Elastic scattering from atomic aggregates
Part 1

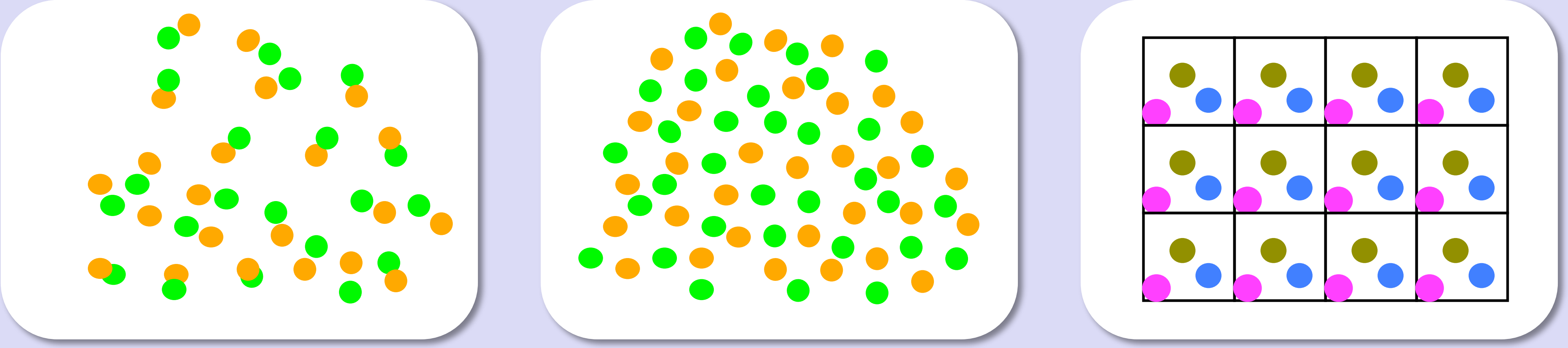
- Atomic aggregates
- X-ray scattering from molecules, Debye formula
- X-ray scattering from non-crystalline materials
- X-ray scattering from crystals
- Synchrotron Radiation and diffraction
- Neutron scattering

Paolo Fornasini
University of Trento
April 2017

Atomic aggregates

Crystalline and non-crystalline materials

Paolo
Fornasini
Univ. Trento



Randomly oriented systems of small size

Molecules in gas phase
Microcrystals

Short-range order

No long-range order

Liquids and non-crystalline solids

Statistical short-range order

No long-range order

Crystalline solids

Short-range order

Long-range order

X-rays, neutron, electrons

Atomic form factors

$$\boxed{f_{\mathrm{a}}\left(\vec{K}\right) =} \begin{cases} \boxed{f_{\mathrm{X}}\left(\vec{K},Z\right) = r_e\, f_0\left(\vec{K},Z\right)} & \text{X-rays} \\[2ex] \boxed{f_{\mathrm{el}}\left(\vec{K},Z\right) = \dfrac{me^2}{2\pi\hbar^2\varepsilon_0}\,\dfrac{Z - f_0\left(\vec{K},Z\right)}{K^2}} & \text{electrons} \\[2ex] \boxed{b_{\mathrm{coh}}(Z)} & \text{neutrons} \end{cases}$$

(neglecting atomic vibrations: zero point + thermal)

Atomic vibrations (zero point + thermal)

Probability density for nuclear positions $w(\vec{r})$

Thermal factor = FT of $w(\vec{r})$

$$f_T(\vec{K}) = \int w(\vec{r})\ \exp(i\vec{K}\cdot\vec{r})\, dV$$

Resultant electron density

$$\rho_T(\vec{r}) = \rho(\vec{r}) * w(\vec{r}) = \int \rho(\vec{r}-\vec{r}\,')\, w(\vec{r}\,')\, dV$$

Atomic thermal factor

$$f_{a,T}(\vec{K}) = f_a(\vec{K})\ f_T(\vec{K})$$

For isotropic harmonic vibrations:

Gaussian
probability density

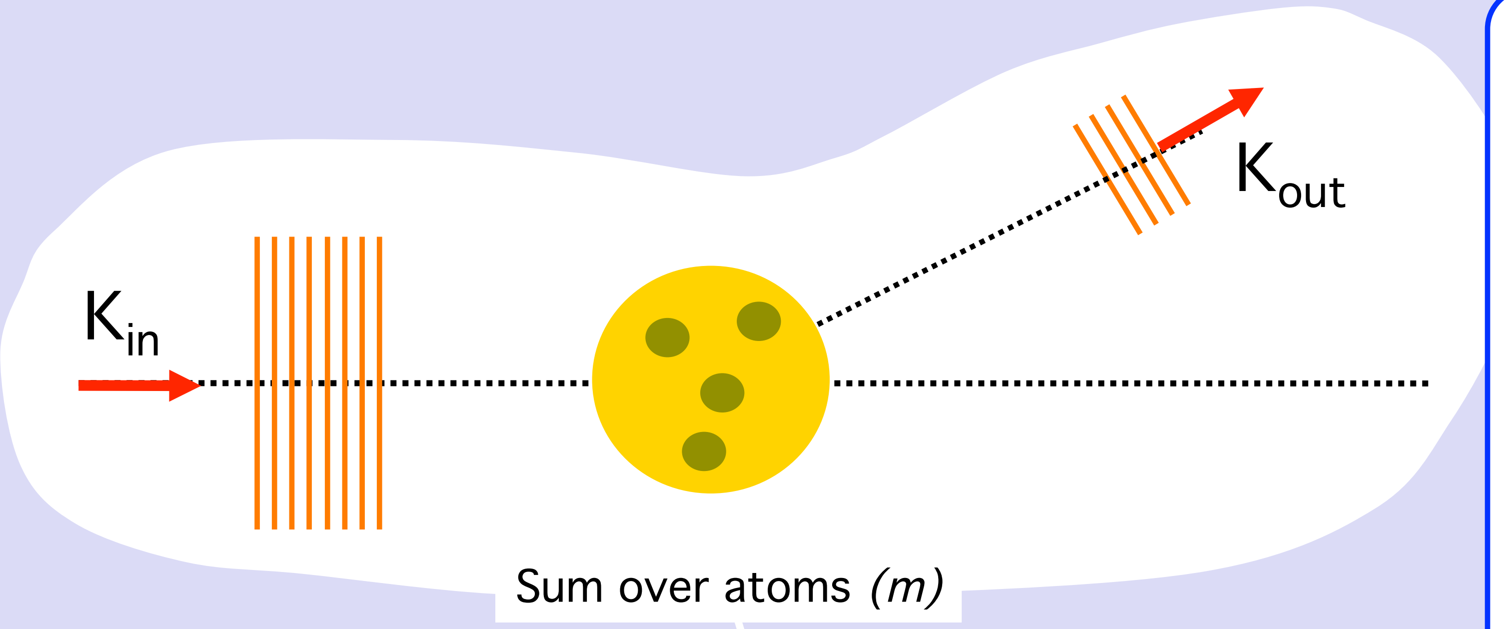
$$w(\vec{r}) = \frac{1}{\left[2\pi\langle u^2\rangle\right]^{3/2}} \exp\left[\frac{-r^2}{2\langle u^2\rangle}\right]$$

Thermal factor:
exponential damping

$$f_T(\vec{K}) = \exp\left[-K^2\langle u^2\rangle/2\right]$$

Scattering amplitude

Paolo
Fornasini
Univ. Trento

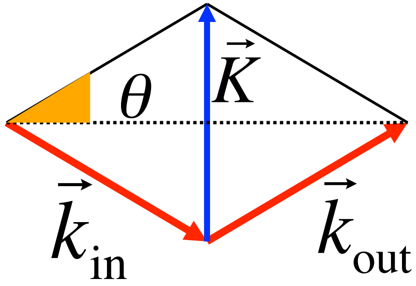


Sum over atoms *(m)*

Scattering vector

$$\vec{K} = \vec{k}_{out} - \vec{k}_{in}$$

$$\left|\vec{K}\right| = 4\pi \frac{\sin\theta}{\lambda}$$



Amplitude $A_{e.u.}\left(\vec{K}\right) = \sum_m f_m\left(\vec{K}\right) e^{i\vec{K}\cdot\vec{r}_m}$

Interference !

X-rays

General formula

X-rays

Intensity

$$I_{\text{e.u.}}\left(\vec{K}\right) = \left|A_{\text{e.u.}}\right|^2 = A_{\text{e.u.}}A^*_{\text{e.u.}}$$

$$= \left(\sum_m f_m\left(\vec{K}\right)e^{i\vec{K}\cdot\vec{r}_m}\right)\left(\sum_n f_n^*\left(\vec{K}\right)e^{-i\vec{K}\cdot\vec{r}_n}\right)$$

$$= \sum_{m=1}^{N}\sum_{n=1}^{N} f_m\left(\vec{K}\right)f_n^*\left(\vec{K}\right)\, e^{i\vec{K}\cdot\vec{R}_{mn}}$$

$$f_m(\vec{K},Z) = f_0(\vec{K},Z)\ f_T(\vec{K})$$

(including the thermal factors)

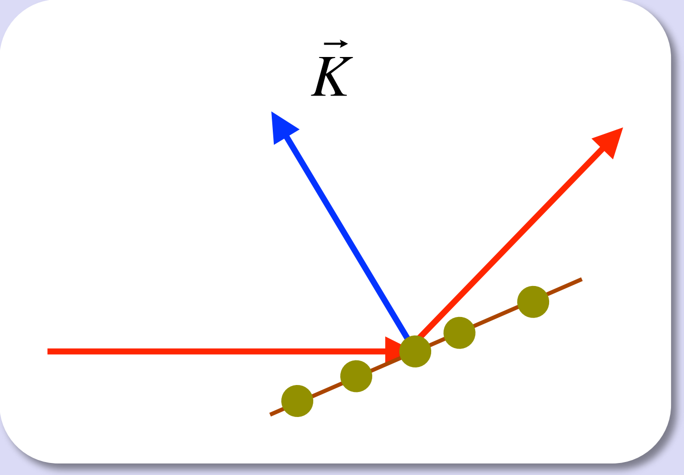
$$\vec{R}_{mn} = \vec{r}_m - \vec{r}_n$$

Inter-atomic distances
(including m=n)

Planar atomic distribution

X-rays

N atoms of the same species



$$I_{\text{e.u.}}(\vec K) = \left(\sum_{m=1}^{N} f(\vec K)\, e^{i\vec K\cdot\vec r_m}\right)\left(\sum_{n=1}^{N} f(\vec K)\, e^{-i\vec K\cdot\vec r_n}\right)$$

$$= N\left|f(\vec K)\right|^2 + \left|f(\vec K)\right|^2 \sum_{m=1}^{N}\sum_{n\neq m}\exp\left(i\vec K\cdot\vec R_{mn}\right)$$

$$= N\left|f(\vec K)\right|^2 + \left|f(\vec K)\right|^2 \sum_{m=1}^{N}\sum_{n\neq m}\left[\cos\left(\vec K\cdot\vec R_{mn}\right) + \cancel{i\sin\left(\vec K\cdot\vec R_{mn}\right)}\right]$$

$$= N\left|f(\vec K)\right|^2 + \left|f(\vec K)\right|^2 \sum_{m=1}^{N}\sum_{n\neq m}\cos\left(\vec K\cdot\vec R_{mn}\right)$$

$$R_{mn} = -R_{nm}$$

N independent terms

N(N-1) interference terms

Max for specular reflection

$$\vec K \perp \vec R_{mn}$$

$$\cos\left(\vec K\cdot\vec R_{mn}\right) = 1$$

$$I_{\text{e.u.}}(\vec K) = N^2\left|f(\vec K)\right|^2$$

X-rays .vs. neutrons

Paolo
Fornasini
Univ. Trento

X-rays

including the thermal factors

$$f_m(\vec{K},Z) = f_0(\vec{K},Z)\; f_T(\vec{K})$$

$$\frac{d\sigma}{d\Omega} = r_e^2 \sum_m \sum_n f_m\left(\vec{K}\right) f_n^*\left(\vec{K}\right) e^{i\vec{K}\cdot\vec{R}_{mn}}$$

m,n = atomic sites & atomic species

Thermal neutrons

without thermal factors

$$\frac{d\sigma}{d\Omega} = \sum_m \sum_n b_m b_n^* \; e^{i\vec{K}\cdot\vec{R}_{mn}}$$

including thermal factors

$$\frac{d\sigma}{d\Omega} = \sum_m \sum_n b_m f_{T,m}(\vec{K}) b_n^* f_{T,n}^*(\vec{K})\; e^{i\vec{K}\cdot\vec{R}_{mn}}$$

m,n = atomic sites, isotopes, spins

$$\vec{R}_{mn} = \vec{r}_m - \vec{r}_n$$

3 types of atomic aggregates

$$I_{\mathrm{e.u.}}\left(\vec K\right) = \sum_m \sum_n f_m\left(\vec K\right) f_n^*\left(\vec K\right) e^{i\vec K\cdot\vec R_{mn}}$$

$$\vec R_{mn} = \vec r_m - \vec r_n$$

Randomly oriented systems of small size

$$I_{\mathrm{e.u.}}\left(\vec K\right) = \sum_{m,n} f_m f_n^* \frac{\sin\left(KR_{mn}\right)}{KR_{mn}}$$

Debye scattering formula

Crystalline solids

$$I_{\mathrm{e.u.}}\left(\vec K\right) = \prod_{i=1}^{3} \frac{\sin^2\left(N_i\vec K\cdot\vec a_i/2\right)}{\sin^2\left(\vec K\cdot\vec a_i/2\right)} \quad \left|F\left(\vec K\right)\right|^2$$

Laue interference function

Structure factor

Liquids and non-crystalline solids

$$I_{\mathrm{e.u.}}\left(\vec K\right) = N\left|f(K)\right|^2 + N\left|f(K)\right|^2 \int_0^\infty 4\pi r^2\left[\rho(r)-\rho_0\right]\frac{\sin Kr}{Kr}\,dr$$

X-rays

- X-ray scattering from small atomic aggregates (molecules, nano-clusters...)

Systems of small size

X-rays

Scattering amplitude

$$A_{\text{e.u.}}\left(\vec{K}\right) = \sum_m f_m(\vec{K})\; e^{i\vec{K}\cdot\vec{r}_m}$$

Scattering intensity

$$\begin{aligned}
I_{\text{e.u.}}\left(\vec{K}\right) &= \left[\sum_m f_m\left(\vec{K}\right) e^{i\vec{K}\cdot\vec{r}_m}\right]\left[\sum_n f_n^*\left(\vec{K}\right) e^{-i\vec{K}\cdot\vec{r}_n}\right] \\
&= \sum_m \left|f_m\left(\vec{K}\right)\right|^2 + \sum_m \sum_{n\neq m} f_m\left(\vec{K}\right) f_n^*\left(\vec{K}\right) e^{i\vec{K}\cdot\vec{R}_{mn}} \\
&= \sum_m \left|f_m\left(\vec{K}\right)\right|^2 + \sum_m \sum_{n\neq m} f_m\left(\vec{K}\right) f_n^*\left(\vec{K}\right) \cos(\vec{K}\cdot\vec{R}_{mn})
\end{aligned}$$

Independent scattering

Interference:
N(N-1) terms

for small systems
it can be calculated

Randomly oriented systems of small size

Random orientation of the molecule

$$I_{\mathrm{e.u.}}(K) \;=\; \sum_m f_m^2(K) \;+\; \sum_m \sum_{n\neq m} f_m(K)\, f_n(K)\, \left\langle e^{\mathrm{i}\vec{K}\cdot\vec{R}_{mn}} \right\rangle$$

Spherical symmetry around each atom

$$\left\langle e^{i\vec{K}\cdot\vec{R}_{mn}} \right\rangle = \frac{\sin(KR_{mn})}{KR_{mn}}$$

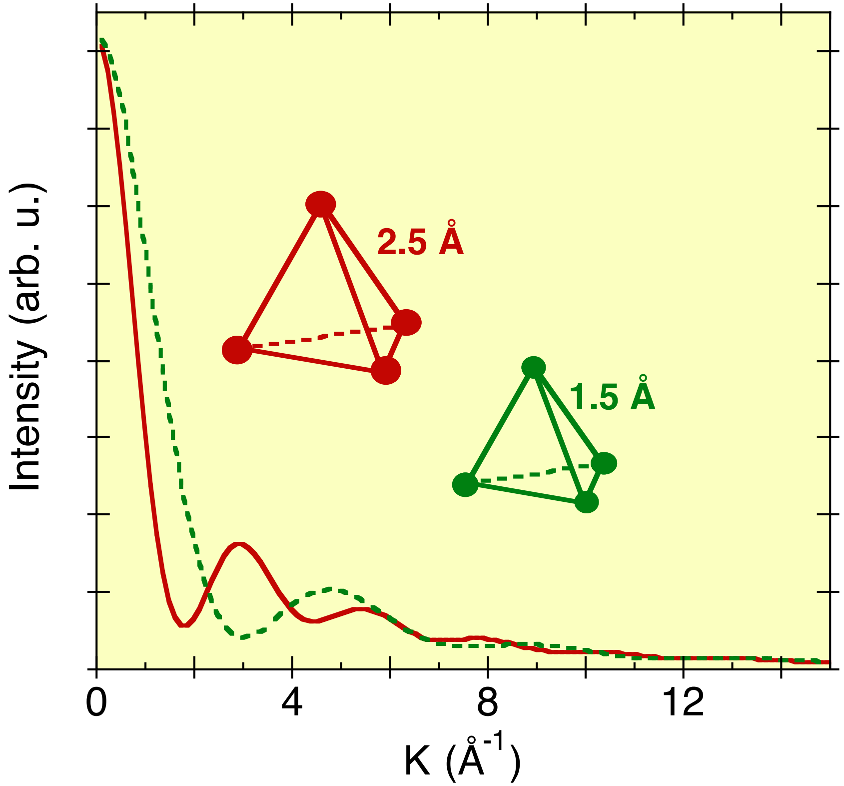
$$I_{\mathrm{e.u.}}(K) \;=\; \sum_m f_m^2(K) \;+\; \sum_m \sum_{n\neq m} f_m(K)\, f_n(K)\, \frac{\sin(KR_{mn})}{KR_{mn}}$$

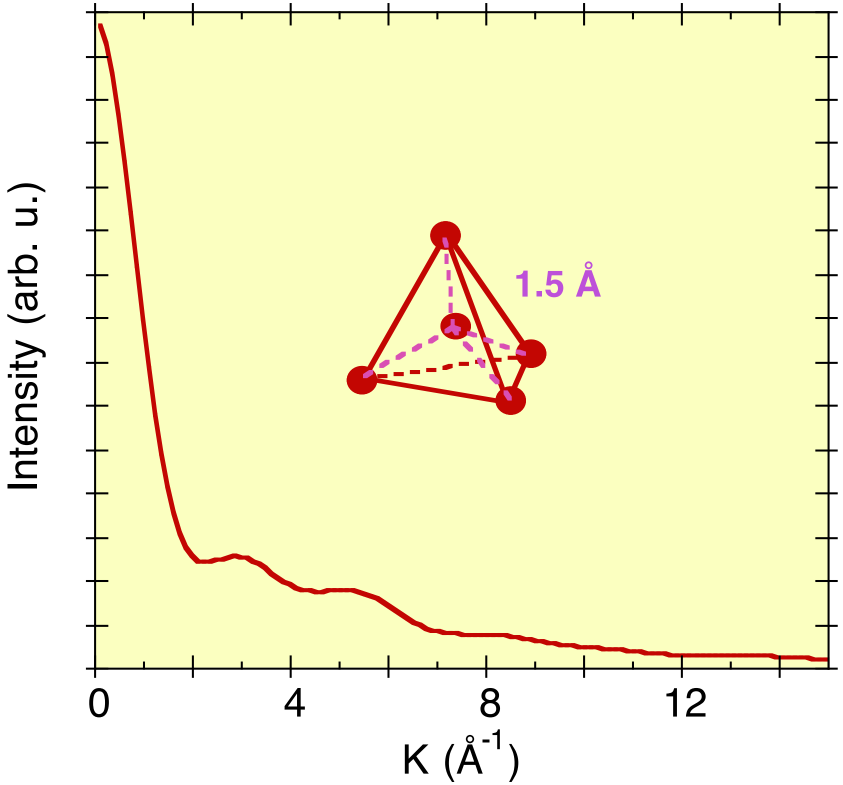
Debye scattering formula
for 1 molecule (1915)

Example 1: system with one atomic species

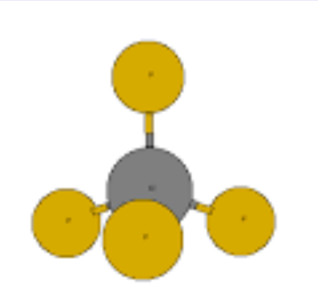
$$I_{\mathrm{e.u.}}(K) \;=\; f^2(K)\;\left[N + \sum_m \sum_{n\neq m} \frac{\sin(KR_{mn})}{KR_{mn}}\right]$$

Example: randomly oriented tetrahedral molecule





Example 2: CF_4 molecule (a)

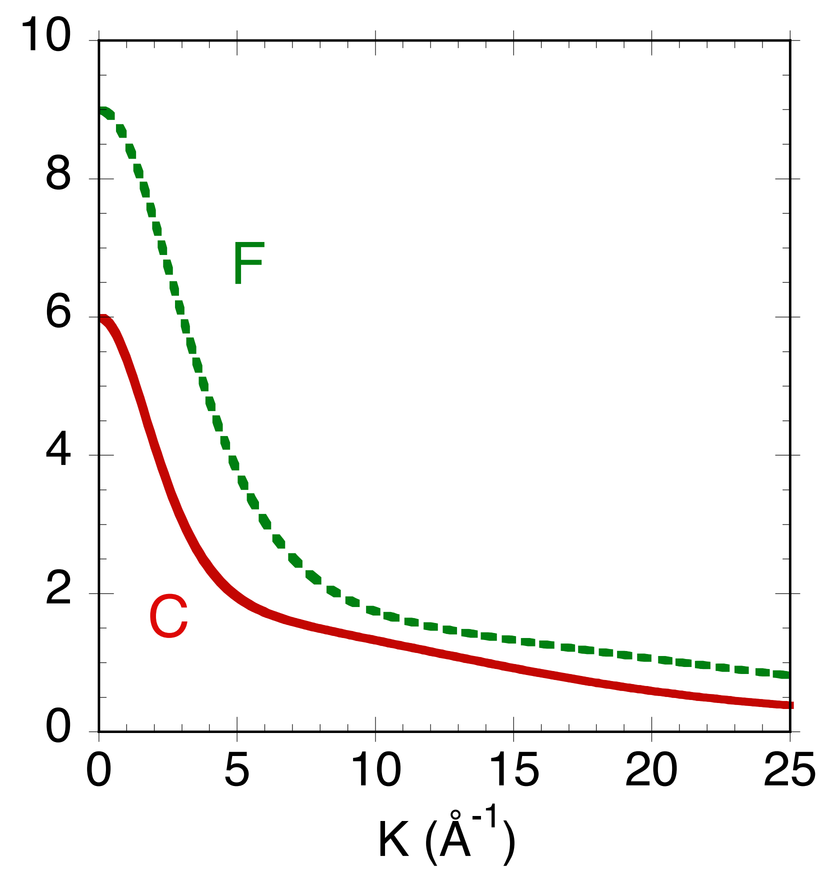


5 independent scattering terms

4 C-F distances = 1.32 Å

6 F-F distances = 2.15 Å

Atomic scattering factors



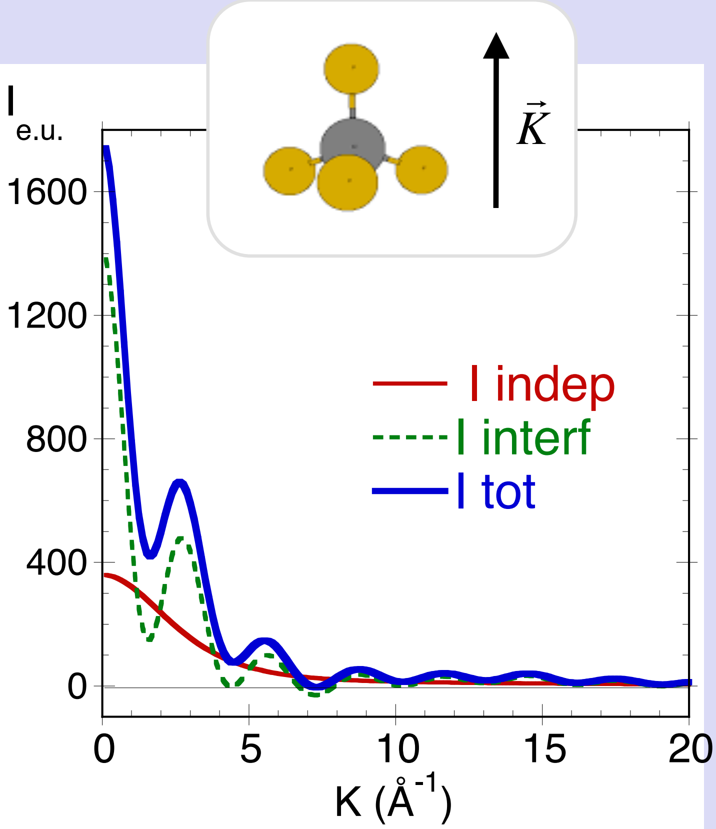
Example 2: CF$_4$ molecule (b)

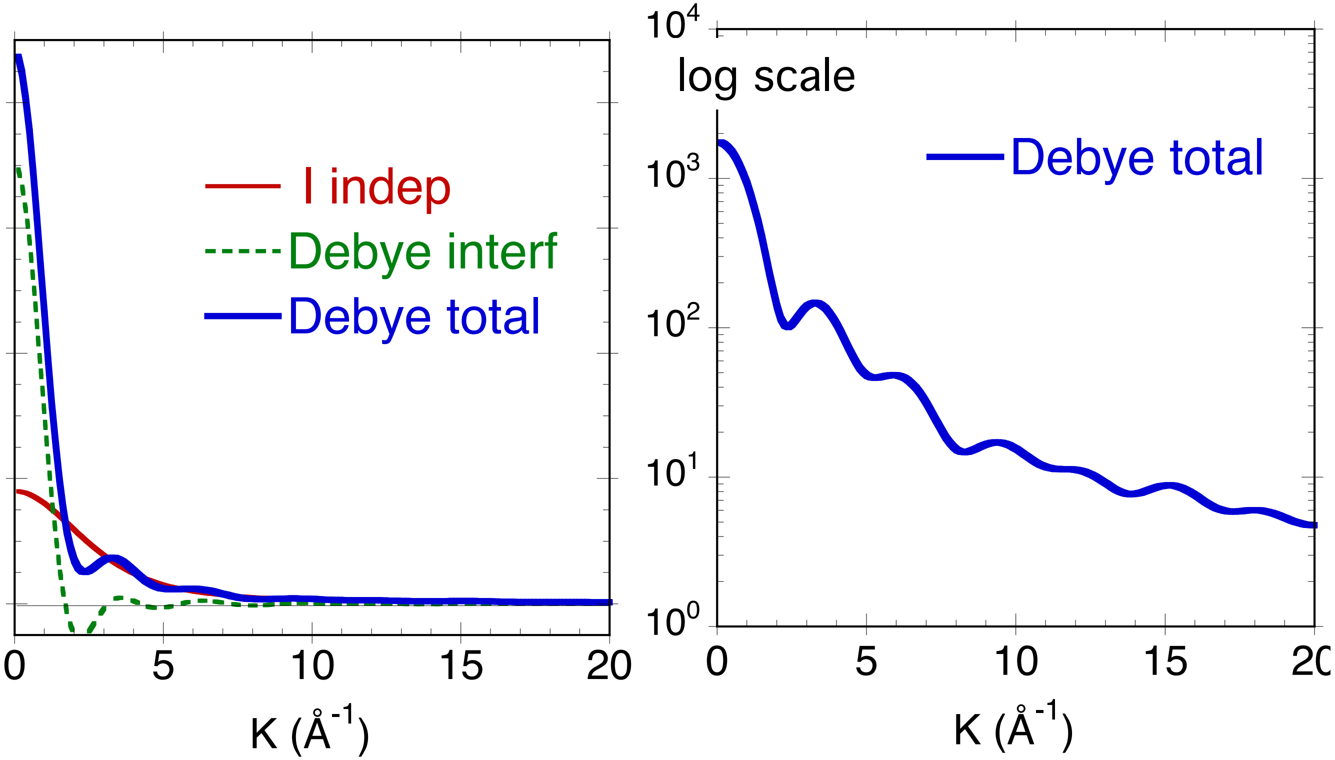
$$I_{\text{e.u.}}\left(\vec{K}\right) = \sum_{m} f_m^2\left(\vec{K}\right) + \sum_{\substack{m \\ n\neq m}} f_m\left(\vec{K}\right) f_n\left(\vec{K}\right) \cos(\vec{K}\cdot\vec{R}_{mn})$$

$$I_{\text{e.u.}}\left(K\right) = \sum_{m} f_m^2\left(K\right) + \sum_{\substack{m \\ n\neq m}} f_m\left(K\right) f_n\left(K\right) \frac{\sin(KR_{mn})}{KR_{mn}}$$

Oriented molecule

Random orientation
Debye equation





Example 2: CF_4 molecule (c)

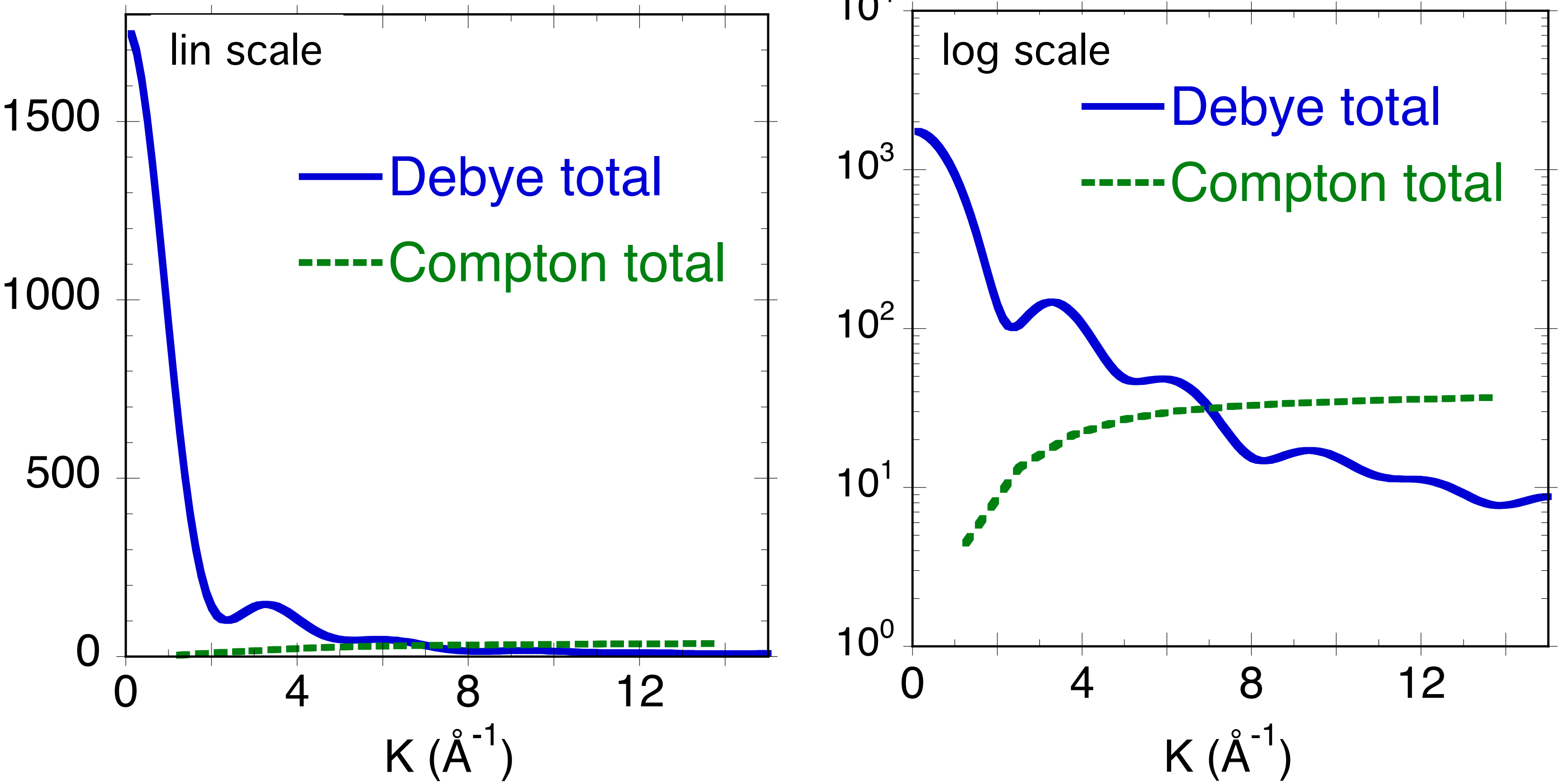
Elastic .vs. inelastic scattering

Debye

$$I_{\text{e.u.}}(K) = \sum_m f_m^2(K) + \sum_{\substack{m \\ n \neq m}} f_m(K) f_n(K) \frac{\sin(KR_{mn})}{KR_{mn}}$$

Compton

$$I_{\text{mod}}(\vec{K}) = Z - \sum_{n=1}^{Z} |f_n|^2$$



Debye formula - comments

- The Debye formula for one molecule has to be multiplied by the number of molecules of the gas
- Experimental intensities include the Compton contribution (standard detectors don't discriminate energy)
- The Debye formula gives only 1-dim info (on inter-atomic distances)
- The Debye formula directly connects the 1-dim structural info to the scattering intensity (by sin-transform)
- Information accuracy increases by increasing the maximum K value

Debye formula – the method

A) <u>Simple systems</u>: sin-transform reciprocal space → real space (next slide)

B) <u>Relatively large systems</u>

Diffraction patterns are calculated from atomistic descriptions via the Debye function, and refined against measured data to obtain detailed microstructural information.

The number of terms to be calculated is proportional to N^2

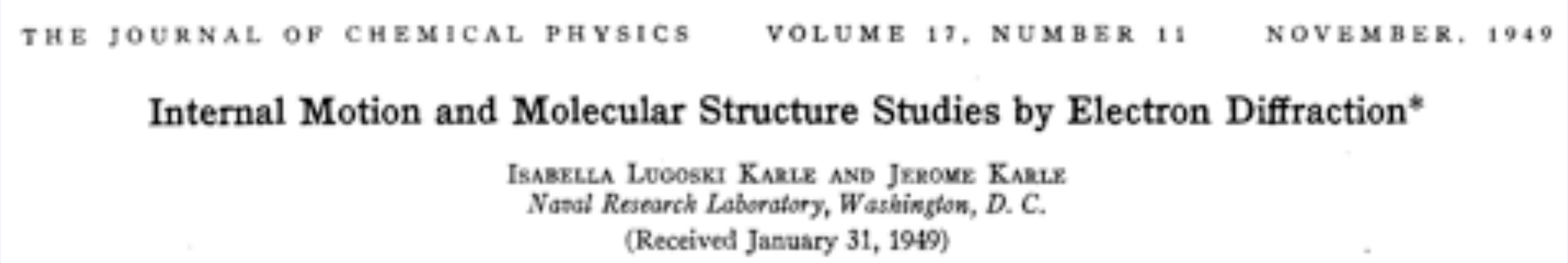
→ Originally suitable only for small molecules

At present

- Interest in nano-technology
- Available computing power available

→ Debye function revisited

Debye formula: sin-transform



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 17, NUMBER 11 NOVEMBER, 1949

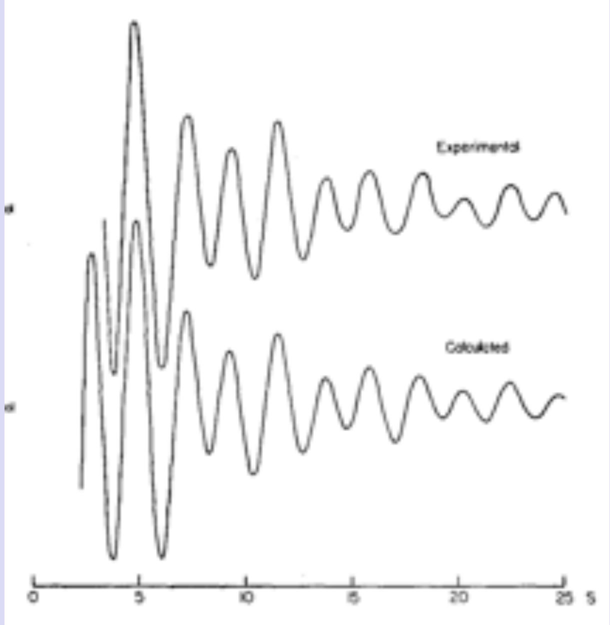
Internal Motion and Molecular Structure Studies by Electron Diffraction*

ISABELLA LUGOSKI KARLE AND JEROME KARLE
Naval Research Laboratory, Washington, D. C.

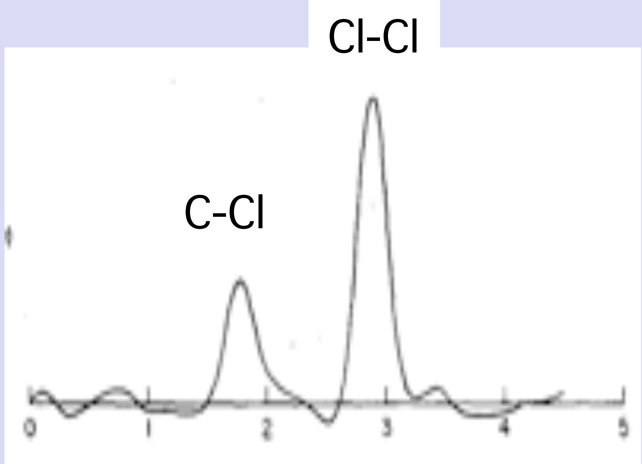
(Received January 31, 1949)

C Cl_4

Experimental spectrum



Experimental and calculated oscillations



RDF from sin-transform

X-ray scattering from liquids and non-crystalline solids

Large non-crystalline systems

General formula...

$$I_{\text{e.u.}}(\vec{K}) = \left(\sum_m f_m(\vec{K})\, e^{i\vec{K}\cdot\vec{r}_m}\right)\left(\sum_n f_n^*(\vec{K})\, e^{-i\vec{K}\cdot\vec{r}_n}\right)$$

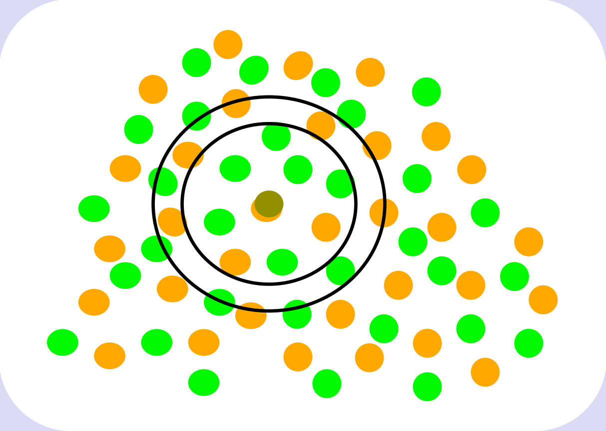
$$= \sum_m \sum_n f_m(\vec{K})\, f_n^*(\vec{K})\, e^{i\vec{K}\cdot\vec{R}_{mn}}$$

?

No long-range order
no Laue interference function

Large systems – no defined structure
Debye formula impracticable

Random orientations



Radial Distribution Function

Paolo
Fornasini
Univ. Trento

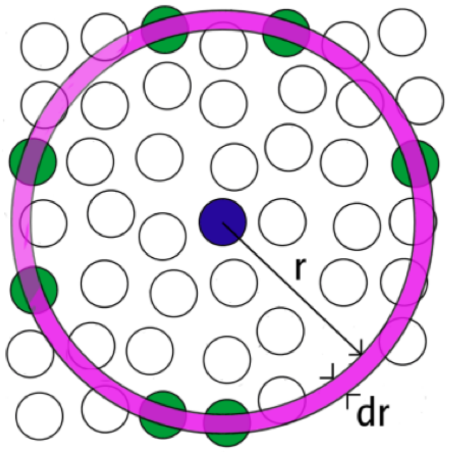
$$R(r) = \frac{1}{N} \sum_{m} \sum_{n \neq m} \delta\left(r - r_{mn}\right)$$

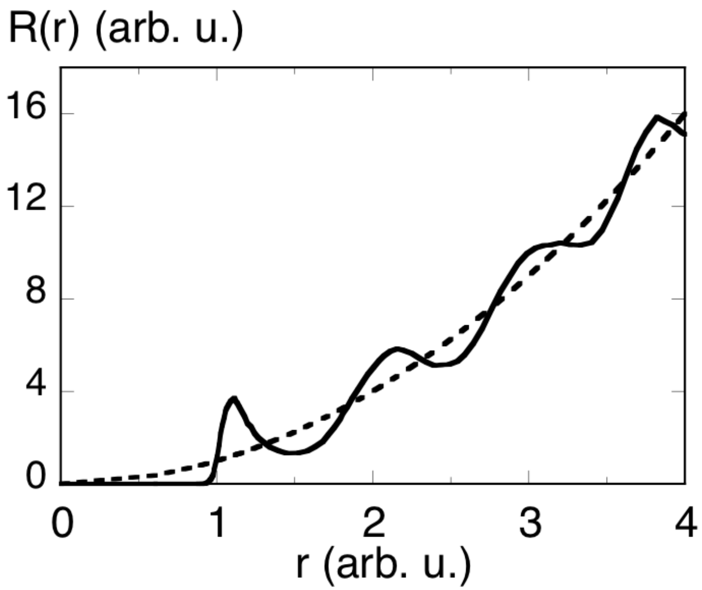
average density

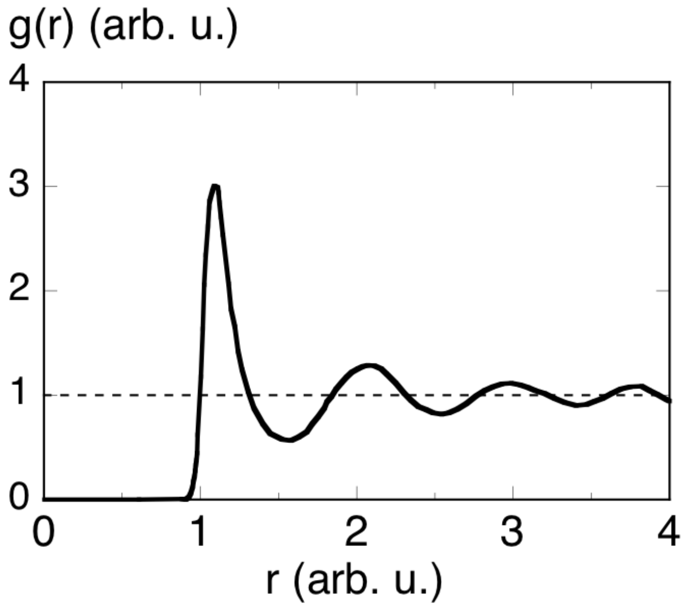
$$R(r) = 4\pi r^2 \rho(r) = 4\pi r^2 \rho_0 \, g(r)$$

Radial distribution function

Pair distribution function







Monatomic non-crystalline systems (a)

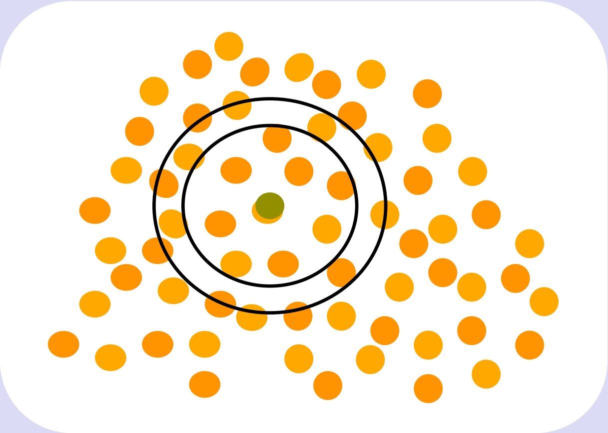
General formula

$$I_{\text{e.u.}}\left(\vec{K}\right) = \sum_m \left|f_m\left(\vec{K}\right)\right|^2 + \sum_m \sum_{n\neq m} f_m\left(\vec{K}\right) f_n^*\left(\vec{K}\right)\, e^{i\vec{K}\cdot\vec{R}_{mn}}$$

Only 1 atomic species

$$I_{\text{e.u.}}\left(\vec{K}\right) = \underbrace{N\left|f\left(\vec{K}\right)\right|^2}_{\text{Independent scattering}} + \underbrace{\left|f\left(\vec{K}\right)\right|^2 \sum_m \sum_{n\neq m} e^{i\vec{K}\cdot\vec{R}_{mn}}}_{\text{Interference: N(N-1) terms}}$$

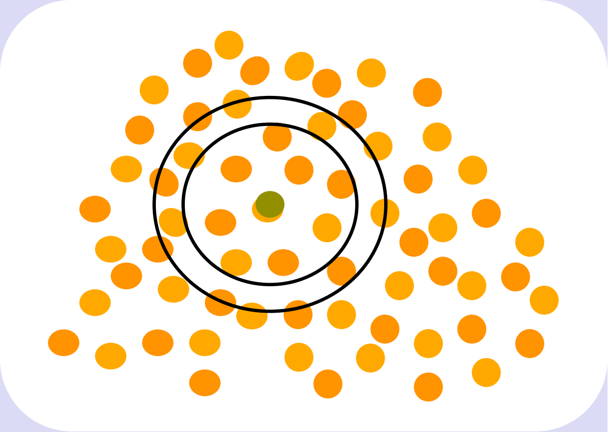
Disordered system



$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(\vec{K})\right|^2 + \left|f(\vec{K})\right|^2 \sum_m \int_V \underbrace{\rho_m\left(\vec{r}_{mn}\right) e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n}_{\text{Integral over distribution of distances from atom m}}$$

Monatomic non-crystalline systems (b)

$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(\vec{K})\right|^2 + \left|f(\vec{K})\right|^2 \sum_m \int_V \underbrace{\rho_m\left(\vec{r}_{mn}\right) e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n}_{\text{Subtract and add the average density}}$$



$$\Big\Downarrow$$

$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(\vec{K})\right|^2 + \left|f(\vec{K})\right|^2 \sum_m \int_V \overbrace{\left[\rho\left(\vec{r}_{mn}\right) - \rho_0\right]}^{\text{Oscillation of the distribution around the average density}} e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n$$

$$\boxed{+ \left|f(\vec{K})\right|^2 \sum_m \int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n}$$

Small-angle scattering only at very small K

Monatomic non-crystalline systems (c)

Neglecting the small-angle term:

$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(\vec{K})\right|^2 + \left|f(\vec{K})\right|^2 \sum_m \int_V \left[\rho\left(\vec{r}_{mn}\right) - \rho_0\right] e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n$$

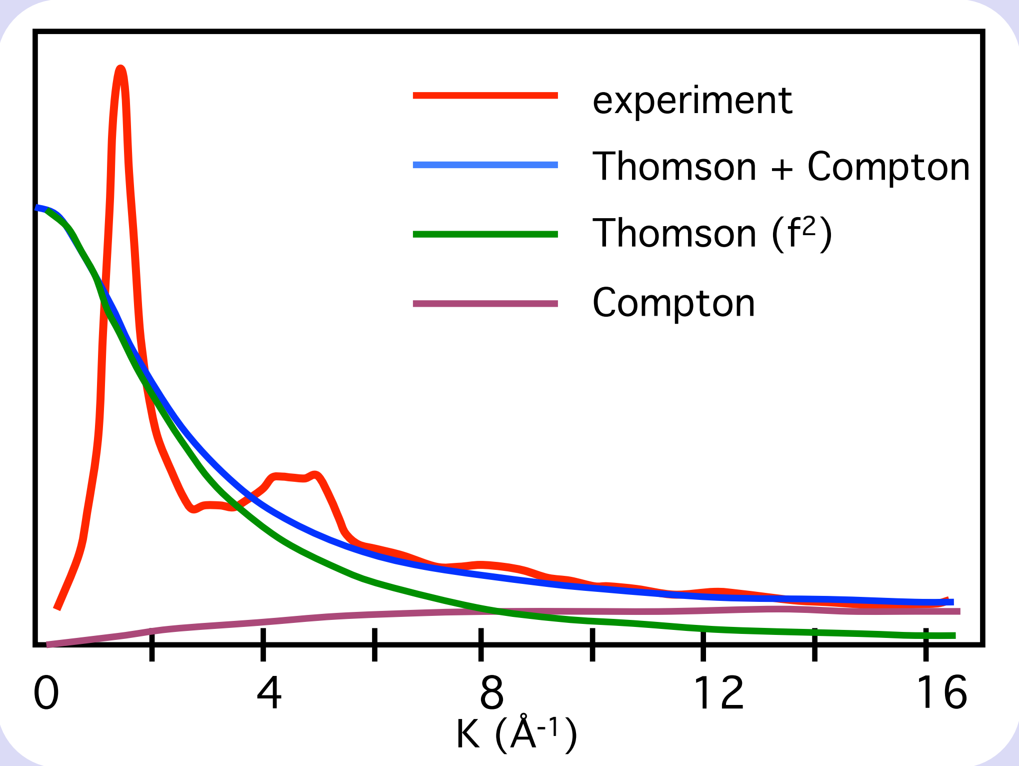
Averaging over the central atom and considering spherical symmetry:

$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(K)\right|^2 + N\left|f(K)\right|^2 \underbrace{\int_0^\infty 4\pi r^2\left[\rho(r) - \rho_0\right]\frac{\sin Kr}{Kr}\, dr}$$

$$\Big\downarrow \quad \rho(r) = \rho_0\, g(r)$$

$$\boxed{4\pi\rho_0 \int_0^\infty r^2\left[g(r) - 1\right]\frac{\sin Kr}{Kr}\, dr}$$

Experimental data: Interference function

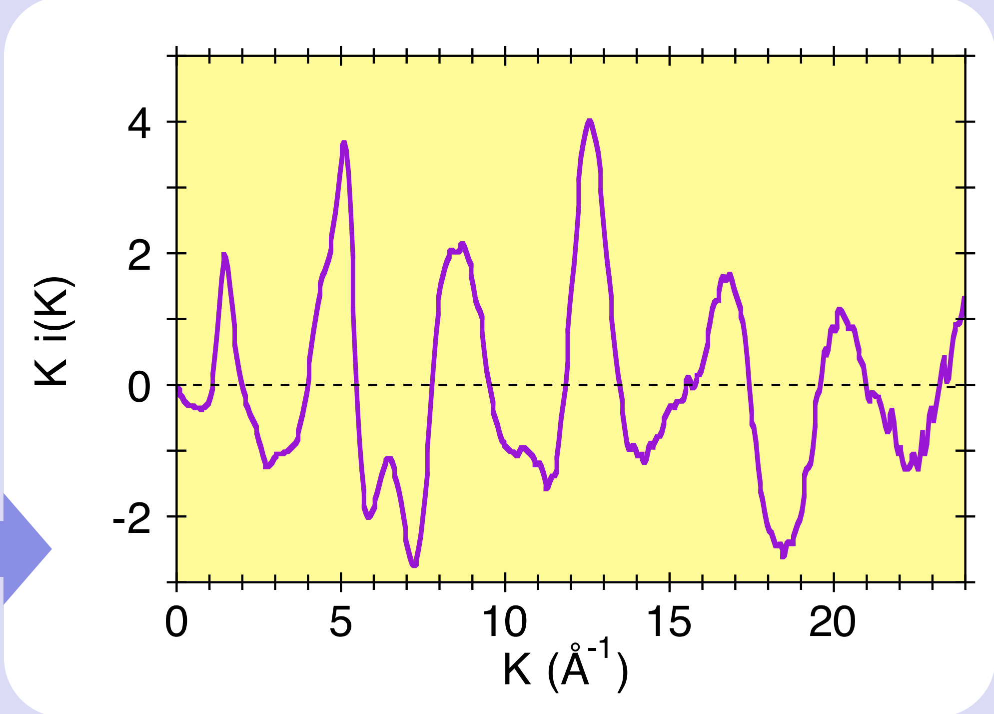


$$I_{\mathrm{e.u.}}(K) = I_{\exp}(K) - I_{\mathrm{Compton}}(K)$$
$$= Nf^2(K)\ \boxed{S(K)}$$

Structure factor

Interference function

$$i(K) = \frac{I_{\mathrm{eu}}(K)/N - f^2(K)}{f^2(K)} = S(K) - 1$$



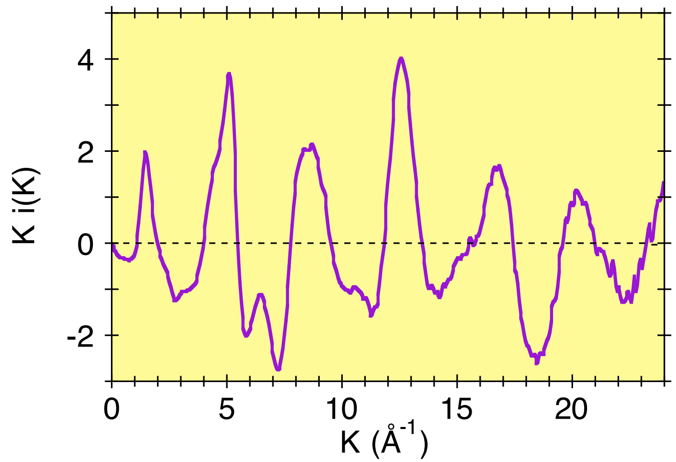
Fourier sin-transform

$$I_{\text{e.u.}}(\vec{K}) = N|f(K)|^2 + N|f(K)|^2\; 4\pi\rho_0 \int_0^\infty r^2\left[g(r)-1\right]\frac{\sin Kr}{Kr}\,dr$$

Interference function

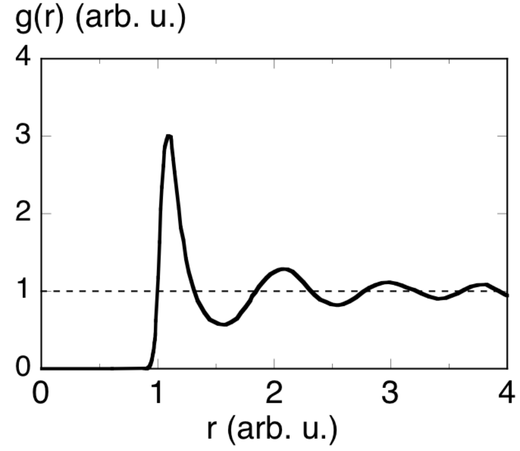
$$K\,i(K) = \frac{I_{\text{eu}}(K)/N - f^2(K)}{f^2(K)}$$

$$K\,i(K) = 4\pi\rho_0 \int_0^\infty r\left[g(r)-1\right]\sin Kr\,dr$$



Pair distribution function

$$g(r)-1 = \frac{1}{2\pi^2 r\rho_0}\int_0^\infty i(K)\,\sin(Kr)\,K\,dK$$



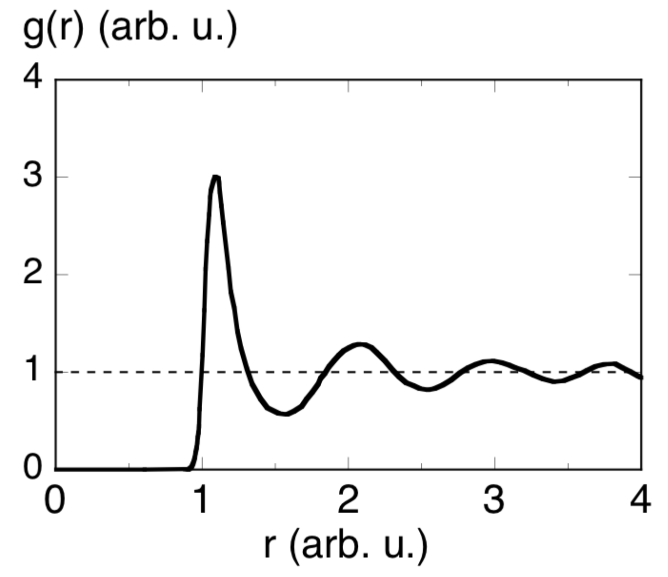
Distribution functions

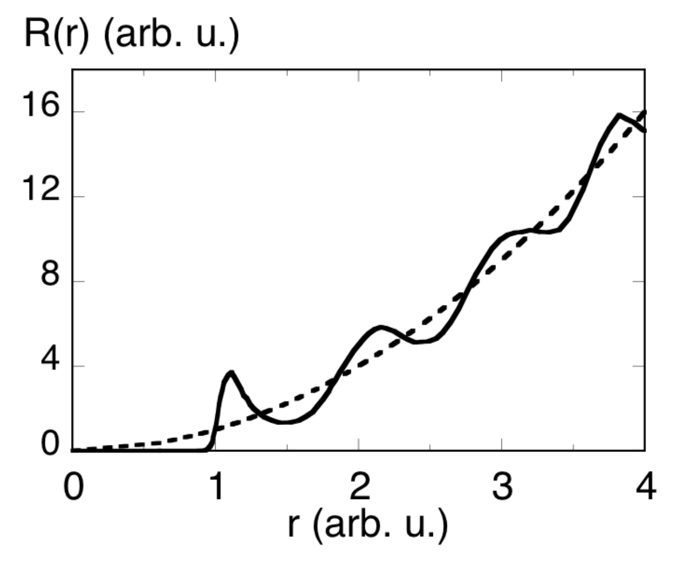
Pair distribution function

$$g(r) = 1 + \frac{1}{2\pi^2 r \rho_0} \int_0^\infty i(K) \sin(Kr)\, K\, dK$$

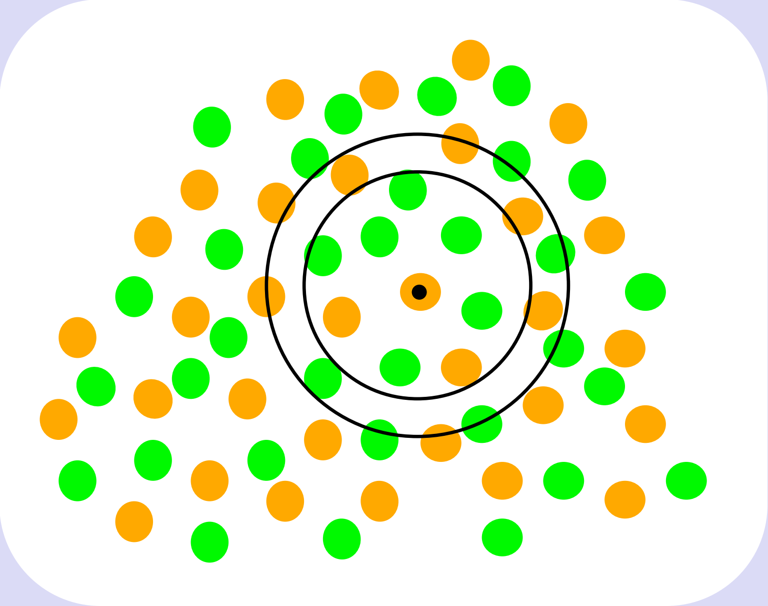
Radial distribution function

$$R(r) = 4\pi r^2 \rho_0\, g(r) = 4\pi r^2 \rho(r)$$





Many-atomic amorphous systems



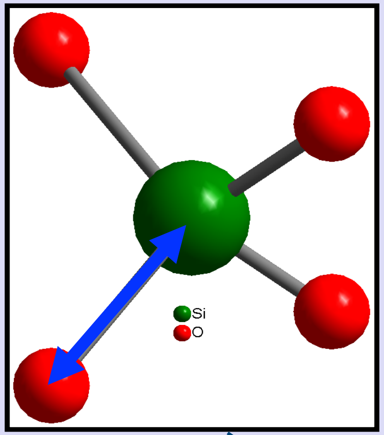
M atomic species

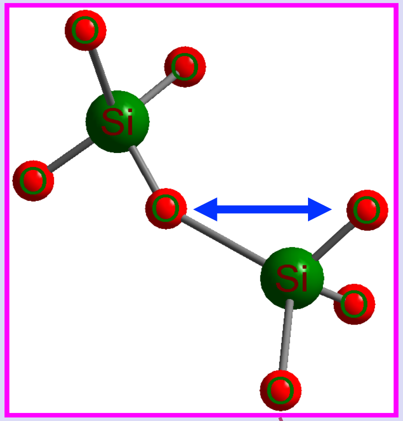
$$\underbrace{\frac{M(M-1)}{2}}_{m \neq n} + \underbrace{M}_{m = n} = \frac{M(M+1)}{2}$$

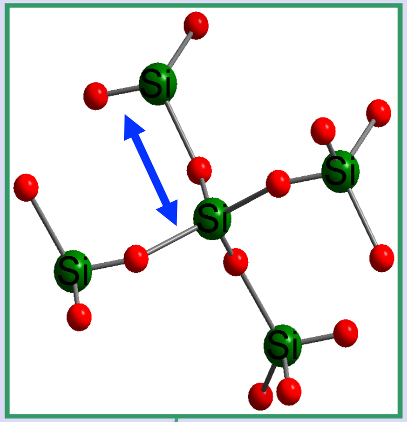
- partial RDFs $g_{mn}(r)$
- partial structure factors $S_{mn}(K)$

Partial RDFs - Amorphous silica

Paolo
Fornasini
Univ. Trento

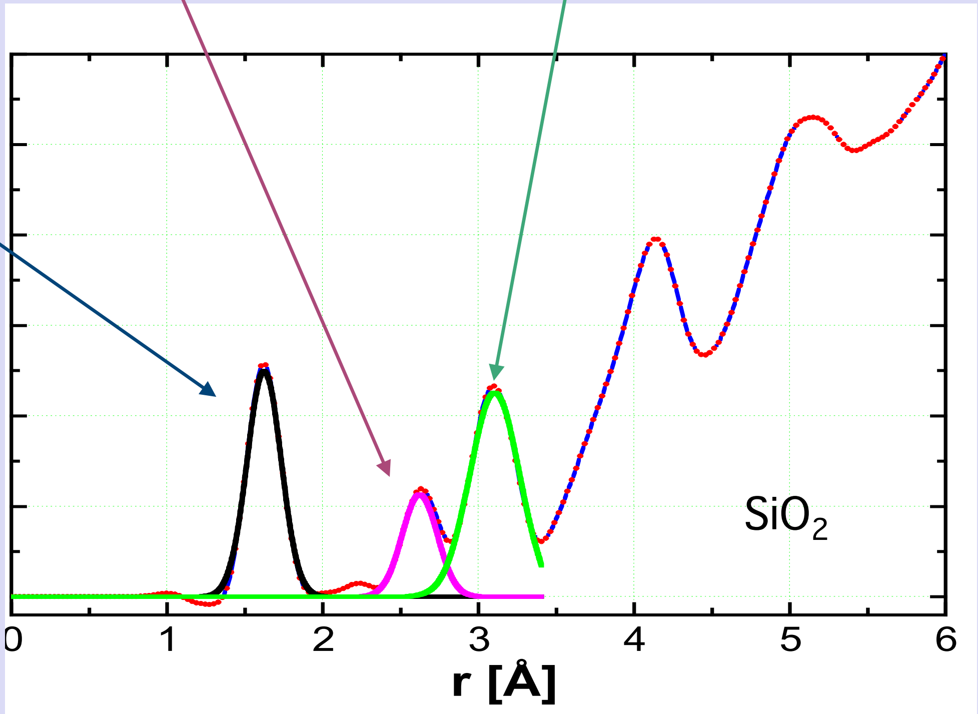




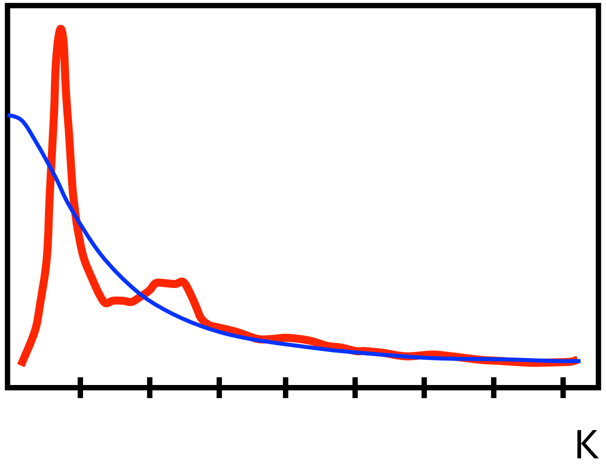


Peaks positions
→ interatomic distances

Peaks area
→ coordination numbers



Partial structure factors



$$M \begin{cases} \text{atomic species} \\ \text{scattering factors} & f_m \\ \text{relative concentrations} & c_m \end{cases}$$

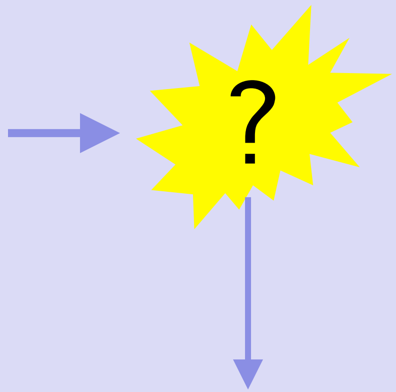
$$I_{eu}(K) = \underbrace{\sum_m c_m f_m^2(K)}_{\text{independent scattering}} + \underbrace{\sum_{m,n\neq m} c_m c_n f_m(K) f_n(K) \left[S_{mn}(K) - 1 \right]}_{\text{interference function}}$$

$\frac{M(M+1)}{2}$ partial structure factors $S_{mn}(K)$

m,*n* = atomic species

Partial distribution functions

- Neutron isotopic substitution
- X-ray anomalous diffraction (MAD)
- Approximate methods



$$I_{eu}(K) = \sum_{m} c_m f_m^2(K) + \sum_{m,n\neq m} c_m c_n f_m(K) f_n(K) \left[S_{mn}(K) - 1\right]$$

$$g_{mn}(r) - 1 = \frac{1}{2\pi^2 \rho_0} \int_0^\infty \left[S_{mn}(K) - 1\right] \sin(Kr)\, K\, dK$$

m,*n* = atomic species

Method of compositional units

Approximate method for molecular systems

uc = unit of composition

SiO_2: 1 Si + 2 O

$$I_{\mathrm{e.u.}}\left(\vec{K}\right) = \sum_{m,n} f_m f_n \, e^{i\vec{K}\cdot\vec{R}_{mn}}$$

$$= \sum_{m} f_m^2 + \sum_{m} f_m \sum_{n\neq m} f_n e^{i\vec{K}\cdot\vec{R}_{mn}}$$

$$= \sum_{m} f_m^2 + f_e^2 \sum_{m} K_m \sum_{n\neq m} K_n e^{i\vec{K}\cdot\vec{R}_{mn}}$$

$$= N\sum_{uc} f_j^2 + N f_e^2 \sum_{uc} K_j \int_0^{\infty} 4\pi R^2 \left[\rho_j(r) - \rho_0\right] \frac{\sin KR}{KR} \, dR + \left[\text{small angle term}\right]$$

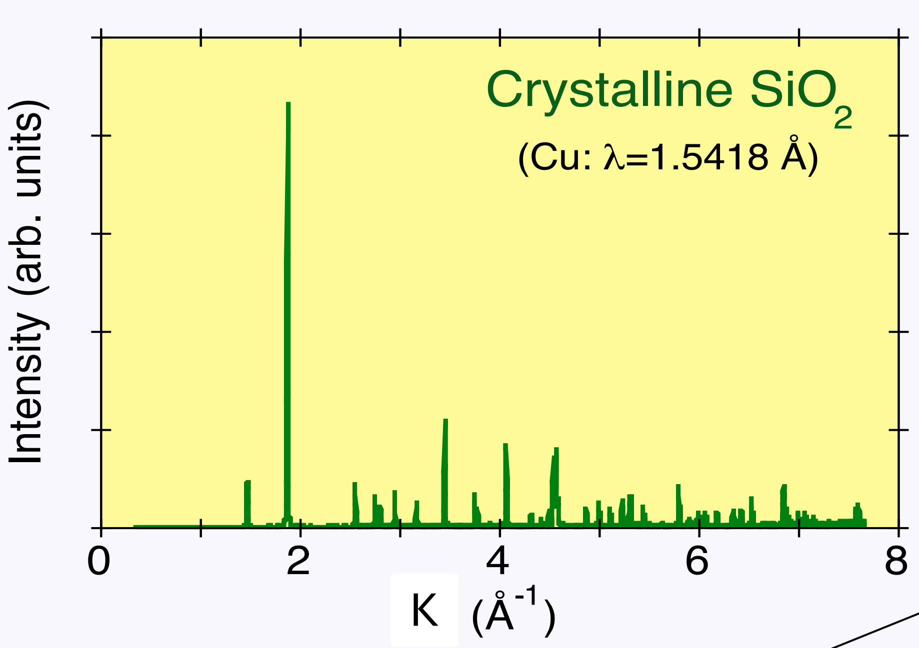
$$\boxed{\text{average } f_e = \frac{\sum_{uc} f_m}{\sum_{uc} Z_m}}$$

$$\boxed{K_m = f_m / f_e}$$

m,n = atomic species

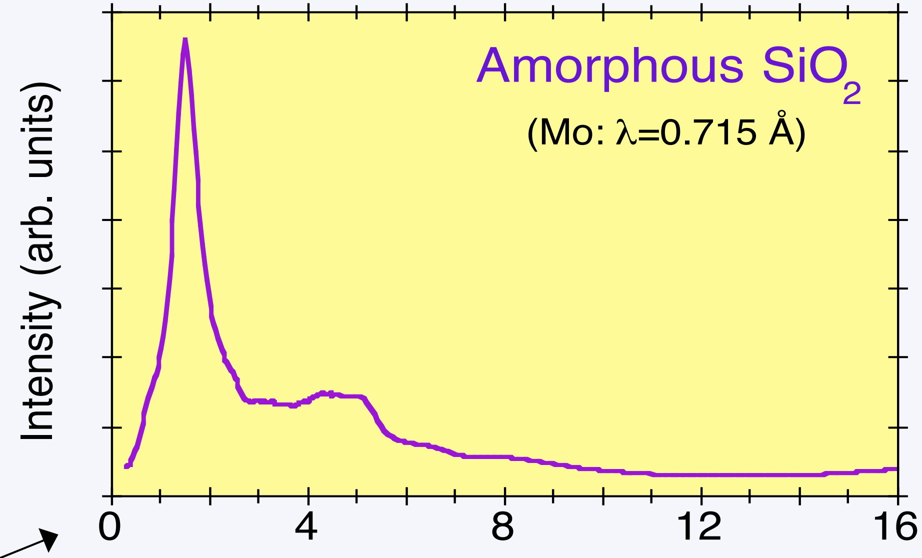
Crystalline .vs. amorphous systems.

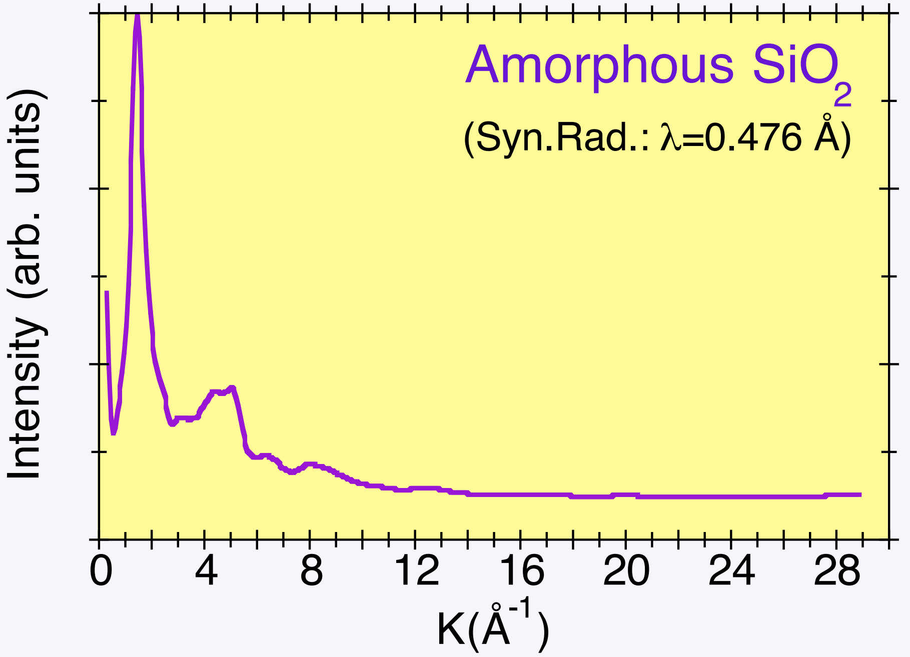
Paolo
Fornasini
Univ. Trento



- Cu anode
- Mo anode
- Sychr. Radiation

$\lambda \Rightarrow$ scattering range





Structure factors

Crystalline solids

$$\frac{d\sigma}{d\Omega} = r_e^2 \prod_{i=1}^{3} \boxed{\frac{\sin^2\left(N_i \vec{K}\cdot\vec{a}_i/2\right)}{\sin^2\left(\vec{K}\cdot\vec{a}_i/2\right)}} \; \boxed{\left|F\left(\vec{K}\right)\right|^2}$$

Laue interference function

Structure factor

Non-crystalline systems

$$\frac{d\sigma}{d\Omega} = r_e^2 \; \left|f(K)\right|^2 \boxed{S(K)}$$

Structure factor

Small angle X-ray scattering
SAXS

Small angle scattering (a)

$$I_{\text{e.u.}}\left(\vec{K}\right) = N\left|f(\vec{K})\right|^2 + \left|f(\vec{K})\right|^2 \sum_m \int_V \left[\rho\left(\vec{r}_{mn}\right) - \rho_0\right] e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n$$

$$\boxed{+ \left|f(\vec{K})\right|^2 \sum_m \int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}_{mn}}\, dV_n}$$

⇓

$$I_{e.u.}^{SAXS}\left(\vec{K}\right) = f^2(\vec{K}) \sum_m e^{i\vec{K}\cdot\vec{r}_m} \int_V \rho_0\, e^{-i\vec{K}\cdot\vec{r}_n}\, dV_n$$

$$= f^2(\vec{K}) \int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}_m}\, dV_m \int_V \rho_0\, e^{-i\vec{K}\cdot\vec{r}_n}\, dV_n$$

$$= f^2(\vec{K}) \left| \int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}}\, dV \right|^2$$

Small angle scattering (b)

$$I^{SAXS}_{e.u.}\left(\vec{K}\right) = f^{\,2}(\vec{K})\left|\int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}}\, dV\right|^2$$

Fourier Transform of the average density:
constant at the length scale of the pdf fluctuations.

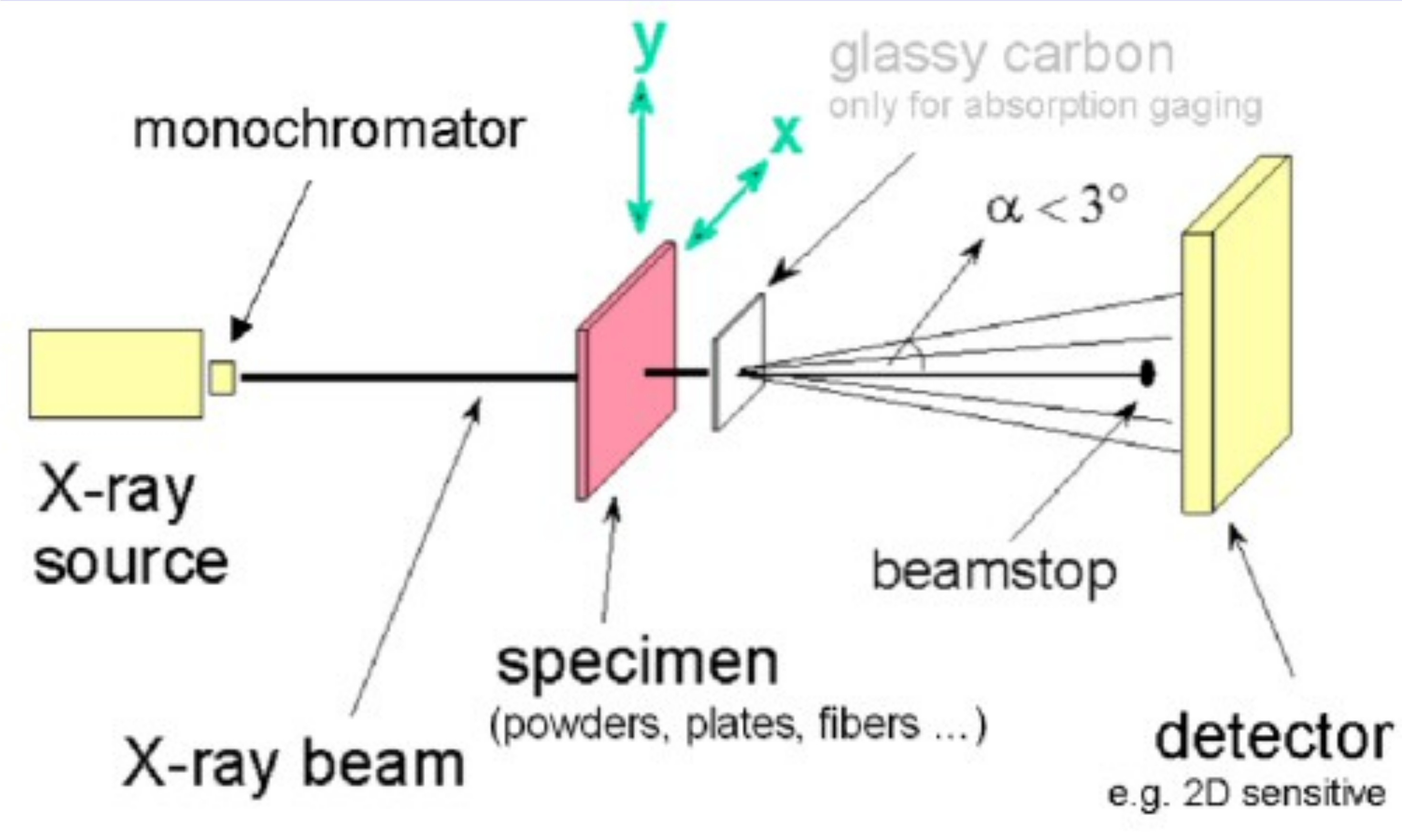
Narrow peak near the origin, typically for K < 0.02 $Å^{-1}$

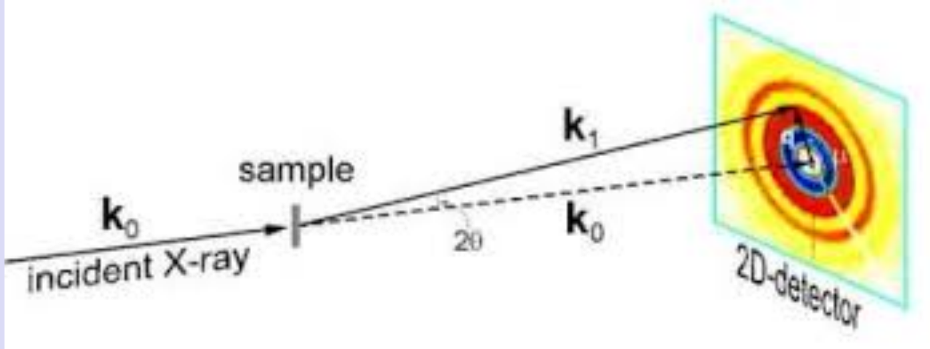
Structures of the small-angle peak
> info on long-range density fluctuations (~100 Å)

Approximate relation between
object dimension, wavelength and angle

$$d \approx \frac{\lambda}{\sin\theta_B} \approx \frac{\lambda}{\theta_B}$$

SAXS experimental layout





Small angle scattering (c)

Independent particles in vacuum

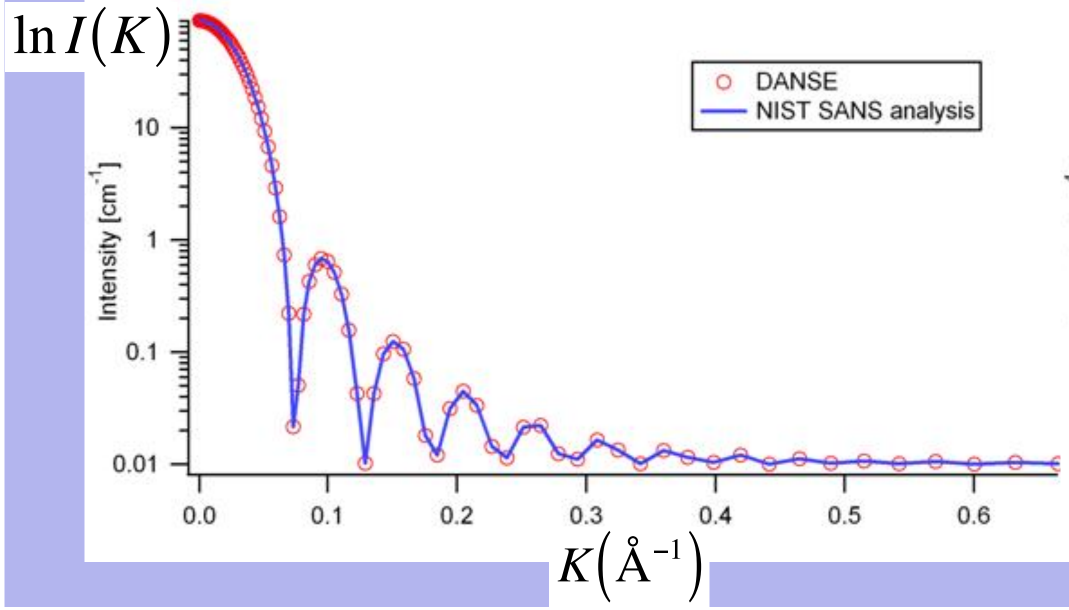
$$I_{e.u.}^{SAXS}\left(\vec{K}\right) = f^2(\vec{K})\left|\int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}} dV\right|^2$$

Form factor of one particle

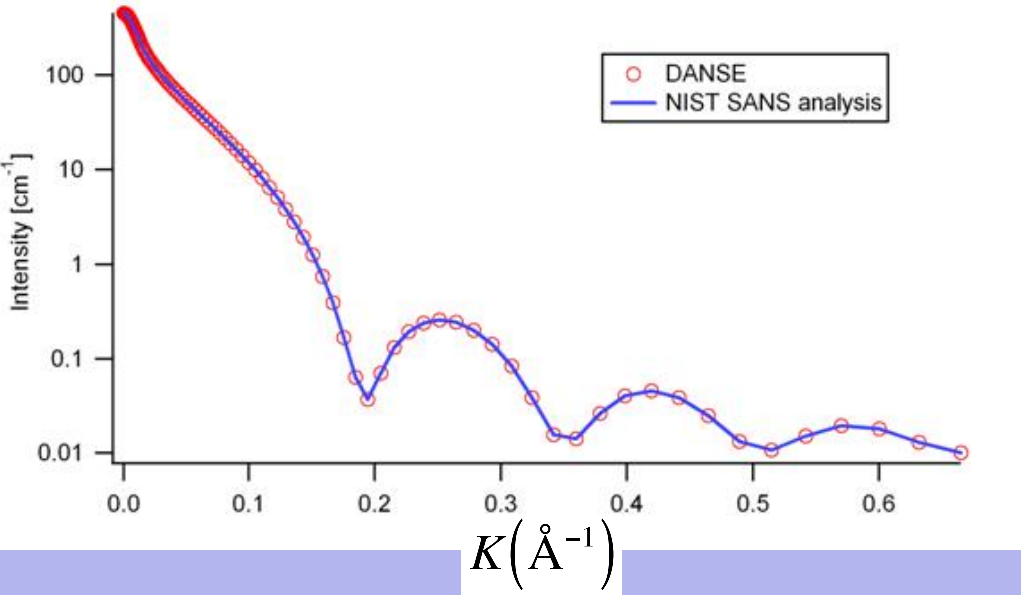
$$\int_V \rho_0\, e^{i\vec{K}\cdot\vec{r}} dV$$

Simple examples

Uniform sphere, radius 60 Å



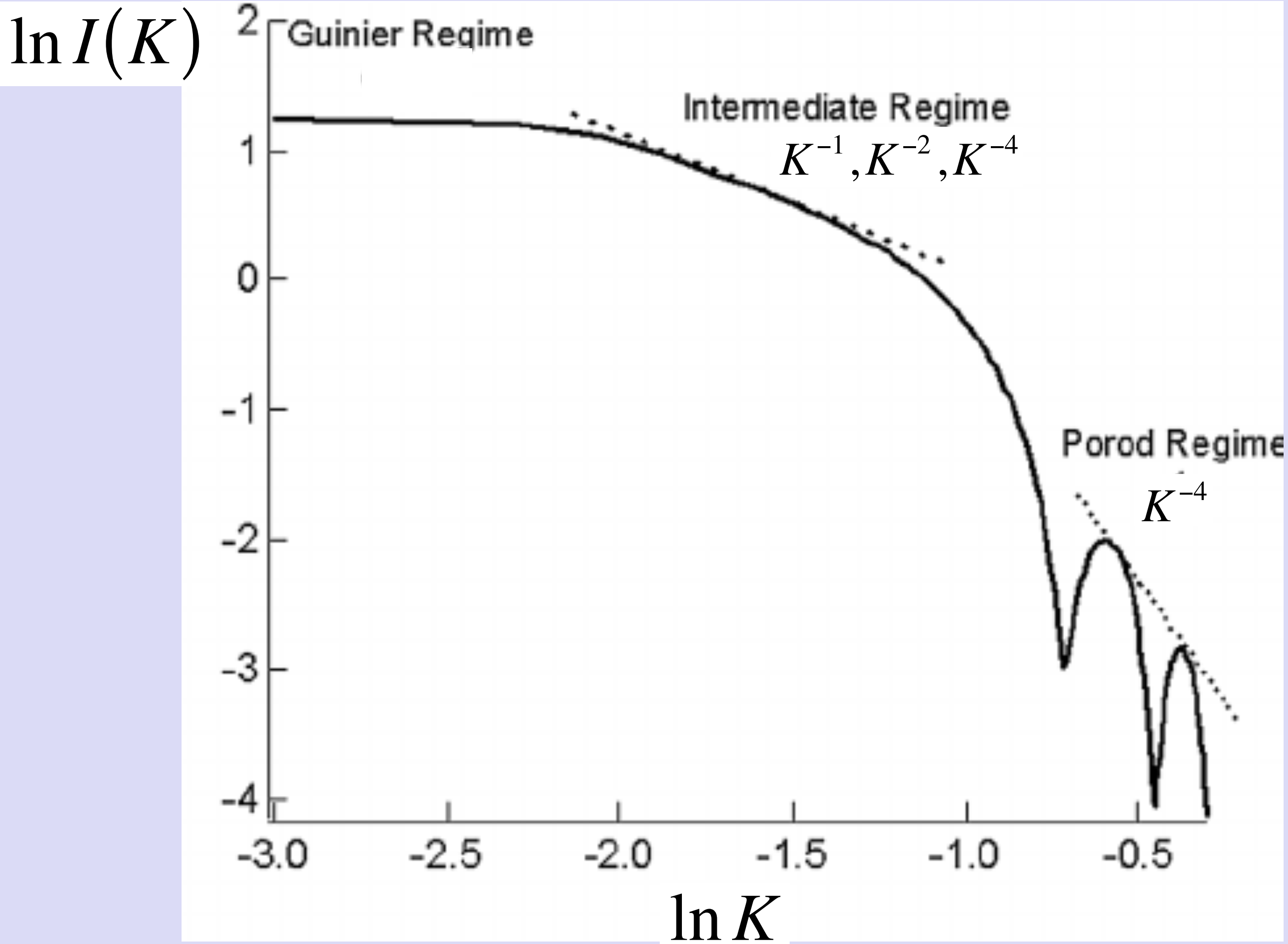
Uniform cylinder, radius 20 Å, length 400 Å



Small angle scattering (d)

Long-wavelength limit

$\text{slope} \propto -R^2/5$



$KR < 1$

Short-wavelength limit

$I \propto \text{surface}/K^4$

SAS applications

SAS of X-rays and neutrons

Study of large-scale structures from 10 Å
up to thousands and even several tens of thousands of angstroms.

Examples:

- Critical opalescence in critical phase transitions
- Colloidal aggregations
- Nano-clusters
- Defects in materials
- Polymers
- Proteins, viruses, ribosome

Basic references

- J. Als-Nielsen and D. McMorrow: Elements of modern X-ray Physics, Wiley, 2011
- S. Mobilio, F. Boscherini, C. Meneghini editors: Synchrotron Radiation: basics, methods and applications, Springer 2014
- B.E. Warren: X-ray diffraction, 1969
- B.K. Vainshstein: Modern Crystallography, vol. 1, Springer 1981.
- S. Chen and M. Kotlarchyk: Interaction of photons and neutrons with matter. World Scientific, 1997
- International Tables for X-ray Crystallography, vol. 3 (Physical and Chemical Tables), D. Reidel Pub. Co.,1985