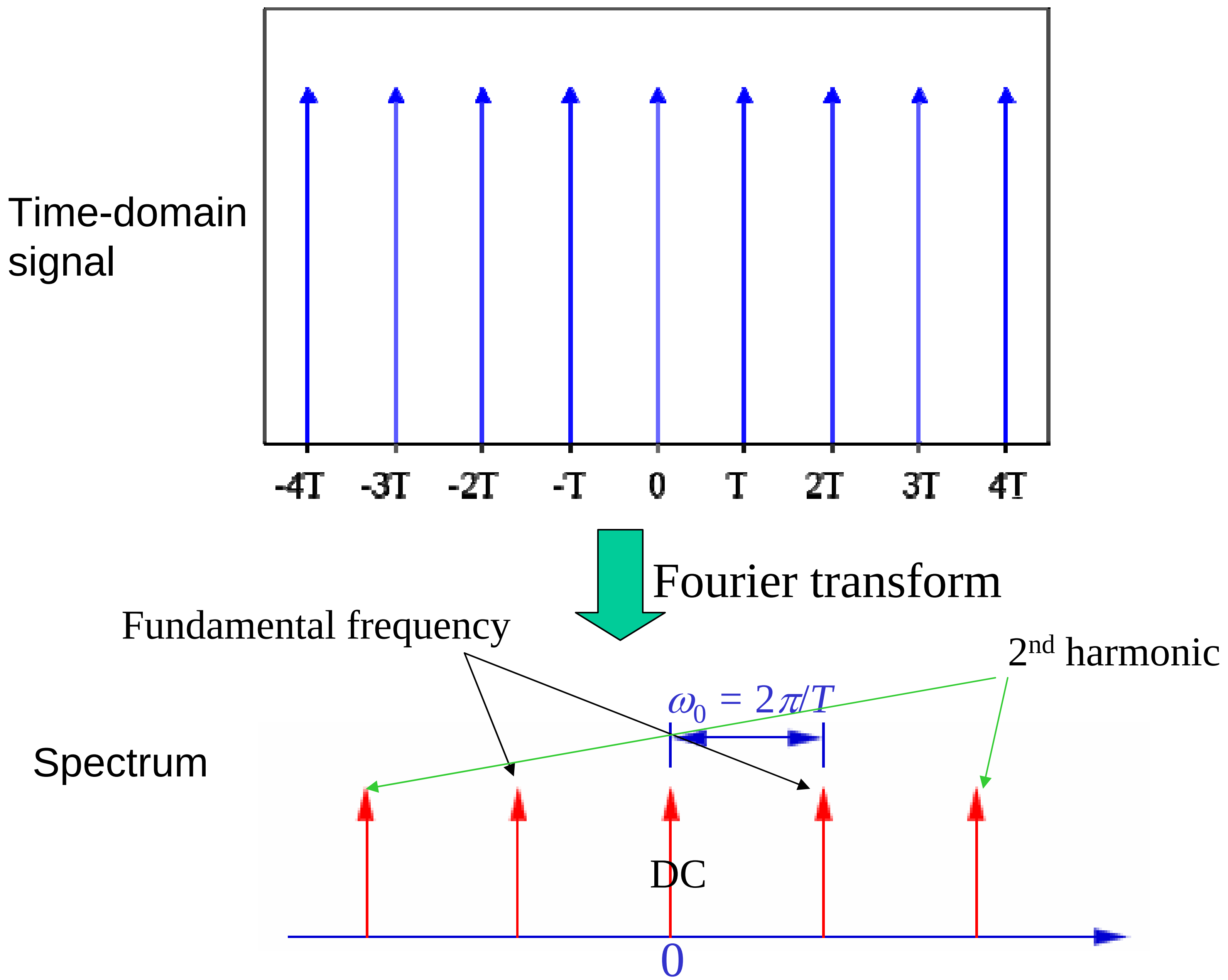
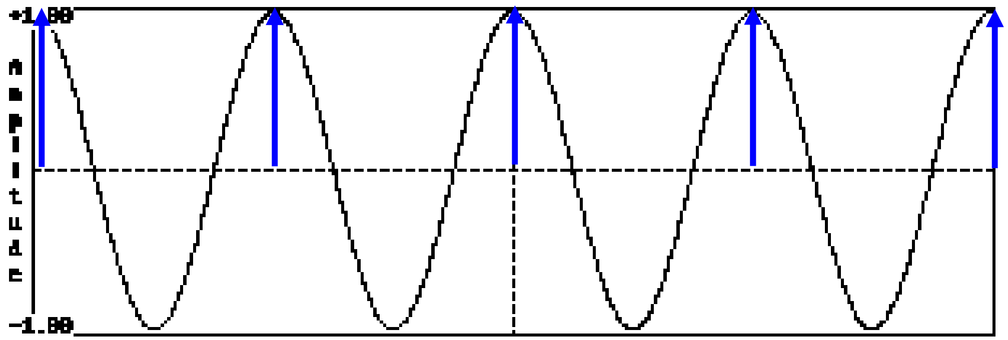


Time-domain signal
-4T
-3T
-2T
-T
0
T
2T
3T
4T
Fourier transform
Fundamental frequency
2nd harmonic
$\omega_0 = 2\pi/T$
Spectrum
DC
0

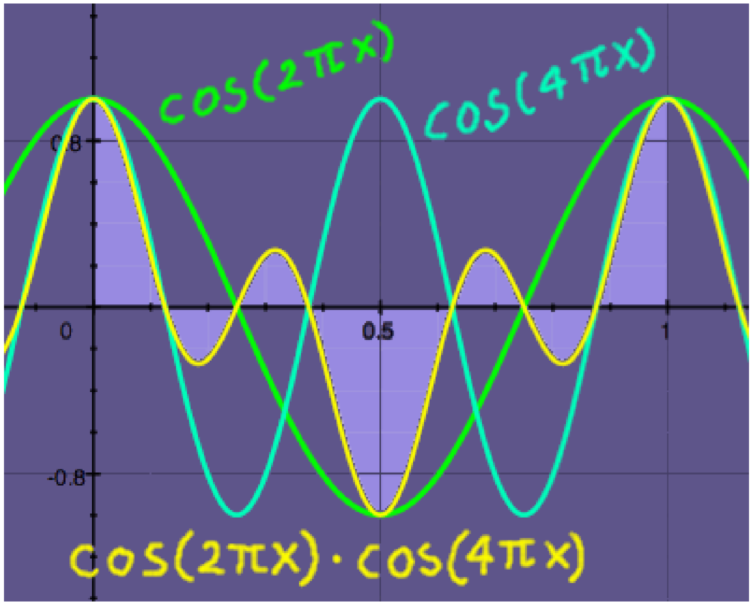


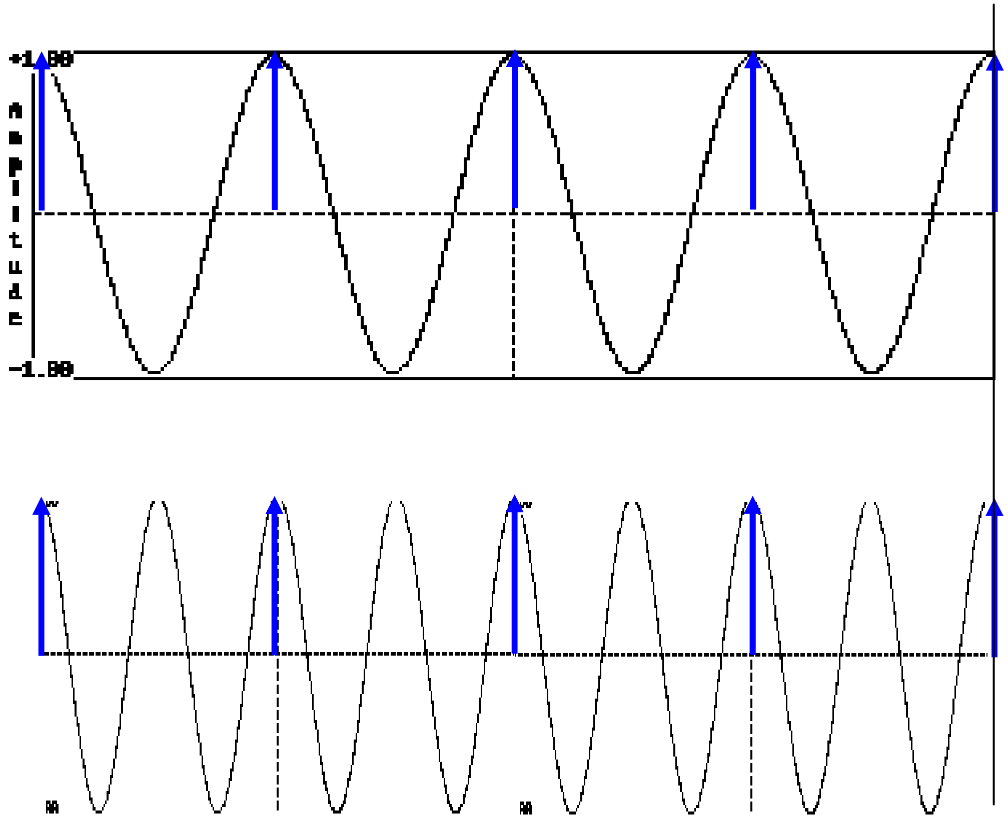
To find the fundamental frequency component: $\int_{-\infty}^{+\infty} \delta(t - nT)\cos\omega_0 t dt$

In contrast,

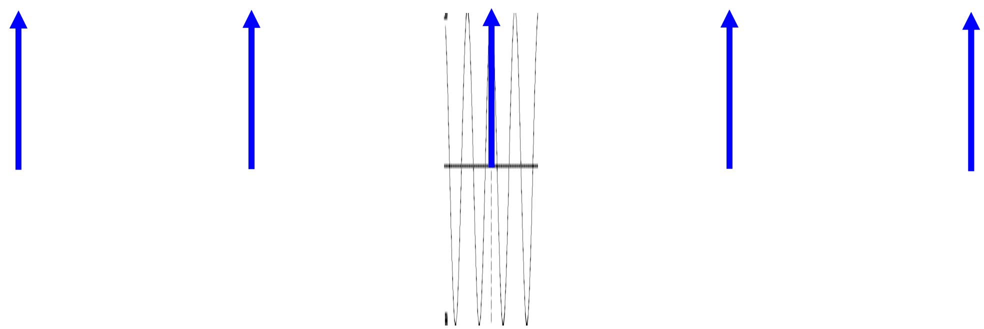
$$\int_{-\infty}^{+\infty} \cos 2\omega_0 t \cos\omega_0 t dt = 0$$

The 2nd harmonic is orthogonal to the fundamental.





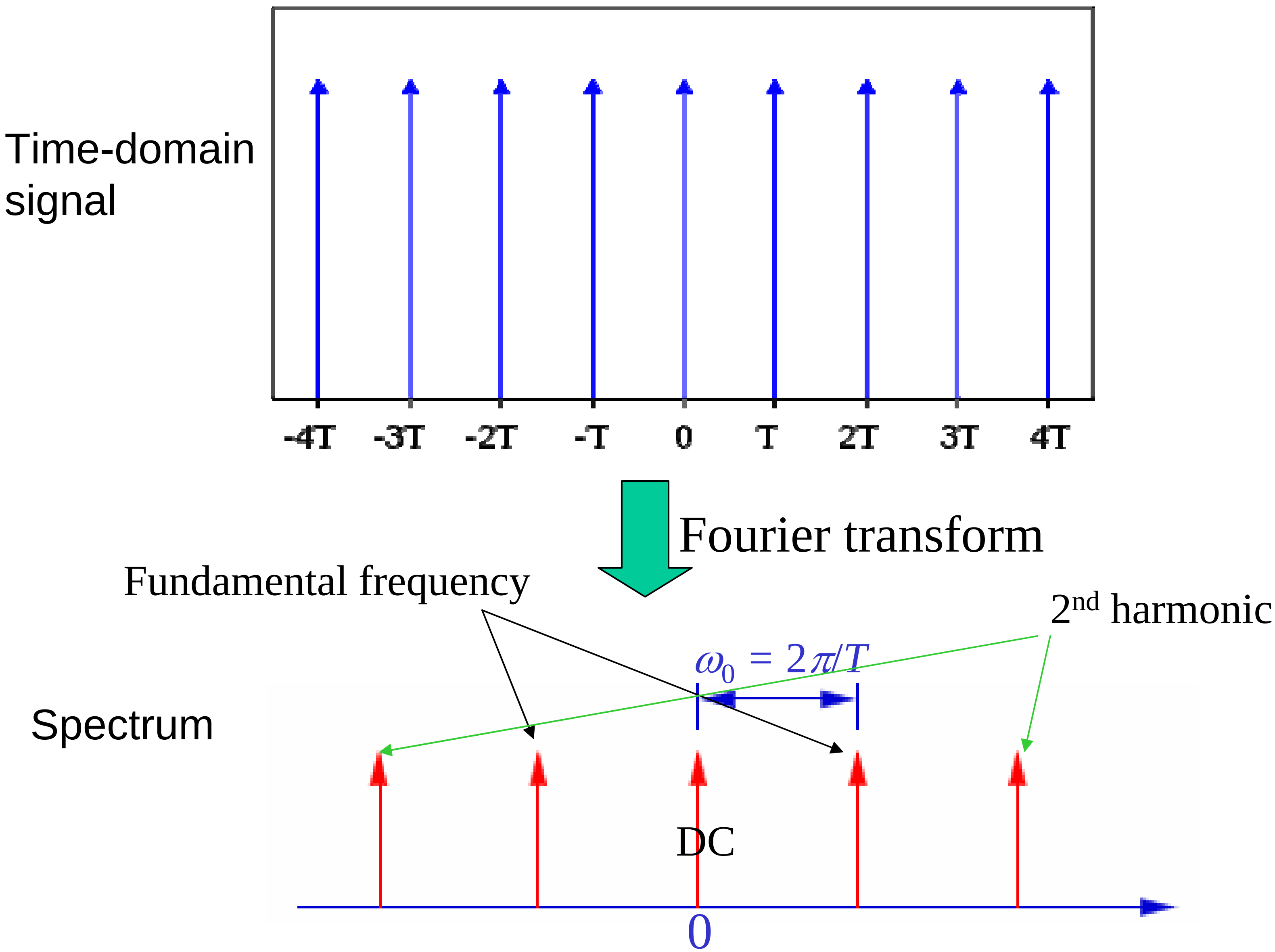
To find the 2nd harmonic: $$\int_{-\infty}^{+\infty} \delta(t-nT)\cos 2\omega_0 t\,dt$$



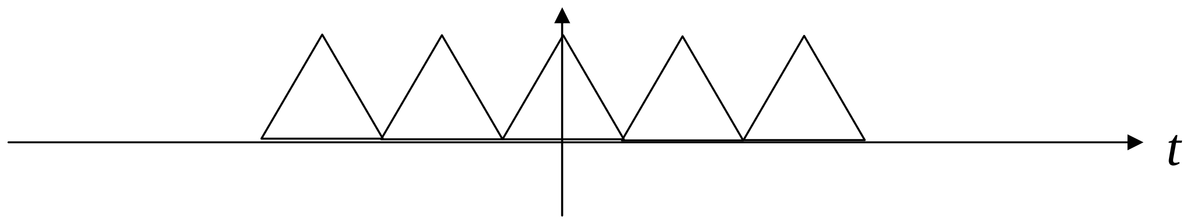
Since the spike is infinitely sharp, we have the *n*th harmonic as a spike in the frequency domain, no matter how big *n* is.

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

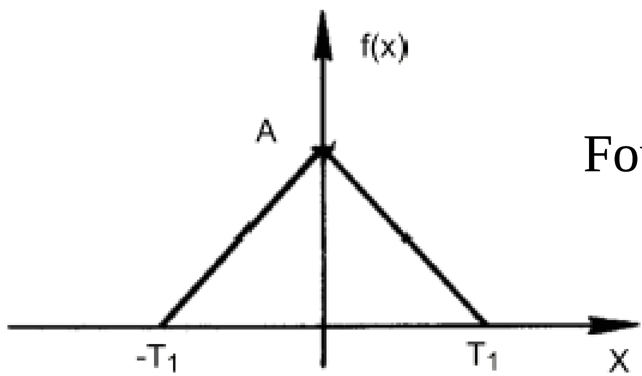
Therefore,


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

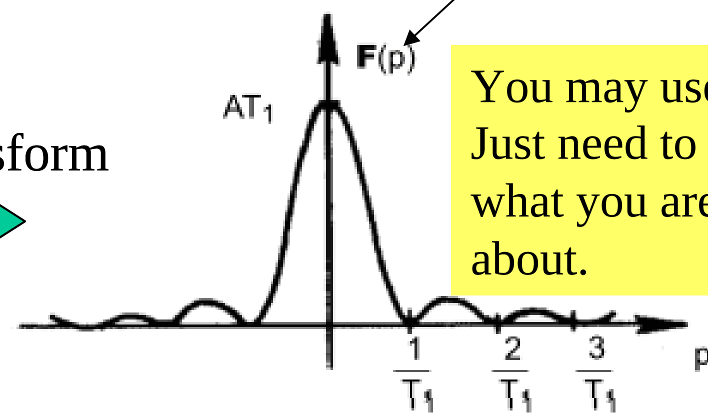


$$f(x) = -\frac{A}{T_1}|x| + A$$

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

Fourier Transform

p is frequency



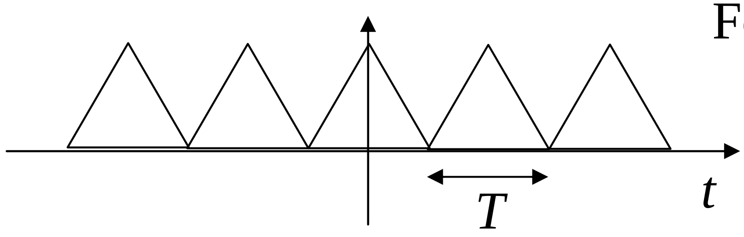
$$\mathbf{F}(p) = AT_1\left[\frac{\sin(\pi T_1 p)}{\pi T_1 p}\right]^2 = AT_1 \operatorname{sinc}^2(\pi T_1 p)$$

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

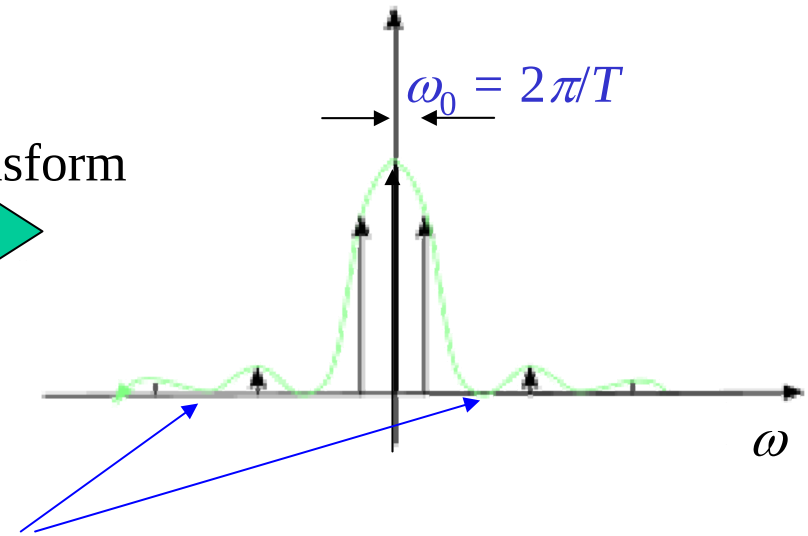
(Figures taken from http://www.roymech.co.uk/Useful_Tables/Maths/fourier/Maths_Fourier_transforms.html)

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

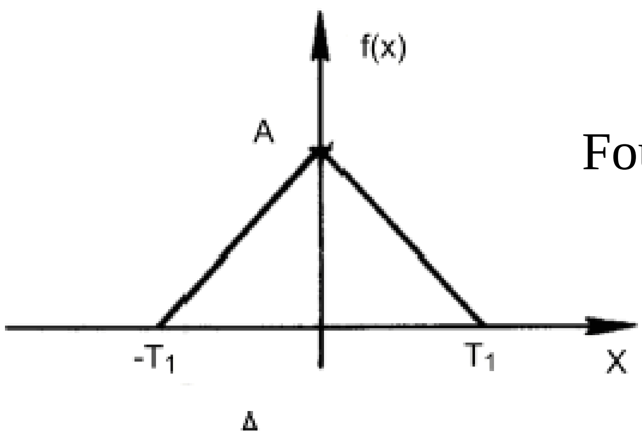


Fourier Transform

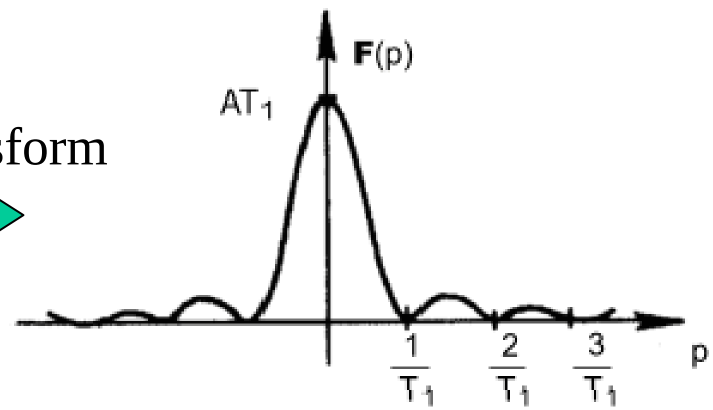


Spikes disappear. We’ll revisit this when we talk about diffraction patterns.

because

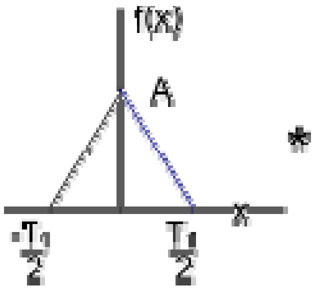


Fourier Transform

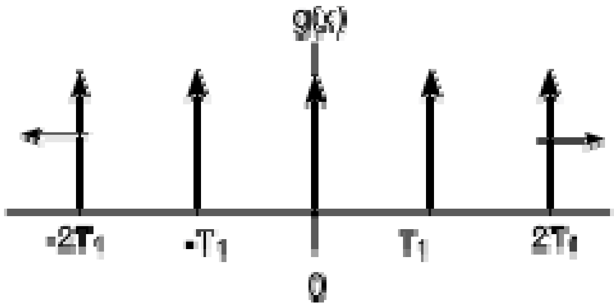


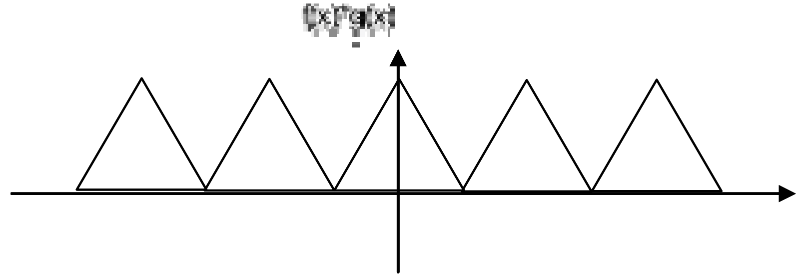
A bit more math if you were into signals and systems:

In the time (or space) domain:



$*$

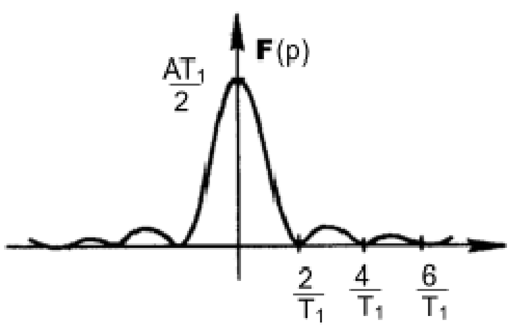


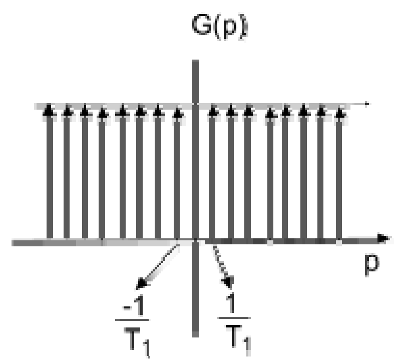


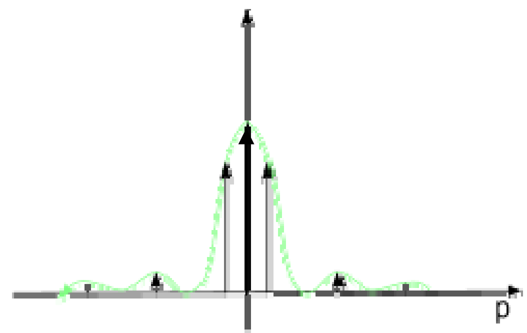
$$f(x) = -\frac{2A}{T_1}|x| + A \qquad g(x) = III_{T_1}(x) = \sum_{n=-\infty}^{\infty} \delta(x - nT_1) \qquad y(x) = f(x) * g(x)$$

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

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

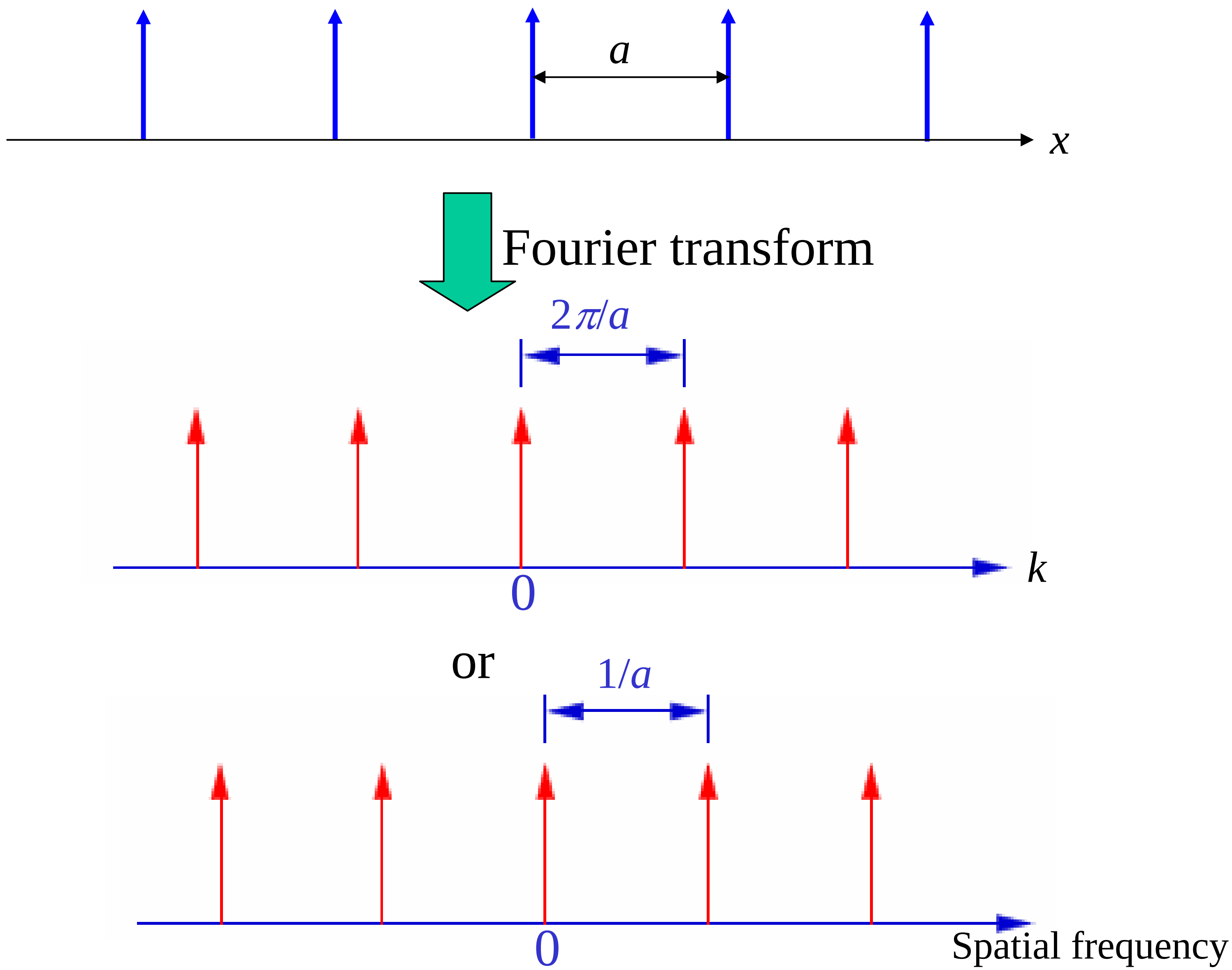






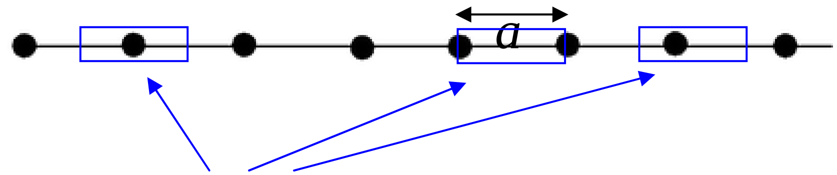
$f_1(t) * f_2(t)$ Fourier Transform $F_1(\omega)F_2(\omega)$

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



You may replace the spikes with points

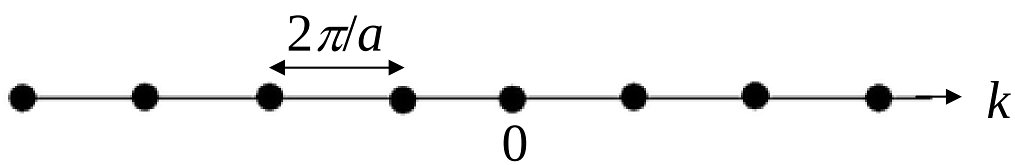
In real space:



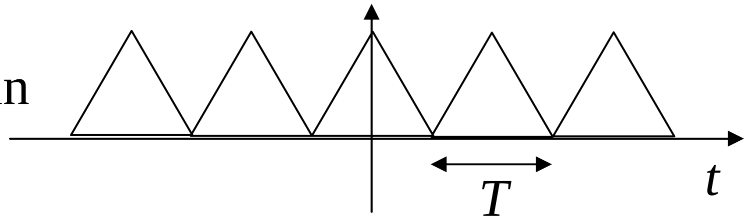
We call a period a “unit cell.” Infinite choices for the unit cell.

Fourier transform

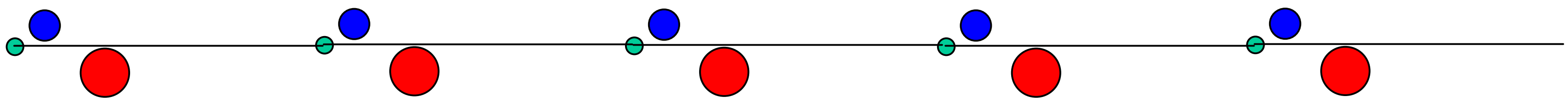
In reciprocal (or *k*-) space:

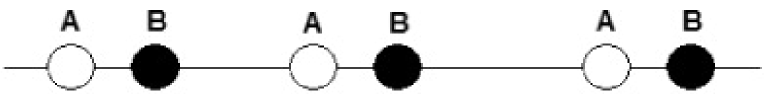


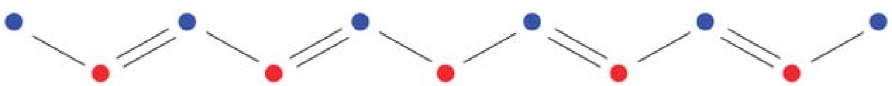
Just like you can have a pulse train in time domain



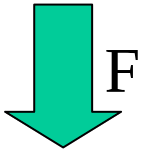
the unit cell can have an internal structure

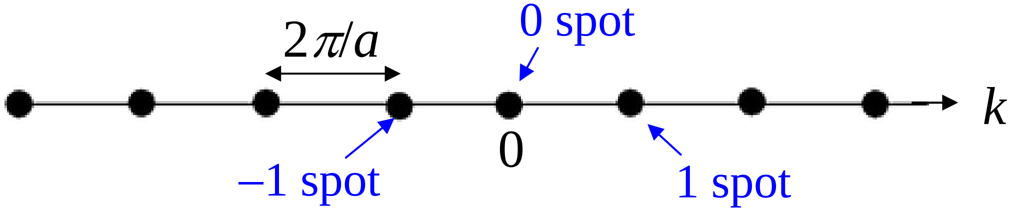




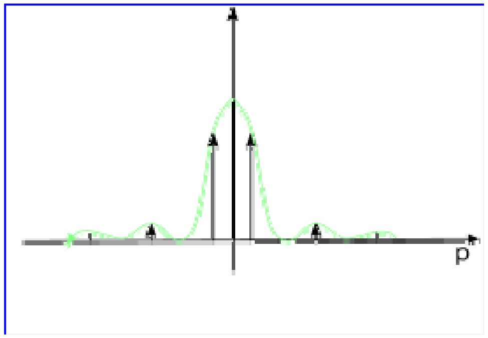


Again, you have infinite choices defining the unit cell.

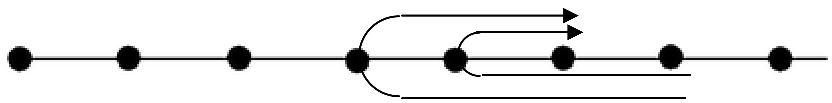




The intensities of the spots vary due to the unit cell internal structure, just like in the spectrum of a time-domain pulse train:



Nature’s way of doing Fourier transform: Diffraction



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

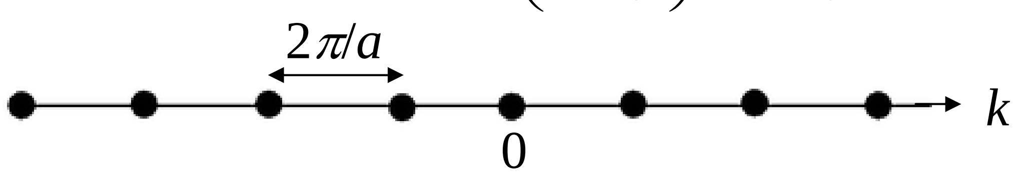
To have constructive interference between reflections by all atoms/unit cells:

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

The k of the photon

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

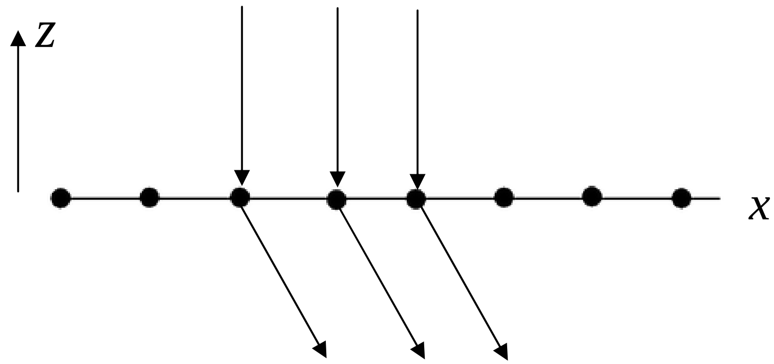
$$|\Delta \boldsymbol{k}| = |\boldsymbol{k}_f - \boldsymbol{k}_i| = 2\left(n\frac{2\pi}{2a}\right) = n\frac{2\pi}{a}$$

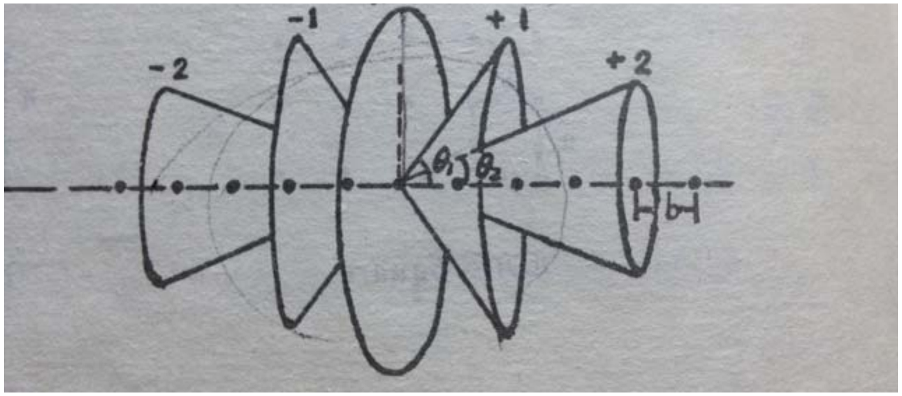


You see, the Fourier transform is just a “spectrum” of $\Delta\boldsymbol{k}$.

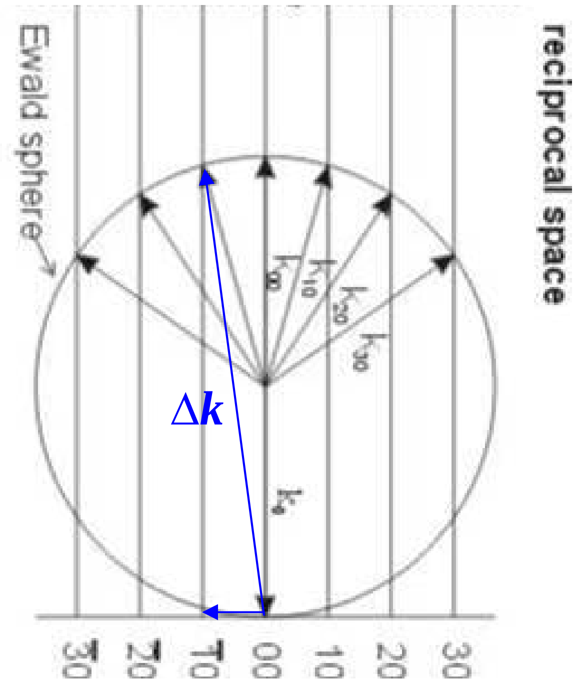
It feels like the lattice gives the photons momenta $n(2\pi/a)$. You have a kind of “momentum conservation.”

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

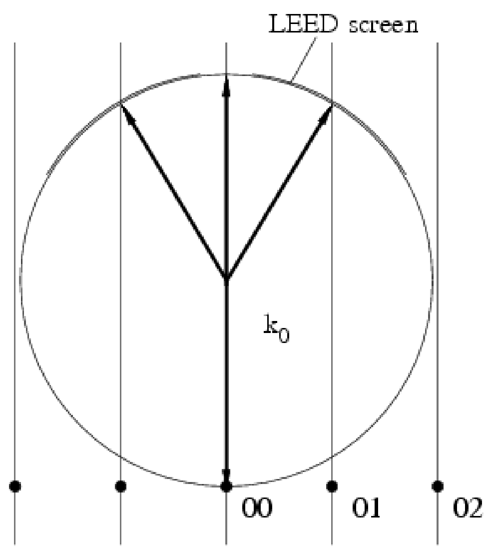




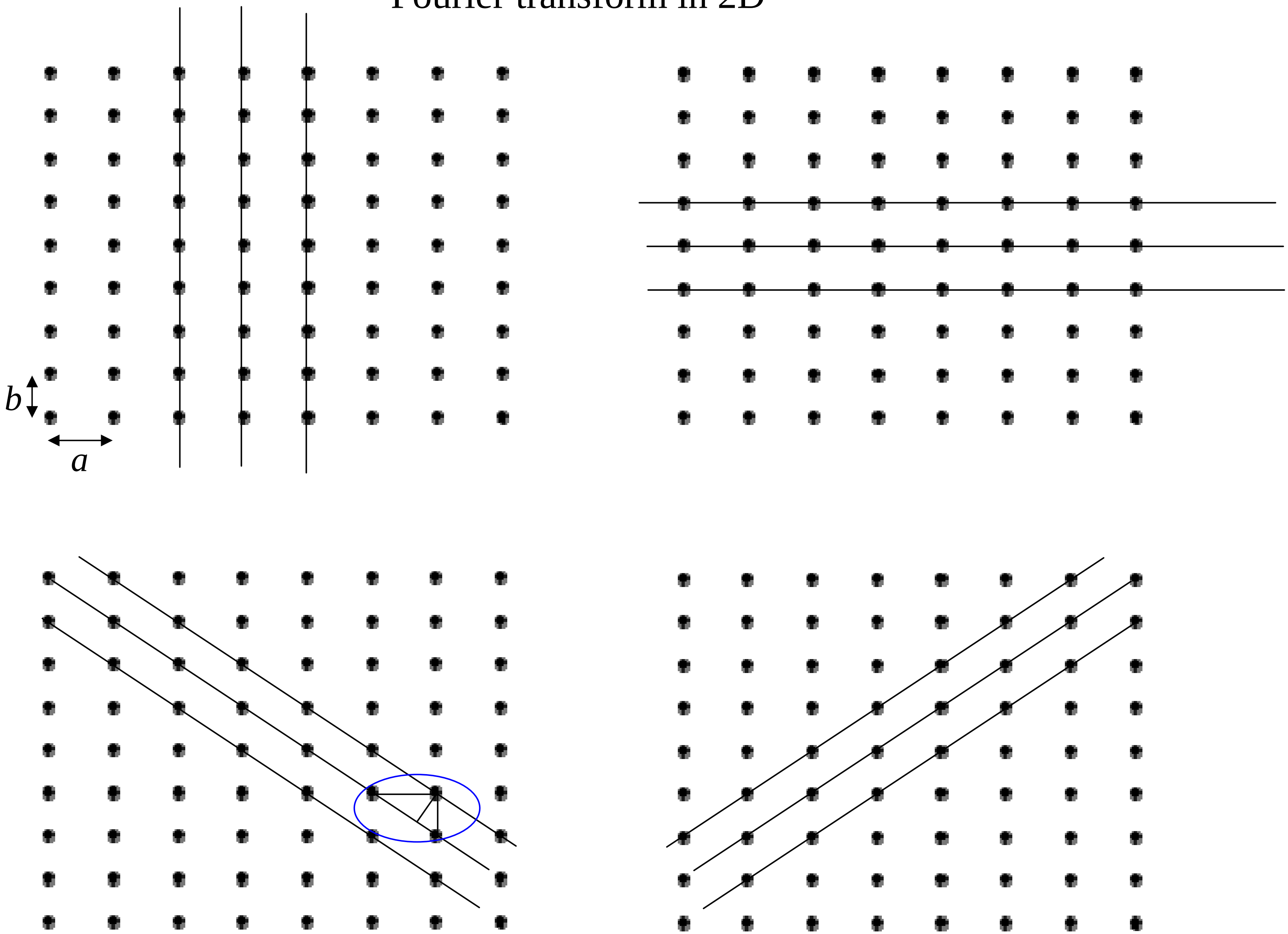
In some directions, you have the right $\Delta \boldsymbol{k}$ for constructive diffraction.

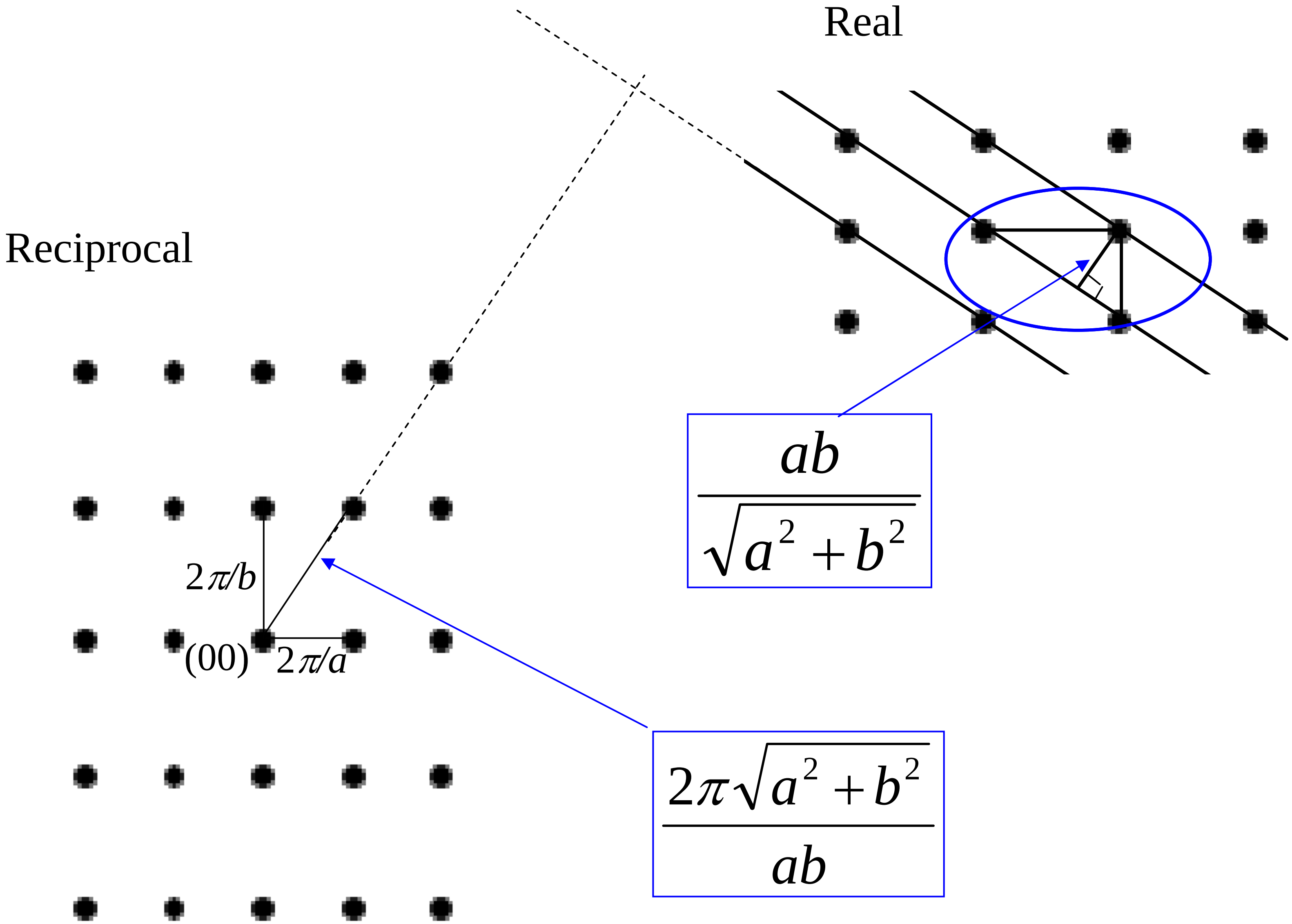


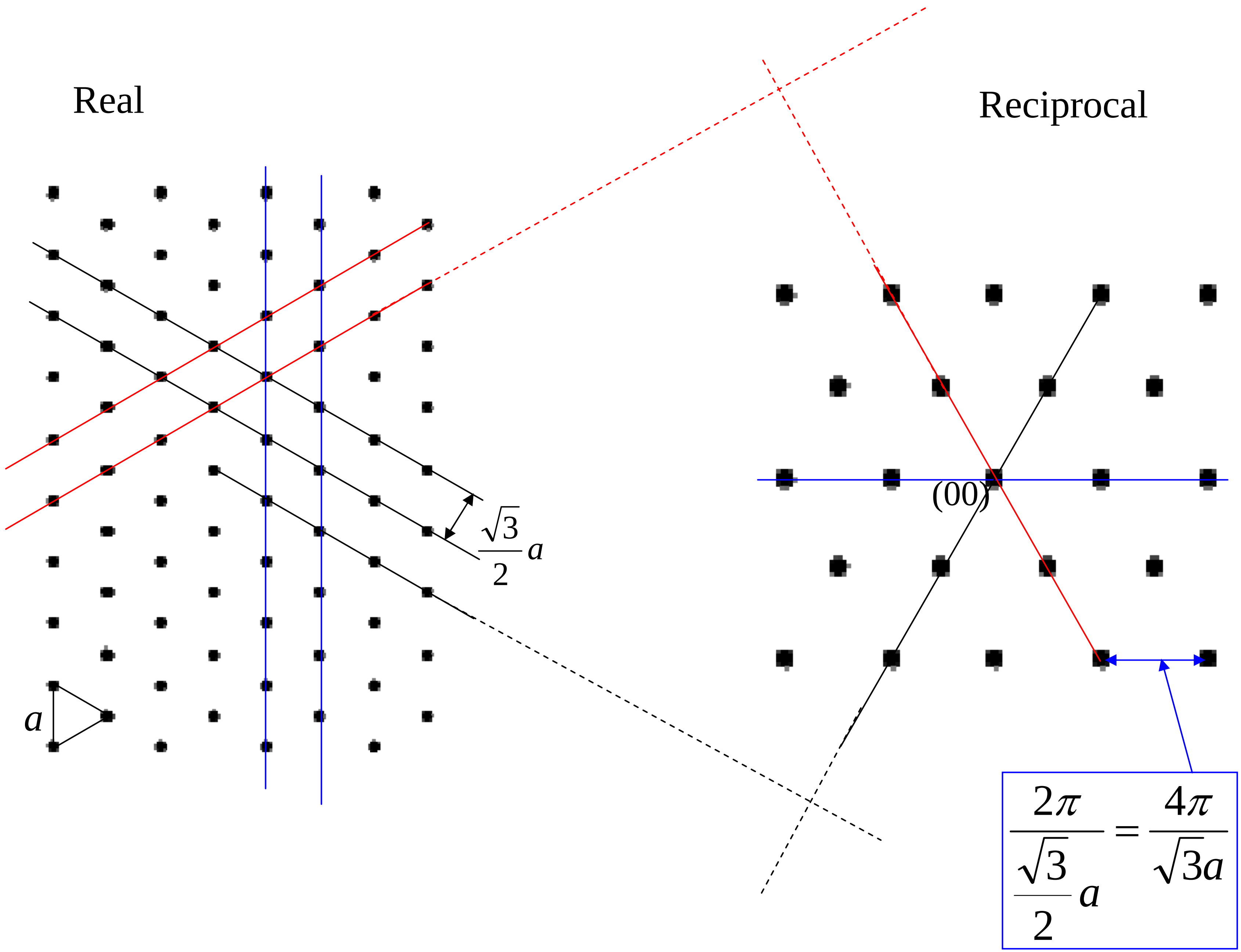
- Momentum conserves only in the x direction.
- k_z is free to keep $k_f = k_i$.
- The pattern is a bunch of parallel lines,
- Each standing for a Δk_x,
- Set by the lattice.
- The pattern is a spectrum of Δk_x,
- Representing the spatial frequencies (momenta) of the lattice.



Fourier transform in 2D

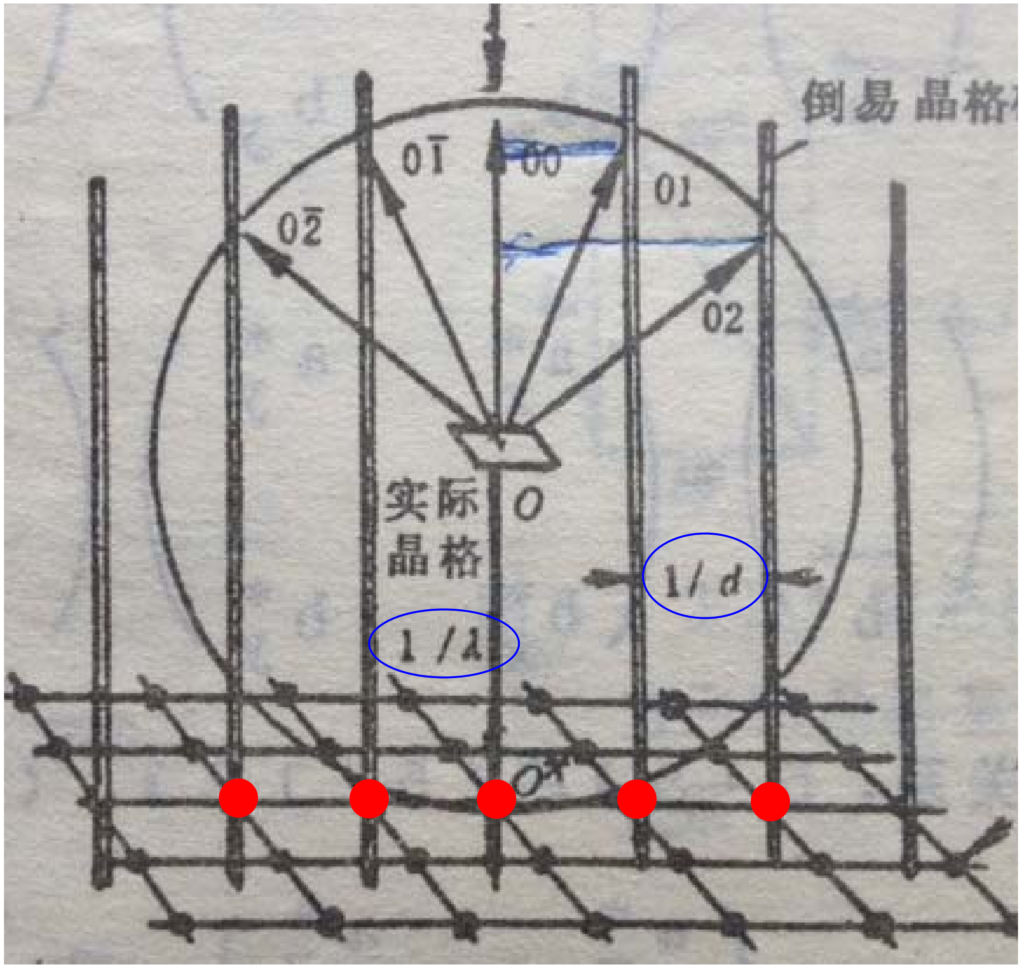



Real
Reciprocal
$2\pi/b$
(00)
$2\pi/a$
$\frac{ab}{\sqrt{a^2+b^2}}$
$\frac{2\pi\sqrt{a^2+b^2}}{ab}$

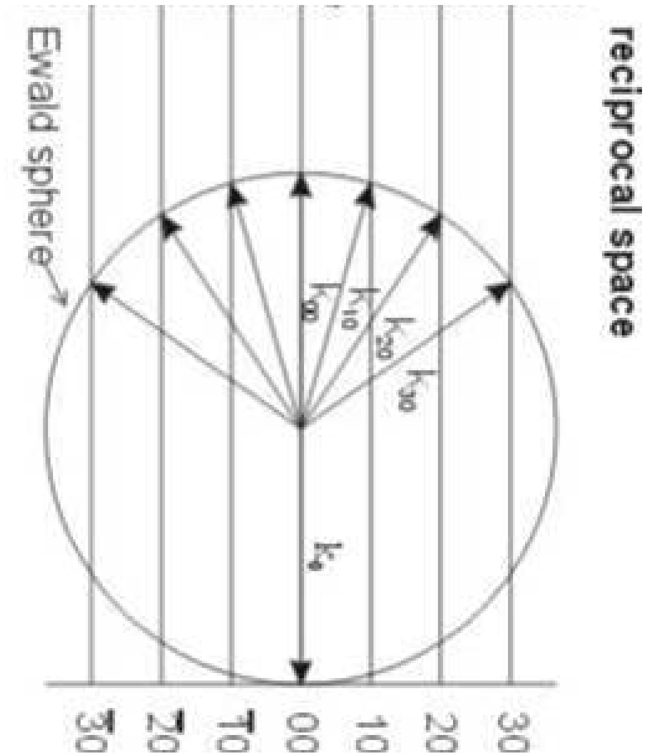


Real
Reciprocal
$\frac{\sqrt{3}}{2}a$
a
(00)
$\frac{2\pi}{\frac{\sqrt{3}}{2}a} = \frac{4\pi}{\sqrt{3}a}$

Diffraction by 2D Lattice

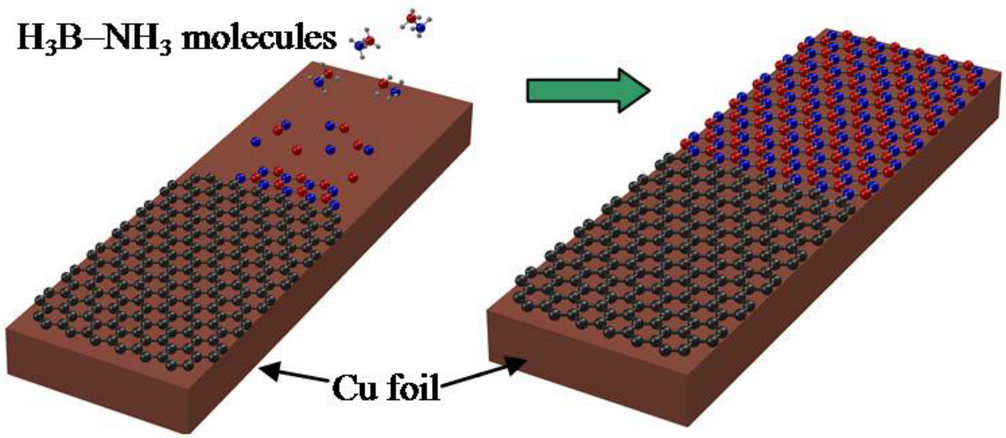


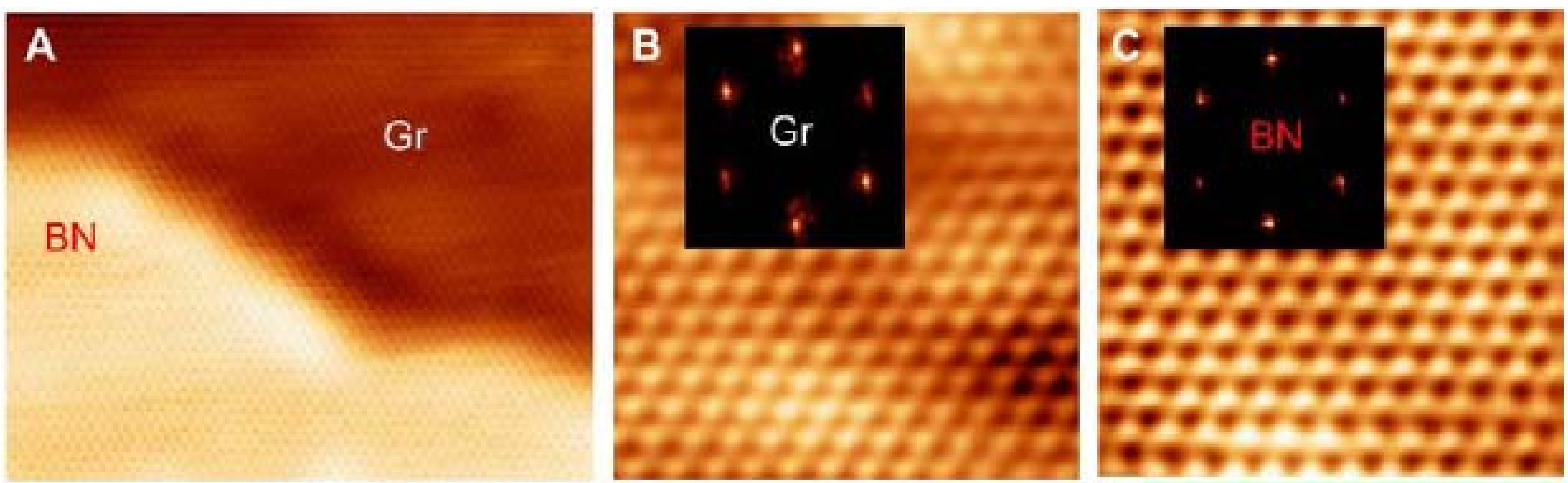
The wave may be an electron beam.
We have talked about the very basics. Now it should be easy for you to read about the details of LEED and SAED.



- 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 $k_f = k_i$.

Examples from my group's research

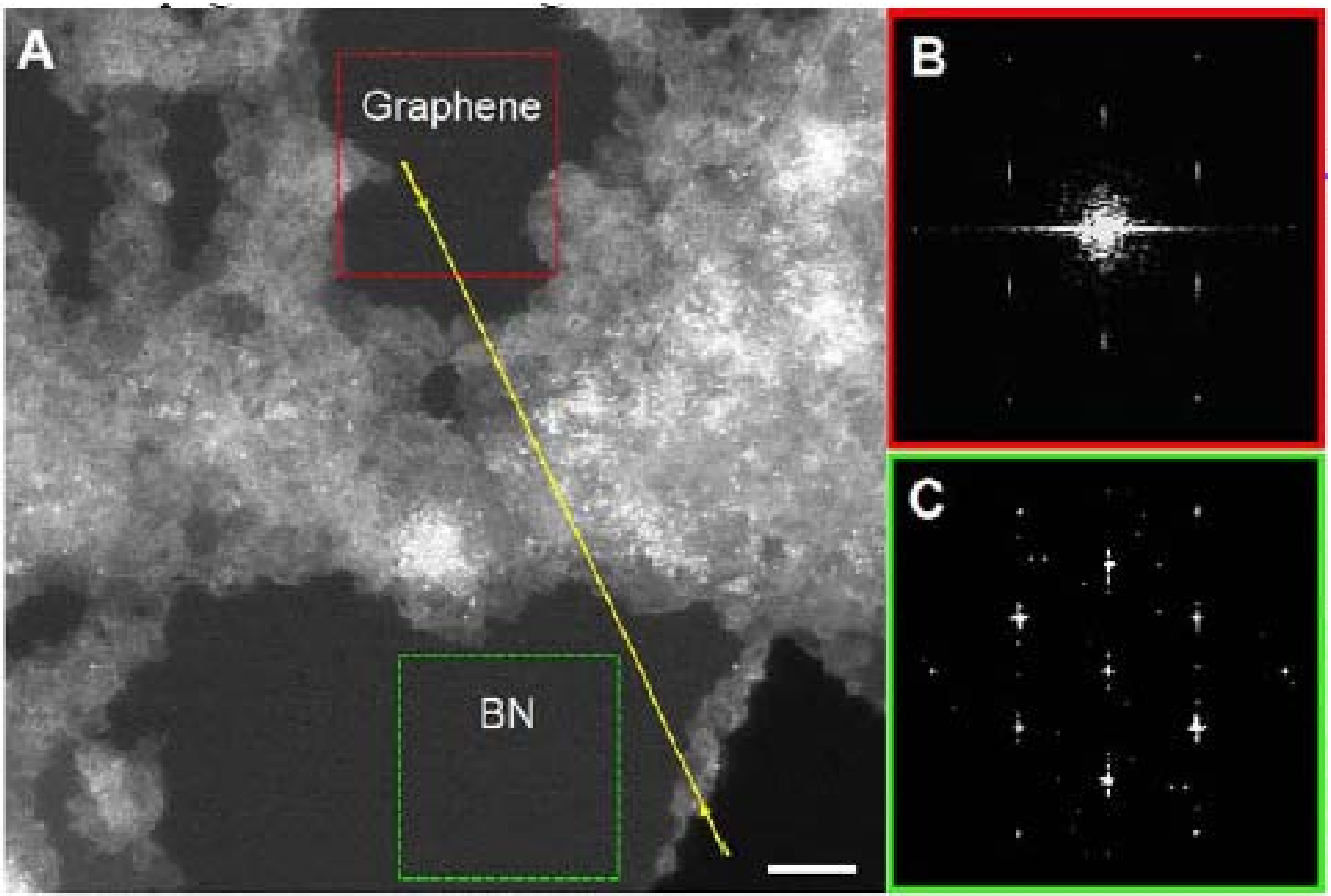




Lei Liu *et al*, *Science* **343**, 163 (2014).

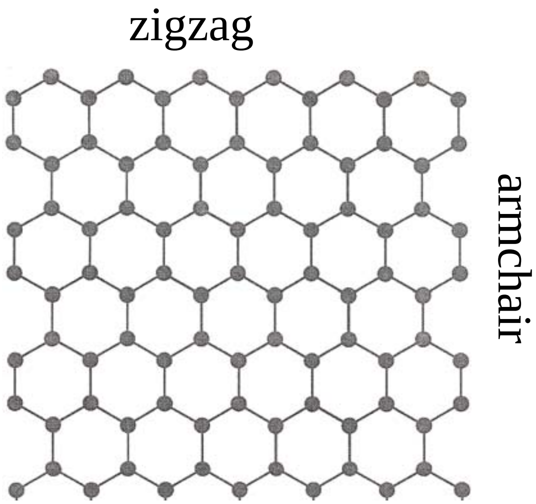
STM images.

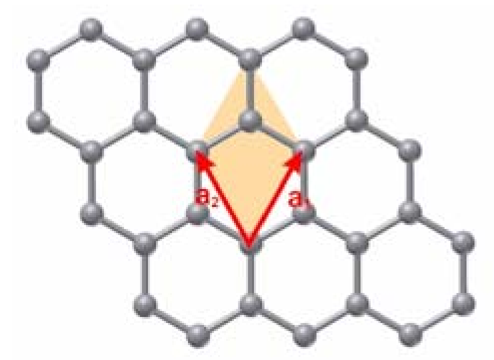
The computer does the Fourier transform (FFT) to the atomic-resolution images.

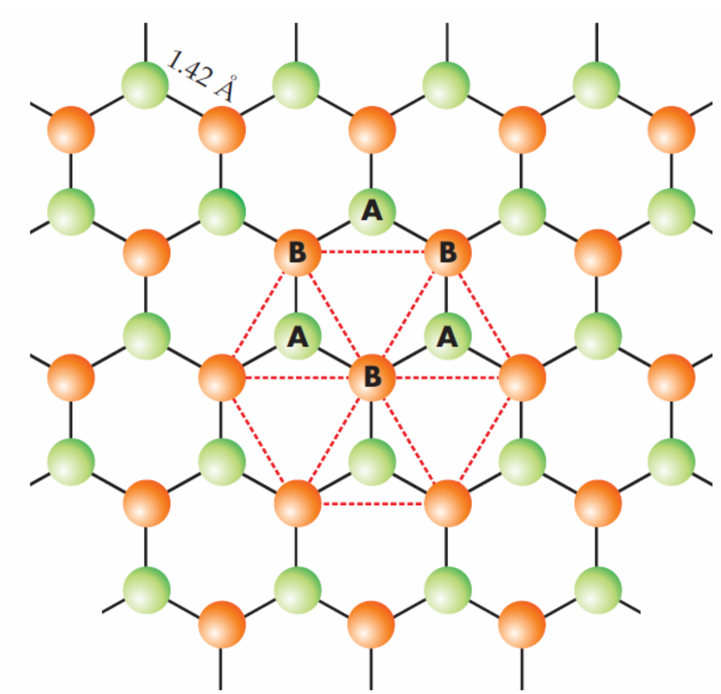


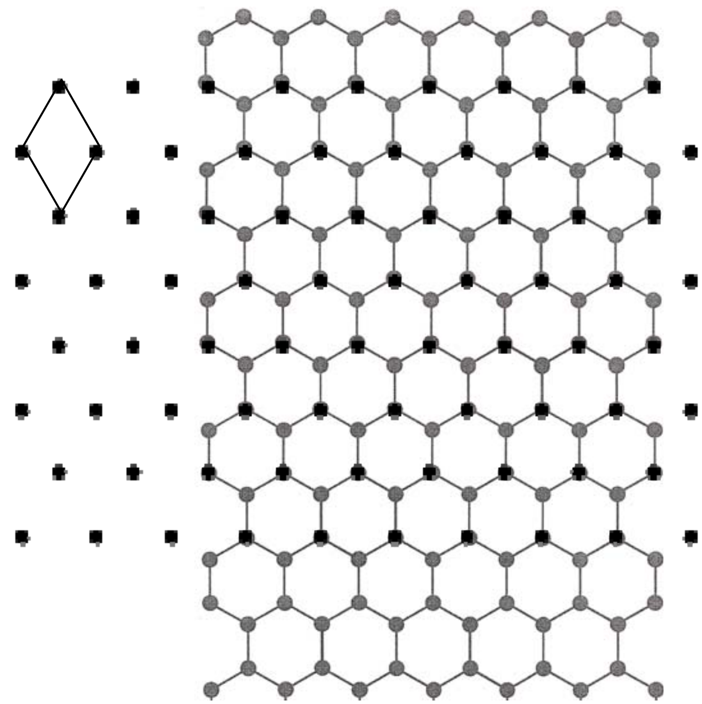
STEM image. Not really atomically resolved, but FFT shows pattern.

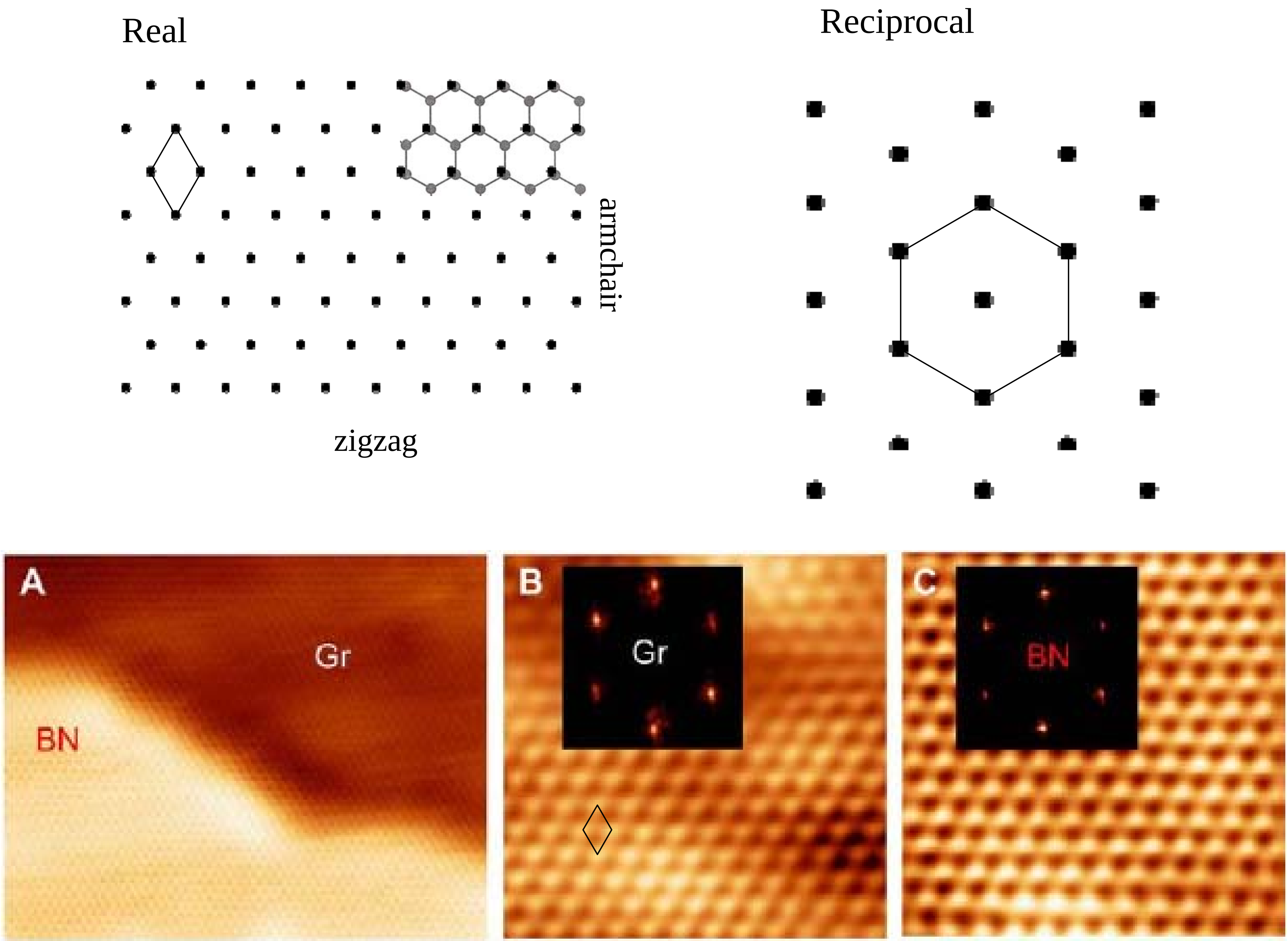
Wait a minute, is the graphene “lattice” a lattice?





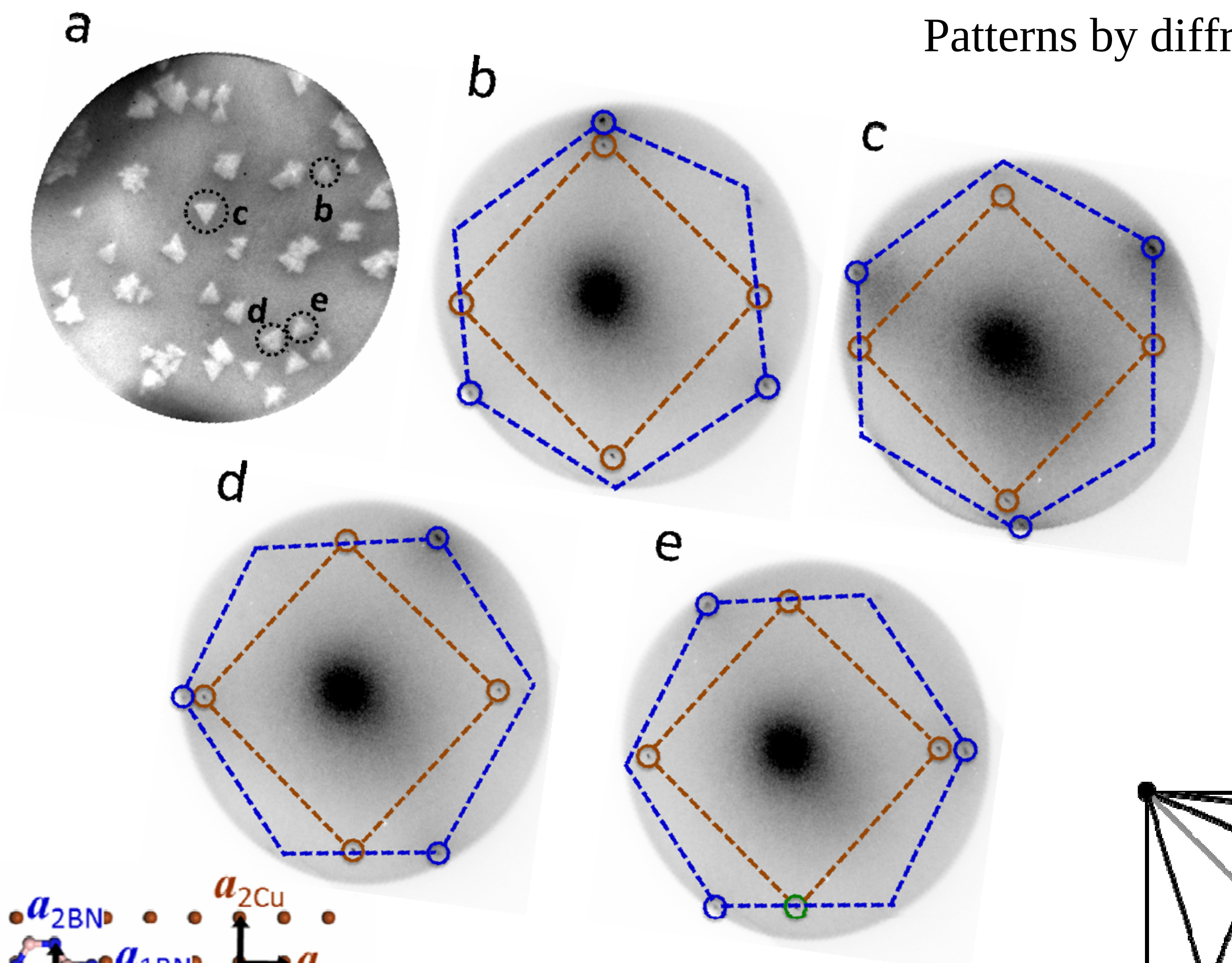


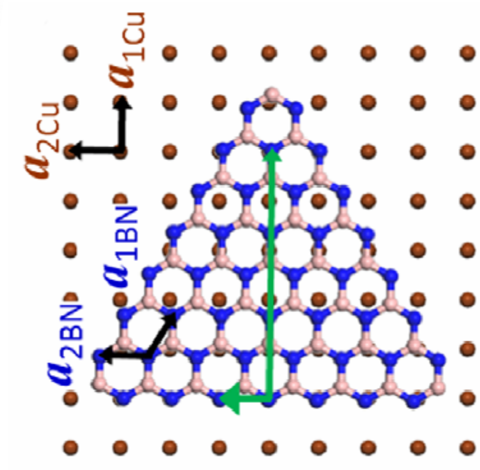


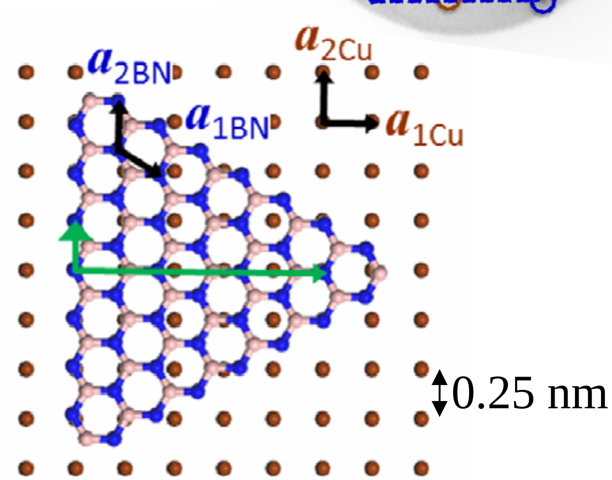

Real
Reciprocal
armchair
zigzag
A
Gr
BN
B
Gr
C
BN

Patterns by diffraction

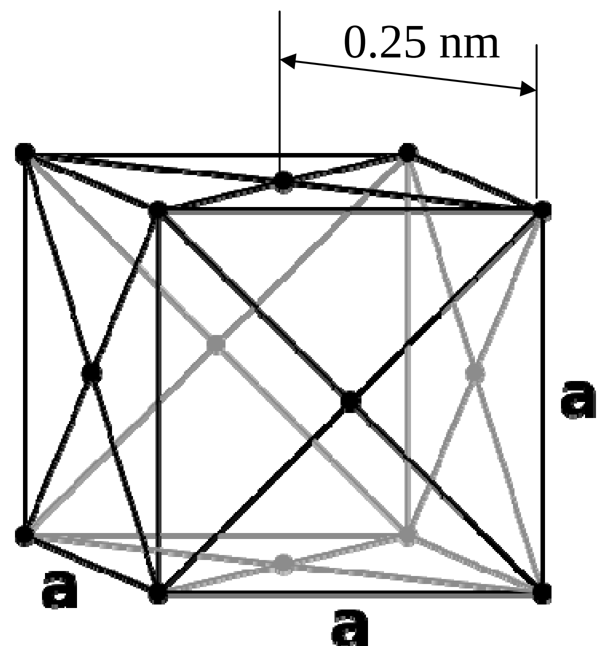
BN on Cu(100)





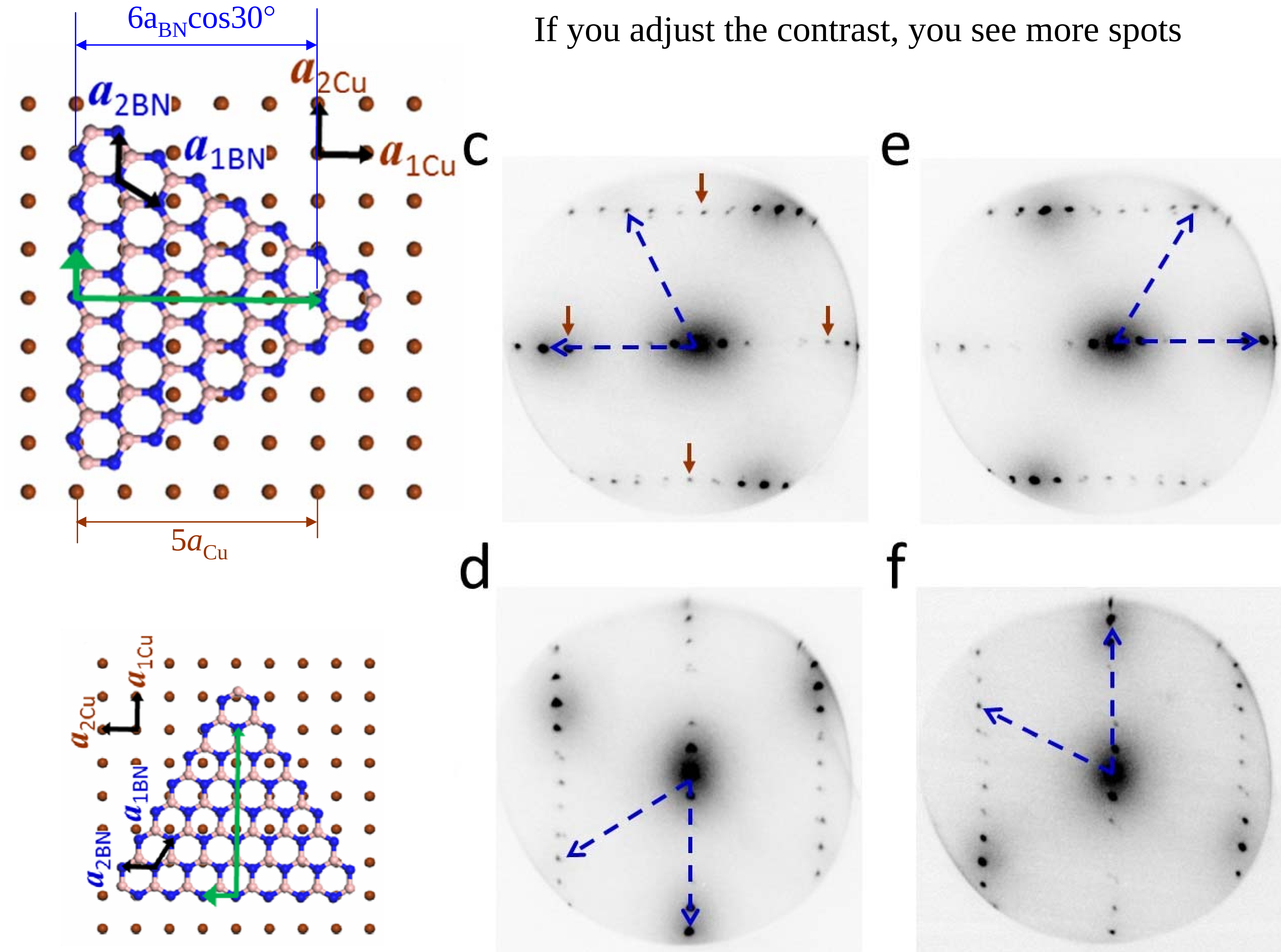


Only 3 of the 6 spots can be seen

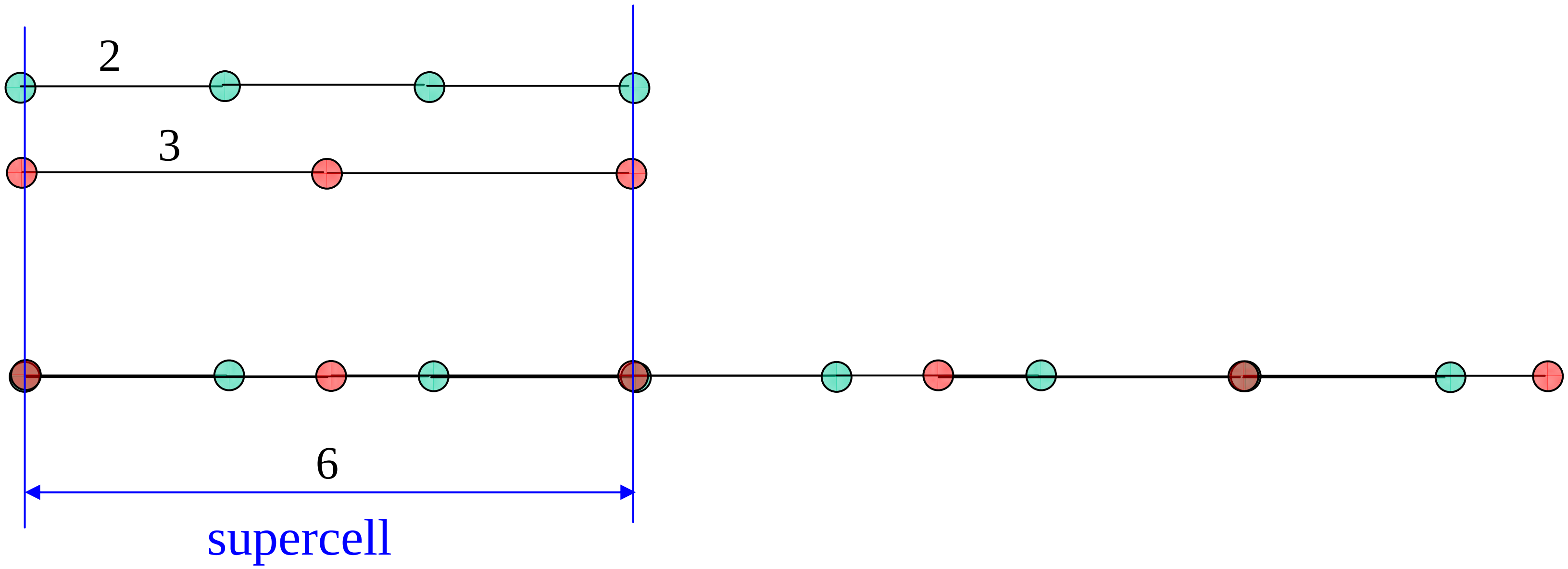


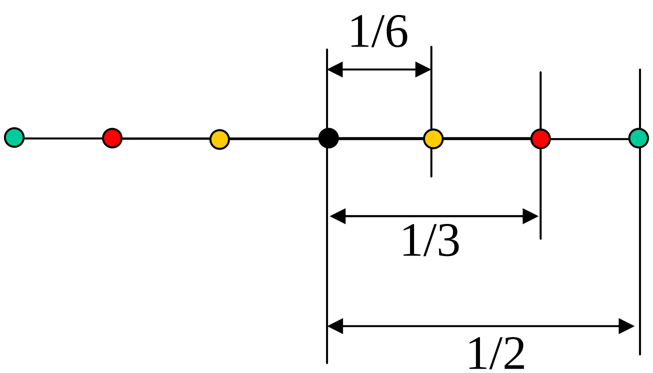
Lei Liu *et al*, *PNAS* (under revision review).

If you adjust the contrast, you see more spots

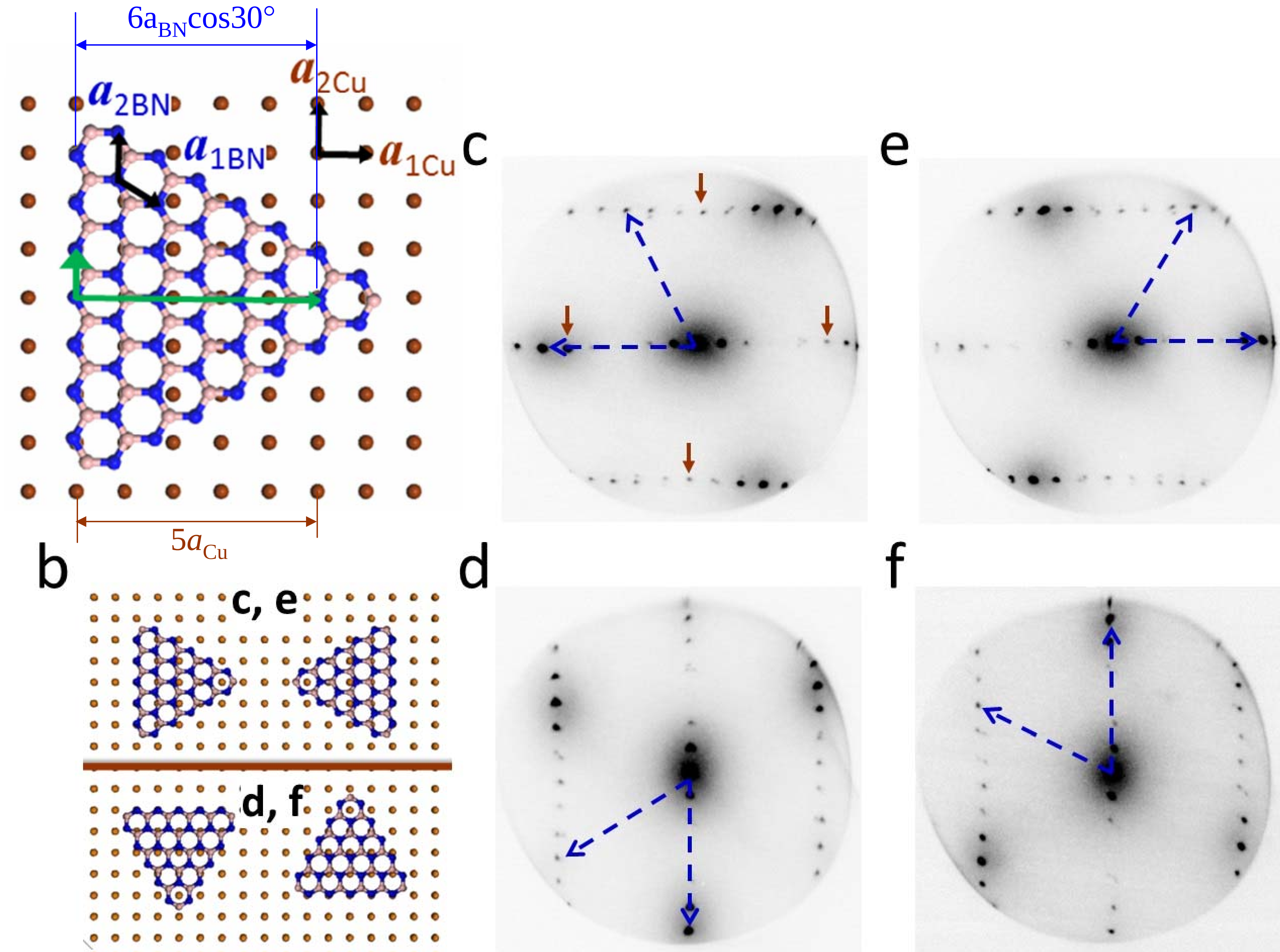


Moiré Patterns and Supercells





Supercell, larger period, smaller frequency.



$6a_{BN}\cos 30°$
a_{2BN}
a_{1BN}
a_{2Cu}
a_{1Cu}
$5a_{Cu}$
c
e
b
c, e
d, f
d
f

Macroscopic Moiré in Min H. Kao Building

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."

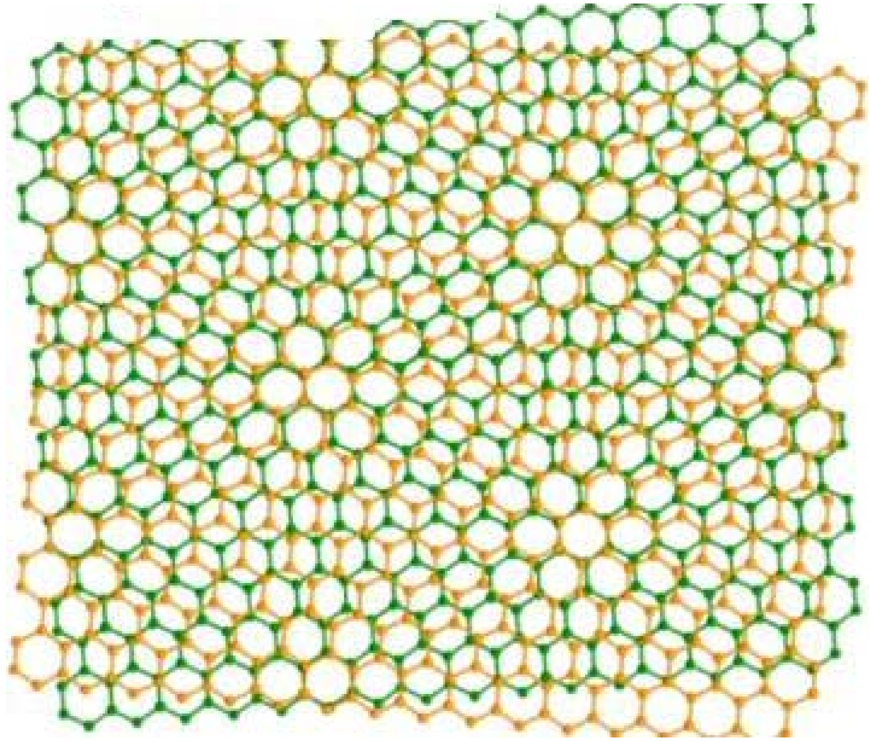
What the physicist calls "yucky and squishy things" may outperform the "beautiful" ordered things.
That squishy thing in Sheldon's head runs on only 20 W and outperforms any supercomputer.

From last lesson

Macroscopic Moiré in Min H. Kao Building

How does this pattern form?

Two identical honeycomb patterns, rotated with regard to each other



Adapted from http://www.physics.rutgers.edu/~aluican/research.html

nature physics

LETTERS

PUBLISHED ONLINE: 29 NOVEMBER 2009 | DOI: 10.1038/NPHYS1463

Observation of Van Hove singularities in twisted graphene layers

Guohong Li[1], A. Luican[1], J. M. B. Lopes dos Santos[2], A. H. Castro Neto[3], A. Reina[4], J. Kong[5] and E. Y. Andrei[1*]

Two (slightly) mismatched honeycomb patterns orientationally aligned to rotated from each other

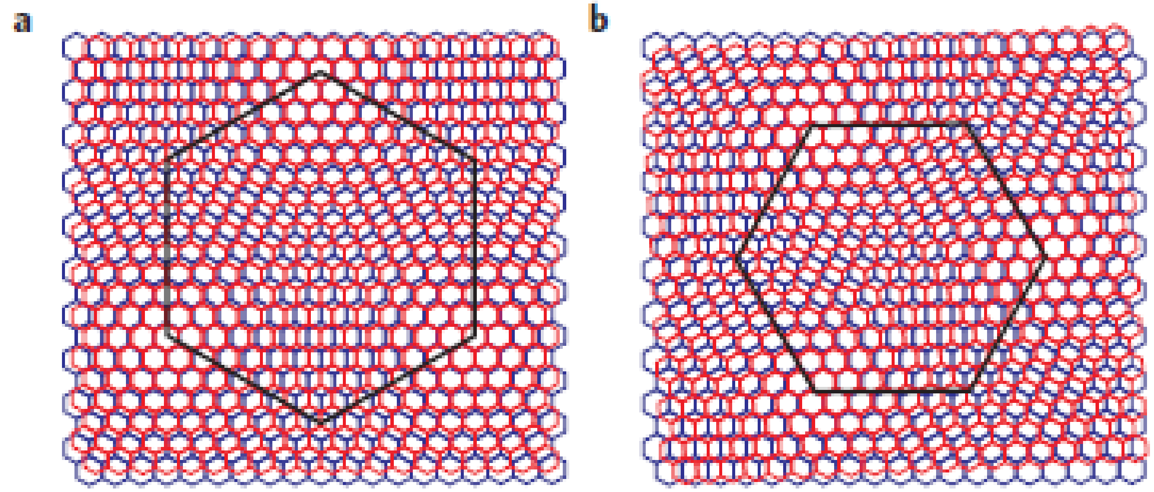


Figure 1 | Schematic representation of the moiré pattern of graphene (red) on hBN (blue). a Relative rotation angle between the crystals $\varphi = 0°$. **b** Relative rotation angle between the crystals $\varphi = 3° \approx 0.052$ rad. The mismatch between the lattices is exaggerated (~10%). Black hexagons mark the moiré plaquette.

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Moiré, superlattice: Larger period over small periods

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L. A. Ponomarenko[1], R. V. Gorbachev[2], G. L. Yu[1], D. C. Elias[1], R. Jalil[2], A. A. Patel[3], A. Mishchenko[1], A. S. Mayorov[1], C. R. Woods[1], J. R. Wallbank[3], M. Mucha-Kruczynski[3], B. A. Piot[4], M. Potemski[4], I. V. Grigorieva[1], K. S. Novoselov[1], F. Guinea[5], V. I. Fal'ko[3] & A. K. Geim[1,2]

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Matthew Yankowitz[1], Jiamin Xue[1], Daniel Cormode[1], Javier D. Sanchez-Yamagishi[2], K. Watanabe[3], T. Taniguchi[3], Pablo Jarillo-Herrero[2], Philippe Jacquod[1,4] and Brian J. LeRoy[1*]

and many more high-profile publications... The importance of periodicity.
We will talk about electrons in periodic things.