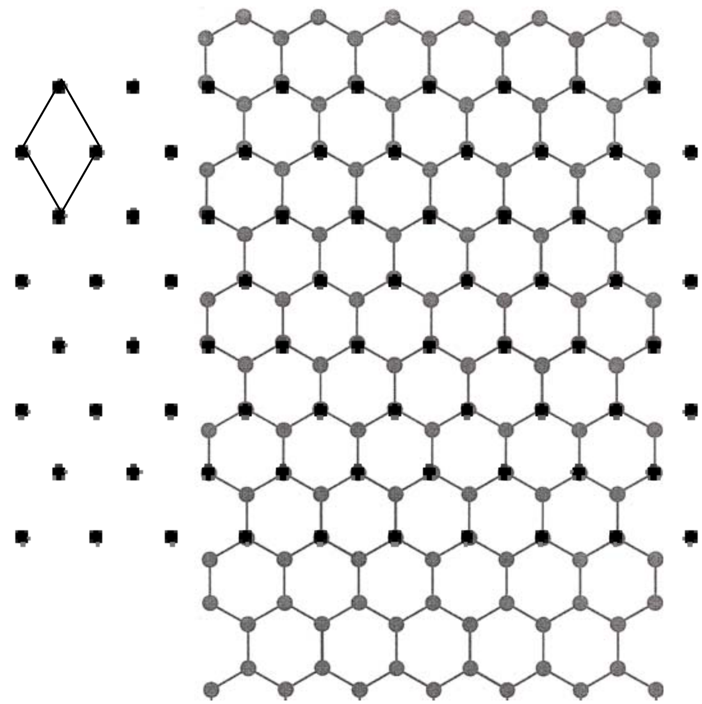
- The pattern is an array of spots,
- Each standing for a $\Delta\boldsymbol{k}_{//}$,
- Set by the lattice.
- The pattern is a spectrum of $\Delta\boldsymbol{k}_{//}$,
- Representing the spatial frequencies (momenta) of the lattice.
- Momentum conserves only in the *xy* plane.
- k_z is free to keep $k_f = k_i$.

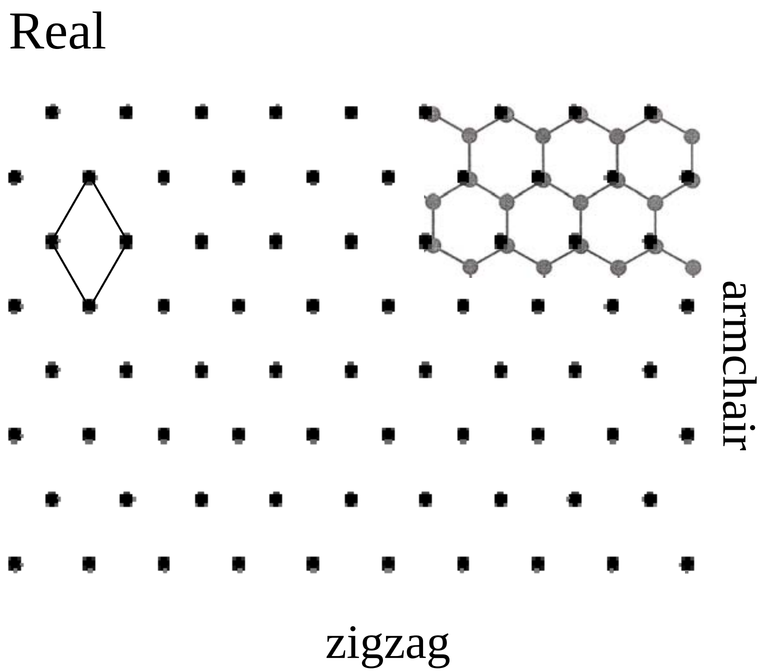
Wait a minute, is the graphene "lattice" a lattice?

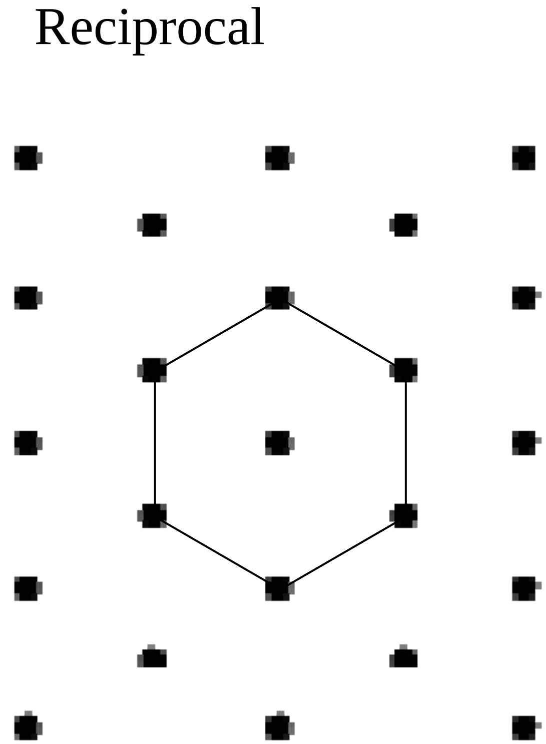












The reciprocal lattice of a 3D lattice is just a 3D array of reciprocal lattice points.

Disclaimer

We’ve seen the beauty of periodic things.
We study them probably just because they are simple and we have the mathematical tools, not necessarily because they are “better.”

What the physicist calls “yucky and squishy things” may outperform the “beautiful” ordered things.
That squishy thing in Sheldon’s head runs on only 20 W and outperforms any supercomputer.

Review of Semiconductor Physics

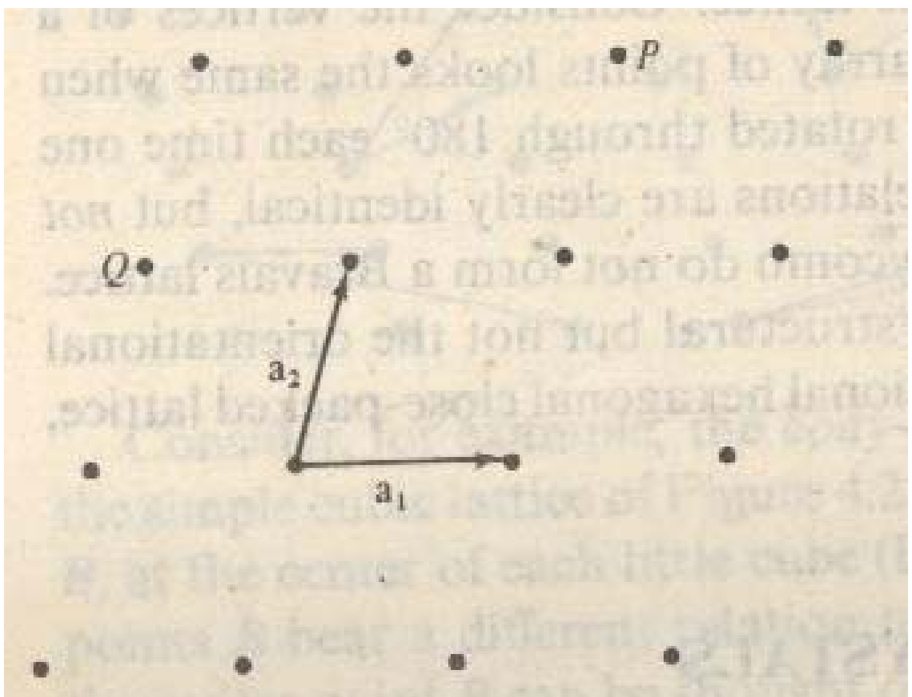
Crystal structures

Bravais Lattices

A mathematical concept:

- No boundary or surface
- No real (physical) thing – just points, hence no defects
- No motion

Unit cells (or primitive unit cells) -- The **smallest** unit that repeats itself.



For this lattice, how many “atoms” are there in each unit cell?

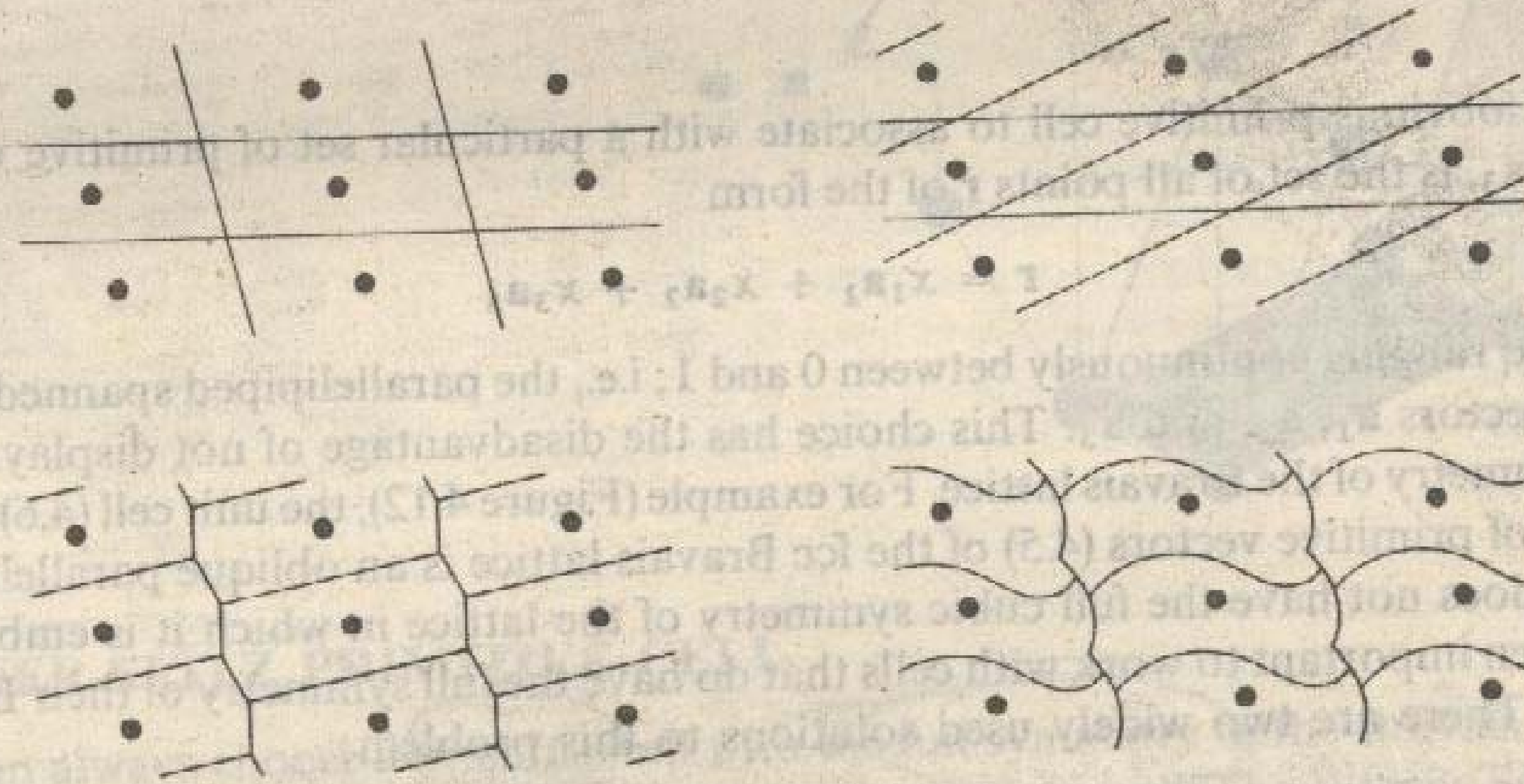
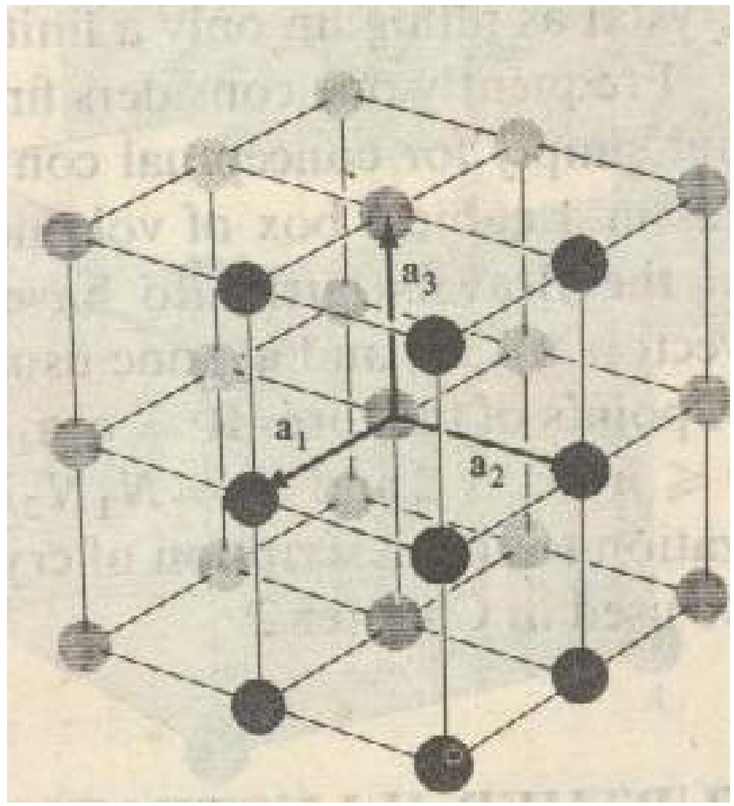


Figure 4.10
Several possible choices of primitive cell for a single two-dimensional Bravais lattice.

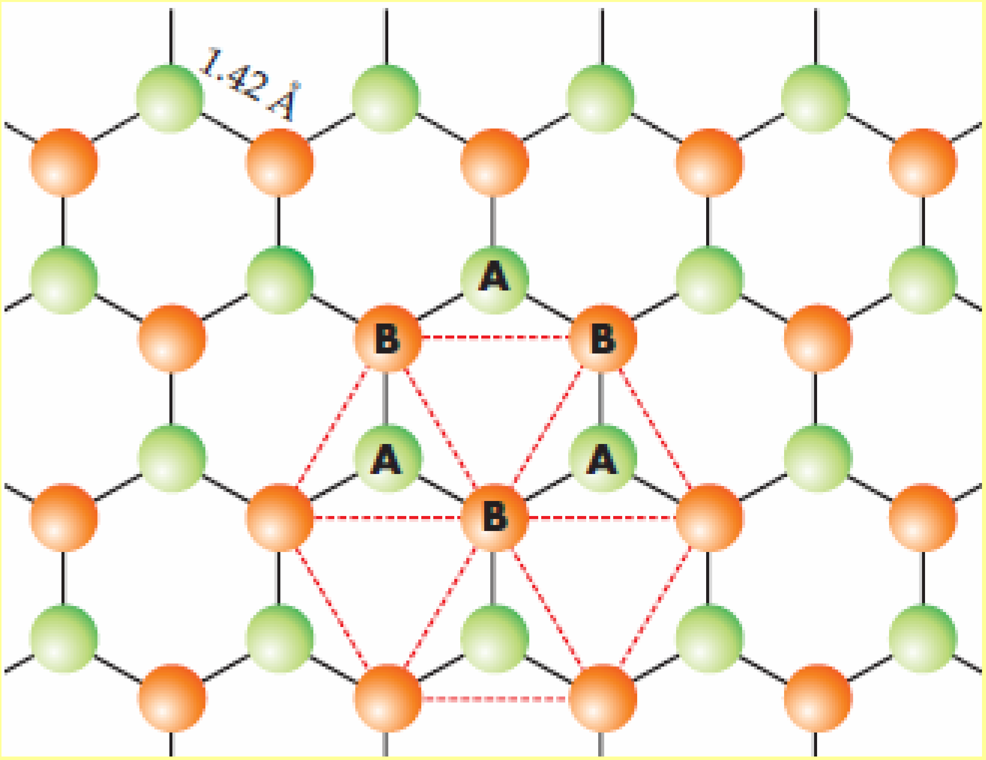
The 3D case



Simple cubic

Crystal structure = lattice + basis

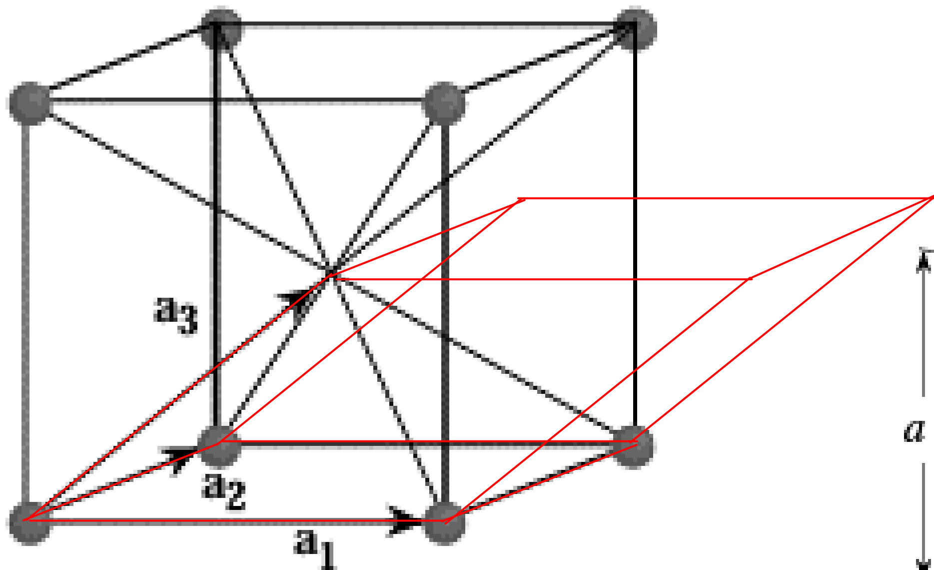
Honeycomb



From Geim & McDonald, Phys Today Aug 2007, 35.

Lattices

Conventional & primitive unit cells



BCC

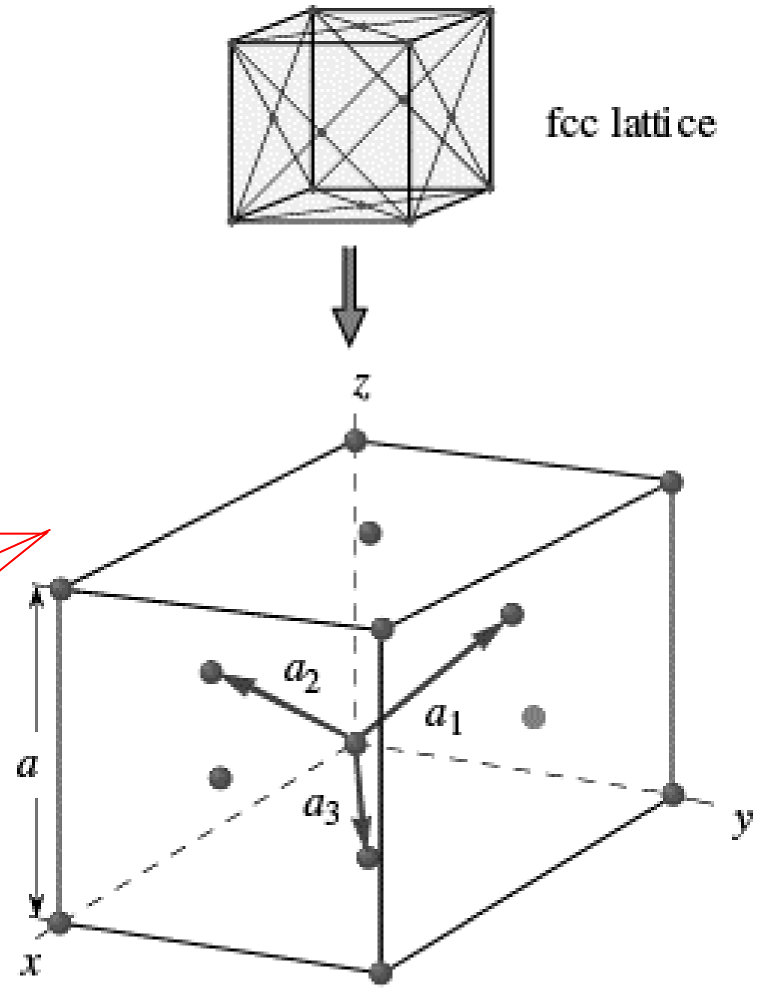


Figure 1.3: Primitive basis vectors for the face centered cubic lattice.

FCC

How many atoms in the conventional unit cell?

BCC & FCC **are** Bravais Lattices.

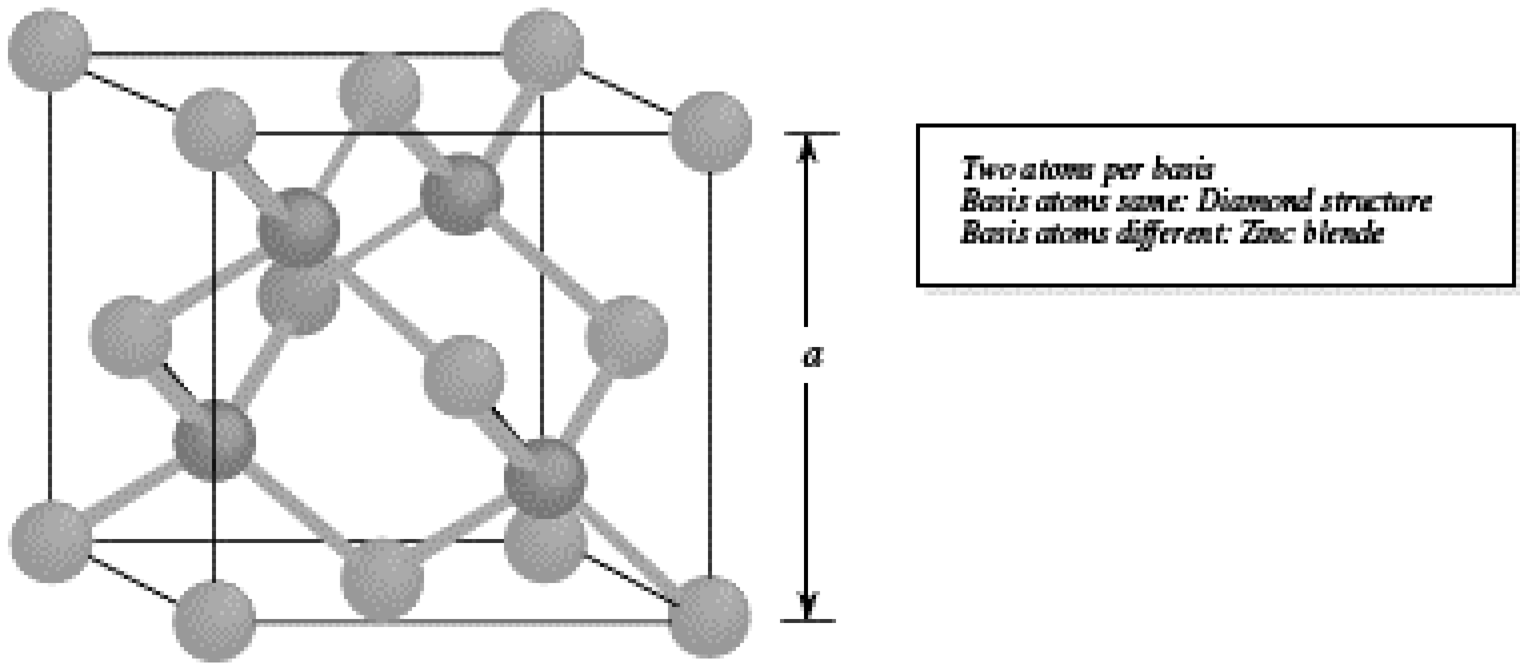


Figure 1.2: The body centered cubic lattice along with a choice of primitive vectors.

U. K. Mishra & J. Singh, *Semiconductor Device Physics and Design*

E-book available on line thru UT Lib.

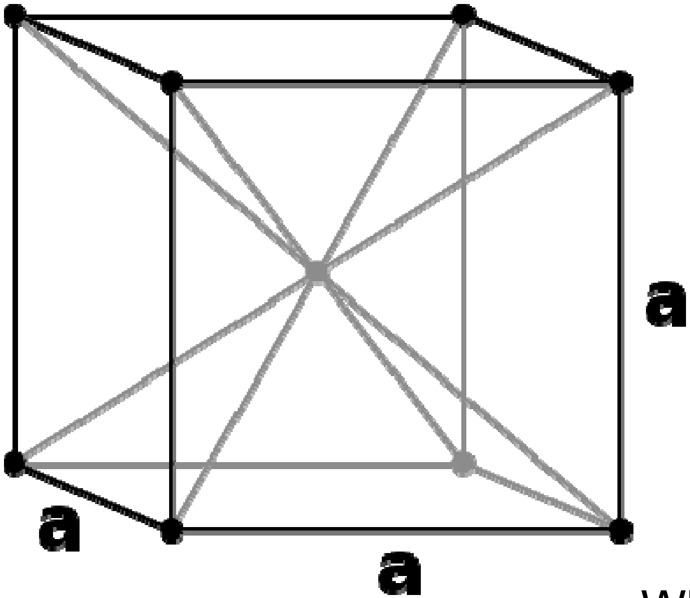
Fast production of e-books. The caption is NOT for this figure.

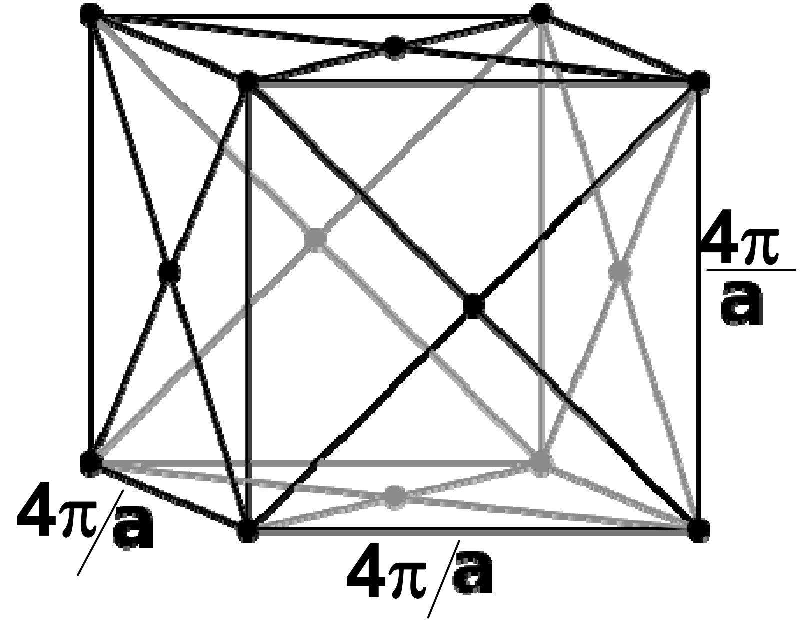
Try not to be confused when reading fast generated books/papers nowadays.

Bragg diffraction and the reciprocal lattice

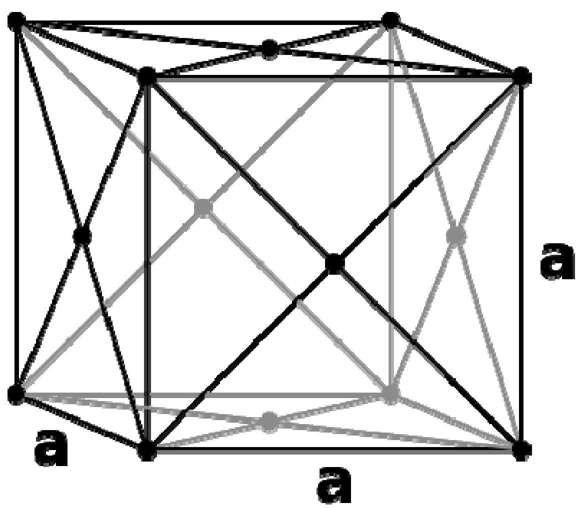
- Bragg diffraction
- Definition of the reciprocal lattice
- 1D, 2D, and 3D
  The 1D & 2D situations are not just mathematical practice or fun, they can be real in this nano age…

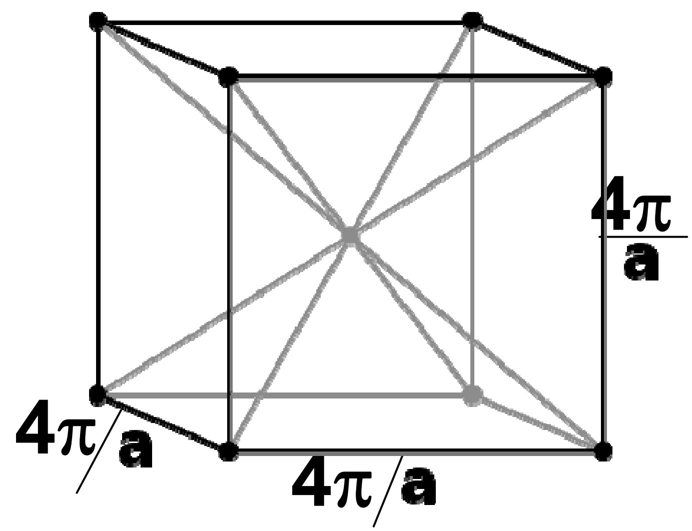
- BCC & FCC are reciprocal lattices of each other





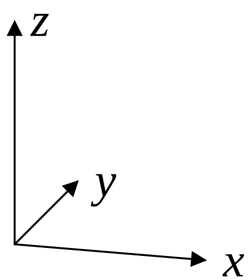
Why not $2\pi/a$?

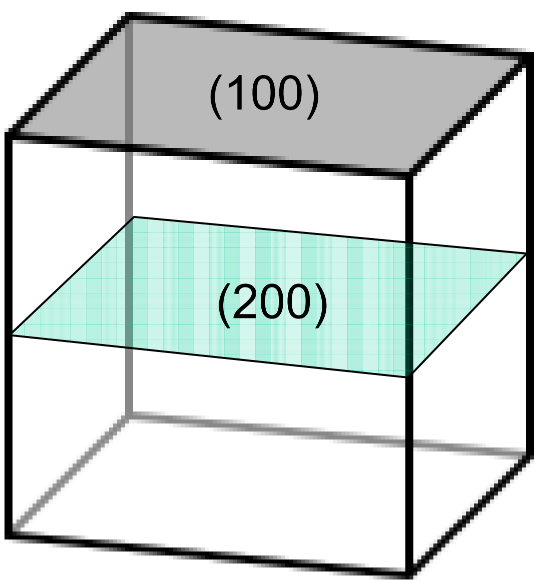




- Miller indices

  Referring to the origin of the reciprocal lattice's definition, i.e, Bragg diffraction, a reciprocal lattice vector ***G*** actually represents a plane in the real space





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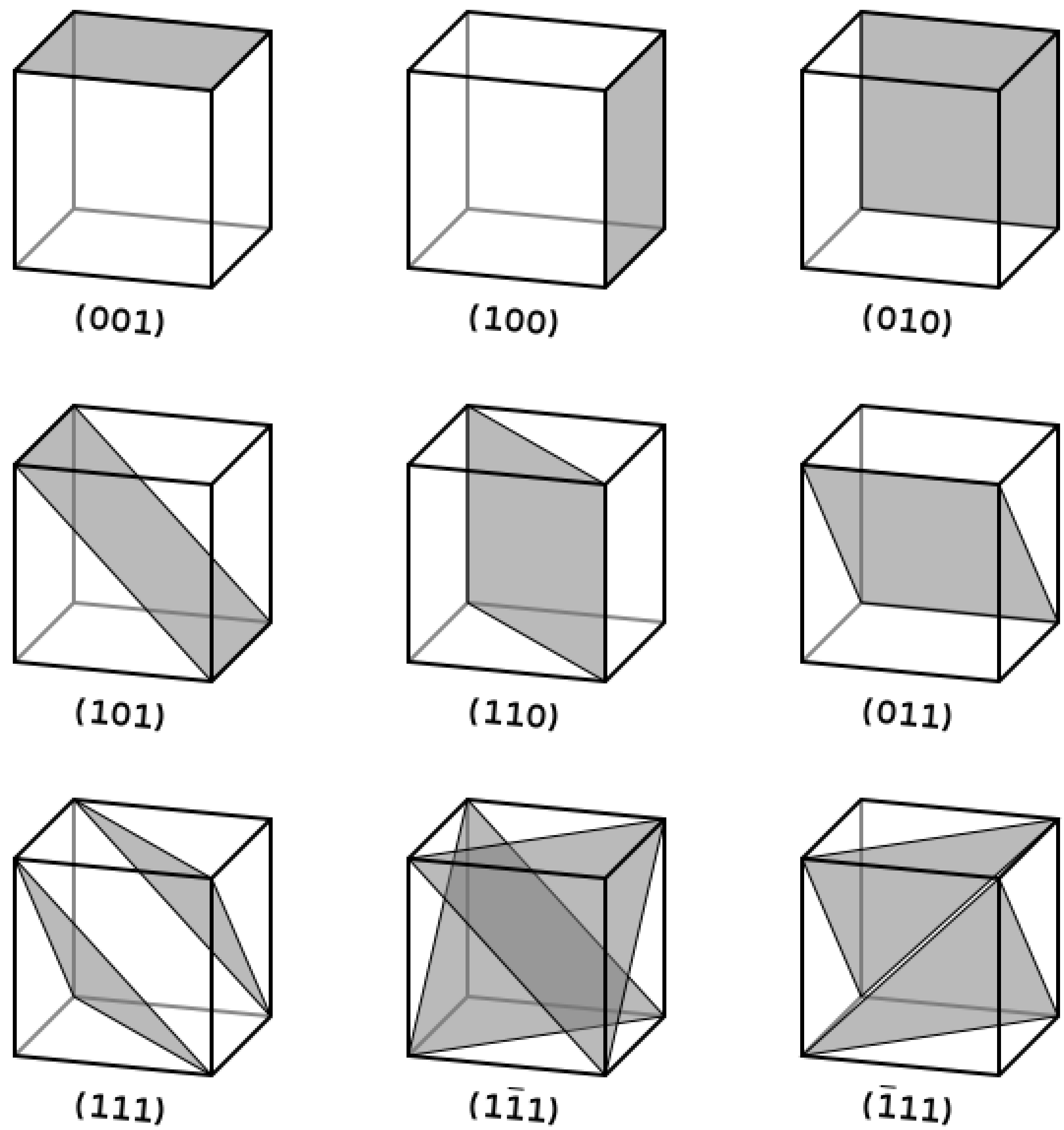


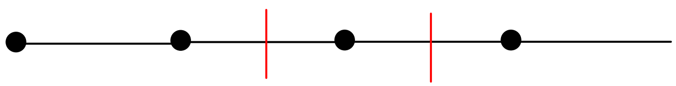
Easier way to get the indices:
Reciprocals of the intercepts

- Wigner-Seitz primitive unit cell and first Brillouin zone

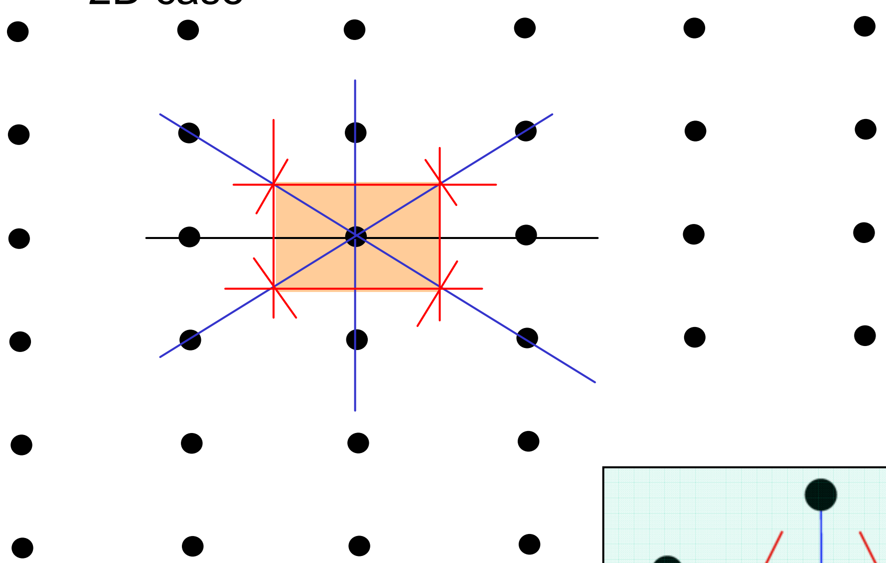
The Wigner–Seitz cell around a lattice point is defined as the locus of points in space that are closer to that lattice point than to any of the other lattice points.

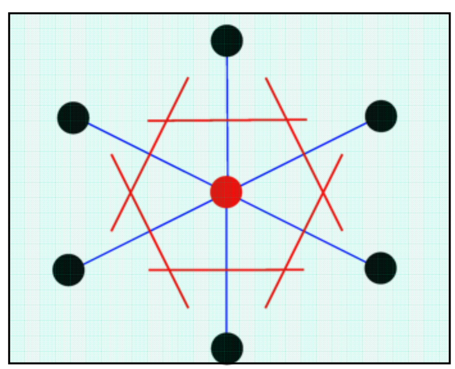
The cell may be chosen by first picking a lattice point. Then, lines are drawn to all nearby (closest) lattice points. At the midpoint of each line, another line (or a plane, in 3D) is drawn normal to each of the first set of lines.

1D case



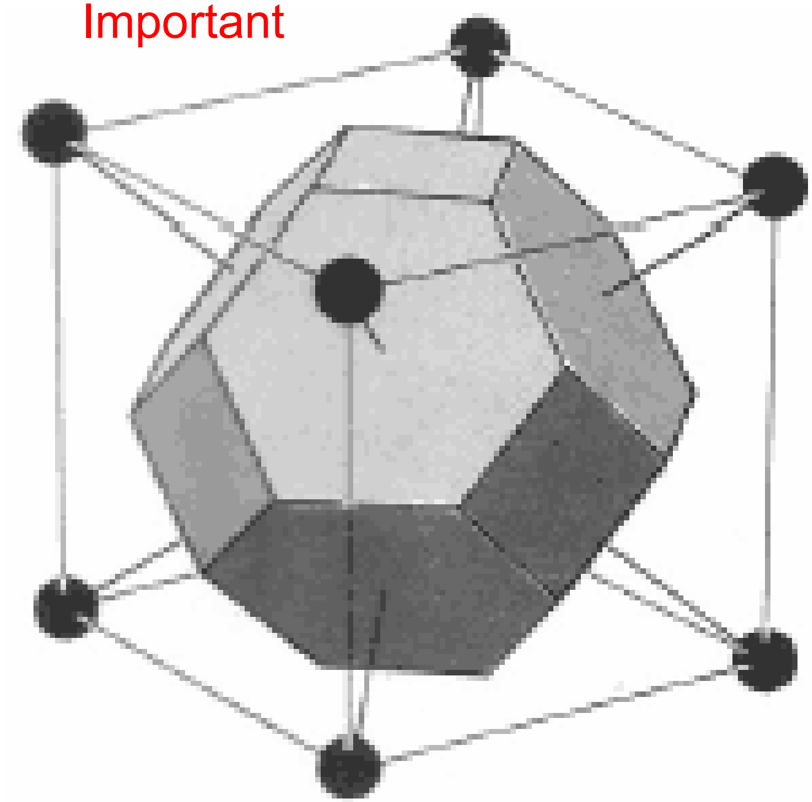
2D case





3D case: BCC

Important

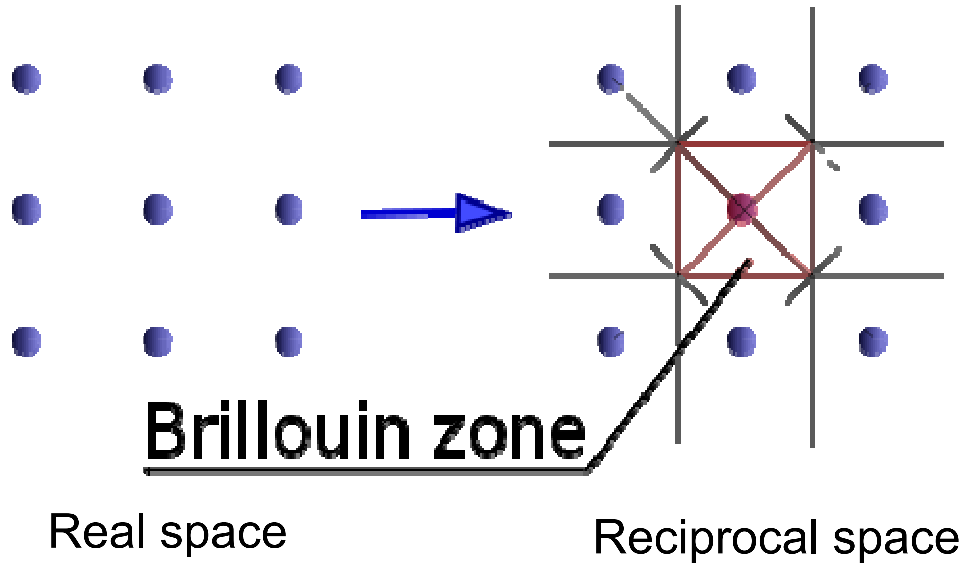


The first Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice

1D

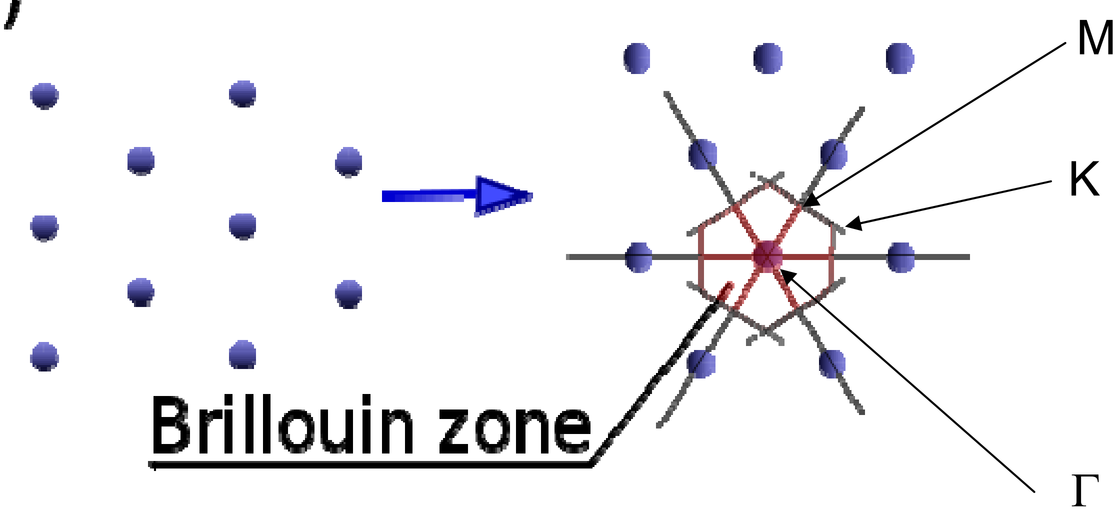
2D

a)

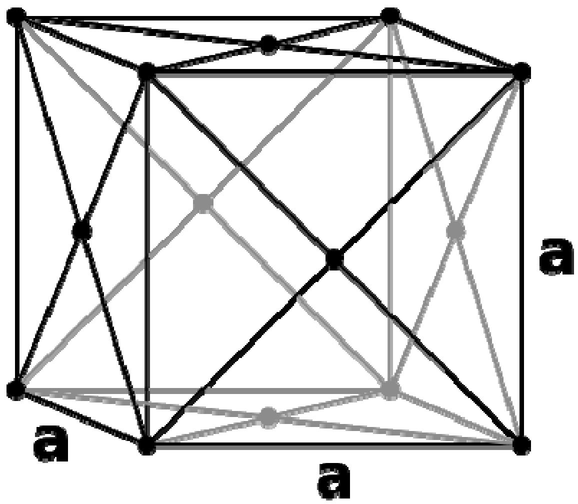


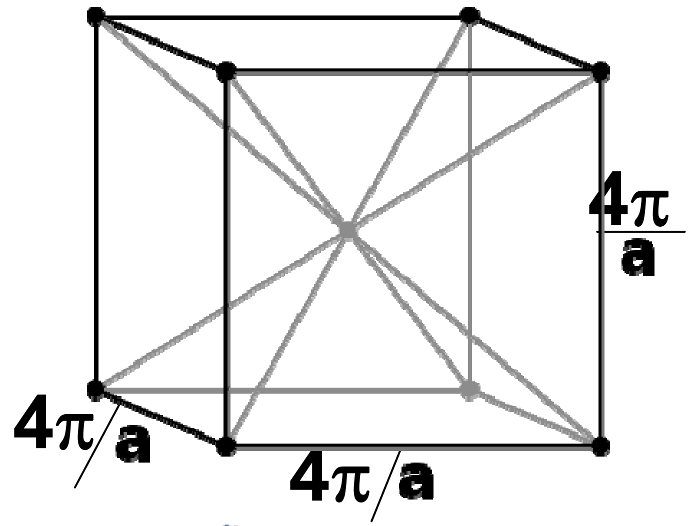
b)

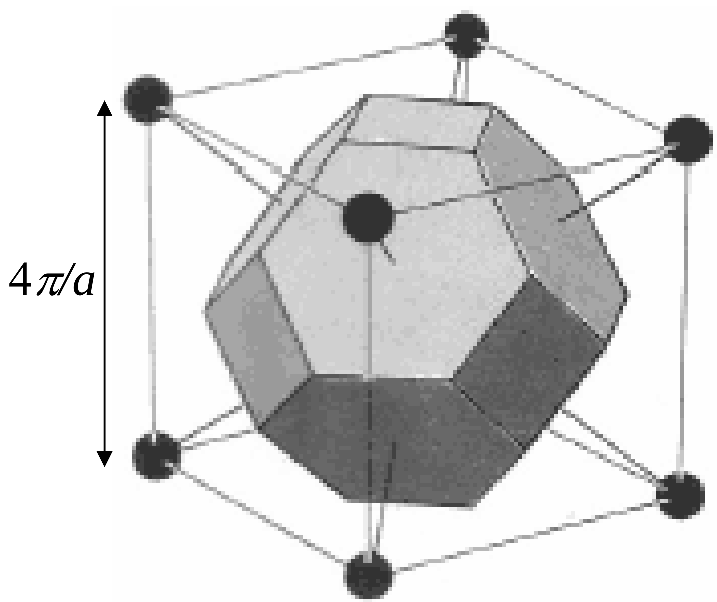
Note: this figure is updated.

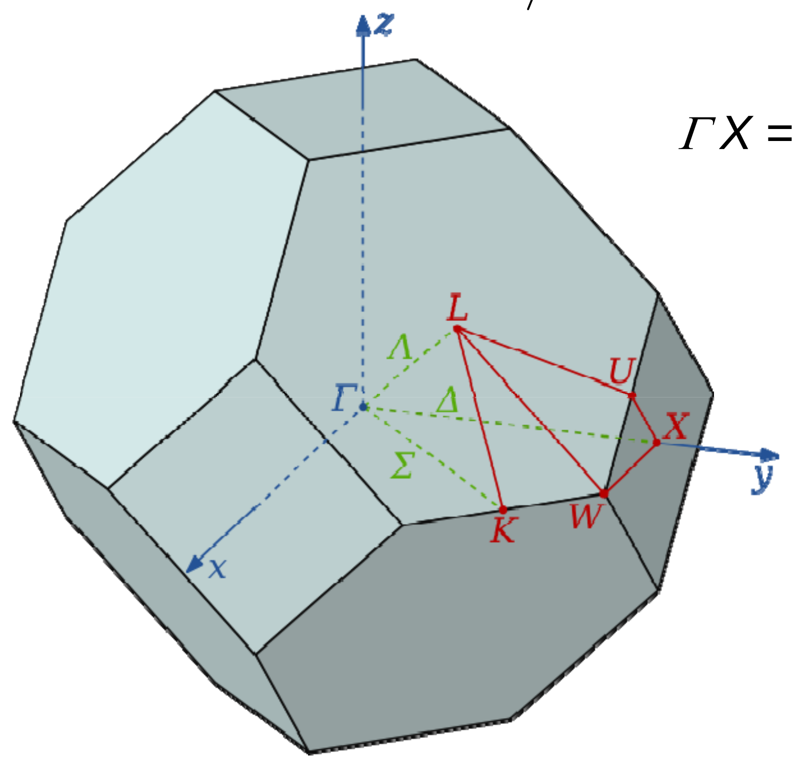


3D:
Recall that the reciprocal lattice of FCC is BCC.







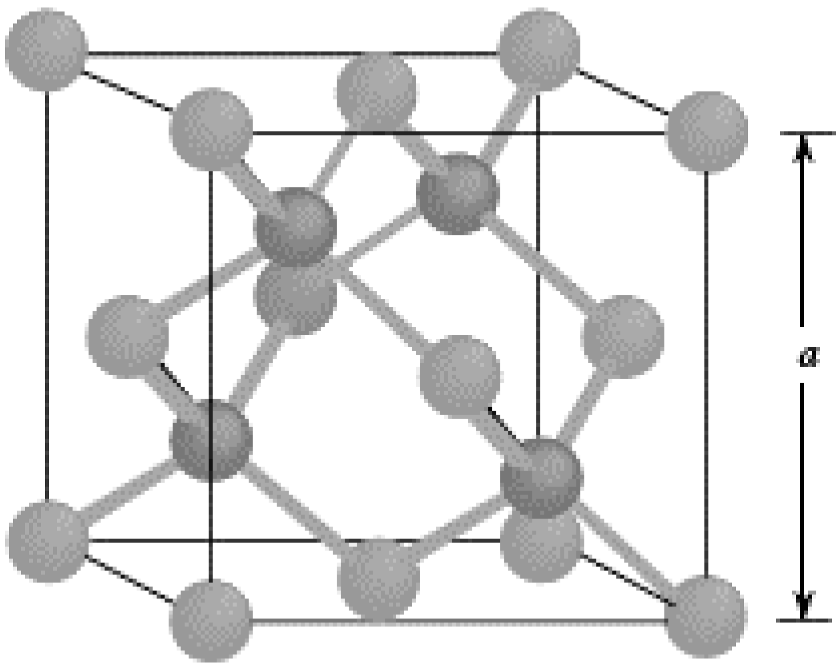


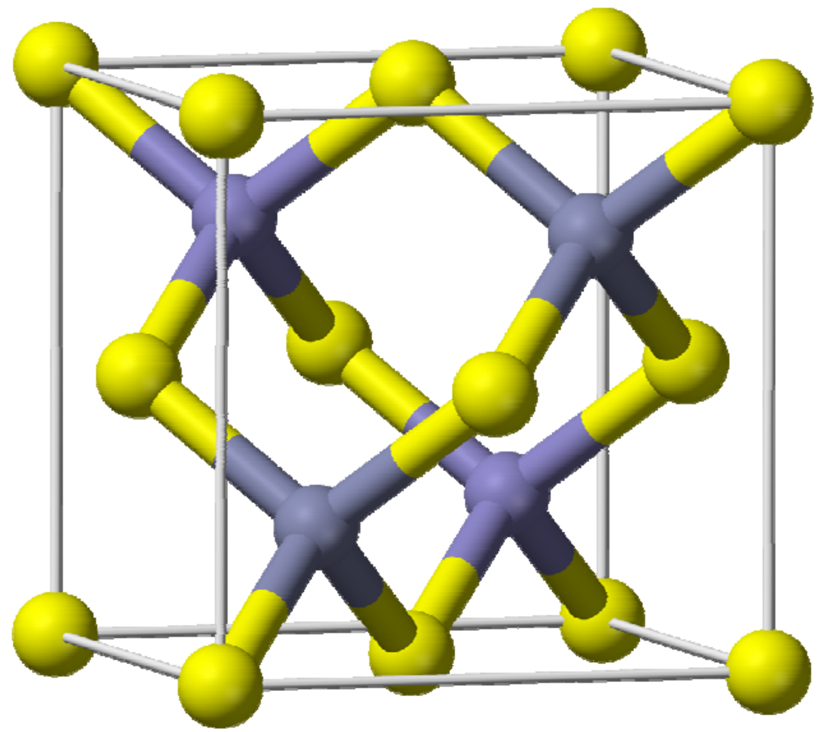
ΓX = ???

Why is FCC so important?

Why is FCC so important?

It's the lattice of Si and many III-V semiconductors.





Si: diamond, a = 5.4 Å
GaAs: zincblende

Crystal structure = lattice + basis

Modern VLSI technology uses the (100) surface of Si.

Which plane is (100)? Which is (111)?

Defined w.r.t. the conventional unit cell.

Review of Semiconductor Physics

Crystal structures

Bravais Lattices

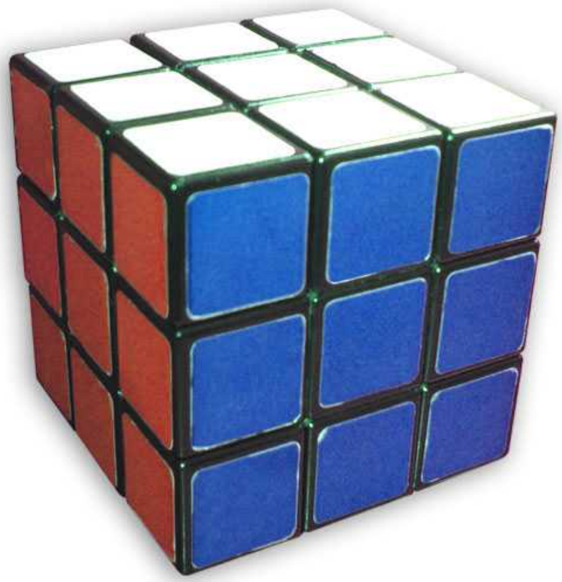
A mathematical concept:

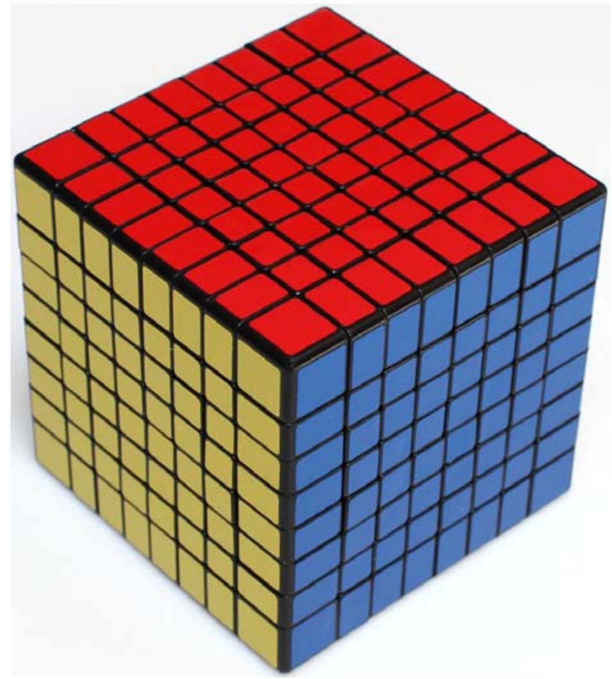
- No boundary or surface
- No real (physical) thing – just points, hence no defects
- No motion

What do you mean by “infinitely large”?

A big cube is made of 10 X 10 X 10 small cubes. How many of them are on the faces?

Unit cells (or primitive unit cells)
The smallest unit that repeats itself.





$3^3 = 27$

$(3-2)^3 = 1$

$10^3 = 1000$

$(10-2)^3 = 512$

Half of the small cubes are on the surface!