Intorduction to Pair Distribution Function

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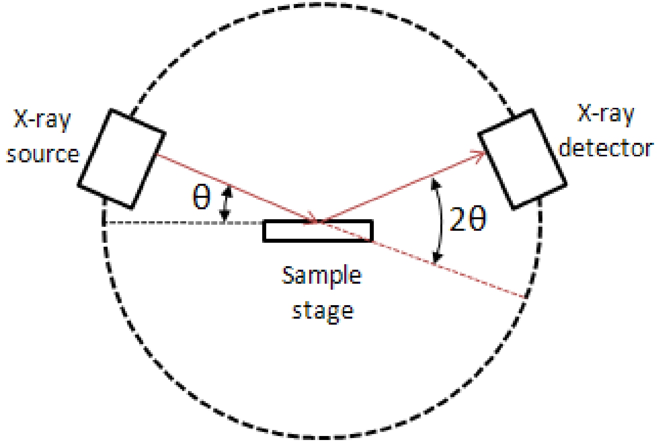
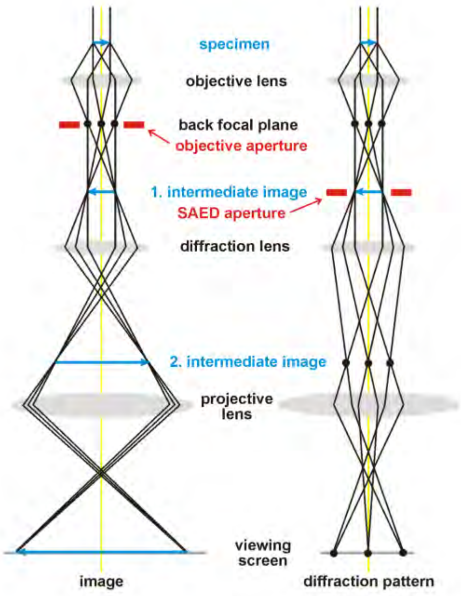
Vocabulary

- $S(Q)$ - Structure Function
- $F(Q)$ - Reduced Structure Function
- $G(r)$ - Reduced pair distribution function
- $g(r)$ - Pair distribution function

Specimen → Pattern





$$F_{hkl} = \sum_{j=1}^{n} f_j\, e^{2\pi i[hx+ky+lz]}$$

$$\left(\frac{d\sigma}{d\Omega}\right) \alpha\ |F_{hkl}|^2$$

$$I_{obs} = I_0 N\, \Delta\Omega \left(\frac{d\sigma}{d\Omega}\right)$$

$$I_{obs}\, \alpha\ |F_{hkl}|^2$$

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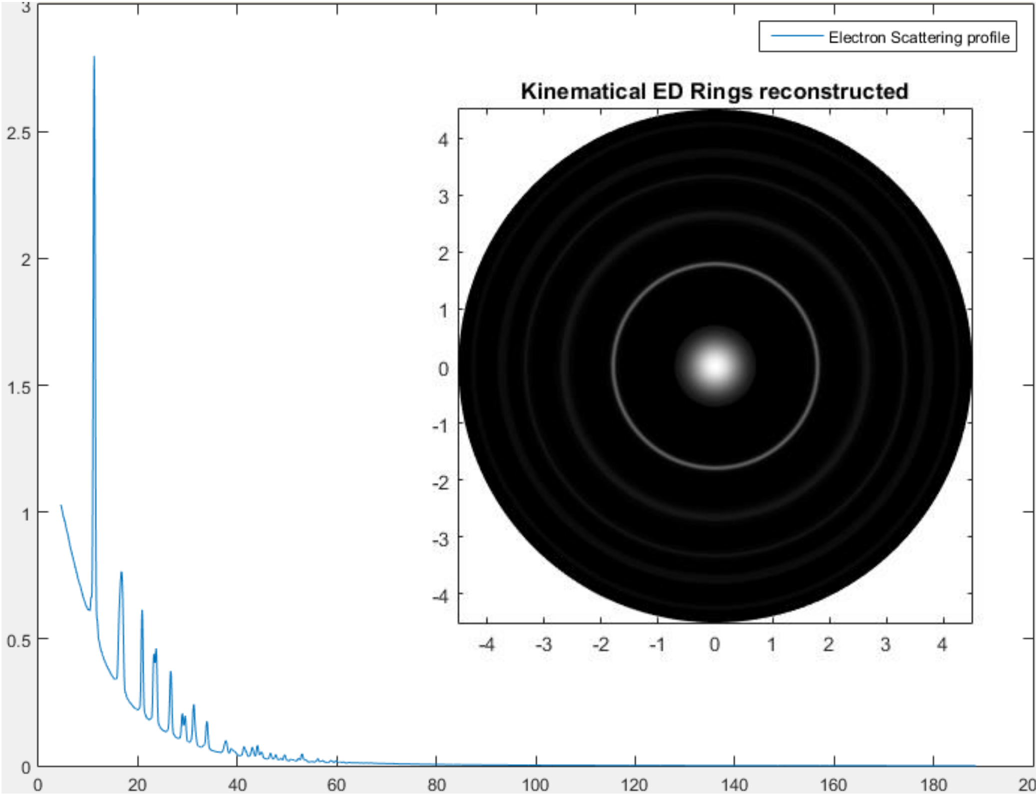
Pattern ⟶ PDF

$$S(Q) = 1 + \frac{\boldsymbol{I(Q)} - \langle f^2(Q) \rangle_{composition}}{\langle f(Q) \rangle^2_{composition}}$$

$$F(Q) = Q[S(Q) - 1]$$

$$G(r) = \frac{2}{\pi}\int_0^\infty F(Q)\sin(Qr)dQ$$

$$g(r) = \gamma(r) + \frac{G(r)}{4\pi\rho_0 r}$$



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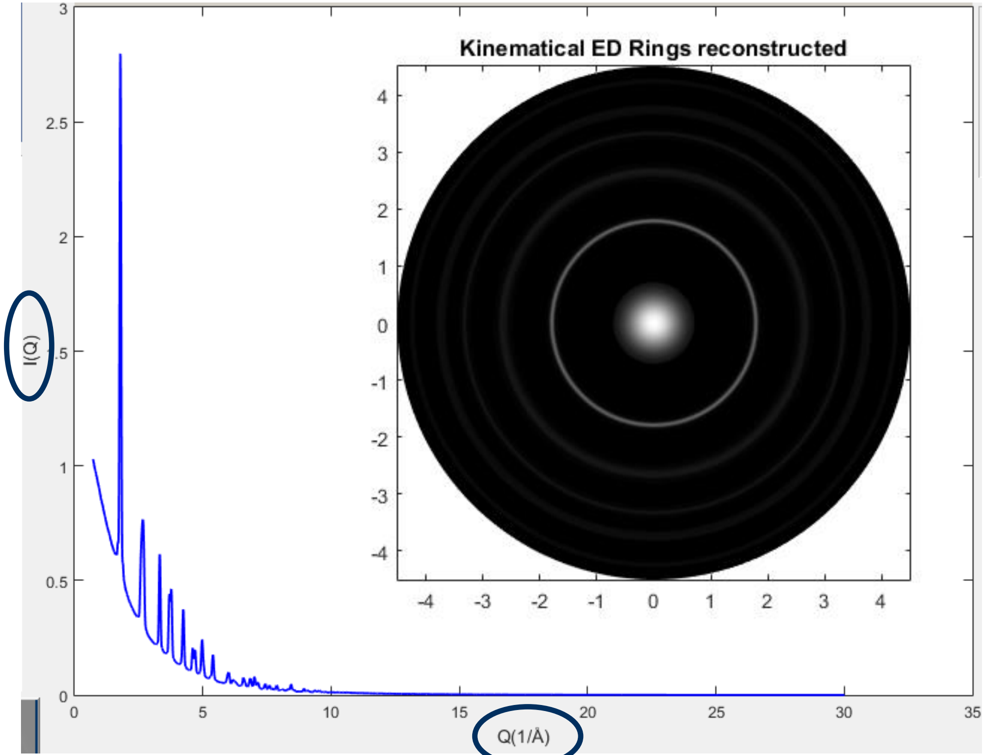

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Pattern ⟹ PDF

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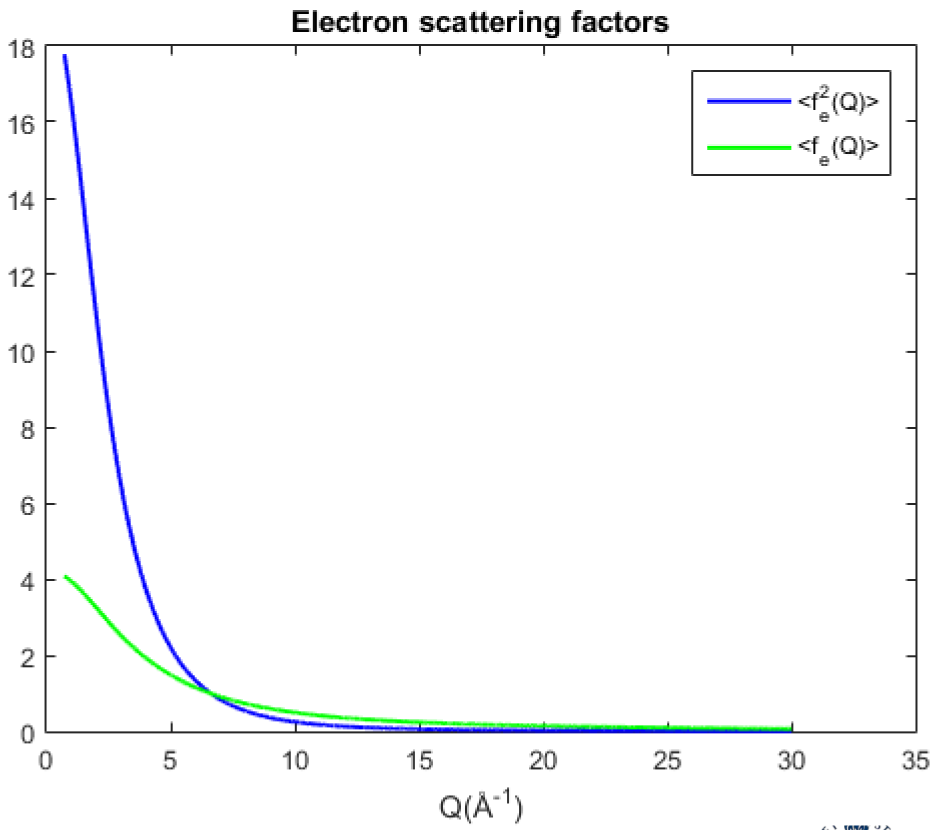

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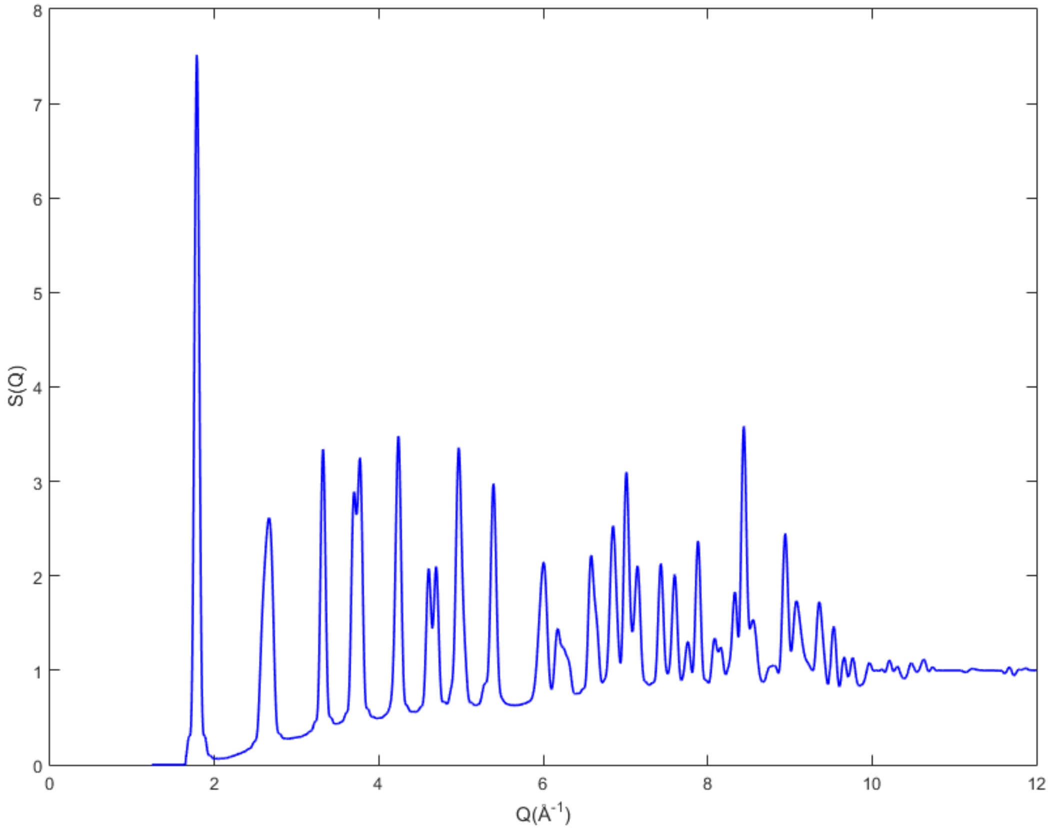

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Pattern → PDF

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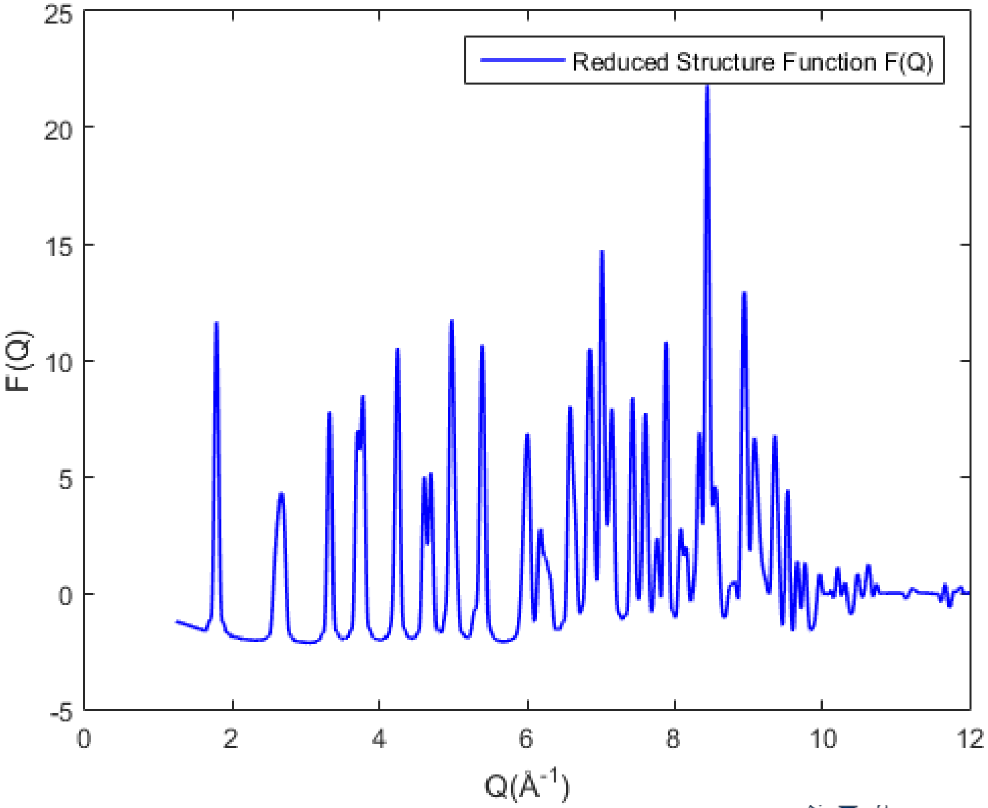

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Pattern ⟹ PDF

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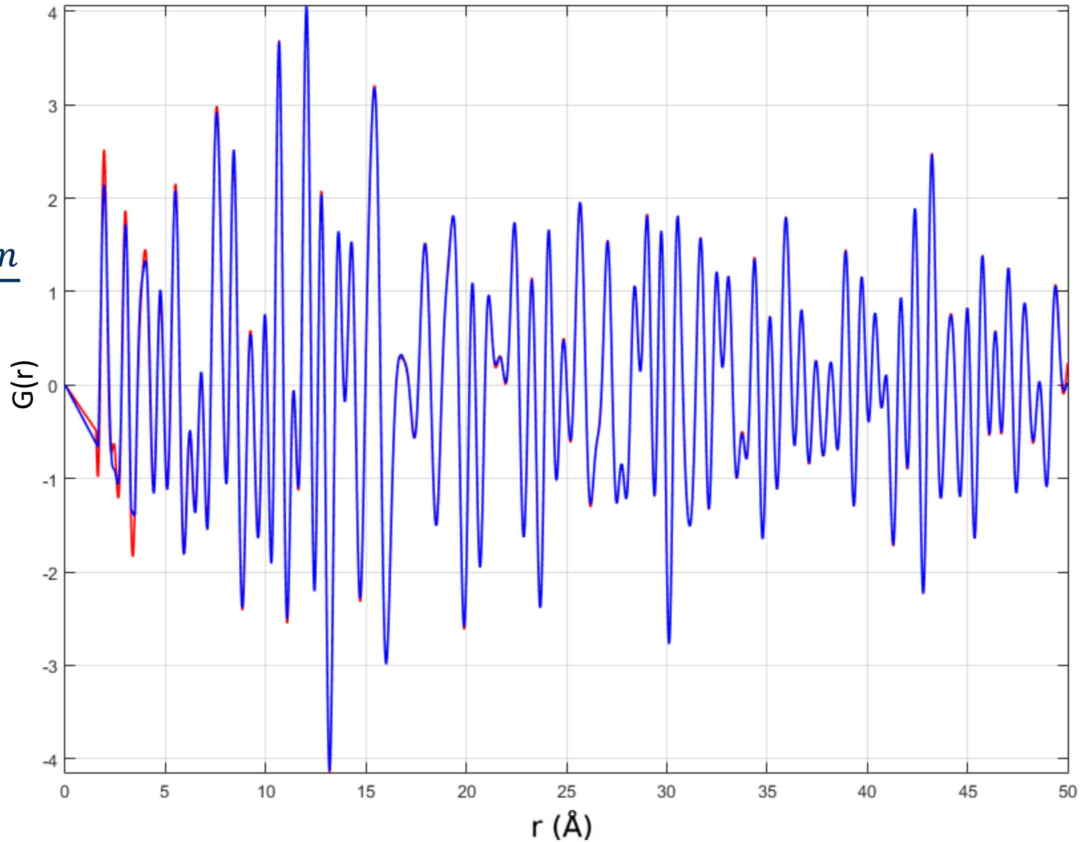

Terban, Maxwell W., Billinge, Simon J. L., Structural Analysis of Molecular Materials Using the Pair Distribution Function, doi: 10.1021/acs.chemrev.1c00237

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Reading ePDF

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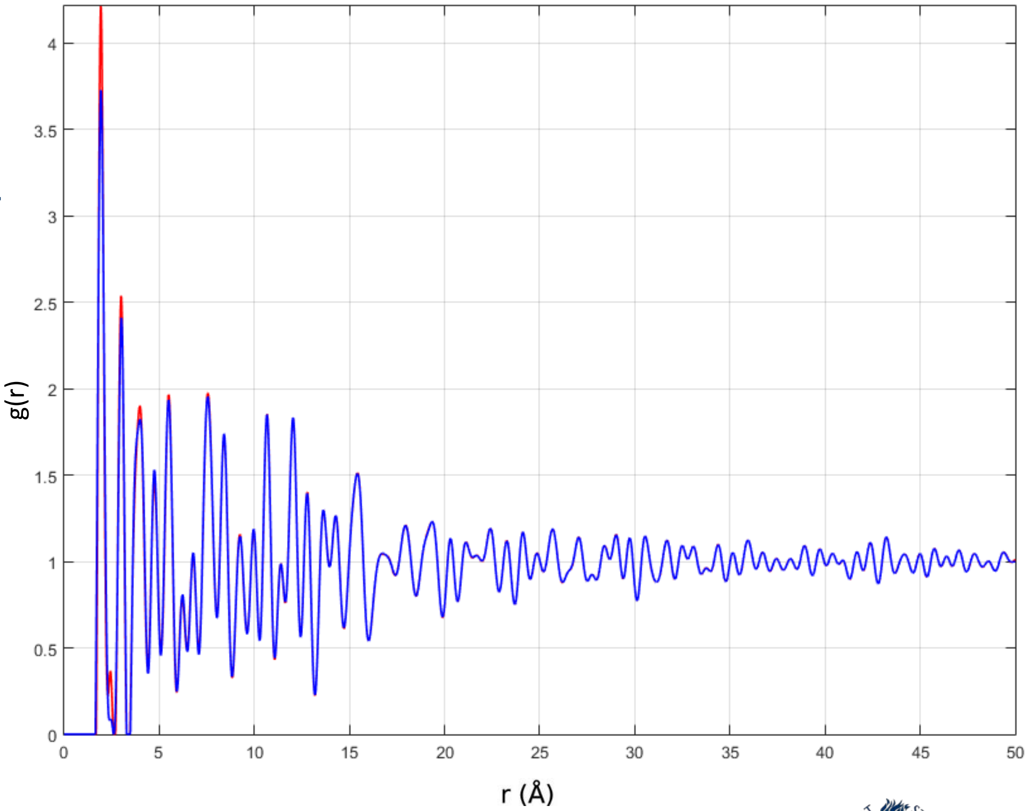

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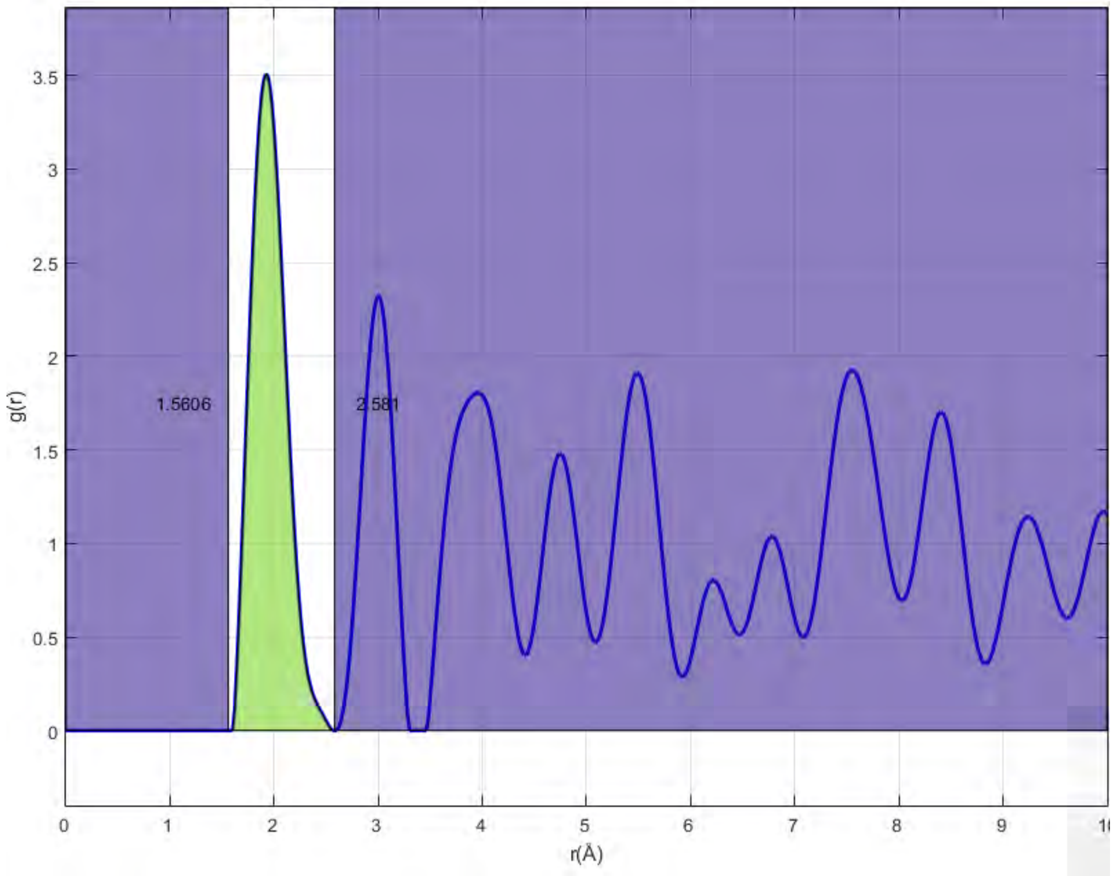
Reading ePDF



$$N_{Coord} = \int_{r_1}^{r_2} R(r)dr$$

$$= \int_{r_1}^{r_2} 4\pi\rho_0 r^2 g(r)dr$$

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Summary

- PDF – “FT of scattering intensity”
- No Phase
- Interatomic distances/bond lengths
- Disorder
- Coordination number
- Particle size

Thank you for the attention!

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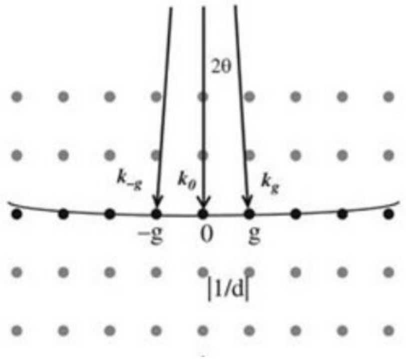
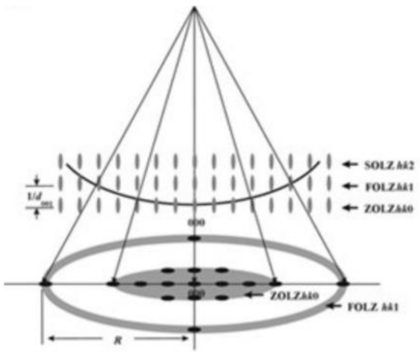
Few notes

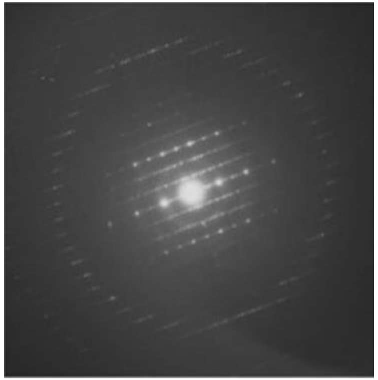
- Electron scattering factors - softwares
- Calibration according to known distance
- Subtract background
- Correct S(Q) tail (oscilation around 1)
- Nanoparticle form factor (in the softwares for simple ones) – bulk: unity

Sample ⟶ Pattern

Source ➔ Specimen ➔ **Diffraction**







- g - 0 = **Q** (scattering vector)

Zou, Xiaodong. - Electron crystallography : electron microscopy and electron diffraction / Xiaodong Zou, Sven Hovmöller, Peter Oleynikov. - 2011. - ISBN: 978-0-19-958020-0

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Non Math

- $f(r;Q_{min}) = \left(\frac{2}{\pi}\right)\int_{Q_{min}}^{\infty} F(Q)\sin(Qr)\mathrm{d}Q;$
- $f(r;Q_{min}) = 4\pi r\rho(r) - \left(\frac{2}{\pi}\right)\int_{0}^{Q_{min}} F(Q)\sin(Qr)\mathrm{d}Q;$
- $f(r;Q_{min}) = 4\pi r\rho(r) - L(r);\qquad L(r) = 4\pi r\rho_0\gamma_0(r);\ \ \gamma_0(r) = \left(\frac{1}{V}\right)\int s(r')\,s(r'+r)\mathrm{d}r'$
- $f(r;Q_{min}) = G'(r) = 4\pi r\left[\rho_{obj.} - \rho_0\gamma_0(r)\right] \rightarrow$ generalized reducedPDF
  - $F(Q) = Q[S(Q)\ - 1]$
  - Only true when small angle scattering below Q_{min} and all wide-andle diff. is above Q_{min}.
- *sdfs*
- In reality:
  - $(\frac{R(r)}{r} = (\frac{2}{\pi})\int_{0}^{\infty} F(Q)\sin(Qr)\mathrm{d}Q)$

Non Math

- Intensity observed
- $I_T = I_C + I_{IC} + I_{MC} + I_{BG}$
    - Coherent + incoherent + multiple + background
  - Correct for seccondary reffects
  - Num reproduce normalized intensity using a struct. Model
    - It is like fitting (kind of)

Non Math

- $G(r) = (\frac{2}{\pi}) \int_0^\infty F(Q)\sin(Qr)\mathrm{d}Q$
  - $F(Q) = Q[S(Q) \ - 1]$
  - Only true when small angle scattering below Q_{min} and all wide-andle diff. is above Q_{min}.
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- In reality:
  - $(\frac{R(r)}{r} = (\frac{2}{\pi}) \int_0^\infty F(Q)\sin(Qr)\mathrm{d}Q)$