Unifying the Concepts of Scattering and Structure Factor in Ordered and Disordered Samples

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Scattering methods are widely used in many research areas to analyze and resolve material structures. Given the importance, a large number of full textbooks are devoted to this topic. However, technical details in experiments and disconnection between explanations from different perspectives often confuse and frustrate beginner students and researchers. To create an effective learning path, we review the core concepts about scattering and structure factor in this article in a self-contained way. Classical examples of scattering photography and spectroscopy are calculated. Sample CPU and GPU codes are provided to facilitate the understanding and application of these methods.

1. INTRODUCTION

Scattering methods, using a source of photons, electrons, X-rays, neutrons, etc., are powerful tools to examine microscopic structural and dynamical properties of matter, which have been successfully applied to study subatomic particles, crystals, liquids, glasses, surfactants, biomolecules and polymers. The rule of thumb is that the wavelength of the radiation should be comparable to the length scale of the structure to be observed. To detect ordering of the radiation, the wavelength $\lambda$ of the incident radiation can be tuned to fit the scale of the structure to be observed. To detect ordering of the radiation, the wavelength $\lambda$ of the incident radiation can be tuned to fit the scale of the structure to be observed. To detect ordering of the radiation, the wavelength $\lambda$ of the incident radiation can be tuned to fit the scale of the structure to be observed. To detect ordering of the radiation, the wavelength $\lambda$ of the incident radiation can be tuned to fit the scale of the structure to be observed. To detect ordering of the radiation, the wavelength $\lambda$ of the incident radiation can be tuned to fit the scale of the structure to be observed.

Given the richness of material structures, varieties of experimental methods have been developed during the last century, with the scattering being hard or soft, monochromatic or polychromatic, elastic or inelastic. Despite the diversity of experimental setups, they can largely be grouped into two categories. The first category is photography of ordered samples, which are recorded as spotted scattering signals on a two-dimensional (2D) film. The second category is spectroscopy of disordered or partially ordered samples, in which scattering intensity is plotted against one variable (a scalar) that characterizes the existence of periodicities in the system. In both types, the quantitative measurement of the signal is scattering intensity $I(q)$, or its normalized version, structure factor $S(q)$, which is often expressed as a function of scattering vector $q$. The central tasks of structural analysis with scattering methods are then

- the forward problem $\rho(r) \rightarrow I(q)$: given the electron density profile $\rho(r)$ or particle positions $(r_1, r_2, \ldots, r_N)$, to predict the scattering pattern $I(q)$; and
- the inverse problem $I(q) \rightarrow \rho(r)$: given the scattering pattern $I(q)$, to resolve the electron density profile $\rho(r)$ or particle positions $(r_1, r_2, \ldots, r_N)$.

In this article, we only focus on the forward problem, which could still shed light on some basic structural information. Sometimes, the forward method may also be used to solve $\rho(r)$ iteratively, through a trial-and-error process. That is, one keeps modifying a proposed structure $\rho(r)$ until the theoretically computed $I(q)$ matches the experimentally observed one. The full solution to the inverse problem is, however, challenged by the notorious “phase problem”.

Concepts about scattering and structure factor are often discussed across different disciplines including condensed-matter physics, materials science, polymer physics, structure biology, etc. The same idea can take different forms in different areas, causing confusions and misconceptions. Graduate or advanced undergraduate students in need of applying these concepts to their research problems can be frustrated by the convoluted experimental details covered in traditional textbooks. It is thus the purpose of this article to unify the concepts about scattering and structure factor, giving junior researchers an effective pathway to quickly grasp the key ideas in this field without taking a whole course or reading a full textbook.

To fulfill this task, we first elaborate the fundamentals about scattering (Section 2), crystallography (Section 3) and liquid state theory (Section 4) based on Fourier transform and reciprocal lattice. Using concrete examples, we then discuss the photography of ordered samples in Section 5 as well as spectroscopy of isotropic samples in Section 6. Relevant CPU and GPU source codes are provided online at https://github.com/statisticalmechanics/scatter. Finally, a brief introduction to 2D structure factor is given in Section 9 before the conclusion in Section 10.
According to Fermi’s golden rule, the scattering intensity is proportional to the square of the transition probability amplitude from state $\psi_{k_0}(\mathbf{r})$ to state $\psi_{k_1}(\mathbf{r})$, after interacting with the overall scattering potential $\rho(\mathbf{r})$. That is,

$$I(q) \propto |\langle k_0 | \rho(\mathbf{r}) | k_1 \rangle|^2 = \left| \int d\mathbf{r} \psi_{k_0}^* \rho(\mathbf{r}) \psi_{k_1}(\mathbf{r}) \right|^2$$

Neglecting the coefficient of proportionality, one can write

$$I(q) = \hat{\rho}_q \delta_{q,-q}, \quad (4)$$

where

$$\hat{\rho}_q = \int d\mathbf{r} \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \quad (5)$$

is the Fourier transform of the density profile and $\hat{\rho}_{-q}$ is its complex conjugate (Appendix A).

Unless $\rho(\mathbf{r})$ has a symmetry center, $\hat{\rho}_q$ is generally a complex number, i.e., $\hat{\rho}_q = |\hat{\rho}_q|e^{i\phi_q}$. If $\hat{\rho}_q$ is known exactly, $\rho(\mathbf{r})$ can in principle be reconstructed through inverse Fourier transform Eq. (A2) \[15\]. However, in experiment, only the scattering intensity $I(q) = |\hat{\rho}_q|^2 e^{i\phi_q} e^{-i\phi_q} = |\hat{\rho}_q|^2$ is directly measurable. This allows us to compute the magnitude of $\hat{\rho}_q$ by $|\hat{\rho}_q| = \sqrt{I(q)}$. Unfortunately, information about the phase angle $\phi_q$ is lost during this process, which gives rise to the “phase problem” in crystallography. Special techniques \[14\] \[16\] \[17\] have been designed to trace $\phi_q$, which are beyond the scope of this article.

In a system of $N$ atoms or particles at positions $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ inside a region of volume $V$, the density profile consists of the contributions from each particle $i$ with a scattering potential $f_i(\mathbf{r} - \mathbf{r}_i) \ (i = 1, 2, \cdots, N)$, i.e.,

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} f_i(\mathbf{r} - \mathbf{r}_i) = \sum_{i=1}^{N} f_i(\mathbf{R}_i), \quad (\mathbf{R}_i \equiv \mathbf{r} - \mathbf{r}_i). \quad (6)$$

In this case

$$\hat{\rho}_q = \int d\mathbf{r} \sum_{i=1}^{N} f_i(\mathbf{r} - \mathbf{r}_i) e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$= \sum_{i=1}^{N} \int d\mathbf{R}_i f_i(\mathbf{R}_i) e^{i\mathbf{q}\cdot\mathbf{R}_i} e^{i\mathbf{q}\cdot\mathbf{r}_i}, \quad (7)$$

$$= \sum_{i=1}^{N} \hat{f}_i(q)e^{i\mathbf{q}\cdot\mathbf{r}_i},$$

where

$$\hat{f}_i(q) = \int d\mathbf{r} f_i(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \quad (8)$$

is the atomic form factor, or scattering factor, of particle $i$. 

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**SCATTERING**

2.1. Scattering Vector

In a scattering experiment, the incident beam of wavevector $\mathbf{k}_0$, after hitting the sample, is deflected from its straight path by a scattering angle $2\theta$ and becomes the diffracted beam of wavevector $\mathbf{k}_1$ (Fig. 1). In case of elastic and monochromatic scattering (of a fixed wavelength $\lambda$), $|k_0| = |k_1| = \frac{2\pi}{\lambda}$. The change of wavevector, called scattering vector, is

$$\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_0 \quad (1)$$

with a magnitude

$$q = 2|k_0| \sin \theta = \frac{4\pi}{\lambda} \sin \theta. \quad (2)$$

Let $s_0 = k_0/|k_0| = k_0\lambda/(2\pi)$ and $s_1 = k_1/|k_1| = k_1\lambda/(2\pi)$ be the unit vectors of the incident and diffracted beam, then scattering vector can also be written as

$$\mathbf{q} = \frac{2\pi}{\lambda}(s_1 - s_0). \quad (3)$$

2.2. Scattering Intensity

When a screen is placed behind the sample in the path of $\mathbf{k}_1$, the diffracted beam may be detected. The strength of such signals is quantified by the scattering intensity $I(q)$ of the ray, which changes with $\mathbf{k}_1$, or equivalently, with $\mathbf{q}$. The scattering pattern, or the distribution of $I(q)$ on the detection screen, is determined by the structure features of the sample, for instance, the electron density profile $\rho(\mathbf{r})$ in the case of X-ray scattering by atoms.

Both the incident and the diffracted rays can be viewed as a plane wave of the form $\psi_{k_0}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k} \rangle \propto e^{i\mathbf{k}\cdot\mathbf{r}}$. According to Fermi’s golden rule, the scattering intensity $I(q)$ is proportional to the square of the transition probability amplitude from state $\psi_{k_0}(\mathbf{r})$ to state $\psi_{k_1}(\mathbf{r})$, after interacting with the overall scattering potential $\rho(\mathbf{r})$. That is,

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In this case

$$\hat{\rho}_q = \int d\mathbf{r} \sum_{i=1}^{N} f_i(\mathbf{r} - \mathbf{r}_i) e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$= \sum_{i=1}^{N} \int d\mathbf{R}_i f_i(\mathbf{R}_i) e^{i\mathbf{q}\cdot\mathbf{R}_i} e^{i\mathbf{q}\cdot\mathbf{r}_i}, \quad (7)$$

$$= \sum_{i=1}^{N} \hat{f}_i(q)e^{i\mathbf{q}\cdot\mathbf{r}_i},$$

where

$$\hat{f}_i(q) = \int d\mathbf{r} f_i(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \quad (8)$$

is the atomic form factor, or scattering factor, of particle $i$. 

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**FIG. 1.** Scattering vector $\mathbf{q}$ defined as the difference between the diffracted wavevector $\mathbf{k}_1$ and the incident wavevector $\mathbf{k}_0$, of a magnitude $2\pi/\lambda$ during elastic scattering.
If the scattering potential of each particle \( f_i(r - r_i) \) is symmetric about \( r_i \), which should be true for atoms and most particles, \( \hat{f}_i(q) \) is real and even, i.e. its complex conjugate, \( \hat{f}_i^*(q) = \hat{f}_i(-q) = \hat{f}_i(q) \) (Appendix A). Under this circumstance, the scattering intensity

\[
I(q) = \sum_{i=1}^{N} \hat{f}_i(q) e^{iqr_i} = \sum_{i=1}^{N} \hat{f}_i(q) e^{iqr_i} \sum_{j=1}^{N} \hat{f}_j(-q)e^{-iqr_j} \\
= \sum_{i=1}^{N} \hat{f}_i(q) e^{iqr_i} \sum_{j=1}^{N} \hat{f}_j(q)e^{-iqr_j} \\
= \left| \sum_{i=1}^{N} \hat{f}_i(q) \cos(q \cdot r_i) \right|^2 + \left| \sum_{i=1}^{N} \hat{f}_i(q) \sin(q \cdot r_i) \right|^2
\]

(9)
or equivalently,

\[
I(q) = \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) e^{iqr_{ij}} \\
= \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) \cos(q \cdot r_{ij}) \\
= \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) \cos(q \cdot r_{ij}) \\
= \sum_{i=1}^{N} \hat{f}_i^2(q) + \sum_{i=1}^{N} \sum_{j \neq i} \hat{f}_i(q) \hat{f}_j(q) \cos(q \cdot r_{ij}).
\]

Equation (9) and Eq. (10) are mathematically equivalent because \( \cos(q \cdot r_{ij}) = \cos(q \cdot (r_i - q \cdot r_j)) = \cos(q \cdot r_i) \cos(q \cdot r_j) + \sin(q \cdot r_i) \sin(q \cdot r_j) \). However, in numerical computation of \( I(q) \) at a given \( q \), Eq. (9) has a lower cost with a computational complexity \( O(N) \), while Eq. (10) is of complexity \( O(N^2) \). Nevertheless, when there is an appropriate symmetry in the system, the expression \( r_{ij} \) in Eq. (10) allows it to be further simplified and thus to become computationally efficient, as will be discussed in later sections.

### 2.3. Atomic Form Factor

For realistic scattering potentials, the atomic form factor \( \hat{f}_i(q) \) changes with scattering vector \( q \) and often drops as scattering angle \( \theta \) increases (Fig. 2). If the scattering potential is further to be spherically symmetric, i.e. \( f_i(r) = f_i(r) \), we can write

\[
\hat{f}_i(q) = \frac{4\pi a_i/(\pi \sigma^3/6)}{q^3} [\sin(q\sigma/2) - q\sigma/2 \cos(q\sigma/2)] \\
= \frac{3a_i}{(q\sigma/2)^3} [\sin(q\sigma/2) - q\sigma/2 \cos(q\sigma/2)].
\]

(14)

\[ f_i(r - r_i) \] is Gaussian-like with standard deviation \( \sigma/2 \),

\[
f_i(r - r_i) = a_i \left( \frac{1}{\sqrt{2\pi}(\sigma/2)^2} \right) e^{-\frac{(r - r_i)^2}{2(\sigma/2)^2}} \\
= \frac{a_i}{\sigma^3(\pi/2)^{3/2}} e^{-\frac{R_i^2}{2\pi\sigma^2}} (R_i = |r - r_i|)
\]

(15)

and

\[
\hat{f}_i(q) = a_i e^{-\frac{q^2\sigma^2}{8}}.
\]

(16)

In all numerical results shown below, we will assume \( \hat{f}_i(q) = 1 \) for all particles.

![FIG. 2. Atomic form factor \( \hat{f}_i(q) \) of a uniform spherical (red solid, Eq. 14) and a Gaussian scattering center (blue dashed, Eq. 16) as a function of \( q \).](image)
3. CRYSTALLOGRAPHY

We now review concepts and theories about scattering methods used for crystal samples. The earlier theory of von Laue [18] that considers diffraction of parallel beams by arrays of atoms is skipped here. Instead, we apply the more intuitive Bragg’s law that envisages crystallographic planes as reflective mirrors to understand the principle, although there is no such reflection in the physical sense.

3.1. Bragg’s Law

For an incident ray of wavelength $\lambda$ to generate a strong constructive scattering signal by a family of crystallographic planes ($hkl$) of interplanar spacing $d_{hkl}$ (Appendix B), the scattering angle $2\theta$ needs to obey Bragg’s law [19] (Fig. 3)

$$n\lambda = 2d_{hkl}\sin \theta, \quad n = 1, 2, 3, \ldots.$$  \hspace{1cm} (17)

This is because the path difference of the two scattering rays “reflected” by two neighboring lattice planes is

$$l(\cos \alpha + \cos \beta) = l[\cos \alpha + \cos(\pi - 2\theta - \alpha)]
= l[\cos \alpha - \cos(2\theta + \alpha)]
= l\sin(\theta + \alpha) \sin \theta
= d_{hkl} \sin \theta.$$

The rescaled scattering vector $s_1 - s_0 = \frac{\lambda}{2\pi} q$ (of a length of $2\sin \theta$) is parallel to the normal vector, or reciprocal vector $d_{hkl}^*$ (of length $1/d_{hkl}$), of the lattice planes ($hkl$). Thus, it is sometimes convenient to express Bragg’s law in a vector form, for instance, for the primary $n = 1$ scattering, as

$$\frac{s_1 - s_0}{\lambda} = d_{hkl}^*.$$  \hspace{1cm} (18)

Using Eq. (3), the necessary condition to receive a strong signal for scattering vector $q$ in crystals is thus

$$q = 2\pi d_{hkl}^*.$$  \hspace{1cm} (19)

3.2. Ewald’s Sphere

Bragg’s law needs to be satisfied to have a strong scattering signal in the direction of $s_1$. However, this does not mean that, given an arbitrary experimental setup, Bragg’s law is guaranteed to be satisfied somewhere. In particular, if a monochromatic incident beam ($\text{fixed } \lambda$) is applied upon a single crystal at an arbitrarily fixed position ($\text{fixed } \theta$’s and $d_{hkl}$’s), it is possible that none of the lattice planes will be able to produce a strong scattering signal. If this happens, either $\lambda$ (polychromatic) or $\theta$ (rotate the sample or use polycrystals) has to be tuned to satisfy Eq. (17-19).

An alternative view to check the satisfaction of Bragg’s law is to use Ewald’s sphere in the reciprocal space [20, 21]. Here, each point at vector $d_{hkl}^*$ represents a family of parallel planes ($hkl$) in the direct space. When the orientation of the crystal sample is fixed, the relative position of the incident beam and reciprocal lattice points are also fixed. One can align the end point of the incident wavevector $k_0$ (in practice $k_0/2\pi$) with the origin $O$ of the reciprocal lattice, then draw a sphere of radius $1/\lambda$. The center of the sphere is found by moving from point $O$ by a vector displacement $-k_0/2\pi$ (Fig. 4). It can be seen that, the end point of the scattering vector $q$, normalized by $2\pi$, falls on the surface of this Ewald’s sphere. According to the vector form of Bragg’s law Eq. (19), a strong scattering from certain lattice planes ($hkl$) is possible, only when the corresponding reciprocal vector point $d_{hkl}^*$ falls on the surface of Ewald’s sphere. If wavelength and crystal orientation are not appropriately chosen, this condition may not be met at all and no scattering signal is generated by the sample.

3.3. Crystal Structure Factor $F_{hkl}$

Bragg’s law is actually the necessary (not sufficient) condition to have a strong scattering signal. Even if Bragg’s law is obeyed by lattice planes ($hkl$), it is still possible that the scattering signal cancels due to special lattice symmetries. In fact, when Bragg’s law is presented as in Fig. 3, a simple square or oblique lattice structure is often used, which misses the complexity in other three-dimensional lattices. Generally, not every family of lattice planes ($hkl$) can produce a constructive scattering.
For crystals, only structure factor $\rho$ system. In crystallography, it is customary to define $\hat{\rho}$

$$
\hat{\rho} = \frac{N}{m} \int_{V_{cell}} d\mathbf{r} \rho(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}},
$$  

(20)

where $N/m$ is the number of unit cells in the $N$-particle system. In crystallography, it is customary to define $\hat{\rho}$ per unit cell as the structure factor,

$$
\mathbf{F}_q = \int_{V_{cell}} d\mathbf{r} \rho(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}}.
$$

(21)

For crystals, only $\mathbf{q}$’s satisfying Bragg’s law can possibly generate a large $\hat{\rho}_q$ or $\mathbf{F}_q$. Therefore, we only need to consider $\mathbf{q}$’s of the form

$$
\mathbf{q} = 2\pi \mathbf{d}^{*}_{hkl} = 2\pi (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*),
$$

where $\mathbf{d}^{*}_{hkl}$ represents a family of lattice planes $(hkl)$ of spacing $d_{hkl} = 1/|\mathbf{d}^{*}_{hkl}|$ (Appendix B). The associated structure factor can thus be denoted as $F_{hkl}$

$$
F_{hkl} = \int_{V_{cell}} d\mathbf{r} \rho(x, y, z) e^{2\pi i(hx + ky + lz)}.
$$

(22)

Inversely, density profile within each unit cell is

$$
\rho(\mathbf{r}) = \frac{1}{V_{cell}} \sum_{hkl} F_{hkl} e^{-2\pi i(hx + ky + lz)}.
$$

(23)

For point-like scattering centers $\rho(\mathbf{r}) = \sum_{i=1}^{m} a_i \delta(\mathbf{r} - \mathbf{r}_i)$, Eq. (22) reduces to

$$
F_{hkl} = \sum_{i=1}^{m} a_i e^{2\pi i(hx_i + ky_i + lz_i)},
$$

(24)

after substituting Eq. (12) and following steps in Eq. (7), where $(x_i, y_i, z_i)$ are coordinates of the $m$ atoms inside one unit cell and are expressed as fractions of lattice vectors. The strength of $F_{hkl}$ by planes $(hkl)$ is the vector sum of each term $a_i e^{2\pi i(hx_i + ky_i + lz_i)}$ in Eq. (24), where the phase angle $hx_i + ky_i + lz_i$ defines the direction of each vector. For typical crystal lattices of point-like atoms, $F_{hkl}$ can be easily computed.

- **Simple Cubic (SC)**
  
  $$
  m = 1 \text{ and } (x_1, y_1, z_1) = (0, 0, 0)
  $$

  $$
  F_{hkl}^{SC} = a_1 e^{2\pi i(hx_0 + ky_0 + lz_0)} = a_1
  $$

  (25)

  for any $h, k, l$.

- **Body-Centered Cubic (BCC)**

  $$
  m = 2 \text{ and } (x_1, y_1, z_1) = (0, 0, 0) \text{ and } (x_2, y_2, z_2) = (1/2, 1/2, 1/2)
  $$

  $$
  F_{hkl}^{BCC} = a_1 e^{2\pi i(hx_0 + ky_0 + lz_0)} + a_2 e^{2\pi i(hx_1 + ky_1 + lz_1)}
  $$

  $$
  = a_1 + a_2 e^{\pi i(h + k + l)}.
  $$

  (26)

- **Face-Centered Cubic (FCC)**

  $$
  m = 4 \text{ and } (x_1, y_1, z_1) = (0, 0, 0) \text{ and } (x_2, y_2, z_2) = (1/2, 1/2, 0) \text{ and } (x_3, y_3, z_3) = (0, 1/2, 1/2) \text{ and } (x_4, y_4, z_4) = (1/2, 0, 1/2)
  $$

  $$
  F_{hkl}^{FCC} = a_1 e^{2\pi i(hx_0 + ky_0 + lz_0)} + a_2 e^{2\pi i(hx_1 + ky_1 + lz_1)} + a_3 e^{2\pi i(hx_2 + ky_2 + lz_2)} + a_4 e^{2\pi i(hx_3 + ky_3 + lz_3)}
  $$

  $$
  = a_1 + a_2 e^{\pi i(h + k + l)} + a_3 e^{\pi i(h + k + l)} + a_4 e^{\pi i(h + k + l)}.
  $$

  (27)

In cases of BCC and FCC lattices, $F_{hkl}$ may completely vanish for certain $h, k, l$. If all $m$ atoms are the same, it can be verified that, successive reflection Miller indices should be $(110), (200), (211), (220), (310), (222) \cdots$ for BCC and $(111), (200), (220), (311), (222), (400) \cdots$ for FCC crystals.

### 3.4. Finite-Size Crystals and Bragg Peak Broadening

When Bragg’s law is satisfied by wavelength $\lambda$ at an incident angle $\theta$, a small deviation $\delta \theta$ from $\theta$ only slightly changes the path difference between two rays reflected by a pair of neighboring planes (of spacing $d_{hkl}$), which still add constructively. If we consider two reflection planes
that are $2d_{hkl}$, $3d_{hkl}$, · · · , apart, the change in path difference due to $\delta \theta$ increases, and at large enough spacing, becomes $\lambda/2$ such that the two rays completely cancel. For a beam reflected by a crystallographic plane in large crystal samples, it is always possible to find another remote plane whose reflected beam interferes destructively, even for very small $\delta \theta$. Therefore, diffraction signals in large samples at fixed $\lambda$, if there are any, should in principle be of infinitely small size (in terms of the range of $\theta$).

For small crystal samples, it is possible that the change in path difference due to $\delta \theta$ is much less than $\lambda/2$ such that Bragg’s law is still approximately satisfied at $\theta + \delta \theta$ and the diffraction signal is broadened by an amount $\sim \delta \theta$. The quantitative relationship between the broadening $2\delta \theta$ of the signal and the linear dimension $L$ of a finite-size crystal can be found by considering all pairs of planes that are $L/2$ apart. When $\theta$ changes to $\theta + \delta \theta$, the path difference for such a pair of planes increases by $2\lambda/2 \left[ \sin(\theta + \delta \theta) - \sin \theta \right] = L \cos \theta \delta \theta$ (Fig. 5). The diffraction signal broadens until destructive interference occurs at $\delta \theta = \frac{\lambda}{2L\cos \theta}$, which gives the Scherrer equation

$$2\delta \theta = \frac{\lambda}{L\cos \theta} = \frac{2 \tan \theta}{L/d_{hkl}}.$$  

Thus diffraction signals tend to be larger in smaller systems or at larger scattering angle.

4. LIQUID STATE THEORY

According to liquid state theory, static structure factor $S(q)$ can be used to address short-range order [22,24] and glass transition [21] in amorphous samples. In a N-particle system, it is defined as

$$S(q) = \frac{1}{N} \sum_{i=1}^{N} \langle \hat{f}^2(q) \rangle = \frac{1}{N} \sum_{i=1}^{N} f_i^2(q)$$

where the ensemble average $\langle \cdots \rangle$ is usually taken over configurations at thermal equilibrium [25].

If scattering centers are point-like, i.e. $\rho(r) = \sum_{i=1}^{N} a_i \delta(r - r_i)$, then $\hat{f}_q = N_\delta q_0$ and

$$S(q) = \frac{1}{N} \sum_{i=1}^{N} a_i^2 \left\langle \left( \sum_{i=1}^{N} a_i \cos(q \cdot r_i) \right)^2 + \left( \sum_{i=1}^{N} a_i \sin(q \cdot r_i) \right)^2 \right\rangle.$$  

For monodisperse systems ($a_i$ is the same for all particles), $S(0) = N$.

In the case of $a_i = 1$, $S(q)$ is related to the radial distribution function $g(r)$ or the pair correlation function $h(r) = g(r) - 1$ by

$$S(q) = 1 + \rho_0 \int dr(g(r) - 1)e^{iqr} + \rho_0 \rho_0 \int dr e^{iqr} = 1 + \rho_0 \int V dr h(r) e^{iqr} + N \delta_{q,0} \text{ (finite } V \text{)}$$

$$= 1 + \rho_0 \int V h(q) e^{iqr} + N \delta_{q,0}$$

where the global number density $\rho_0 = N/V$ and the Fourier transform $\hat{h}_q = \int V dr h(r)e^{iqr}$. Note that $S(q)$ is singular or discontinuous at $q = 0$, i.e. $\lim_{q \to 0} S(q) \neq S(0) = N$. Correspondingly, $\lim_{q \to 0} \hat{h}_q \neq \hat{h}_0 = -1/\rho_0$.

The radial distribution function can be obtained from structure factor by inverse Fourier transform

$$g(r) = 1 + \frac{1}{(2\pi)^3} \int dq S(q) - 1 \frac{e^{-iqr}}{\rho_0}.$$  

where the value $\lim_{q \to 0} S(q)$ should be used at $q = 0$ in the integration. When the system is uniform, i.e. $g(r) = g(r)$, more convenient relationships can be arrived

$$S(q) = 1 + 4\pi \rho_0 \int_0^\infty dr(g(r) - 1)r^2 \frac{\sin(qr)}{qr},$$

$$g(r) = 1 + \frac{1}{2\pi^2} \int_0^\infty dq \frac{S(q) - 1}{\rho_0} q^2 \frac{\sin(qr)}{qr}.$$
where \( \lim_{x \to 0} \frac{\sin x}{x} = 1 \) should be used in the integration.
The limit value of \( S(q) \) as \( q \) approaches zero is related to the isothermal compressibility \( \kappa \) by \[ (35) \]

\[
\lim_{q \to 0} S(q) = \rho_0 k_B T \kappa.
\]

5. EXPERIMENTAL SETUPS IN PHOTOGRAPHY

In this section, we discuss some technical details about photography methods, which collects signals of \( I(q) = I(X, Y) \) on a two-dimensional film with coordinates \((X, Y)\). Three popular experimental setups are often used as described below, which map \( q \) onto \((X, Y)\) differently.

5.1. Back-reflection and Transmission Methods

In back-reflection and transmission methods, the recording film is a rectangular plane, which is placed either before (back-reflection) or after (transmission) the sample as shown in Fig. 6. In both methods, it can be seen that the ratio \( q_x / q_y \) equals \( X/Y \). If the incident wave number is \( |k_0| = 2\pi/\lambda \), then

\[
(q_x, q_y) = \frac{2\pi}{\lambda} \left( \frac{X}{L}, \frac{Y}{L} \right),
\]

where \( L^2 = R^2 + D^2 \) and \( R^2 = X^2 + Y^2 \). The difference remains in the \( z \) component \( q_z \).

In back-reflection method, because \( \alpha = \frac{\pi}{2} - \theta \) satisfies \( \cos(2\alpha) = D/L \), it follows that

\[
q_z = -\frac{2\pi}{\lambda} \cos \alpha \cos \alpha = -\frac{2\pi}{\lambda} \cos(2\alpha)
\]

\[
= -\frac{2\pi}{\lambda} \left( 1 + D/L \right).
\]

Therefore,

\[
(q_x, q_y, q_z) = \frac{2\pi}{\lambda} \left( \frac{X}{L}, \frac{Y}{L}, D + L \right) \quad \text{(back-reflection)}
\]

(37)

In contrast, one can show that, in transmission method,

\[
(q_x, q_y, q_z) = \frac{2\pi}{\lambda} \left( \frac{X}{L}, \frac{Y}{L}, -L - D \right) \quad \text{(transmission)}.
\]

(38)

5.2. Cylindrical Method

Compared with above two setups, cylindrical method collects signals from all azimuthal angles \( \phi \) and is thus more informative (Fig. 7). In fact, a cylindrical film can be considered as the sum of an infinitely wide back-reflection film and an infinitely wide transmission film with certain deformation due to curvature.

To map \( q \) onto the film, one can unfold the cylinder into a plane with coordinates \((X, Y) = (D \sin \phi, Y)\) with
the azimuthal angle $\phi \in (-\pi, \pi)$. The relationship is

$$(q_x, q_y, q_z) = \frac{2\pi}{\lambda} \left( D \sin \phi, Y \frac{D \cos \phi - D}{L} \right).$$ \hspace{1cm} (39)

6. PHOTOGRAPHY OF SINGLE CRYSTALLINE SAMPLES

The illustration of Bragg’s law using Ewald’s sphere suggests two ways to make reciprocal lattice points fall on the sphere thus to generate constructive scattering signals from specific crystallographic planes. One is to tune the wavelength and the other is to change the orientation of the sample. These correspond to two experimental strategies in designing photography methods for single crystals – Laue method and rotation method.

6.1. Varying Wavelength at Fixed Angle – Laue Method

In Laue method, one fixes the orientation of the sample (thus the angle $\theta$ in Bragg’s law) and changes the wavelength of incident beam over a certain range $\lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}]$, which is thus called “white color”.

For each pixel $(X, Y)$ on the film, the scattering intensity is thus the sum of contributions from all wavelengths, or equivalently, all scattering vectors $q$, which can be formally written as

$$\bar{I}(X, Y) = \sum_q I(q) = \sum_q \left[ \left| \sum_{i=1}^N \hat{f}_i(q) \cos(q \cdot r_i(\Omega)) \right|^2 + \left| \sum_{i=1}^N \hat{f}_i(q) \sin(q \cdot r_i(\Omega)) \right|^2 \right].$$ \hspace{1cm} (40)

We demonstrate the photography results using perfect SC, BCC and FCC samples. The incident beam is along the [001] direction and the nearest neighbor distance $\sigma$ is set as the unit of length. The code to compute $\bar{I}(X, Y)$ numerically implementing Eq. (40) is provided online. The value of $D$ can be chosen arbitrarily, with all other lengths calculated accordingly, because it only leads to a scaling of the photograph. Here, we set $D = 100\sigma$ for numerical convenience. If the total number of pixels on the film is $N_{XY}$ and the number of wavelengths scanned is $N_{\lambda}$, then the computational complexity using Eq. (40) is $O(N_{XY} N_{\lambda} N)$.

6.2. Varying Angle using Fixed Wavelength – Rotation Method

We use the conventional setup – cylindrical film – to explain the rotation method in the same SC, BCC and FCC crystalline samples as above (Fig. 9). The wavelength $\lambda$ of incident beam is fixed in this method and the sample placed at the central axis of cylinder is rotated by a full circle of $2\pi$ to probe all possible orientations and scattering angle $2\theta$ for given crystallographic planes.

The scattering intensity at coordinates $(X, Y)$ is then

$$\bar{I}(X, Y) = \sum_{\Omega} \left[ \left| \sum_{i=1}^N \hat{f}_i(q) \cos(q \cdot r_i(\Omega)) \right|^2 + \left| \sum_{i=1}^N \hat{f}_i(q) \sin(q \cdot r_i(\Omega)) \right|^2 \right].$$ \hspace{1cm} (41)

where $\Omega$ represents orientation of the sample due to rotation. For a given sample, we apply a rotational matrix about its $y$-axis to transform particle coordinates into new values. The accumulated signal $\bar{I}(X, Y)$ on the cylinder is then unfolded onto a rectangle. If a total number $N_\Omega$ of rotation angles within $(0, 2\pi)$ are scanned, the
FIG. 8. Back-reflection (left column) and transmission (right column) photography of SC (a-b) ($N = 3375$), BCC (c-d) ($N = 4394$) and FCC (e-f) ($N = 5324$) crystals. The range of wavelength $\lambda$ is 0.35-1.0$\sigma$ for SC back-reflection, 0.199-0.35$\sigma$ for SC transmission, 0.4-1.2$\sigma$ for BCC back-reflection, 0.23-0.4$\sigma$ for BCC transmission, 0.5-1.42$\sigma$ for FCC back-reflection and 0.23-0.49$\sigma$ for FCC transmission.

computational complexity to implement Eq. (41) to produce results on $N_{XY}$ pixels is then $O(N_{XY}N_{D}N)$.

6.3. Broadening due to Finite-size Effect

So far we assume that either varying wavelength or varying sample orientation is needed to satisfy Bragg’s
law and produce nonvanishing scattering signals on photograph. However, this is only true for infinitely large systems and in our small samples \((N \sim 10^3)\), signal broadening allows us to observe certain scattering patterns when wavelength \(\lambda\) is fixed at appropriate values.

For example, in the previously mentioned SC crystals, we can see four scattering spots in back-reflection method at fixed wavelength \(\lambda = 0.55\sigma\), which correspond to the (113) planes and alike (Fig. 10). When the system size is varied from \(N = 7^3\) to \(30^3\), the size of each spot decreases.

It can be confirmed that the relationship between box size \(L = \sqrt[3]{N}\) and spot size \(2\delta\theta\) roughly satisfies the Scherrer equation \(2\delta\theta \propto 1/L\). An empirically scaling factor \(\sqrt{2}\) is needed on \(L\) to estimate the actual dimension of the sample perpendicular to (113) planes and to agree with the theoretical slope \(\lambda/\cos\theta\).
6.4. DNA Double Helix

One of the most successful and famous applications of scattering methods is the determination of DNA structure, whose X-ray photography shows a characteristic “X”-shape pattern with horizontal stripes \([27]\). The form of the pattern can be understood analytically by diffraction from the 2D projected sinusoidal waves of the single or double helix \([28] [29]\). Here we produce the transmission photography of a model DNA fiber with only backbone particles. Each helix has \(N = 70\) particles with 10 particles per turn (pitch). The parameters of the right-handed B-DNA, \(3\sigma\) for pitch and \(20\sigma\) for helix diameter, are used (Fig. 11). The unit of length \(\sigma\) can be mapped onto the real length unit \(\AA\).

All the four photographs, with the fiber being single or double strand, 2D projected or 3D stereoscopic, have a “X”-shape pattern at the center and are made of horizontal broken stripes (Fig. 11a). The two branches of the “X” pattern can be viewed as scattering signals from the two series of parallel particles on the sinusoidal wave (Fig. 11b). Because each pitch of the helix has 10 particles, the pattern has a vertical period of 10 stripes \([28]\). The brightness and darkness along each horizontal stripe depends sensitively on the relative position between different particles \([30]\). For example, the level 4 stripe disappears when two double strands with a phase difference of 3/8 pitch are present. The bright level 8 signal of 3D samples at \(X = 0\) is missing for 2D structures.

7. SCATTERING VECTOR \(q\) IN SPECTROSCOPY

In this section, we discuss the choice of scattering vector \(q\) in case of disordered or partially ordered samples that are spatially isotropic or approximately isotropic. When samples are isotropic, the scattering intensity \(I(q)\) or its normalized version, structure factor \(S(q)\), only depends on the magnitude \(q\) of the scattering vector, thus does not generate isolated spotty signals as in photography of ordered samples. The photography \(I(X, Y)\), often of less interest in this context, should ideally exhibit concentric circular patterns. The spectroscopy \(I(q)\) or \(S(q)\) as a function of \(q\) is the primary method used for isotropic samples.

7.1. One Vector \(q\) to Represent Magnitude \(q\) in Isotropic Systems

In experiment, one can vary \(q\) by observing signals at continuously changing scattering angle \(2\theta\) using a fixed incident wavelength \(\lambda\). Because experimental samples are generally large enough, a well-averaged scattering signal can be detected along one particular direction at \(2\theta\), as in powder method with a diffractometer.

For example, consider a polycrystal with \(M\) randomly oriented crystalline grains (domains), each of \(N\) particles. The scattering intensity at \(q\) computed from Eq. (9), assuming \(\hat{f}_i(q) = 1\), is

\[
I(q) = \left[ \sum_{n=1}^{M} \sum_{i=1}^{N} \cos(q \cdot r_{n,i}) \right]^2 + \left[ \sum_{n=1}^{M} \sum_{i=1}^{N} \sin(q \cdot r_{n,i}) \right]^2,
\]

where \(r_{n,i}\) is the position vector of particle \(i\) in grain \(n\). If \(M\) is large and crystalline grains are uniformly oriented in all directions, \(I(q)\) at the particular vector \(q\) can be accurate enough to represent \(I(q)\) at the magnitude \(q\), without averaging over all directions of \(q\). Similar argument applies to bulk liquids or glasses, in which \(I(q)\) is also well self-averaged.

7.2. Random Rotation of a Small Anisotropic Sample

The above method of using a scattering vector \(q\) at one direction to represent that magnitude \(q\) does not work well for simulation samples, which are usually small and anisotropic (single crystal instead of polycrystal). To simulate experimental results, we can fix the direction of the incident ray but randomly rotate the small sample to many orientations. This is done by applying a three-dimensional rotation matrix to the original particle coordinates \(r_i\), whose rotation axis is uniformly distributed on a sphere and rotation angle is uniformly chosen from \([0, 2\pi]\). Then the signal \(I(q)\) in Eq. (12) can be approximated by accumulating intensities from all those orien-
FIG. 11. Transmission photography of single-strand (a,c) and double-strand (b,d) 2D sinusoidal waves (a-b) and 3D DNA helices (c-d) using $\lambda = 1.54\sigma$. Each helix is made of a backbone of $N = 70$ particles with a pitch of $p = 34\sigma$ and a diameter of $20\sigma$. There are 10 particles per pitch. The two helices in the double strand structure is offset by $3/8$ pitch. Particle size in insets is set as $5\sigma$ to enhance visibility.

The positions of these virtual grains generated by rotation do not reflect the absolute positions of grains in the real polycrystal. According to the equivalency of Eq. (9) and Eq. (10), Eq. (43) is an approximation to Eq. (42) by only considering relative positions of particles within each grain $r_i(\Omega) - r_j(\Omega)$. Therefore, the difference between coordinates of particles $i$ and $j$ at two different orientations, $r_i(\Omega) - r_j(\Omega')$, does not affect the result of Eq. (43), but will lead to different and wrong results, if the sum is taken as $\left| \sum_{\Omega} \sum_{i=1}^{N} \cdots \right|^2$.

For small and nearly isotropic liquids or glasses, one can replace random rotations of the sample by averaging over many thermally equilibrated configurations. For
anisotropic systems, however, rotations are needed to sample different directions.

7.3. Scattering Vector \( q \) on a Lattice

An alternative and more convenient way to match experiment in simulation is to fix the sample coordinates and choose \( q \) of a given \( q \) from all directions. It is often suggested to select \( q \) from a 3D orthorhombic lattice, \( q = \Delta q (n_x, n_y, n_z) \), with integers \( n_x, n_y, n_z \) and increment \( \Delta q = \frac{2\pi}{L} \), where \( L \) is the linear dimension of the cubic simulation box \([31]\). The motivation here is that \( L \) sets the maximum periodicity of the simulation sample that is still physically meaningful thus the resolution of \( q \). The integers \( n_x, n_y, n_z \) may be chosen to run from negative to positive values to sample spherically symmetric \( q \)'s, or to start from zero to sample only \( q \)'s on 1/8 of the sphere. At the expense of symmetry and averaging, the latter choice can reach a higher magnitude \( q \) with the same number of lattice points.

There are multiple \( q \)'s on this lattice that correspond to the same magnitude \( q \), from which we can compute an average \( S(q) \). The number of \( q \)'s for a given magnitude \( q \) tends to, but not necessarily, increase with \( q \). For example, in a 2D system with \( q \)'s on a square lattice, there are \( 1, 2, 4, 8 \) \( q \) points on the lattice at magnitude \( q/\Delta q = 0, 1, \sqrt{2}, 2, \sqrt{2}, 3, \sqrt{2}, 4, \sqrt{2}, 5, \sqrt{2}, 6 \) respectively (Fig. [12]). When reporting the result of \( S(q) \), one can assign \( q \)'s into bins of equal size or just use the original \( q \) values visited by the lattice points. In both cases, the \( S(q) \) should be the mean value averaged over all the \( q \)'s at that \( q \).

If the sample is crystalline and \( L \) is an integer multiple of the crystallographic lattice constant \( a \), then the \( q \) lattice contains the reciprocal lattice points of the crystal (subject to a \( 2\pi \) factor difference). If \( L = 5a \) in the above 2D example, then \( q \) points \( \Delta q (0,0), \Delta q (0,5), \Delta q (5,0), \Delta q (5,5) \) correspond to reciprocal lattice points \( (0,0), (1/a,0), (0,1/a), (1/a,1/a) \) respectively (Fig. [12]). These lattice points are where Bragg’s law Eq. [19] are obeyed. Therefore, according to the discussion in Section 3.3, if all atomic form factors are unity, then \( I(q) = |F_{hkl}|^2 = N^2 \) and \( S(q) = N \) at each of these reciprocal lattice points. The spectroscopy result \( S(q) \) needs to be an average over all \( q \) points at that \( q \), some of which are not reciprocal lattice points and thus have \( S(q) = 0 \). For example, at \( q = 5\Delta q \) of the 2D system, two points have \( S(q) = N \) and two have \( S(q) = 0 \). The average \( S(q = 5\Delta q) \) is thus \( (N + N + 0 + 0)/4 = N/2 \) (Fig. [12]).

Using lattice points to approximate \( q \)'s from all directions is problematic, when \( L \) is small and thus increment \( \Delta q \) is large such that only a few \( q \)'s are available at each \( q \). The issue is severer at small \( q \) or towards corners of the cubic lattice at high \( q \). The calculated signal \( S(q) \) can then be quite noisy because \( q \) is not averaged enough over all directions.

![FIG. 12. Scattering vector \( q = \Delta q (n_x, n_y) \) on a square lattice used for a 2D system of box size \( L \). \( q \) points at the same magnitude \( q \) are connected by concentric quarter circles up to \( q = 8\Delta q \). If the system is a crystal of lattice constant \( a = L/5 \), then four points shown in red correspond to reciprocal lattice points.](image)

7.4. Scattering Vector \( q \) on a Sphere and Debye’s Scattering Equation

In order to obtain a smooth curve of \( S(q) \) that better matches experimental results, we need to use enough spherically distributed \( q \)'s. To guarantee uniform distribution of points on a sphere, we apply the Fibonacci grid approach to randomly chose \( N_q \) scattering vectors \( q \)'s from a sphere of radius \( q \) [32]. Increasing \( N_q \) improves the effect of averaging. The complexity to compute \( I(q) \) or \( S(q) \) at each \( q \) is then \( O(N_q N) \).

In the limit of \( N_q \to \infty \), using Eq. [10], we can integrate over all \( q \) directions and then normalize it by the full solid angle of \( 4\pi \) to compute the average \( I(q) \)

\[
I(q) = \frac{1}{4\pi} \int_{|q|=q} dq \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) e^{i\mathbf{q} \cdot \mathbf{r}_{ij}}
= \frac{1}{4\pi} \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin \theta d\theta \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) e^{iqr_{ij}} \cos \theta
= \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{f}_i(q) \hat{f}_j(q) \frac{\sin(qr_{ij})}{qr_{ij}}
\]

This is known as the Debye’s scattering equation [33][34], which can also be viewed as the discrete version of the Fourier transform of radial distribution function \( g(r) \) in Eq. [33]. The computational complexity of Debye’s method is \( O(N^2) \) and it becomes more efficient than numerically sampling \( N_q \) vector \( q \)'s on a sphere when \( N < N_q \).
8. PHOTOGRAPHY AND SPECTROSCOPY OF DISORDERED OR PARTIALLY ORDERED SAMPLES

Although spectroscopy, $I(q)$ or $S(q)$ as a function of $q$, gives most useful structural information about isotropic samples, it is sometimes interesting to show the corresponding photography $I(X,Y)$. In fact, spectroscopy can be obtained from photography by moving along a specific radial direction on the $(X,Y)$ film, as in the early days of powder method.

To generate scattering photograph of isotropic samples, we use the rotation or thermal averaging method in Section 7.2. Spectroscopy curves are calculated using the three methods mentioned in Section 7.3 and Section 7.4.

8.1. Liquids and Glasses

If scattering photograph is taken for disordered samples like liquids or glasses using a fixed wavelength, a characteristic ring signal is expected at $q^* \sim \frac{2\pi}{\sigma}$ that corresponds to the molecular size $\sigma$. This ring is regular and clear, when the sample, like most experimental bulk samples, is large enough such that a good average is taken within the system in the calculation of $I(q)$. However, in a small simulation system ($N = 10^3 -10^4$), photography of one static disordered sample gives spotty and noisy signals with certain traces of ring features (Fig. 13a). To
FIG. 14. Powder method. Transmission photography using fixed wavelength $\lambda = 0.4\sigma$ (a,c,d) and structure factor $S(q)$ (b,d,f) of polycrystalline SC (a-b), BCC (c-d) and FCC (e-f) samples. Miller indices $(hkl)$ are labelled next to each signal peak. The photograph is produced by randomly rotate a single crystalline sample in three dimensions and take average of $I(q)$ over 5000 orientations. The small concentric circular pattern at the center of photograph is due to Fraunhofer diffraction from the small simulation box as a circular obstacle, after being randomly rotated. Three methods are used to compute $S(q)$: with $q$’s on a cubic lattice (green vertical lines), with $q$’s on spheres (blue dotted line) and Debye’s scattering equation (red solid line).

To enhance sharpness of the ring, one can either increase the size $N$ of the sample or take ensemble average of $I(q)$ over many configurations (Fig. 13c).

For homogeneous liquids and glasses, the static structure factor $S(q) = S(q)$ varies only with the magnitude $q$ of the scattering vector and exhibits a major peak at $q^* \sim \frac{2\pi}{\sigma}$. Using $q$’s on a sphere numerically or Debye’s equation can generate well-averaged smooth $S(q)$ curves for liquids or glasses (Fig. 13b,d). If only one disordered configuration is analyzed, the $S(q)$ curve is much more
noisy using \( q \)'s on a cubic lattice (Fig. 13b).

### 8.2. Polycrystalline Samples – Powder Method

Powder method is often used to analyze polycrystals, in which a crystalline sample is ground into powder to produce many small randomly oriented crystalline grains. Then, at the scattering angle \( 2\theta \) where strong signal is expected, at least one of the grains has the correct orientation by chance to meet Bragg’s law. The measured spectroscopy \( S(q) \) can be used to calculate interplanar spacing of the crystal and to further derive the lattice type.

It is difficult to produce a well randomized polycrystalline sample in simulation, given the limit of system size. Nevertheless, we can start from a small single crystal sample and use random rotation or \( q \)'s from different directions to simulate scattering signals of a polycrystal. In particular, we use the same SC, BCC, FCC crystals used above to generate photography and spectroscopy results of corresponding polycrystals (Fig. 14).

The sharp concentric rings in photograph \( I(X,Y) \) and the narrow peaks in \( S(q) \) correspond to scattering from different crystallographic planes \( (hkl) \) of the three crystals, as mentioned in Section 3.3.3. \( S(q) \) peaks computed from spherically distributed \( q \)'s are lower and broader than that from cubic lattice \( q \)'s. The peak height using cubic lattice \( q \)'s often scales with system size \( N \). For example, the SC crystal has \( L = 15\sigma \) and \( N = L^3 = 3375 \) particles. Given \( \Delta q = \frac{2\pi}{15\sigma} \), \( S(q) \) peak from \((001)\) planes is expected to occur at six \( q \) points, \( \Delta q(15,0,0), \Delta q(0,15,0), \Delta q(0,0,15), \Delta q(-15,0,0), \Delta q(0,-15,0), \) and \( \Delta q(0,0,-15) \), each has a value \( S(q) = 3375. \) However, there are other \( q \) points with magnitude \( q = 15\Delta q \), which correspond to integer solutions to \( n_1^2 + n_2^2 + n_3^2 = 15^2 \). In total, at \( q = 15 \), there are 6 \((15,0,0)\)-like (considering its permutation and \( \pm \)), 24 \((12,9,0)\)-like, 24 \((10,10,5)\)-like, 48 \((11,10,2)\)-like, and 48 \((14,5,2)\)-like \( q \) points. Out of these 150 points, only 6 has \( S(q) = N \) while others have \( S(q) = 0 \). So the peak height \( S(q = 15\Delta q) = 3375 \times 6/150 = 135 \).

### 8.3. Mesophases – Small Angle Method

Mesophases are states of matter intermediate between liquids and solids found in block copolymers \[35\], liquid crystals \[36\], structural DNAs \[37\], etc., which present mesoscopic ordering of length scales larger than molecular size \( \sigma \). To detect these long wavelength structures, small angle X-ray scattering (SAXS) \[11\] or small angle neutron scattering (SANS) \[38\] methods are needed because scattering signals are expected at small \( q \) (before the peak \( \sim \frac{2\pi}{3\sigma} \)) thus small \( \theta \) as seen from Eq. \[2\]. A logarithmic scale axis is often set for \( S(q) \) in the structure factor plot because at \( q \to 0 \) the signal scales with system size \( N \) \[39\].

![Fig. 15. Small angle structure factor \( S(q) \) for (a) lamellar, (b) cylindrical and (c) BCC spherical mesophases. Three methods are used to compute \( S(q) \): with \( q \)'s on a cubic lattice (green vertical lines), with \( q \)'s on spheres (blue dotted line) and Debye’s scattering equation (red solid line). Debye’s result of \( S(q) \) of a homogeneous glass, after vertically rescaled to align at \( q \to 0 \), is shown for comparison (black dashed line). Black downward arrows mark signature peaks for each structure. The broad peak at \( 7.5\sigma^{-1} \) corresponds to particle size \( \sigma \). Insets show top/side views of the configurations under consideration. Blue solid line in (c) is Debye’s result of \( S(q) \) for BCC sphere mesophase with one particle per domain, obtained by rescaling the curve of BCC crystal.](image-url)
In the lamellar phase, each period is of length $d = 5\sigma$ consisting of a layer with thickness $3.5\sigma$ and a gap with thickness $1.5\sigma$. We found three peaks of $S(q)$ at one time, two times and three times of $2\pi \approx 1.257\sigma^{-1}$, corresponding to the first, second and third order of Bragg diffraction of the superlattice (Fig. 15). The peak height drops as $q$ increases, and when layer thickness equals to gap thickness, peaks at even multiples of $\frac{2\pi}{\sigma}$ disappear.

The cylindrical phase with a disk thickness $1.8\sigma$ resides on a two dimensional triangular superlattice with lattice constant $5\sigma$. By assigning unit cells in two different ways with interplanar spacing $d_1 = \frac{5\sigma^2}{d} \sigma$ and $d_2 = 2.5\sigma$, we can identify two peaks at $q_1 = \frac{2\pi}{d_1} \approx 1.451\sigma^{-1}$ and $q_2 = \frac{2\pi}{d_2} \approx 2.513\sigma^{-1}$ (Fig. 15). The second order peak around $2q_1 \approx 2.9\sigma^{-1}$ is also visible (not marked).

The spherical phase has spheres of radius $2\sigma$ that pack on a BCC superlattice with a lattice constant $7\sigma$. If each sphere domain has only one particle, the structure factor would be the same as a normal BCC crystal besides a change of unit for $q$. We can obtain $S(q)$ of this one-particle spherical phase by rescaling the $q$ axis of $S(q)$ of the BCC crystal, which has a lattice constant $a = \frac{2\pi}{\sqrt{3}} \sigma$, by a factor of $\frac{7\sqrt{3}}{2} \approx 6.062$. This moves the (110) peak from $7.7\sigma^{-1}$ to $12.7\sigma^{-1}$ (Fig. 15). This helps us to identify that only the peak from (110) planes of the BCC superlattice is sharply distinguishable from the background signals.

9. 2D STRUCTURE FACTOR

For 2D samples or 2D projection of 3D samples, it is sometimes useful to express $S(q)$ as a 2D function of $(q_x, q_y)$ or scattering angles $(\theta_x, \theta_y)$. 2D structure factor $S(q_x, q_y)$ is related to the photography $I(X, Y)$ by converting coordinates $(X, Y)$ on the film into components $(q_x, q_y)$ of the scattering vector using Eq. (36). For 3D structures, the component $q_z$ can be expressed as a function of $q_x$ and $q_y$ for example, in case of transmission method (Eq. (38)),

$$q_z = -\frac{2\pi}{\lambda} (1 - D/L)$$

$$= -\frac{2\pi}{\lambda} \left( 1 - \sqrt{1 - \frac{\lambda^2}{(2\pi)^2} q_x^2 - \frac{\lambda^2}{(2\pi)^2} q_y^2} \right)^2$$

$$= -\frac{2\pi}{\lambda} + \sqrt{\left(\frac{2\pi}{\lambda}\right)^2 - q_x^2 - q_y^2}.$$  \hspace{1cm} (45)

Note that knowing $(q_x, q_y)$ does not uniquely determine $q_z$. The constant $\frac{2\pi}{\lambda}$ still needs to be specified. For small angle scattering with $q_x, q_y \rightarrow 0$, an approximation to set $q_z = 0$ is valid if there is no long range periodicity along the $z$ direction.

We compute $S(q_x, q_y)$ for the cylindrical mesophase in Fig. 15b, whose cylinder axis is aligned with the incident ray in the $z$ direction. We first use $q_z$ calculated from
Eq. (45) with \( \lambda = 0.4\sigma \). Besides the isotropic circular signal corresponding to particle size \( \sigma \), a characteristic hexagonal pattern with six-fold symmetry is observed at small \( q \), which results from the cylinders packed on a 2D triangular lattice. We can identify two sets of spots on the vertices of hexagons—one corresponds to the unit cell with spacing \( d_1 \) and the other corresponds to the unit cell with spacing \( d_2 \) (Fig. 16). The second order peak related to \( d_1 \) and first order peak related to \( d_2 \) forms a hexagon together, while the first peak related to \( d_1 \) is mixed with the Fraunhofer diffraction pattern at smaller \( q \).

If we set \( q_z = 0 \), the \( S(q_x,q_y) \) pattern is approximately the same at small \( q \), with certain degree of enhancement (Fig. 16b). Some of higher order peaks become visible at larger \( q \).

10. CONCLUSION

In this article, we give a comprehensive and coherent review of core concepts about scattering methods used to determine the structure of ordered and disordered samples. Scattering photography and spectroscopy of typical examples are calculated that can be used as benchmarks to compare with. Sample CPU codes are provided on Github at https://github.com/statisticalmechanicsscatter to illustrate the mathematics and algorithms. Accelerating GPU codes that can reduce hours of computation to seconds are also provided for efficient simulation of scattering signals.

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Appendix A: Fourier Transform: Continuous and Discrete

The Fourier transform \( \hat{F}_k \) of a function \( F(r) \) defined continuously in three-dimensional real space of infinite volume is

\[
\hat{F}_k = \int dr F(r) e^{-ik \cdot r},
\]

(A1)

where \( k \) is a wavevector used to extract the spatial periodicity of \( F(r) \). For instance, if \( F(r) \) has a periodic pattern of wavelength \( \lambda \) along the \( x \) axis, i.e., \( F(x, y, z) = F(x + \lambda, y, z) \), then the value of \( \hat{F}_k \) is large for the \( k \) of magnitude \( |k| = 2\pi/\lambda \) pointing to the \( x \) direction, i.e., \( k = (2\pi/\lambda, 0, 0) \). Physically, if \( e^{ik \cdot r} \) is viewed as a plane wave traveling in the \( k \) direction, then \( \hat{F}_k \) would exhibit a peak value, when \( F(r) \) has wave-like properties coherent with \( e^{ik \cdot r} \) such that they add constructively in the integral. In this sense, the Fourier transform Eq. (A1) quantifies the existence and the extent of periodicity corresponding to \( k \) in \( F(r) \).

In general, even if \( F(r) \) is a real function, \( \hat{F}_k \) can be complex. However, if \( F(r) \) is real \((F^*(r) = F(r))\) and even \((F(-r) = F(r))\), i.e., with a symmetry center, its Fourier transform \( \hat{F}_k \) is also real and even, because the conjugate of \( \hat{F}_k \) is

\[
\hat{F}^*_k = \int dr F^*(r)e^{-ik \cdot r} = \int dr F(r)e^{-ik \cdot r} = \hat{F}_{-k}
\]

\[
= \int_{-\infty}^{\infty} dr F(-r)e^{-ik \cdot r} = -\int_{-\infty}^{\infty} dr' F(r')e^{ik \cdot r'}
\]

\[
= \int_{-\infty}^{\infty} dr' F(r')e^{ik \cdot r'} = \hat{F}_k.
\]

(A2)

Here the integration limits for the variable vector \( r \), formally denoted as \( \pm \infty \), are to be understood as for each of its component.

The inverse Fourier transform of \( \hat{F}_k \) is an integral in the wavevector space which gives the original real space function

\[
F(r) = \frac{1}{(2\pi)^3} \int dk \hat{F}_ke^{-ik \cdot r}.
\]

(A3)

This expands \( F(r) \) in terms of an infinite number of periodic basis functions \( e^{-ik \cdot r} \) characterized by different \( k \)’s. The coefficient or contribution of each \( k \) is just the Fourier transform \( \hat{F}_k \). In principle, the collection of all \( \hat{F}_k \)’s contains the entire information about the original function \( F(r) \) such that knowing \( \hat{F}_k \)’s allows us to reconstruct \( F(r) \).

In physical systems, \( F(r) \) is often defined within a finite volume \( V \) and the Fourier transform should be integrated over the region \( V \)

\[
\hat{F}_k = \int_V dr F(r)e^{ik \cdot r}.
\]

(A3)

If such a finite system is of a cubic shape with a linear dimension \( L \), i.e., \( V = L^3 \), then any periodicity or wavelength \( \lambda > L \) is unphysical. This imposes a lower bound, \( 2\pi/L \), on the smallest wavevector to be considered. The inverse Fourier transform Eq. (A2) thus should not vary \( k \) continuously as in an integral, but only take discrete values of \( k \) with increments \( (\Delta k_x, \Delta k_y, \Delta k_z) = (\frac{2\pi}{L}, \frac{2\pi}{L}, \frac{2\pi}{L}) \).

The integral then becomes \([43]\)

\[
F(r) = \frac{1}{(2\pi)^3} \sum_k \hat{F}_k e^{-ik \cdot r} \left(\frac{2\pi}{L}\right)^3 = \frac{1}{V} \sum_k \hat{F}_k e^{-ik \cdot r}.
\]

(A4)

Mathematically, for the Fourier transform Eq. (A1) to exist, the function \( F(r) \) needs to be absolutely integrable. If \( F(r) \) equals to some nonzero constants, or without loss of generality, \( F(r) = 1 \), in order to reconcile the singularity, the result of the Fourier transform is formally written
Appendix B: Direct and Reciprocal Lattices

The position vector \( \mathbf{r} \) of particles or atoms residing on a crystal lattice, the direct lattice, can be expressed as a linear combination,

\[
\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c},
\]

of the (direct) lattice vectors \( \mathbf{a}, \mathbf{b}, \mathbf{c} \), which are basis vectors of the unit cell with volume \( V_{\text{cell}} = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \). Generally, \( \mathbf{a}, \mathbf{b}, \mathbf{c} \) may not be orthogonal to each other and thus \( x, y, z \) are not necessarily the projection of \( \mathbf{r} \) in a Cartesian coordinate system. If particles coincide with lattice points, then \( x, y, z \) are integers; if particles are contained inside the unit cell, their coordinates \( x, y, z \) can be fractions [44].

Particles on regular crystal lattices are situated on different families of parallel crystallographic planes, when viewed from different angles. Such parallel planes are denoted by three integers \((hkl)\), the Miller indices, whose reciprocals are proportional to the intercepts of the planes with the axes of the direct lattice. The spacing or distance, \( d_{hkl} \), between neighboring lattice planes in the family \((hkl)\) is a function of the Miller indices and lattice parameters (Fig. 17). In the special case of orthorhombic lattice,

\[
\frac{1}{d^2_{hkl}} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}.
\]

The reciprocal lattice is defined mathematically in a space spanned by the reciprocal lattice vectors \( \mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^* \), which are related to the direct lattice vectors by

\[
\mathbf{a}^* = (\mathbf{b} \times \mathbf{c})/V_{\text{cell}}
\]
\[
\mathbf{b}^* = (\mathbf{c} \times \mathbf{a})/V_{\text{cell}}
\]
\[
\mathbf{c}^* = (\mathbf{a} \times \mathbf{b})/V_{\text{cell}}
\]

It is straightforward to verify that, \( \mathbf{a}^* \) is orthogonal to \( \mathbf{b}, \mathbf{c} \), \( \mathbf{b}^* \) is orthogonal to \( \mathbf{a}, \mathbf{c} \) and \( \mathbf{c}^* \) is orthogonal to \( \mathbf{a}, \mathbf{b} \), i.e.

\[
\mathbf{a}^* \cdot \mathbf{a} = 1, \quad \mathbf{a}^* \cdot \mathbf{b} = 0, \quad \mathbf{a}^* \cdot \mathbf{c} = 0, \quad \text{etc.}
\]

Note that, in general, \( \mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^* \) are not orthogonal to each other. Positions of reciprocal lattice points can be represented by vectors of the form

\[
\mathbf{d}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*
\]

where \( h, k, l \) are integers (Fig. 17).

In crystallography, as the notation here implies, the physical meaning of the reciprocal lattice is related to lattice planes in the direct space as follows [44]:

- Each point with a vector \( \mathbf{d}_{hkl}^* \) on the reciprocal lattice represents a family of lattice planes with Miller indices \((hkl)\);
- The direction of \( \mathbf{d}_{hkl}^* \) is perpendicular to (or normal to) the lattice planes \((hkl)\);
- The magnitude of \( |\mathbf{d}_{hkl}^*| \) equals to the reciprocal of the interplanar spacing \( d_{hkl} \), i.e. \( |\mathbf{d}_{hkl}^*| = 1/d_{hkl} \).
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