Imaging

• Imaging in the TEM
• Diffraction Contrast in TEM Image
• HRTEM (High Resolution Transmission Electron Microscopy) Imaging or phase contrast imaging
• STEM imaging
(a) HRTEM image of gold foil along [001] showing atomic crystal structure
(b), (c) Crystal structure model
Multi-wall Carbon Nano Tube

10nm
• Imaging in the TEM
• What is the contrast?
• In microscopy, contrast is the difference in intensity between a feature of interest (I_s) and its background (I_0). Contrast is usually described as a fraction such as:

\[ C = \frac{I_s - I_0}{I_0} = \frac{\Delta I}{I_0} \]

You won’t see anything on the screen or on the photograph, unless the contrast from your specimen exceeds 5-10%.
**In summary**, BF and DF images (for TEM and STEM) are formed by using the transmitted and diffracted beam respectively. In order to understand and control the contrast in these images, we need to know what features of a specimen cause scattering and what aspects of TEM operation affect the contrast.

**Mechanism of Contrast for TEM/STEM image**

1. **Mass-thickness contrast**: primary contrast source of TEM/STEM image for non-crystalline materials such as polymers and biological materials.

2. **Z-contrast**: High resolution STEM image

3. **Diffraction contrast**: primary contrast source of BF/DF image especially for crystalline materials such as metals. Amplitude of e-wave contributes to the contrast.

4. **Phase contrast**: High/low resolution TEM image (atomic lattice image).

5. **Both the amplitude and the phase contrast**: are primary contrast source of electron holography image for magnetic materials

6. In some situations, image contrast may arise from more than one mechanism and one may dominate.

7. Crystalline sample may generate mass-thickness and diffraction contrast when aperture is removed.
Diffraction contrast

- Diffraction contrast imaging uses the coherent elastic scattering beam to form image.
- Diffraction contrast imaging is controlled by the Bragg diffraction through variation of crystal structure and orientation of specimen.
- Diffraction contrast is simply a special form of amplitude contrast because the scattering occurs at Bragg angle.
- BF and DF image is diffraction contrast image by selecting the direct or diffracted beam as seen figure.
- Beam condition of diffraction contrast imaging: the incident beam must be parallel in order to give the sharp diffraction spots and thereby strong diffraction contrast. So we need to underfocus C2 to spread the beam.

Parallel beam condition
Two-beam conditions for diffraction contrast imaging

BF/DF image pairs along with two-beam diffraction of a series of dislocation and a stacking fault in Cu-15at\%Al.
(a) The [001] zone-axis diffraction pattern showing many planes diffracting with equal strength. In the smaller patterns, the specimen is tilted so there are only two strong beams, the direct [000] on-axis beam and a different one of the \{hkl\} off-axis diffracted beam. (b) and (c) showing the complementary BF and DF image under two-beam conditions. In (b), the precipitates is diffracted strongly and appears dark. In (c), it appears bright.
Beam condition of Imaging

• HRTEM (Phase contrast) Imaging
• Diffraction Contrast Imaging
optic axis

diffraction pattern

lattice image

objective aperture

HRTEM image
How to obtain TEM images

• Using the objective aperture to form BF or DF images
• Using the STEM detector to form BF and DF image
• HRTEM: usually without aperture

To obtain meaningful TEM image

• Careful preparation of sample. Garbage in, and garbage out
• Proper setting-up the optics condition
• Study your materials before TEM session
• Correct operation of instrument
• What’s your question?
• Design the lab plan
• More than one session is necessary
• Please add more tips from your practice, share and discuss your experience.
Incorrect results come from incorrect usage

Very be careful for operation especially in HRTEM mode
1. Delta-function and discontinuities

A Dirac delta function at $x = a$ is defined by

$$\delta(x - a) = \begin{cases} 
0 & \text{for } x \neq a \\
\infty & \text{for } x = a 
\end{cases}$$

and

$$\int_{-\infty}^{\infty} \delta(x - a) \, dx = 1$$

It is represented by an infinitely narrow peak of infinite height at the position $x = a$, the area under the peak is equal to one.
The delta function at \(x=0\), \(\delta(x)\), can be considered as the limit of a set of real continuous functions, such as Gaussians:

\[
\delta(x) = \lim_{a \to \infty} \left[ \frac{a}{\sqrt{\pi}} e^{-a^2 x^2} \right]
\]

The Fourier transform of the constant 1 is equal to delta function

\[
\delta(x) = F(1) = \int_{-\infty}^{\infty} e^{2\pi i x y} \, dy
\]

and

\[
c \delta(x) = F(c) = cF(1) = c \cdot \int_{-\infty}^{\infty} e^{2\pi i x y} \, dy
\]
2. Convolutions

In 1-D, the Convolution integral of two functions, \( f(x) \) and \( g(x) \) is defined as

\[
C(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(X)g(x - X)dX
\]

By simple change of variable, we find that

\[
f(x) * g(x) = \int_{-\infty}^{\infty} g(X)f(x - X)dX = g(x) * f(x)
\]

For two or more dimensions we may use the vector form

\[
f(\vec{r}) * g(\vec{r}) = \int f(\vec{R})g(\vec{r} - \vec{R})d\vec{R}
\]

The identity operation is the convolution with the Dirac delta function

\[
f(x) * \delta(x) = f(x)
\]

\[
f(x) * \delta(x - a) = f(x - a)
\]
Examples of convolutions

\[ C(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(X)g(x-X) dX \] (a)

- Convolutions are fundamental to many different types of experiments.
- For example, a reference signal, \( R(x) \), is created and directed at the material to be investigated (such as electron beam, light or thermal pulse, etc).
- The sample then modifies this reference signal, and ideally we would like to measure the modified signal, \( R'(x) \).
- In practice, the detector system, which converts the modified signal into an observable signal (e.g. visible light, or electron current), introduces its own fingerprint onto the signal, \( R''(x) \).
- In simple case, this would be a linear scaling of \( R'(x) \), but in many case, the relationship between the detected signal \( R''(x) \) and modified signal \( R'(x) \) is nonlinear and can be described by a convolution of \( R'(x) \) with a function \( T(x) \), known as the instrument point spread function \( T \):

\[ R''(x) = T(x) * R'(x) \]

- This means that the instrument impose a resolution limit, which results in blurring of the smallest details in the signal \( R' \), as shown in figure.

The high-frequency details are suppressed by convolution with the wider point spread function.
Fourier transform of a one dimensional function $f(x)$ is defined as

$$F[f(x)] = F(u) = \int_{-\infty}^{\infty} f(x) \cdot e^{2\pi iux} \, dx$$

Fourier inverse transform is defined as

$$f(x) = F^{-1}[F[f(x)]] = \int_{-\infty}^{\infty} F(u) \cdot e^{-2\pi iux} \, du$$
Fourier transform of a 3-D function $f(\mathbf{r})$ is: $\mathbf{r}$ is a vector

$$F(\mathbf{u}) = \int_{-\infty}^{\infty} f(\mathbf{r}) \cdot e^{2\pi i \mathbf{u} \cdot \mathbf{r}} \, d\mathbf{r}$$

If $\mathbf{r}$ has a coordinate $(x,y,z)$ and $\mathbf{u}$ has a coordinate of $(u,v,w)$, then:

$$F(u, v, w) = \iiint_{-\infty}^{\infty} f(x, y, z) \cdot e^{2\pi i (ux + vy + zw)} \, dx \, dy \, dz$$
We may write Fourier transform as

\[ F[f(x)] = F(u) = \int_{-\infty}^{\infty} f(x) \cdot e^{2\pi iux} \, dx \]

\[ F(u) = \int_{-\infty}^{\infty} f(x) \cdot \cos(2\pi ux) \, dx + i \int_{-\infty}^{\infty} f(x) \cdot \sin(2\pi ux) \, dx \]

If the function \( f(x) \) is real and even function, i.e. \( f(-x)=f(x) \), the sine integral is zero, so that

\[ F(u) = \int_{-\infty}^{\infty} f(x) \cdot \cos(2\pi ux) \, dx \]

\[ = 2 \int_{0}^{\infty} f(x) \cdot \cos(2\pi ux) \, dx \]

\( F(u) \) is a real function
Property of Fourier transforms

\[
F[f(x)] = F(u) = \int_{-\infty}^{\infty} f(x) \cdot e^{2\pi iux} \, dx
\]

\[
F[f(-x)] = F(-u)
\]

\[
F[f(ax)] = \frac{1}{a} F\left(\frac{u}{a}\right)
\]

\[
F[f(x) + g(x)] = F(u) + G(u)
\]

\[
F[f(x-a)] = e^{2\pi i au} F(u)
\]
Multiplication and convolution

Multiplication theorem
the Fourier transform of a product of two functions is the convolution of their Fourier transforms.

\[ F[f(x) \cdot g(x)] = F(u) \ast G(u) \]

Convolution theorem: the Fourier transform of the convolution of two functions is the product of their Fourier transforms.

\[ F[f(x) \ast g(x)] = F(u) \cdot G(u) \]
Fourier transform and Diffraction

1. The amplitude distribution of a very small source or the transmission through a very small aperture (slit) in 1-D may be described as $\delta(x)$, or by $\delta(x-a)$ when it is not at the origin. The Fourier transform can be used to derive the diffraction pattern (in general called Fraunhofer diffraction pattern according to wave optics),

$$F[\delta(x)] = 1$$
$$F[\delta(x-a)] = e^{2\pi iua}$$

The amplitude of a diffraction pattern will be proportional to $F(u)$, where $u = l / \lambda$

The intensity observed will be proportional to $|F(u)|^2 = 1$
2. Translation of an object

Translation of the object in real space has effect of multiplying the amplitude in the Fourier transform space (reciprocal space) by a complex exponential. The intensity distribution of the Fraunhofer diffraction pattern is given by $|F(u)|^2$.

$$F[f(x-a)] = F[f(x) \ast \delta(x-a)] = F(u)e^{2\pi i u a}$$
3. Rectangular aperture

In the 2-D, the transmission function of a rectangular aperture is

$$f(x, y) = \begin{cases} 
1 & \text{if } |x| < a/2 \text{ and } |y| < b/2 \\
0 & \text{elsewhere}
\end{cases}$$

Then

$$F(u, v) = \int_{-a/2}^{a/2} e^{2\pi i ux} dx \int_{-b/2}^{b/2} e^{2\pi i uy} dy$$

$$= ab \frac{\sin(\pi au)}{\pi au} \frac{\sin(\pi bv)}{\pi bv}$$

so for a diffraction from a rectangular aperture the intensity distribution is

$$I(u, v) = a^2 b^2 \frac{\sin^2(\pi au)}{(\pi au)^2} \frac{\sin^2(\pi bv)}{(\pi bv)^2}$$
4. Circular aperture

In the 2-D, the transmission function of a circular aperture is

\[ f(x, y) = \begin{cases} 
1 & \text{if } (x^2 + y^2) < (a / 2)^2 \\
0 & \text{elsewhere}
\end{cases} \]

Then

\[ F(u) = \left( \frac{\pi a^2}{2} \right) \frac{J_1(\pi au)}{\pi au} \]

\( u \) is a radial coordinate and \( J_1(x) \) is the first order Bessel function.

the first order Bessel function

\[ J_1(z) = \frac{z}{2} \sum_{k=0}^{\infty} \frac{(-1)^k \cdot z^{2k}}{2^{2k} \cdot k!(k+1)!} \]
1. The imaging process

As a first approximation, we consider coherent image, i.e. a plane parallel, monochromatic electron wave falls in the object, and is scattered, the scattered waves interfere and recombined by an electron lens (objective lens) to form an image.

2. The process consists of two parts: (a) The interaction of the incident wave with the object, defining the exit wave from the object; (b) the action of the objective lens in forming the image.

3. The essential question: how is the image's intensity distribution related to the object structure?

Phase contrast images

- Contrast in TEM images can arise due to the differences in the electron waves scattered through a thin specimen.

- This phase contrast mechanism can be difficult to interpret because it is very sensitive to many factors such as specimen thickness, scattering factors, and properties of lens, etc.

- Phase contrast imaging can be exploited to image the atomic structure of thin specimens.

- The most obvious distinction between phase contrast imaging and other forms of TEM imaging is the number of beams collected by the objective aperture or an electron detector.

  - For BF/DF image only requires a single beam selected by OA for imaging.

  - A phase-contrast image requires the selections of more than one beam. In general, the more beams collected, the higher the resolution of the image.

(A) Schematic many-beam image showing crossing lattice fringes and (B) the diffraction pattern.

7 spots are used for imaging the lattice.
Only two diffraction spots were used for imaging the GaAS lattice showing one set of fringes from the (111) plane (horizontal). Only (111) diffraction contributed the image. The vertical crystal planes are invisible. The information retracted by image is not complete.
Many beams were selected by an aperture (ring) to form an image showing more information about the structure of the specimen.

The question is where are the atoms with respect to the bright and dark contrast dots?

Do the dark spots or bright spot correspond to what atoms (Ga or As), etc.?

Beautiful image sometimes is difficult to interpret.

Correct operation
Beautiful image sometimes is difficult to interpret.