How to assess the structure of glasses ?

CNRS thematic school about glass structure

Structure of disordered materials by neutron diffraction

Gabriel Cuello
Institut Laue Langevin
Grenoble, France

cuello@ill.eu

Characterization of glass structure
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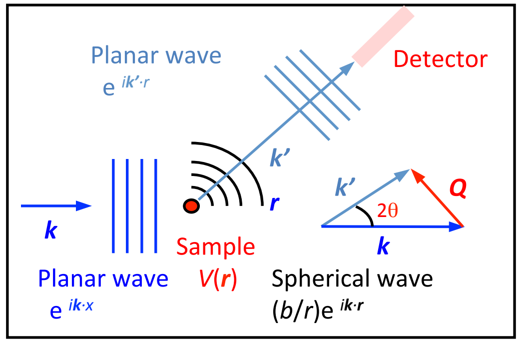
EPN Campus – Grenoble, France

Scattering experiment

Experiment → Microscopic properties



Intensity $I(2\theta,\omega)$ • Scattering Cross Section $d^2\sigma/d\Omega d\omega$ • Dynamical SF $S(\mathbf{Q},\omega)$

$$I(2\theta,\omega) = C\,\Phi_0\,\frac{\mathrm{d}^2\sigma}{\mathrm{d}\sigma\mathrm{d}\omega}(2\theta,\omega)\,\epsilon(k')$$

Beam

Sample

Detector

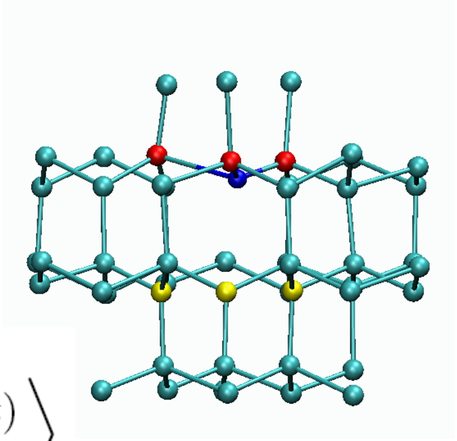
$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\sigma\mathrm{d}\omega}(2\theta,\omega) = N\,\frac{k'}{k}\,\frac{\sigma}{4\pi}\,S(\vec{Q},\omega)$$

Interaction

System

Microscopic properties

Dynamical Structure Factor $S(\boldsymbol{Q},\omega)$



Microscopic Configuration $\{\boldsymbol{r}_1(t), \boldsymbol{r}_2(t), \ldots, \boldsymbol{r}_N(t)\}$

$$S(\vec{Q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\omega t}\, \frac{1}{N}\sum_{i,j}^{N}\left\langle \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{r}_i(0)}\mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{r}_j(t)}\right\rangle$$

$$\delta(\vec{r}) = \frac{1}{(2\pi)^3}\int_{\mathrm{all}\ \vec{Q}} \mathrm{e}^{\mathrm{i}\vec{Q}\cdot\vec{r}}\mathrm{d}\vec{Q}$$

$$\rho(\vec{r},t) = \sum_{i=1}^{N}\delta\left(\vec{r}-\vec{r}_i(t)\right)$$

Microscopic particle density

$$S(\vec{Q},\omega) = \frac{1}{2\pi}\iint \mathrm{d}\vec{r}\mathrm{d}t\ \mathrm{e}^{\mathrm{i}(\vec{Q}\cdot\vec{r}-\omega t)}G(\vec{r},t)$$

Probability density of having a given atom somewhere, *e.g.* at (**0**, 0), and *any* atom at (***r***, *t*)

van Hove's correlation function

$$G(\vec{r},t) = \frac{1}{N}\int \mathrm{d}\vec{r'}\left\langle \rho(\vec{r'},0)\rho(\vec{r}+\vec{r'},t)\right\rangle$$

Coherent and incoherent scattering

$$\frac{d^2\sigma}{d\Omega d\omega}(2\theta,\omega) = N\frac{k'}{k}\left\{\frac{\sigma_{coh}}{4\pi}S(\vec{Q},\omega) + \left(\frac{\sigma_{inc}}{4\pi}\right)S_s(\vec{Q},\omega)\right\}$$

coherent

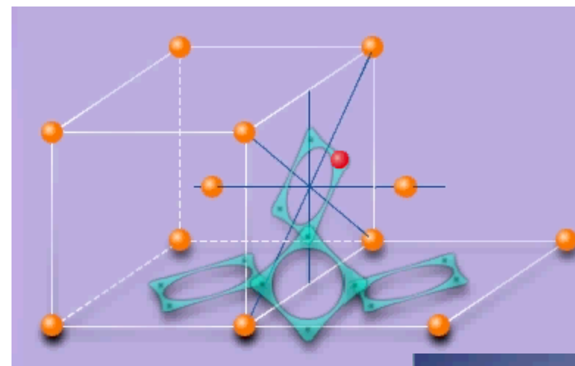
incoherent

Diffusive
Motions
Internal
Dynamics

$\sigma_{coh} = 4\pi\,|\langle b\rangle|^2$ squared mean

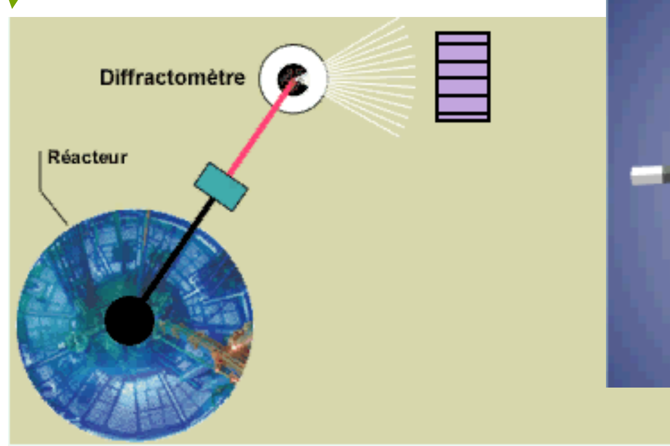
$\sigma_{inc} = 4\pi\left(\langle|b|^2\rangle - |\langle b\rangle|^2\right)$ variance

Scattering cross section $\sigma = \sigma_{coh} + \sigma_{inc}$



Structural information
Collective dynamics

Diffraction
(no energy discrimination)



Static structure factor

$$S(\vec{Q}) = \int_{-\infty}^{+\infty} \mathrm{d}\omega\; S(\vec{Q},\omega) = \int \mathrm{d}\vec{r}\; \mathrm{e}^{\mathrm{i}\vec{Q}\cdot\vec{r}} G(\vec{r},0)$$

Static approximation

S(Q)-1 & g(r)-1 become a FT pair

$$S(\vec{Q}) - 1 = \rho \int_V \mathrm{d}\vec{r}\; [g(\vec{r}) - 1]\; \mathrm{e}^{\mathrm{i}\vec{Q}\cdot\vec{r}}$$

$$\rho\, [g(\vec{r}) - 1] = \frac{1}{(2\pi)^3} \int \mathrm{d}\vec{Q}\; \left[S(\vec{Q}) - 1\right]\; \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{r}}$$

Definition

$$F(\vec{Q}) = S(\vec{Q}) - 1$$

$$G(\vec{r}) = 4\pi\rho r\, [g(\vec{r}) - 1]$$

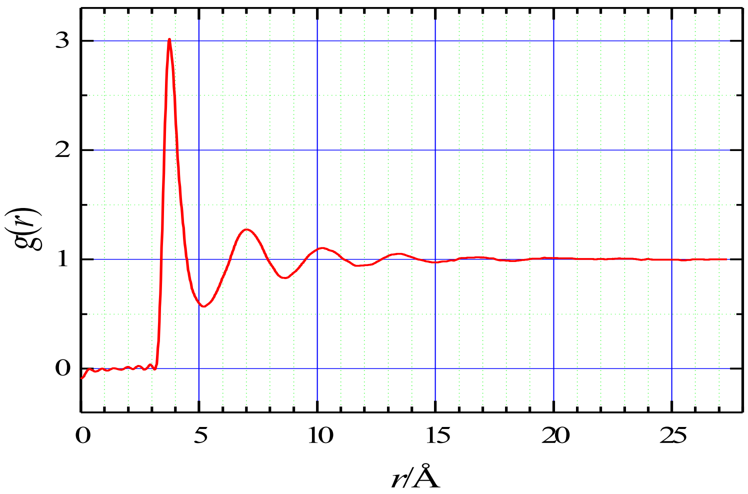
$$F(\vec{Q}) = \int_V \mathrm{d}\vec{r}\; \frac{G(\vec{r})}{4\pi r}\; \mathrm{e}^{\mathrm{i}\vec{Q}\cdot\vec{r}}$$

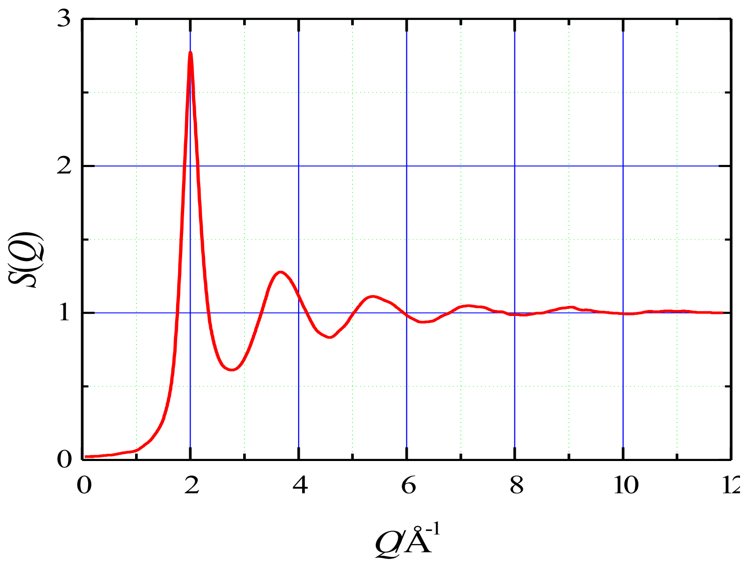
$$\frac{G(\vec{r})}{4\pi r} = \frac{1}{(2\pi)^3} \int \mathrm{d}\vec{Q}\; F(\vec{Q})\; \mathrm{e}^{-\mathrm{i}\vec{Q}\cdot\vec{r}}$$

Isotropic case

$$Q\ F(Q) = \int_0^\infty G(r)\ \sin(Qr)\ \mathrm{d}r$$

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





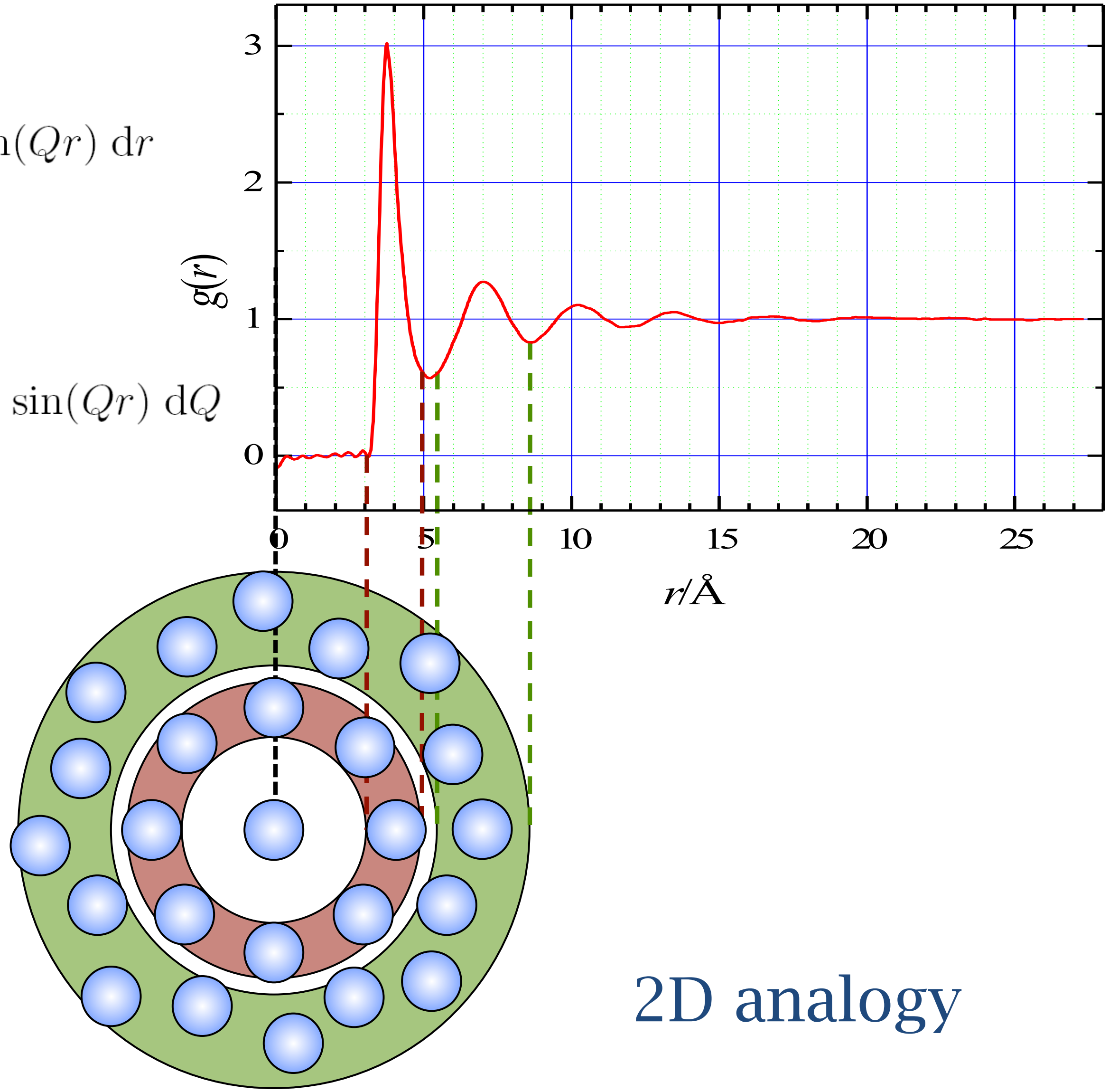
$$S(Q) - 1 = \frac{4\pi\rho}{Q} \int_0^\infty r\ [g(r) - 1]\ \sin(Qr)\ \mathrm{d}r$$

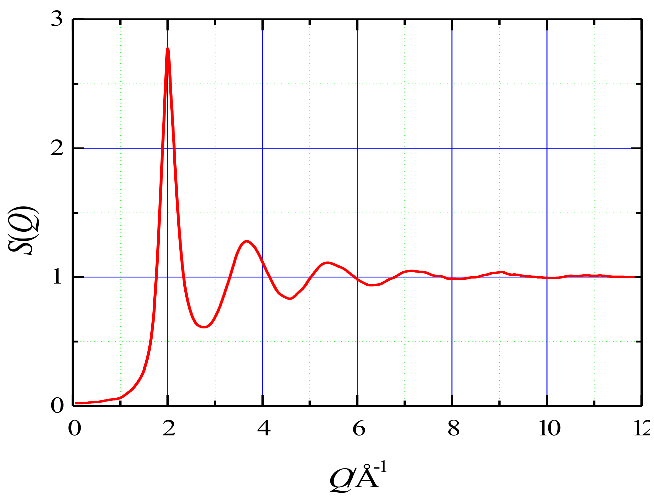
$$g(r) - 1 = \frac{1}{2\pi^2 \rho r} \int_0^\infty Q\ [S(Q) - 1]\ \sin(Qr)\ \mathrm{d}Q$$

Pair distribution function

$$S(Q) - 1 = \frac{4\pi\rho}{Q} \int_0^\infty r\ [g(r) - 1]\ \sin(Qr)\ \mathrm{d}r$$

$$g(r) - 1 = \frac{1}{2\pi^2\rho r} \int_0^\infty Q\ [S(Q) - 1]\ \sin(Qr)\ \mathrm{d}Q$$

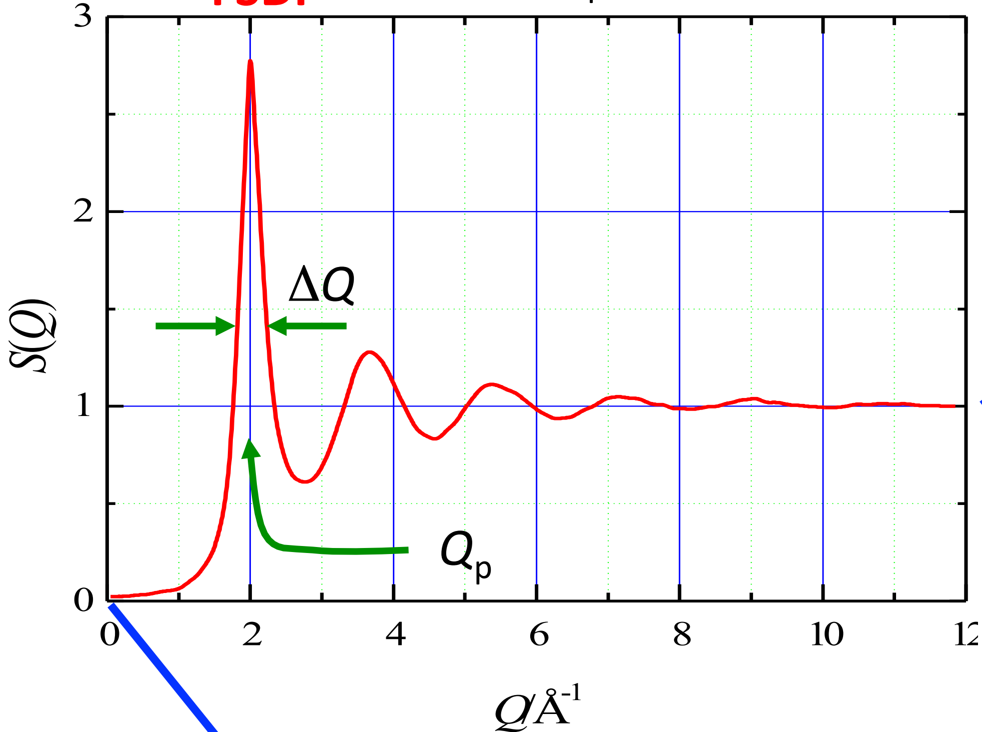




2D analogy

From $S(Q)$ to $g(r)$

FSDP First Sharp Diffraction Peak



Liquid Ar @ 85K

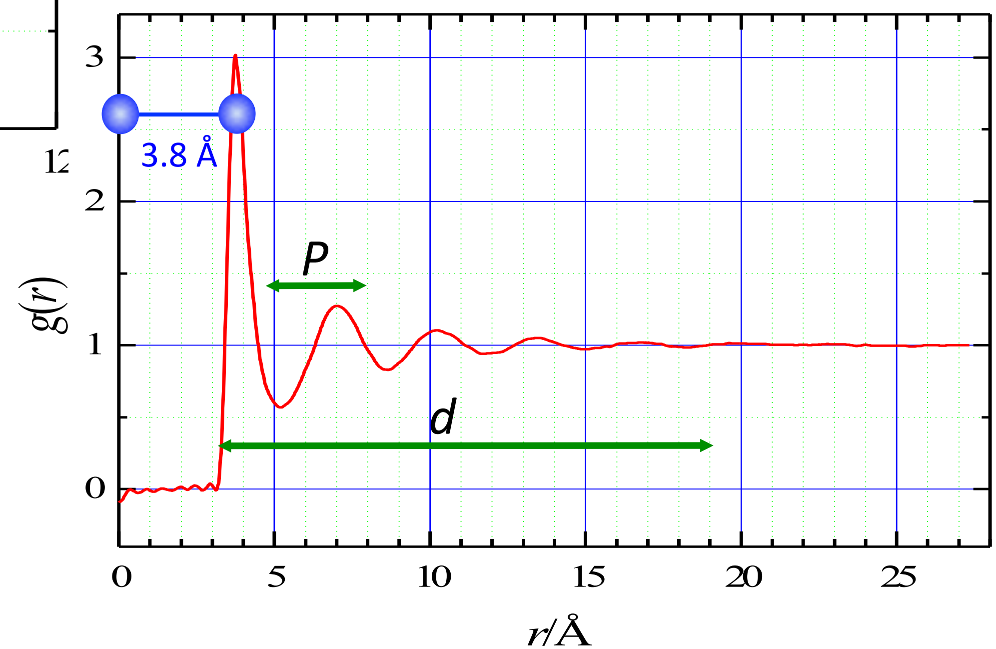
J.L. Yarnell *et al.* (1973) PRA **7**, 2130

$$S(\infty) = 1$$

Fourier Transformation

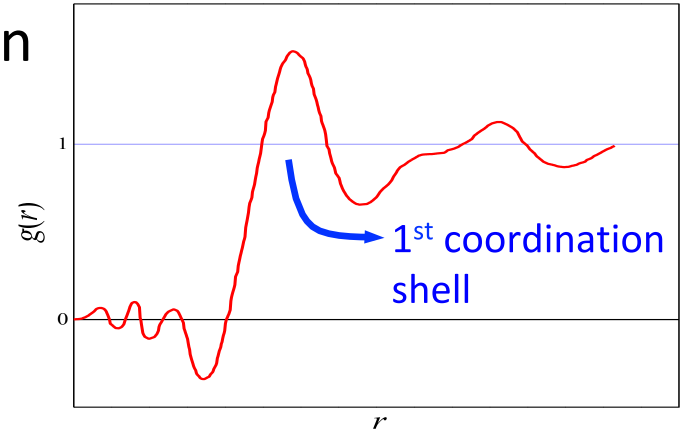
$$S(0) = \rho\, \chi_T\, k_{\mathrm{B}} T$$

Limiting values → Normalisation



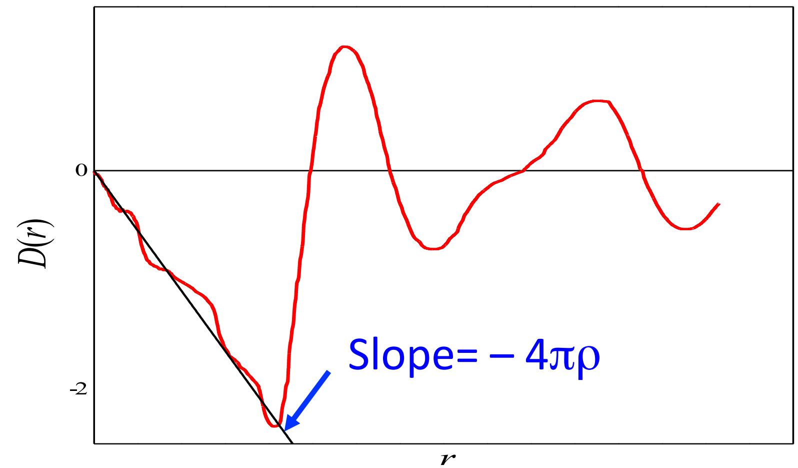
Related functions

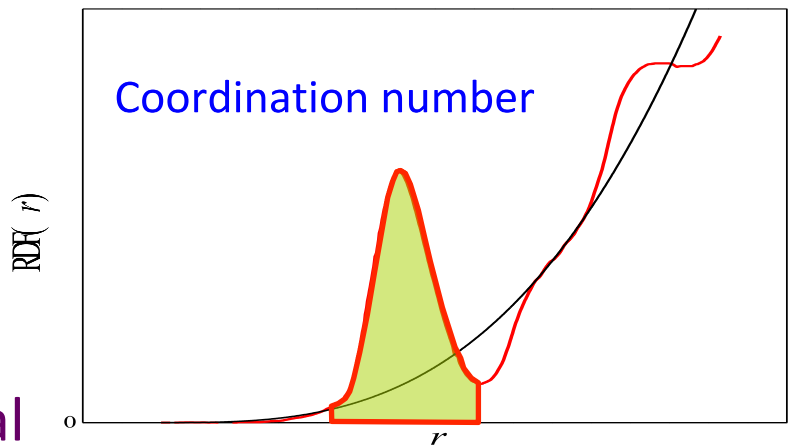
Pair distribution function $g(r)$



Pair correlation function $G(r)$ or density function $D(r)$

$$G(r) = D(r) = 4\pi\, r\, \rho\, [g(r) - 1]$$





Radial distribution function RDF(r)

$$\mathrm{RDF}(r) = 4\pi\, r^2\, \rho\, g(r)$$

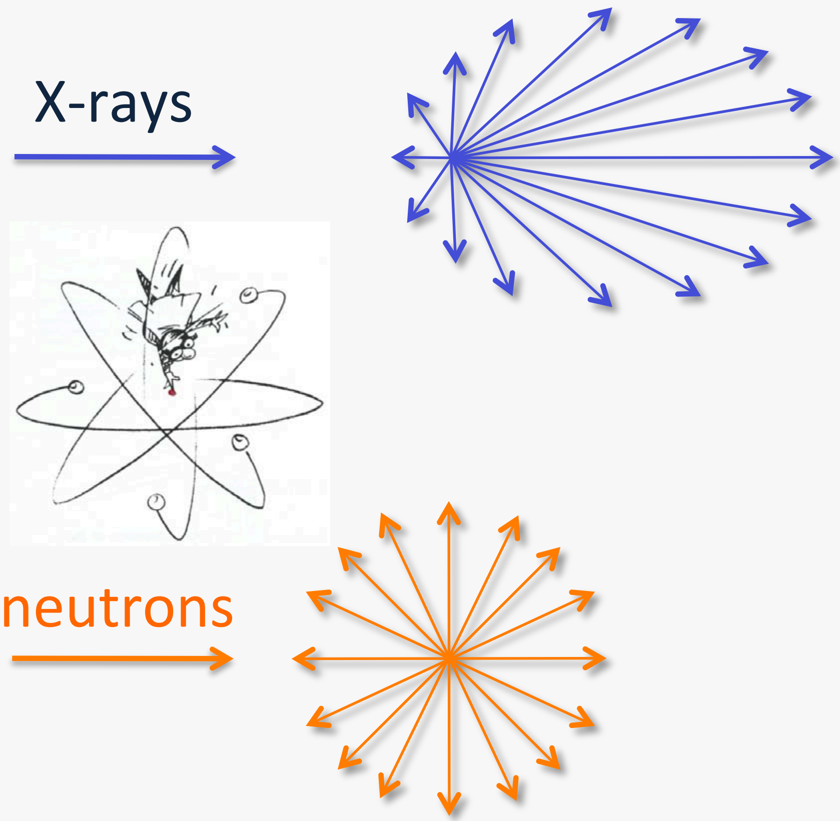
$$T(r) = \mathrm{RDF}(r)/r = 4\pi\, r\, \rho\, g(r) = 4\pi\, r\, \rho + G(r)$$

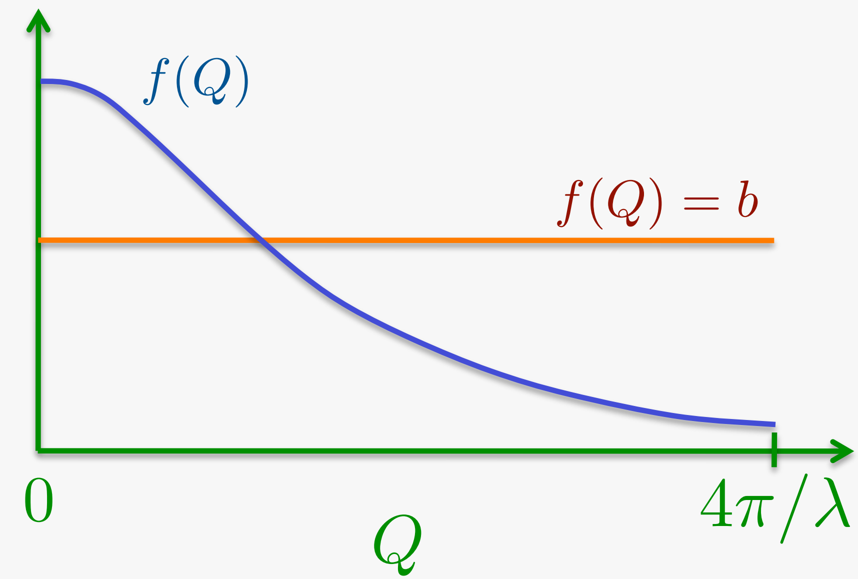
Remember!

$$g(r) - 1 \propto \mathrm{FT}\,\{S(Q) - 1\} / \rho$$

X-rays *vs* neutrons

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right) = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{jj'} f_j(\vec{Q})f_{j'}(\vec{Q})\int_{-\infty}^{\infty}\langle \mathrm{e}^{-i\vec{Q}\cdot\vec{r}_{j'}(0)}\mathrm{e}^{i\vec{Q}\cdot\vec{r}_j(t)}\rangle \mathrm{e}^{-i\omega t}\mathrm{d}t$$





Bragg law $\quad Q = \frac{4\pi}{\lambda}\sin\left(\frac{2\theta}{2}\right)$

Multiatomic systems

System of n chemical species

$$\bar{b}^2 \ \underbrace{[S(Q)-1]}_{F(Q)} = \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} c_\alpha c_\beta b_\alpha b_\beta \ [S_{\alpha\beta}(Q)-1]$$

$n\ (n+1)/2$ independent partial $S_{\alpha\beta}(Q)$

$$\bar{b}^2 = \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} c_\alpha c_\beta b_\alpha b_\beta$$

Change b_α by

- Isotopic substitution
- X-ray experiments
- Anomalous diffraction

$$\mathbf{F}_{\mathrm{exp}}(Q) = \mathbf{A}\ \mathbf{F}_{\mathrm{p}}(Q)$$

NDIS: $|\mathbf{A}| < 0.1$

Binary system:

Two different species: x, y

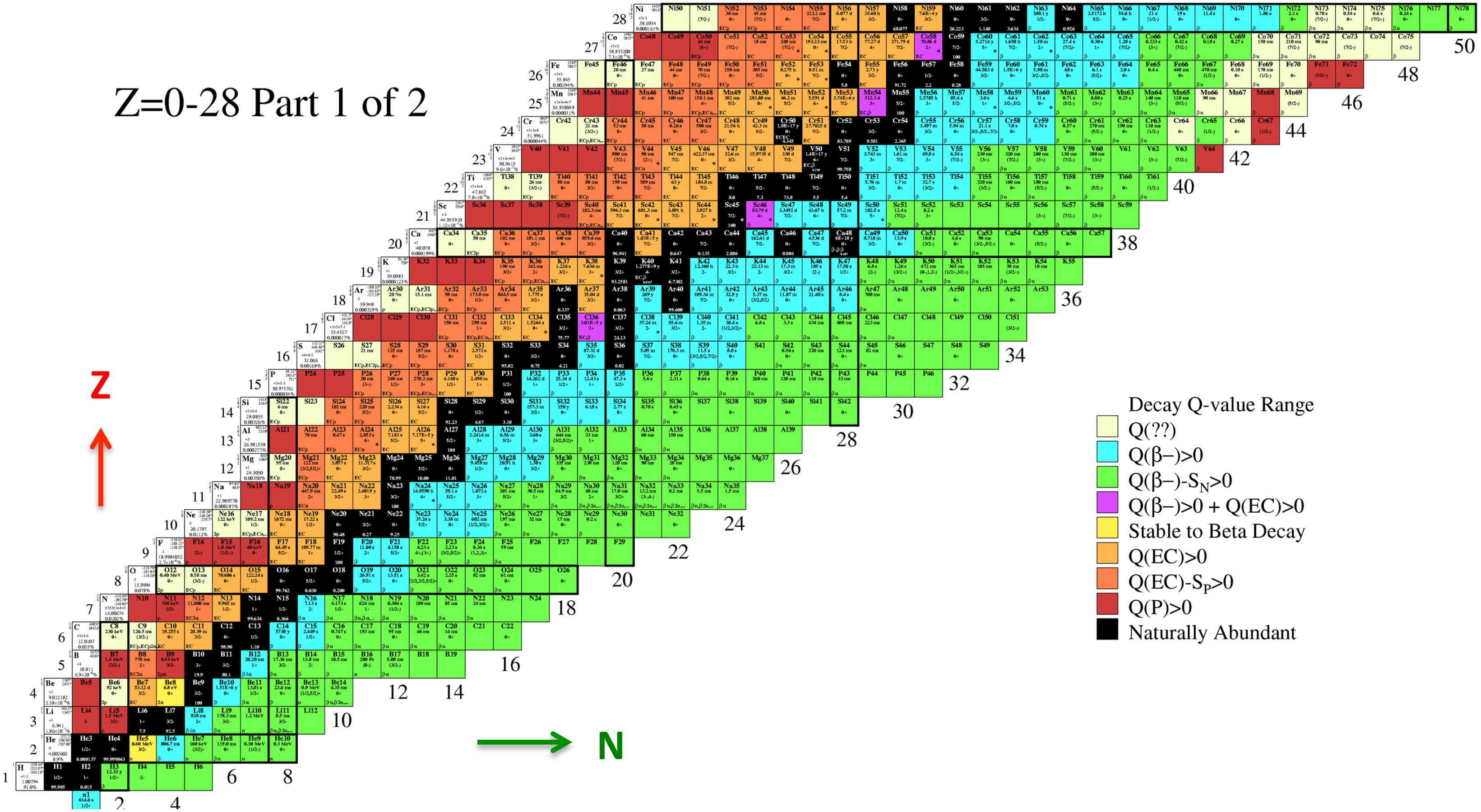
Fixed composition: constant c_x , c_y

Isotopes with good contrast

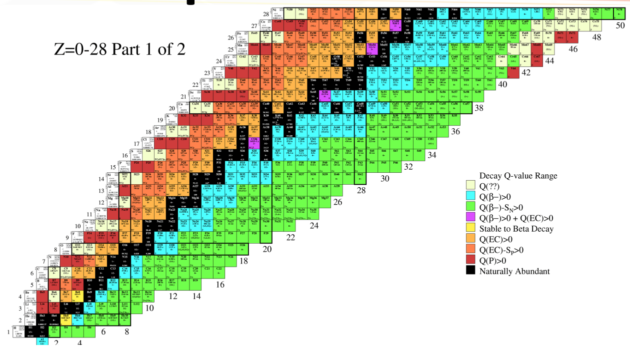
$b_{\alpha i}$: scattering length of isotope i of species α

$$\bar{b}^2 \begin{pmatrix} F_{\mathrm{S1}}(Q) \\ F_{\mathrm{S2}}(Q) \\ F_{\mathrm{S3}}(Q) \end{pmatrix} = \begin{pmatrix} c_{\mathrm{X}}^2 b_{\mathrm{X1}}^2 & c_{\mathrm{Y}}^2 b_{\mathrm{Y1}}^2 & 2c_{\mathrm{X}}c_{\mathrm{Y}}b_{\mathrm{X1}}b_{\mathrm{Y1}} \\ c_{\mathrm{X}}^2 b_{\mathrm{X2}}^2 & c_{\mathrm{Y}}^2 b_{\mathrm{Y2}}^2 & 2c_{\mathrm{X}}c_{\mathrm{Y}}b_{\mathrm{X2}}b_{\mathrm{Y2}} \\ c_{\mathrm{X}}^2 b_{\mathrm{X3}}^2 & c_{\mathrm{Y}}^2 b_{\mathrm{Y3}}^2 & 2c_{\mathrm{X}}c_{\mathrm{Y}}b_{\mathrm{X3}}b_{\mathrm{Y3}} \end{pmatrix} \begin{pmatrix} F_{\mathrm{XX}}(Q) \\ F_{\mathrm{YY}}(Q) \\ F_{\mathrm{XY}}(Q) \end{pmatrix}$$

Isotopic substitution



Isotopic substitution



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw		

20%
5%
1c$
ABS
Abs
Inc
Rad

Appendix

Neutron Scattering Lengths and Cross Sections

Javier Dawidowski, José Rolando Granada, Javier Roberto Santisteban, Florencia Cantargi and Luis Alberto Rodríguez Palomino

Comisión Nacional de Energía Atómica, Consejo Nacional de investigaciones Científicas y Técnicas, Centro Atómico Bariloche and Instituto Balseiro, Bariloche, Río Negro, Argentina

Experimental Methods in the Physical Sciences, Vol. 44.

Periodic table showing elements with isotopes with > 20 % scattering length contrast (orange), 5 - 20 % contrast (blue), mono-isotopic, lack of scattering length contrast or prohibitively expensive isotopes (grey), elements with high absorption coefficients where non-absorbing isotopes are available (green), elements with isotopes to overcome incoherent scattering effects (yellow) and radioactive elements (red).

A binary system

Fast-ion conductor or semiconductor glasses

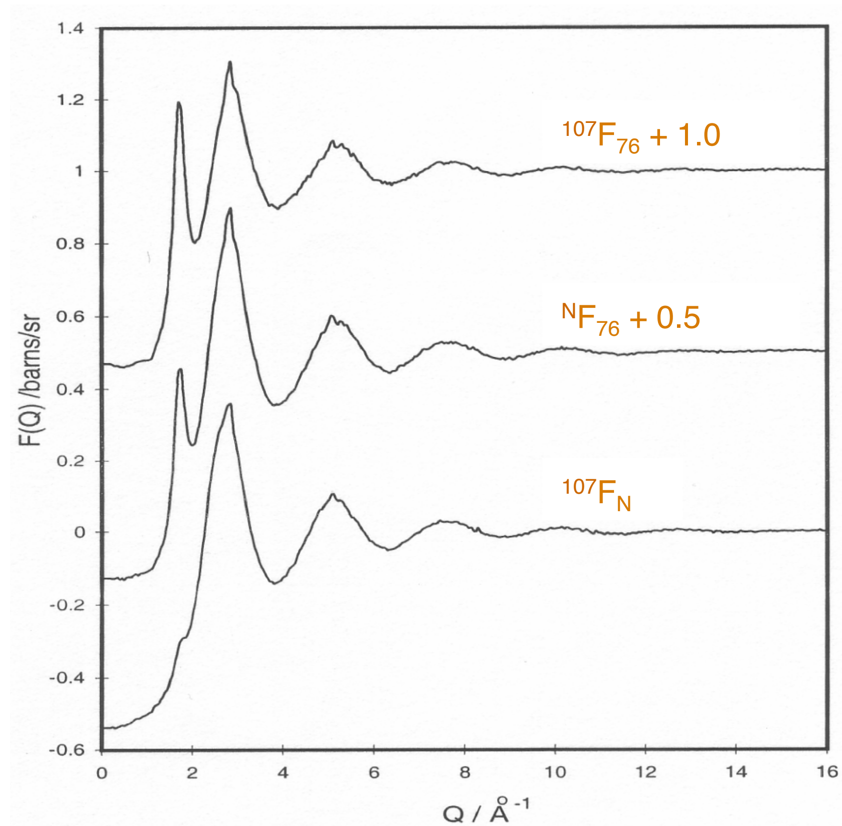
Silver chalcogenides Ag_2X + Network formers AsX or As_2X_3

X= S, Te or Se

Samples: $^{107}Ag_2{}^{nat}Se$, $^{109}Ag_2{}^{76}Se$, $^{nat}Ag_2{}^{76}Se$

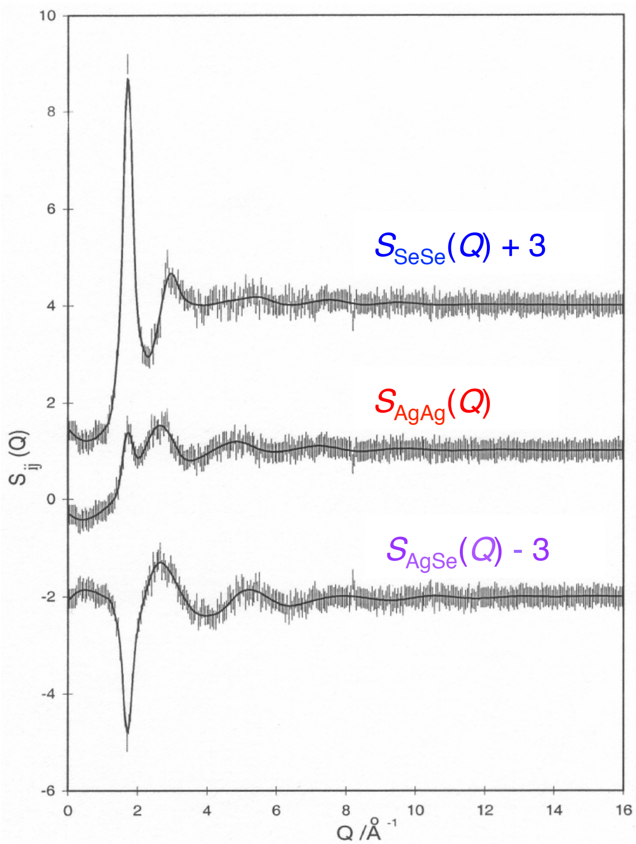
Isotope	*b* (fm)	σ_a (b)	σ_s (b)
^{n}Ag	**5.922**	**24.6**	**4.99**
^{107}Ag	7.64	14.6	7.44
^{109}Ag	4.19	35.4	2.55
^{n}Se	**7.97**	**4.55**	**8.31**
^{76}Se	12.2	33.1	18.7

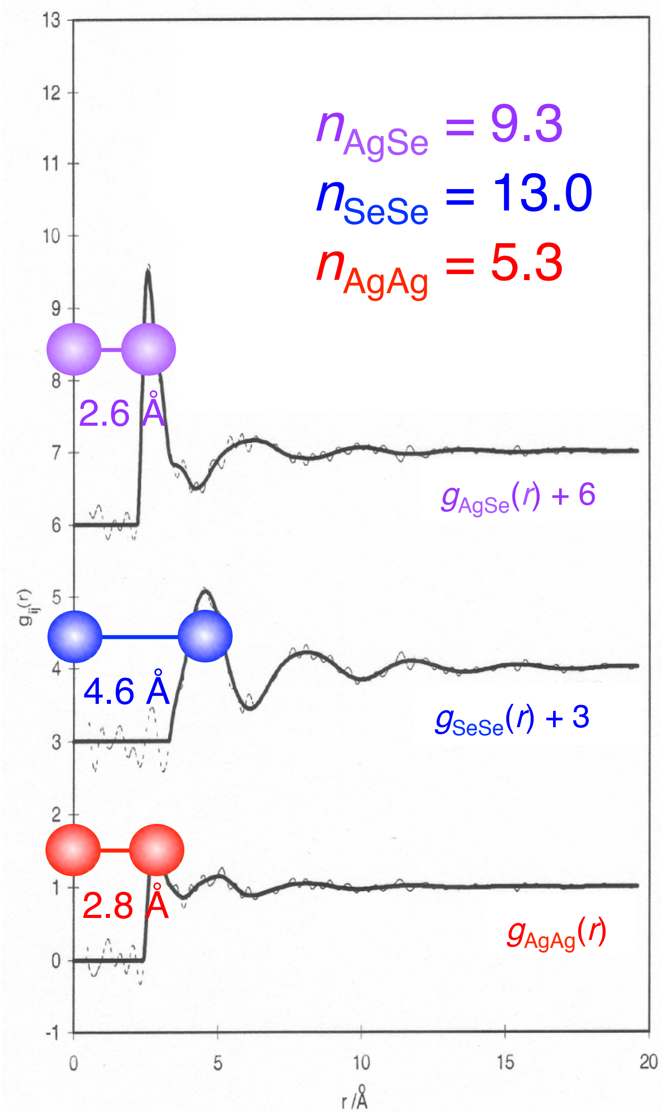
$$\begin{bmatrix} {}^{107}_{nat}F_{S1}(Q) \\ {}^{109}_{76}F_{S2}(Q) \\ {}^{nat}_{76}F_{S3}(Q) \end{bmatrix} = \begin{bmatrix} 0.2594 & 0.0706 & 0.2706 \\ 0.0780 & 0.1654 & 0.2272 \\ 0.1559 & 0.1654 & 0.3211 \end{bmatrix} \begin{bmatrix} F_{AgAg}(Q) \\ F_{SeSe}(Q) \\ F_{AgSe}(Q) \end{bmatrix}$$



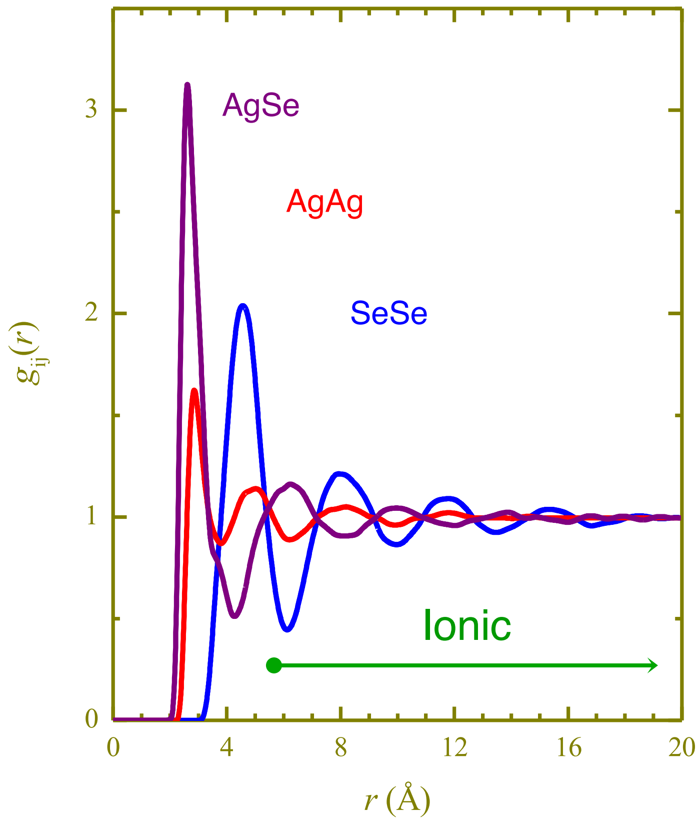
Partial structure factors

$$\begin{bmatrix} F_{\mathrm{AgAg}}(Q) \\ F_{\mathrm{SeSe}}(Q) \\ F_{\mathrm{AgSe}}(Q) \end{bmatrix} = \begin{bmatrix} 12.17 & 17.31 & -22.50 \\ 8.11 & 32.22 & -29.63 \\ -10.09 & -25.00 & 29.30 \end{bmatrix} \begin{bmatrix} {}^{107}_{\mathrm{nat}}F_{S1}(Q) \\ {}^{109}_{76}F_{S2}(Q) \\ {}^{\mathrm{nat}}_{76}F_{S3}(Q) \end{bmatrix}$$





Ionic behaviour



First difference method

$$\bar{b}^2\ F(Q) = \sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} c_\alpha c_\beta b_\alpha b_\beta\ F_{\alpha\beta}(Q)$$

Substitution ------→ γ: γ_1, γ_2

Important! We change scattering lengths but <u>not</u> composition

$$\bar{b}^2\ F_{\gamma 1}(Q) = c_\gamma^2 b_{\gamma 1}^2\ F_{\gamma\gamma}(Q) + c_\gamma b_{\gamma 1} \sum_{\alpha\neq\gamma}^{n} c_\alpha b_\alpha\ F_{\alpha\gamma}(Q) + \sum_{\alpha,\beta\neq\gamma}^{n} c_\alpha c_\beta b_\alpha b_\beta\ F_{\alpha\beta}(Q)$$

$$\bar{b}^2\ F_{\gamma 2}(Q) = c_\gamma^2 b_{\gamma 2}^2\ F_{\gamma\gamma}(Q) + c_\gamma b_{\gamma 2} \sum_{\alpha\neq\gamma}^{n} c_\alpha b_\alpha\ F_{\alpha\gamma}(Q) + \sum_{\alpha,\beta\neq\gamma}^{n} c_\alpha c_\beta b_\alpha b_\beta\ F_{\alpha\beta}(Q)$$

Correlation function of atom γ with all other components

$$\bar{b}^2\ \Delta F_\gamma(Q) = c_\gamma^2 (b_{\gamma 1}^2 - b_{\gamma 2}^2) \boxed{F_{\gamma\gamma}(Q)} + c_\gamma (b_{\gamma 1} - b_{\gamma 2}) \sum_{\alpha\neq\gamma}^{n} c_\alpha b_\alpha \boxed{F_{\alpha\gamma}(Q)}$$

$$\frac{\bar{b}^2\ \Delta F_\gamma(Q)}{c_\gamma^2 (b_{\gamma 1}^2 - b_{\gamma 2}^2)} = F_{\gamma\gamma}(Q) + \frac{\cancel{\sum_{\alpha\neq\gamma}^{n} c_\alpha b_\alpha\ F_{\alpha\gamma}(Q)}}{c_\gamma\ (b_{\gamma 1} + b_{\gamma 2})}$$

small

A ternary system

Li in ND_3

Metal-nonmetal transition at 7 MPM

Class A metals

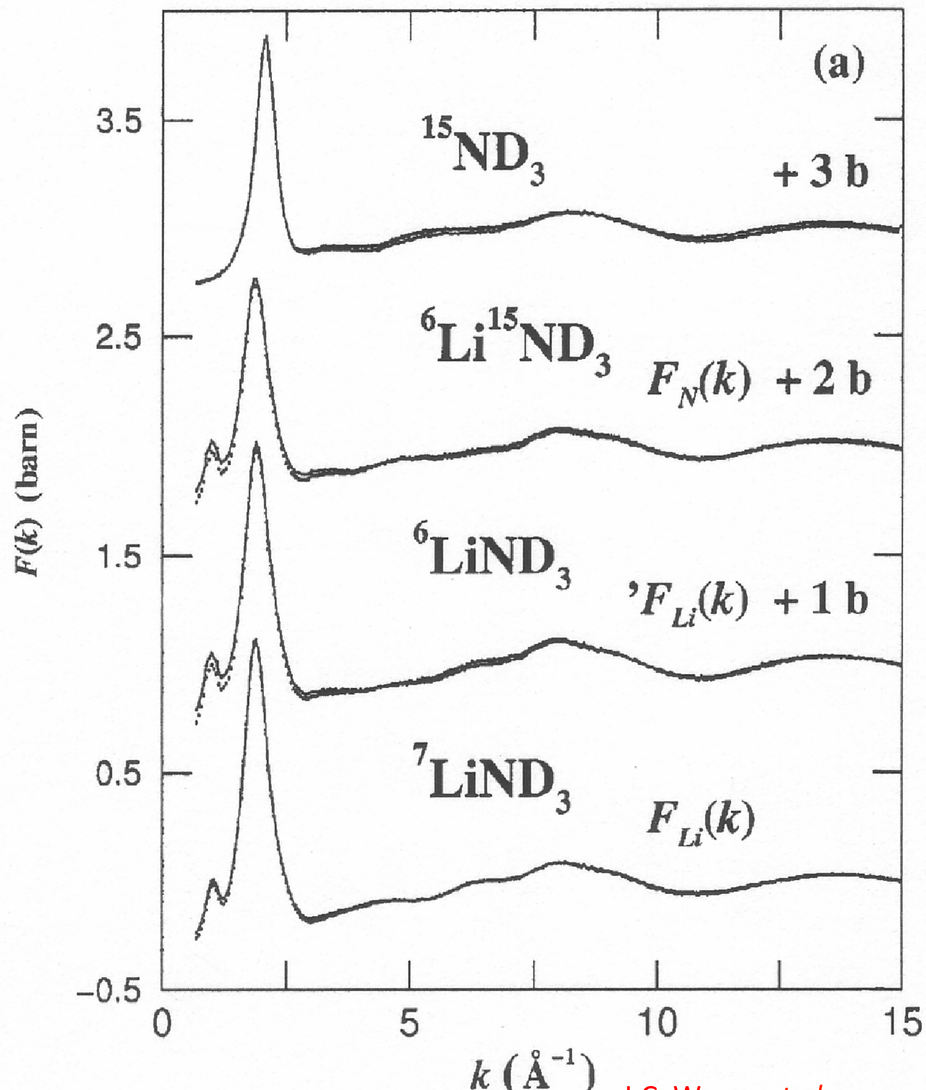
Conductivity 15000 Ω^{-1} cm^{-1} mol^{-1}

3 species $\Rightarrow$ 6 different experiments!

First difference method

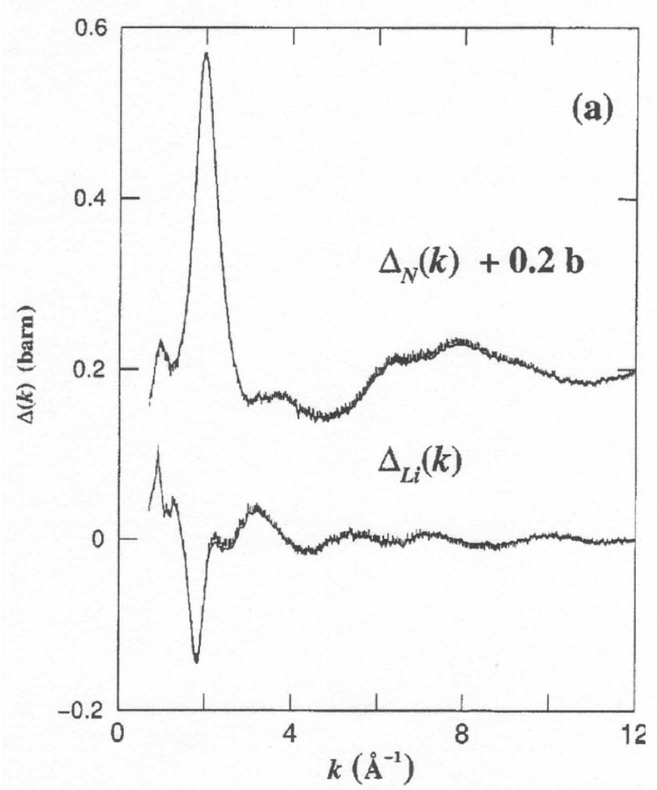
Samples:

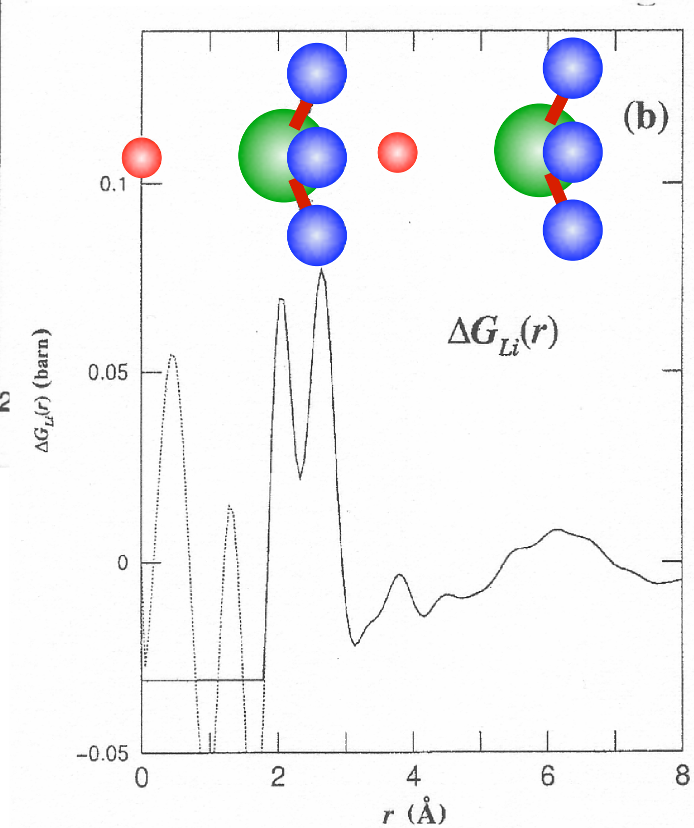
- ^{6}Li in $^{nat}ND_3$
- ^{7}Li in $^{nat}ND_3$
- ^{6}Li in $^{15}ND_3$
- $^{15}ND_3$

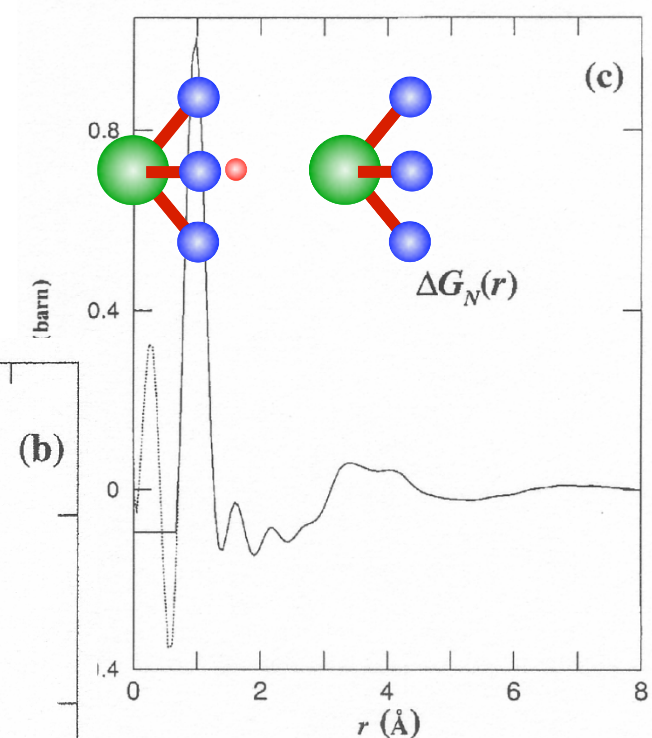


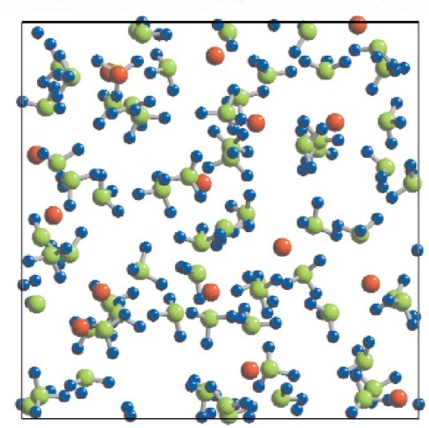
J.C. Wasse *et al.*
PRB **61**, 11993 (2000)

Quasi-partials









J.C. Wasse *et al.*
PRB **61**, 11993 (2000)

Second difference method

New substitution δ: δ_1, δ_2

$$\bar{b}^2\,\Delta F_{\gamma\delta 1}(Q) = c_\gamma^2 (b_{\gamma 1}^2 - b_{\gamma 2}^2)\,F_{\gamma\gamma}(Q) + c_\gamma c_\delta (b_{\gamma 1} - b_{\gamma 2})\,b_{\delta 1} \boxed{F_{\gamma\delta}(Q)} + c_\gamma (b_{\gamma 1} - b_{\gamma 2}) \sum_{\alpha \neq \gamma,\delta}^{n} c_\alpha b_\alpha\,F_{\alpha\gamma}(Q)$$

$$\bar{b}^2\,\Delta F_{\gamma\delta 2}(Q) = c_\gamma^2 (b_{\gamma 1}^2 - b_{\gamma 2}^2)\,F_{\gamma\gamma}(Q) + c_\gamma c_\delta (b_{\gamma 1} - b_{\gamma 2})\,b_{\delta 2} \boxed{F_{\gamma\delta}(Q)} + c_\gamma (b_{\gamma 1} - b_{\gamma 2}) \sum_{\alpha \neq \gamma,\delta}^{n} c_\alpha b_\alpha\,F_{\alpha\gamma}(Q)$$

$$\bar{b}^2\,\Delta^2 F_{\gamma\delta}(Q) = c_\gamma c_\delta (b_{\gamma 1} - b_{\gamma 2})\,(b_{\delta 1} - b_{\delta 2}) \boxed{F_{\gamma\delta}(Q)}$$

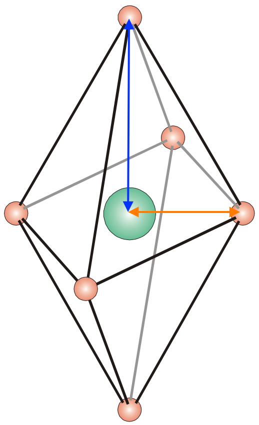
$$F_{\gamma\delta}(Q) = \frac{\bar{b}^2\,\Delta^2 F_{\gamma\delta}(Q)}{c_\gamma c_\delta (b_{\gamma 1} - b_{\gamma 2})\,(b_{\delta 1} - b_{\delta 2})}$$

Partial structure factor
for pairs γ and δ

Cu(II) aqua ion

A. Pasquarello *et al.*
Science **291**, 856 (2001)

Model Octahedral complex $[Cu(H_2O)]^{2+}$
Sixfold coordination



X-ray diffraction
EXAFS
XANES
NDIS

A priori assumptions about structure

Overlap axial Cu-O and Cu-H

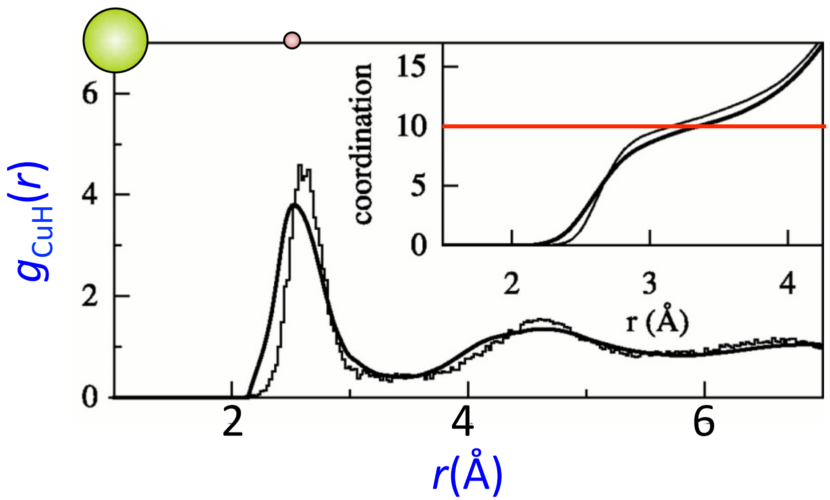
System:
$Cu(ClO_4)_2$+$HClO_4$ in H_2O
→ 10 expts!

Samples:
$^{65}Cu(ClO_4)_2$+$HClO_4$ in H_2O
$^{63}Cu(ClO_4)_2$+$HClO_4$ in H_2O
$^{65}Cu(ClO_4)_2$+$DClO_4$ in D_2O
$^{63}Cu(ClO_4)_2$+$DClO_4$ in D_2O

Second difference method

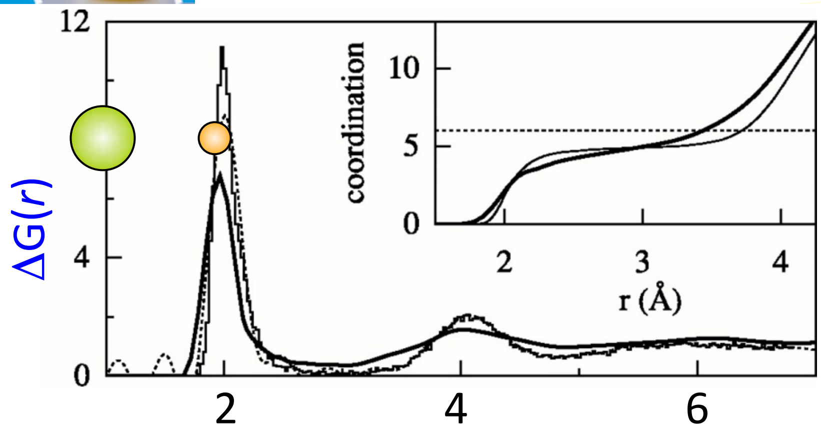
$$\Delta F_{\underset{D}{H}} = c_{Cu}^2 (b_{65}^2 - b_{63}^2) F_{CuCu} + 2 c_{Cu} (b_{65} - b_{63}) \times (c_{Cl} b_{Cl} F_{CuCl} + c_O b_O F_{CuO} + c_H b_{\underset{D}{H}} F_{CuH})$$

$$\boxed{\Delta^2 F = 2 c_{Cu} c_H (b_{65} - b_{63}) (b_D - b_H) F_{CuH}}$$



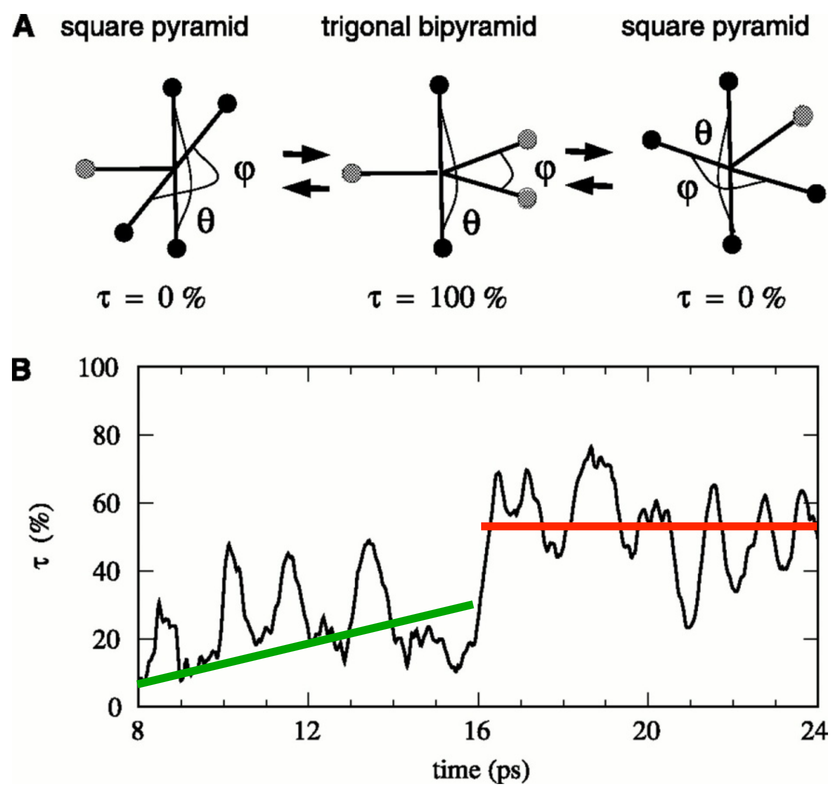
Five-fold coordinated ion

A. Pasquarello *et al.*
Science **291**, 856 (2001)



$$\Delta F = F_{CuO} + 0.044\, F_{CuCu} + 0.102\, F_{CuCl}$$

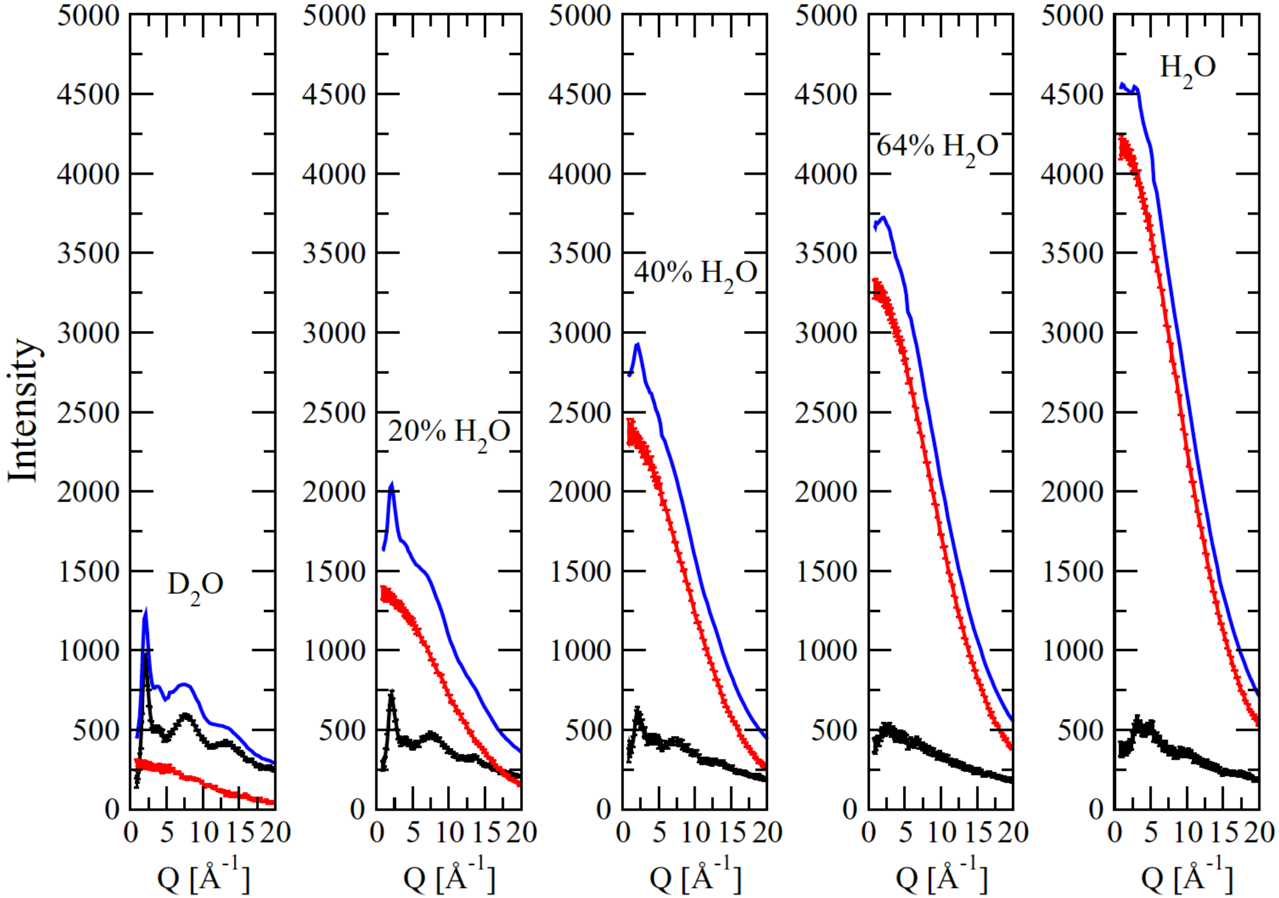
First-principles Molecular Dynamics Simulation



$$\tau = (\theta - \varphi)/60 \times 100\%$$

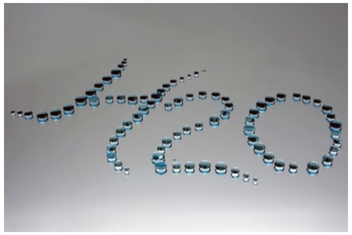
Cu(II) aqua ion is **five-fold** coordinated

H incoherence problem



Neutron diffraction of hydrogenous materials: Measuring incoherent and coherent intensities separately

László Temleitner, Anne Stunault, Gabriel J. Cuello, and László Pusztai
Phys. Rev. B **92**, 014201 – Published 1 July 2015



Isotopes

σ_c	σ_i	σ_s	σ_a
44.89 (4)	0	44.89 (4)	0
1.7568 (10)	80.26(6)	82.02 (6)	0.3326 (7)
1.7589 (11)	79.91(4)	81.67 (4)	0.3326 (7)
5.597 (10)	2.04(3)	7.64(3)	0.000519 (7)
2.89(3)	0.14(4)	3.03(5)	<6E−06

Appendix

Neutron Scattering Lengths and Cross Sections

Javier Dawidowski, José Rolando Granada, Javier Roberto Santisteban, Florencia Cantargi and Luis Alberto Rodríguez Palomino
Comisión Nacional de Energía Atómica, Consejo Nacional de investigaciones Científicas y Técnicas, Centro Atómico Bariloche and Instituto Balseiro, Bariloche, Río Negro, Argentina

Experimental Methods in the Physical Sciences, Vol. 44.
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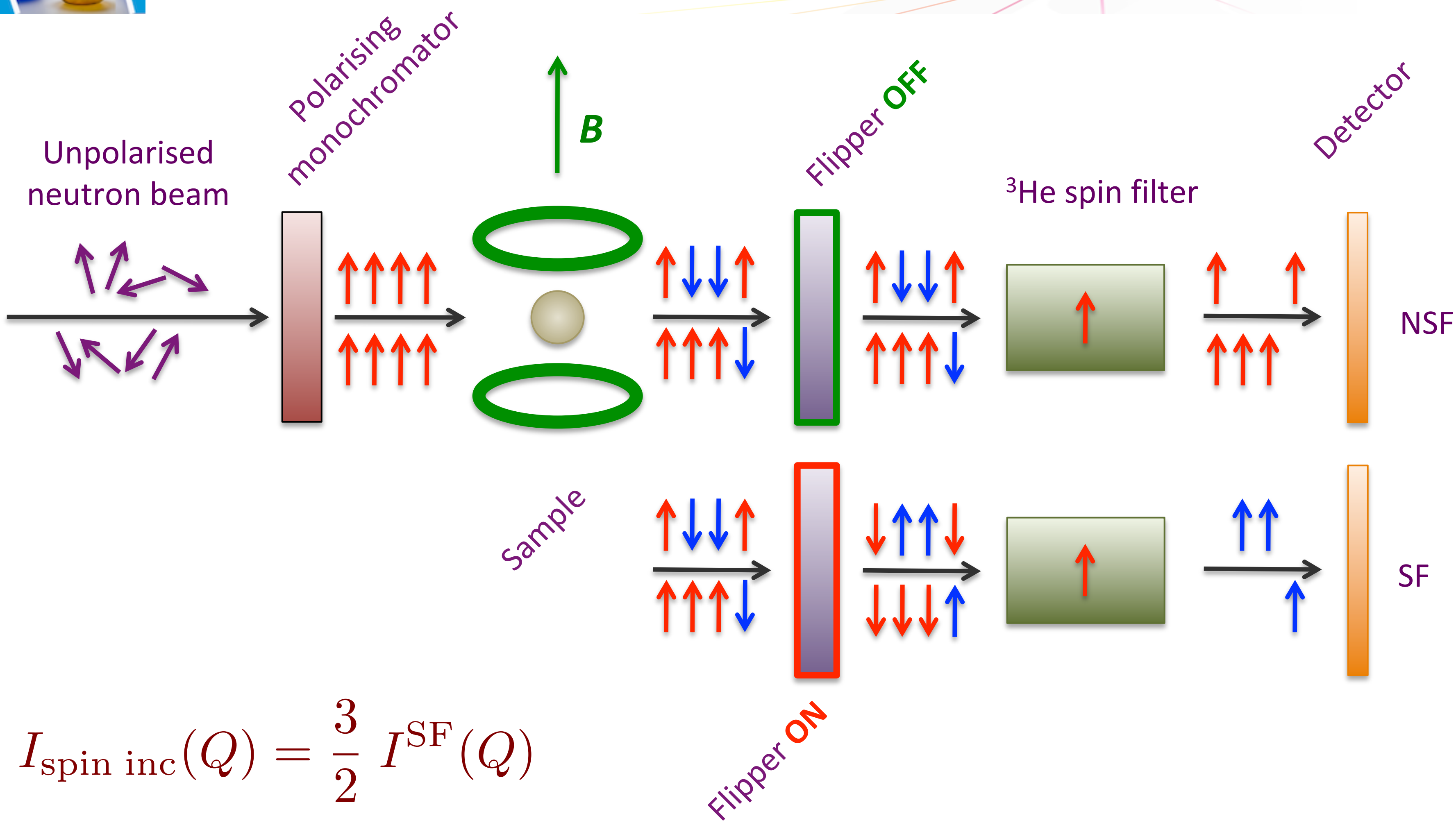
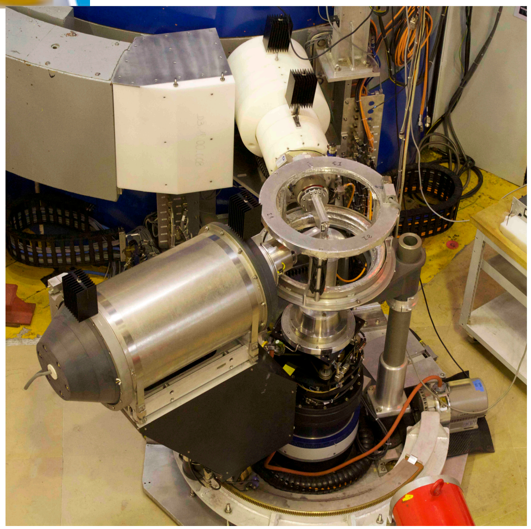
Polarised neutrons



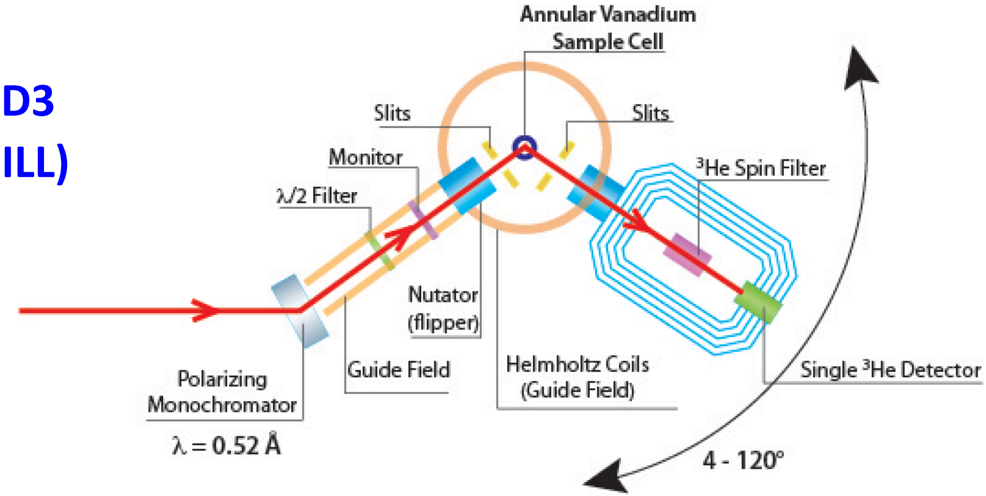
$$I_{\text{spin inc}}(Q) = \frac{3}{2}\, I^{\text{SF}}(Q)$$

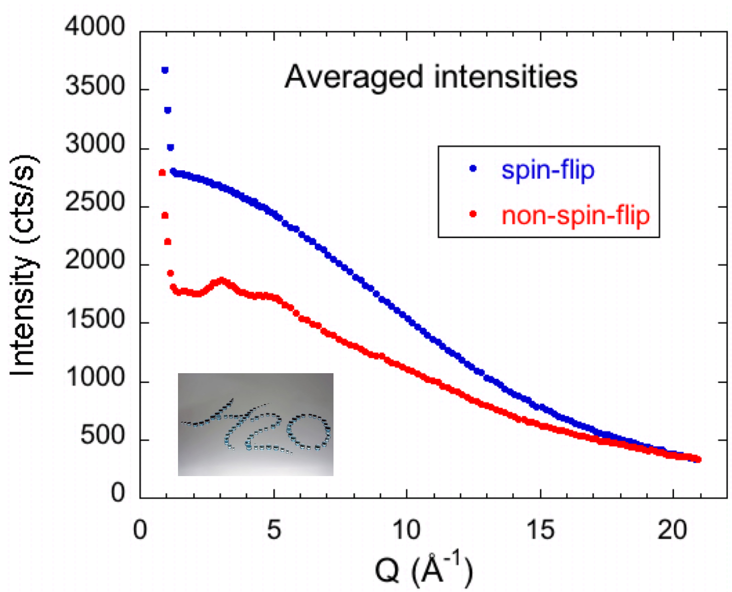
$$I_{\text{coh}}(Q) + I_{\text{isotope inc}}(Q) = I^{\text{NSF}}(Q) - \frac{1}{2}\, I^{\text{SF}}(Q)$$

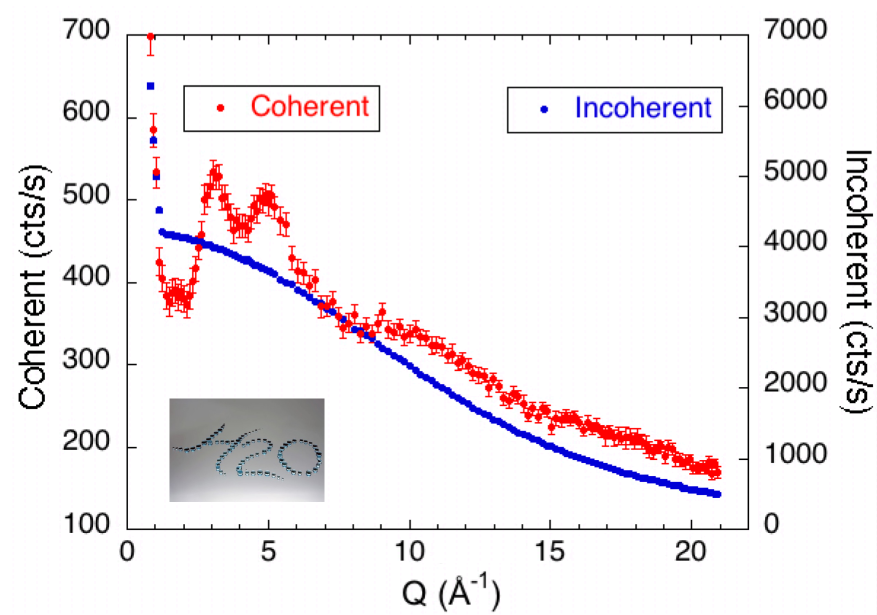
Example: water



D3
(ILL)







Tutorial:
Neutron total scattering

Gabriel Cuello
Institut Laue Langevin
Grenoble, France

cuello@ill.eu

Characterization of glass structure
18 - 22 November 2019
EPN Campus – Grenoble, France

Outline

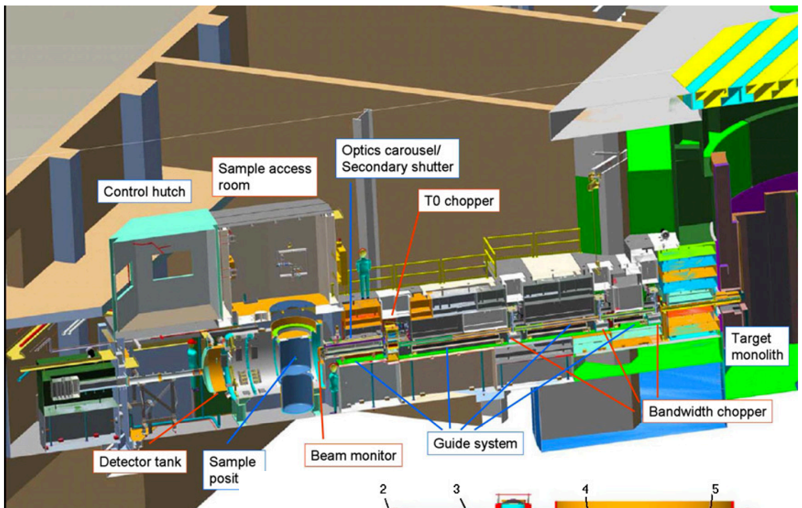
- Instruments
- Raw data
- Background subtraction
- Multiple scattering
- Inelasticity effects
- Normalisation to absolute scale
- Fourier transformation

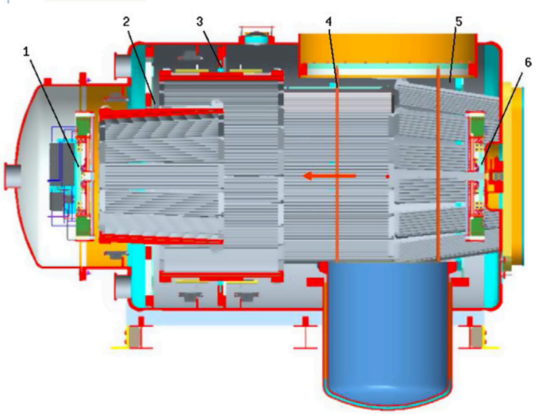
Instruments

Reactor → 2-axis → Scattering angle

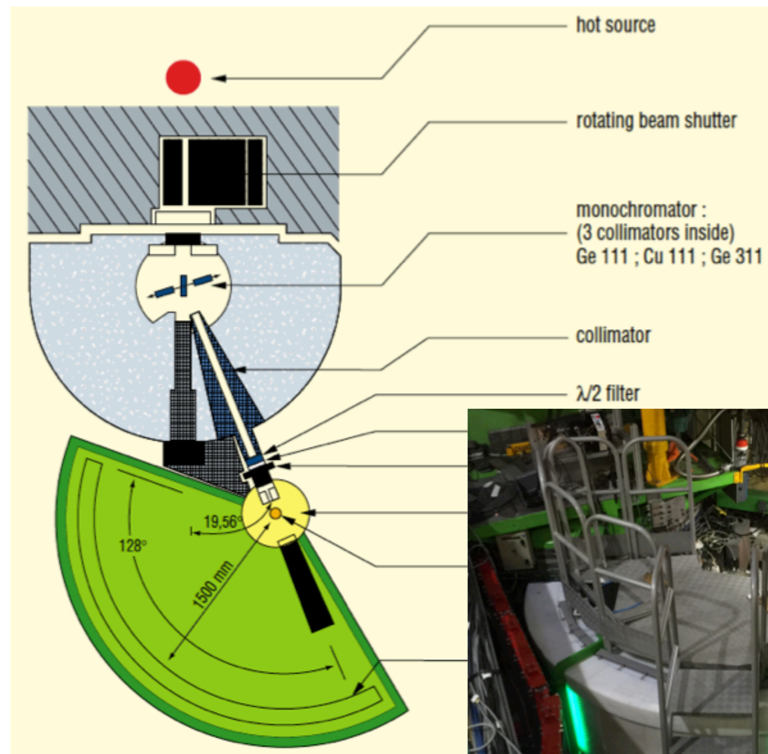
Accelerator → TOF → Time-of-flight

Elastic scattering → *Q*



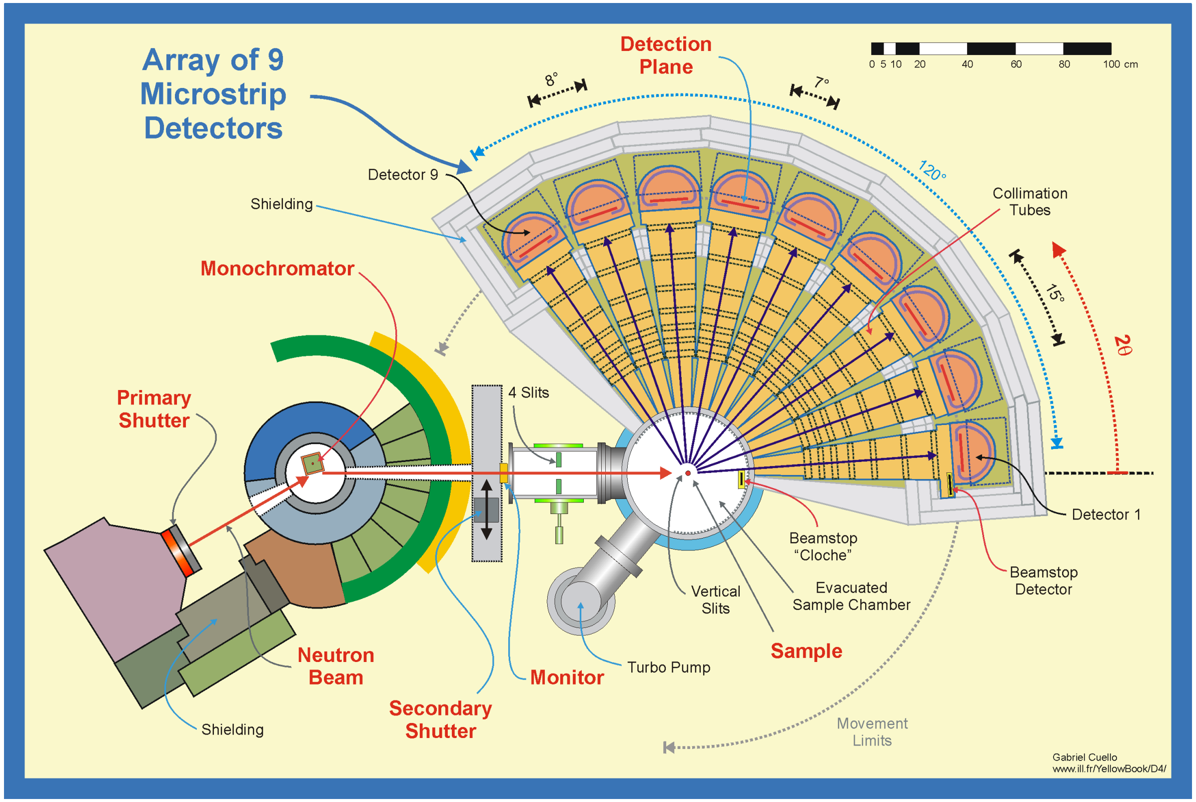


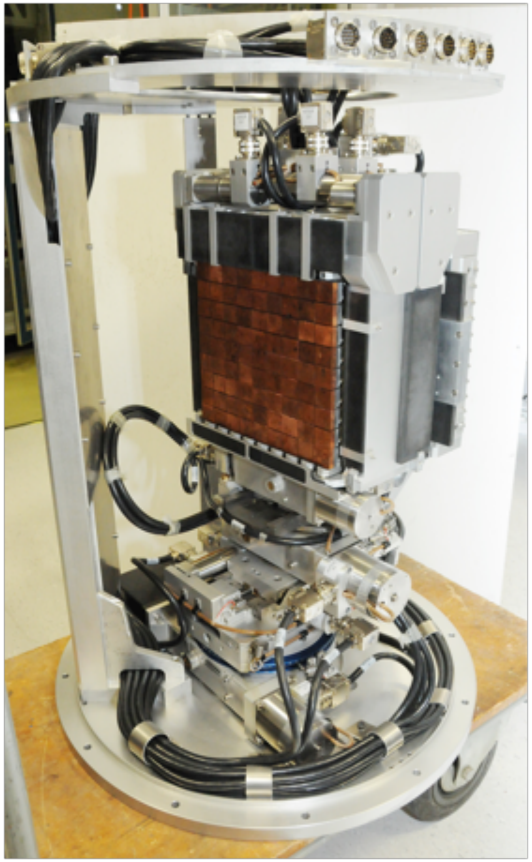
NOMAD
(ORNL)



7C2
(LLB)

D4C @ ILL

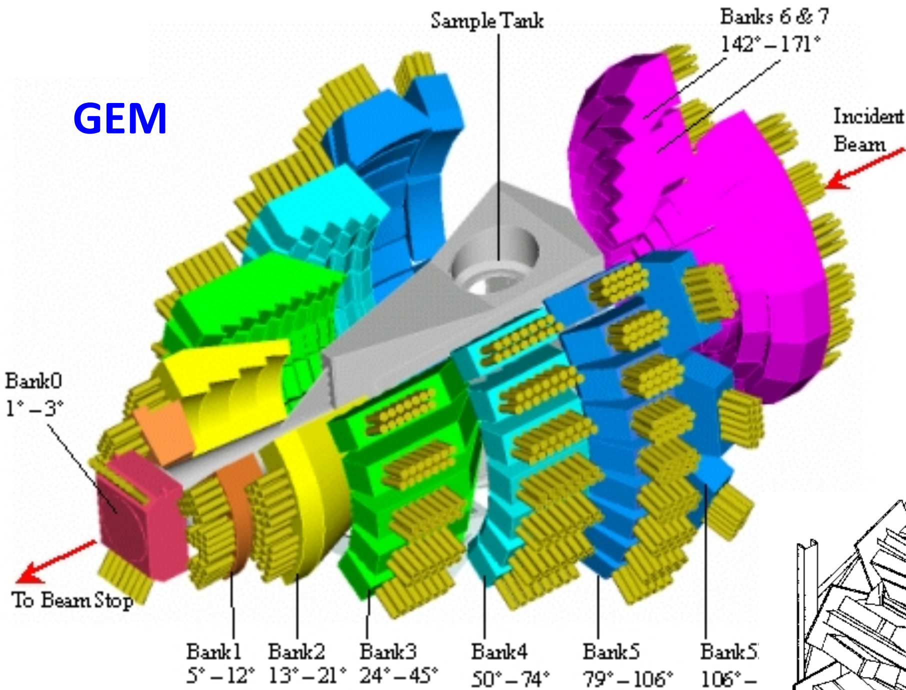


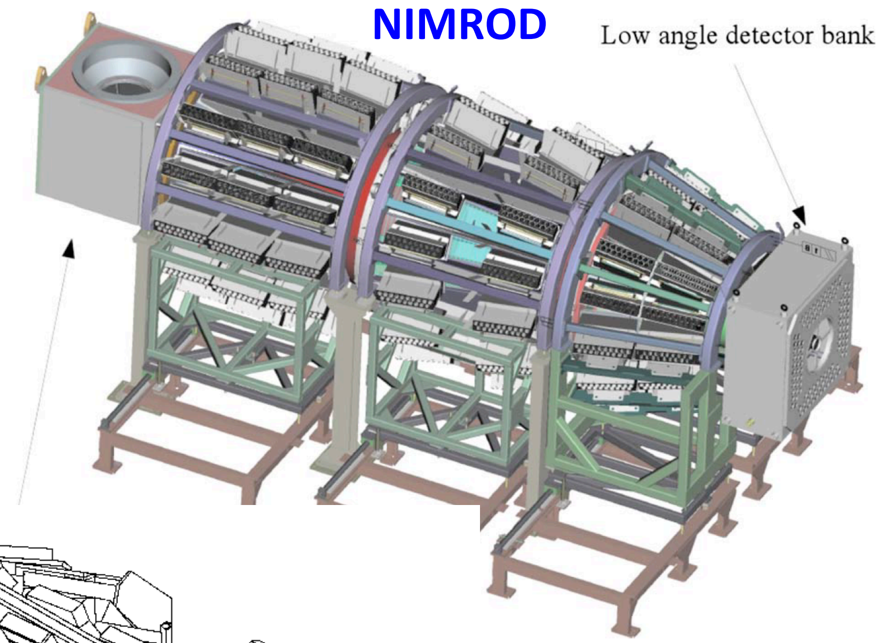


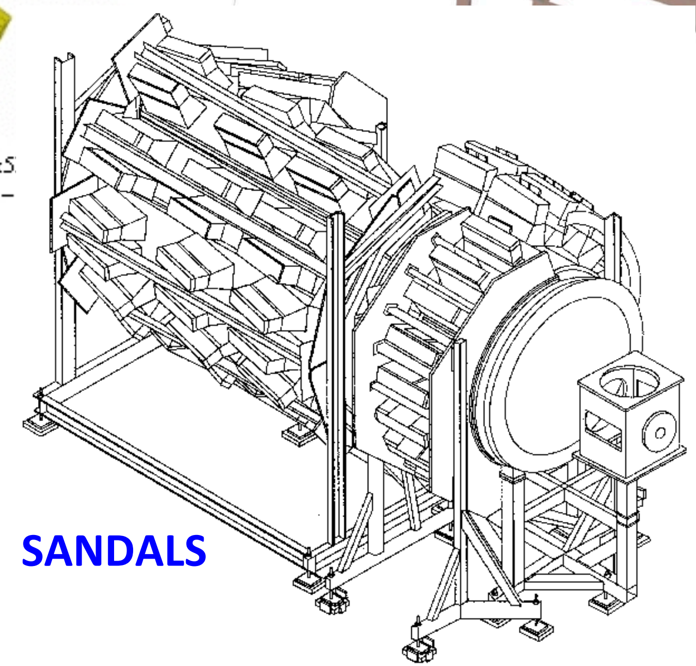
Face	d-spacing (Å)	λ (Å)	Flux (10^7 n cm^{-2} s^{-1})	Filter
Si111	1.807	0.7	5.0	Ir
Cu220	1.278	0.5	4.5	Rh
Cu331	0.829	0.35	0.3	Non

$$Q = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)$$

Instruments @ ISIS







Data reduction

$$I(2\theta,\omega) = C\,\Phi_0\,N\,\frac{k'}{k}\,\frac{\sigma}{4\pi}\,S(\vec{Q},\omega)\,\epsilon(k')$$

$$I(2\theta) = C\,\Phi_0\,N\,\frac{\sigma}{4\pi}\int_{\substack{-\infty \\ \text{constant } 2\theta}}^{E_{\max}} \mathrm{d}\omega\,\frac{k'}{k}\,S(\vec{Q},\omega)\,\epsilon(k')$$

Formal aspects

- Elastic scattering (diffraction) — Bragg's law (for *Q*); Integration limits ($\pm\infty$)
- Stationary beam
- Constant efficiency detector
- One interaction processes (single scattering)

$$I(2\theta) = C\,\Phi_0\;N/4\pi\;(\sigma_{coh}\,S(Q) + \sigma_{inc})\,\varepsilon(k)$$

Practical aspects

- Monochromatic beam
- No background
- No attenuation
- Single scattering

No beam
No container
No sample
No environment
No detector

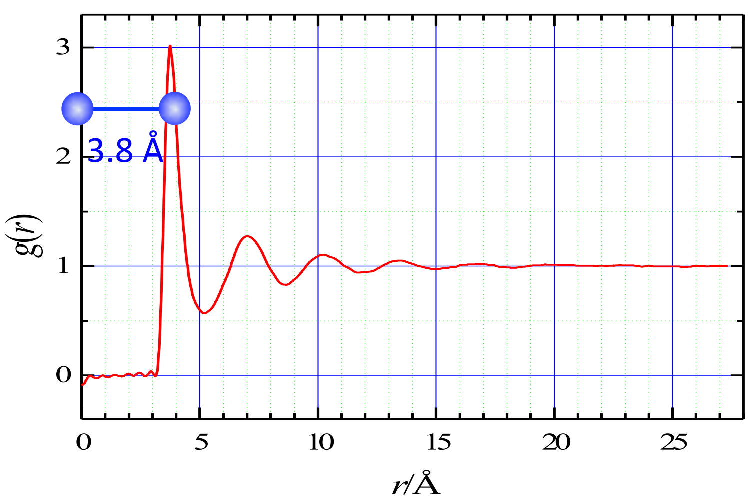
No problem!

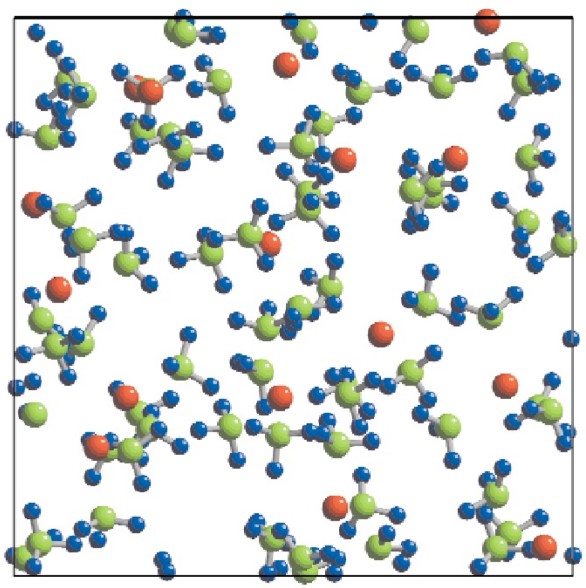
Final analysis

$I_{exp}(2\theta)$ → Corrections → $S(Q)$ → FT → $g(r)$

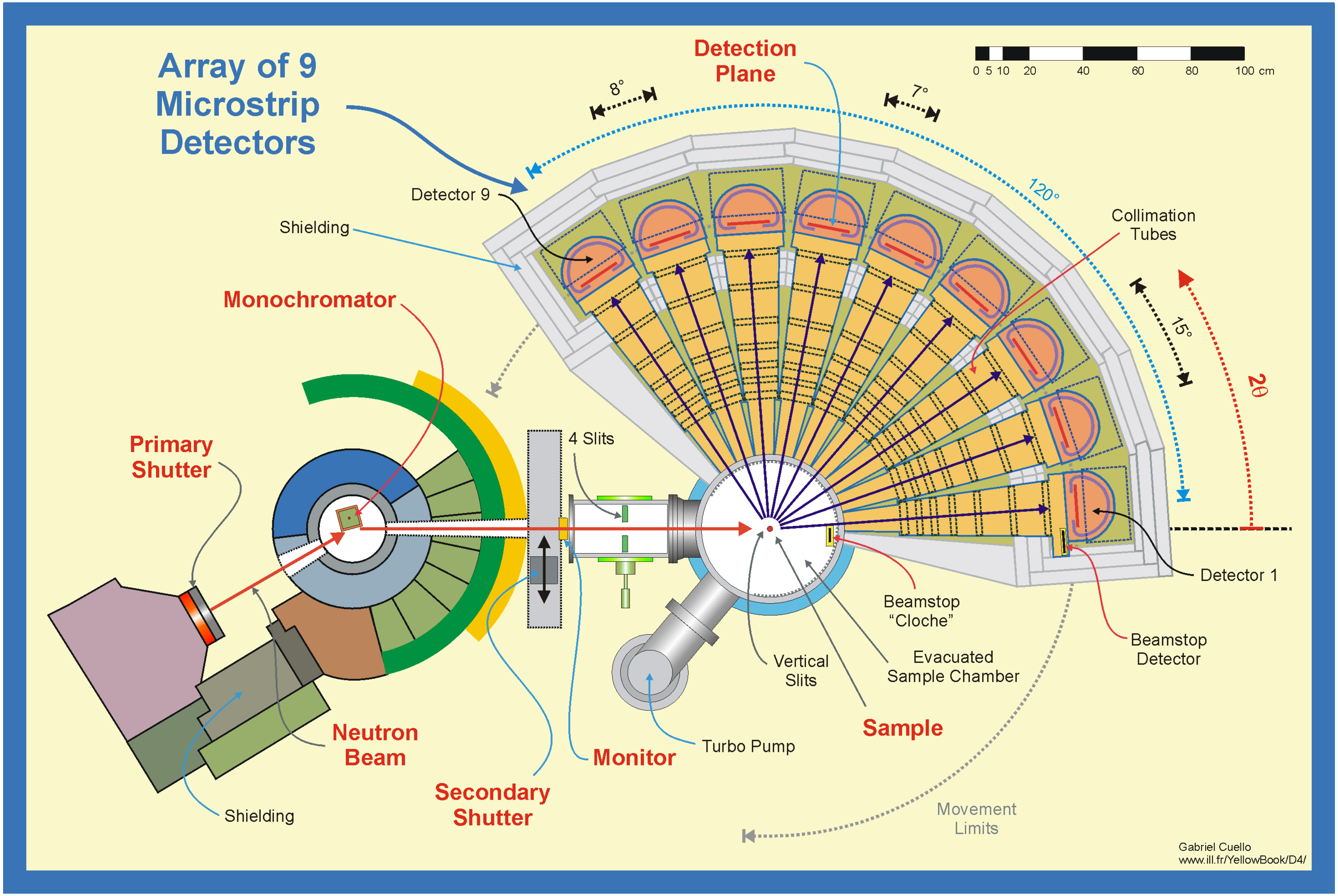
Truncation effects
Window functions

Interpretation
- Model
- Simulation, *e.g.* RMC, EPSR, MD, etc.





Instrument (D4@ILL)



Heavy atoms

SeTe alloys: different compositions and temperatures

We have measured 3 samples with compositions Se_xTe_{1-x} with $x = 0.15$, 0.20 and 0.25 at different temperatures:

$Se_{15}Te_{85}$: T = 425 C, 485 C and 550 C.
$Se_{20}Te_{80}$: T = 380 C, 400 C, 450 C, 550 C and 650 C.
$Se_{25}Te_{75}$: T = 400 C, 520 C and 650 C.

Quartz sample containers, at T = 350 C, 450 C, 550 C and 650 C.

We assume we have two diffractograms D_1 and D_2 measured at the temperatures T_1 and T_2, respectively, with $T_2 > T > T_1$.

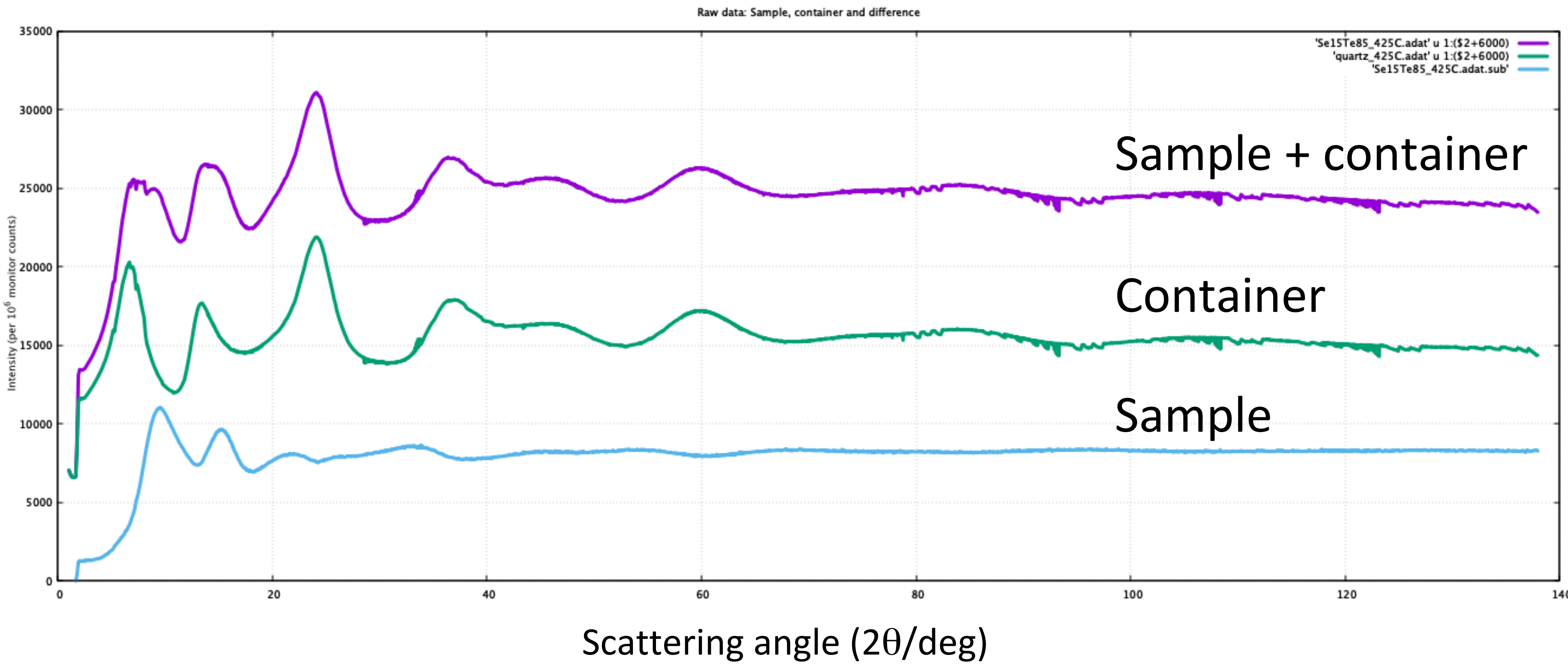
The interpolated diffractogram is then

$$D = f_1 D_1 + f_2 D_2$$

where $f_1 = (T_2 - T)/(T_2 - T_1)$ $f_2 = (T - T_1)/(T_2 - T_1)$.

Raw data

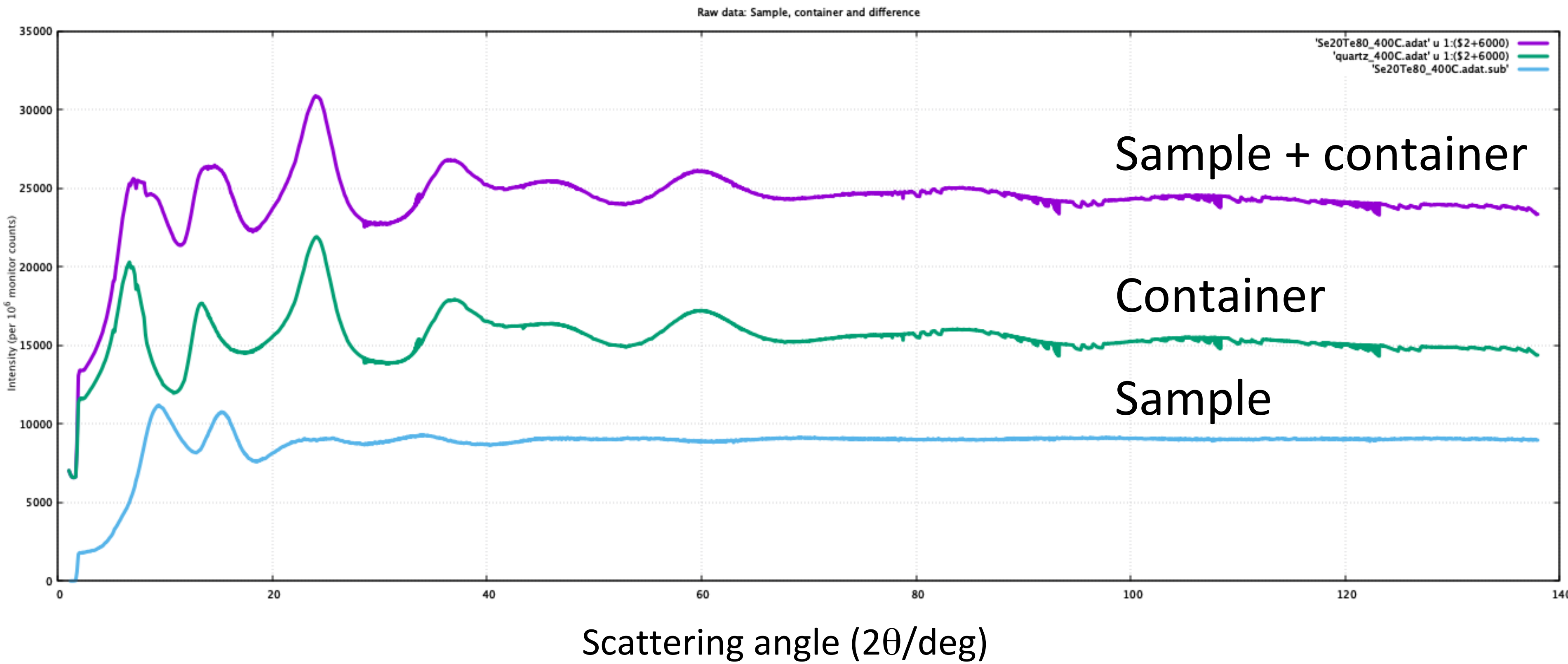
$Se_{15}Te_{85}$ @ 425 C



Sample = (Sample+container) − Container

Raw data

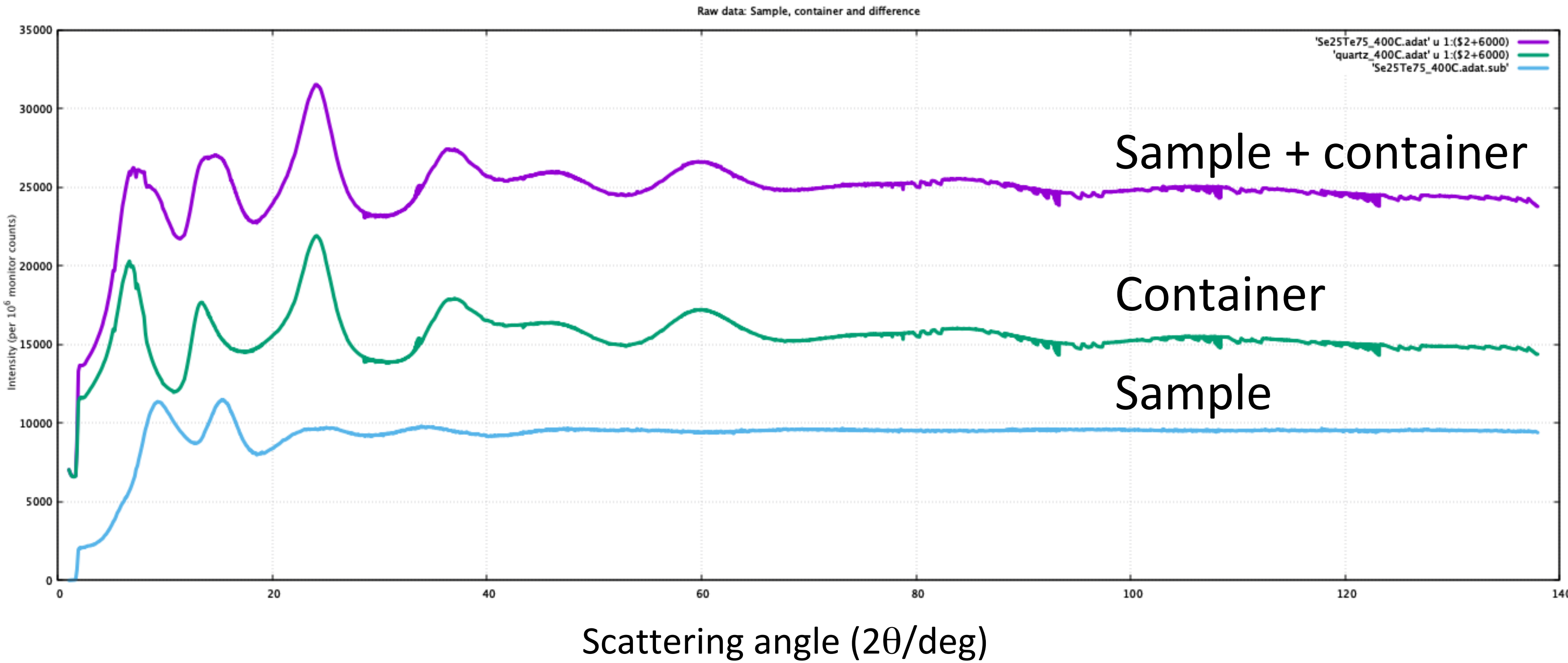
$Se_{20}Te_{80}$ @ 400 C



Sample = (Sample+container) − Container

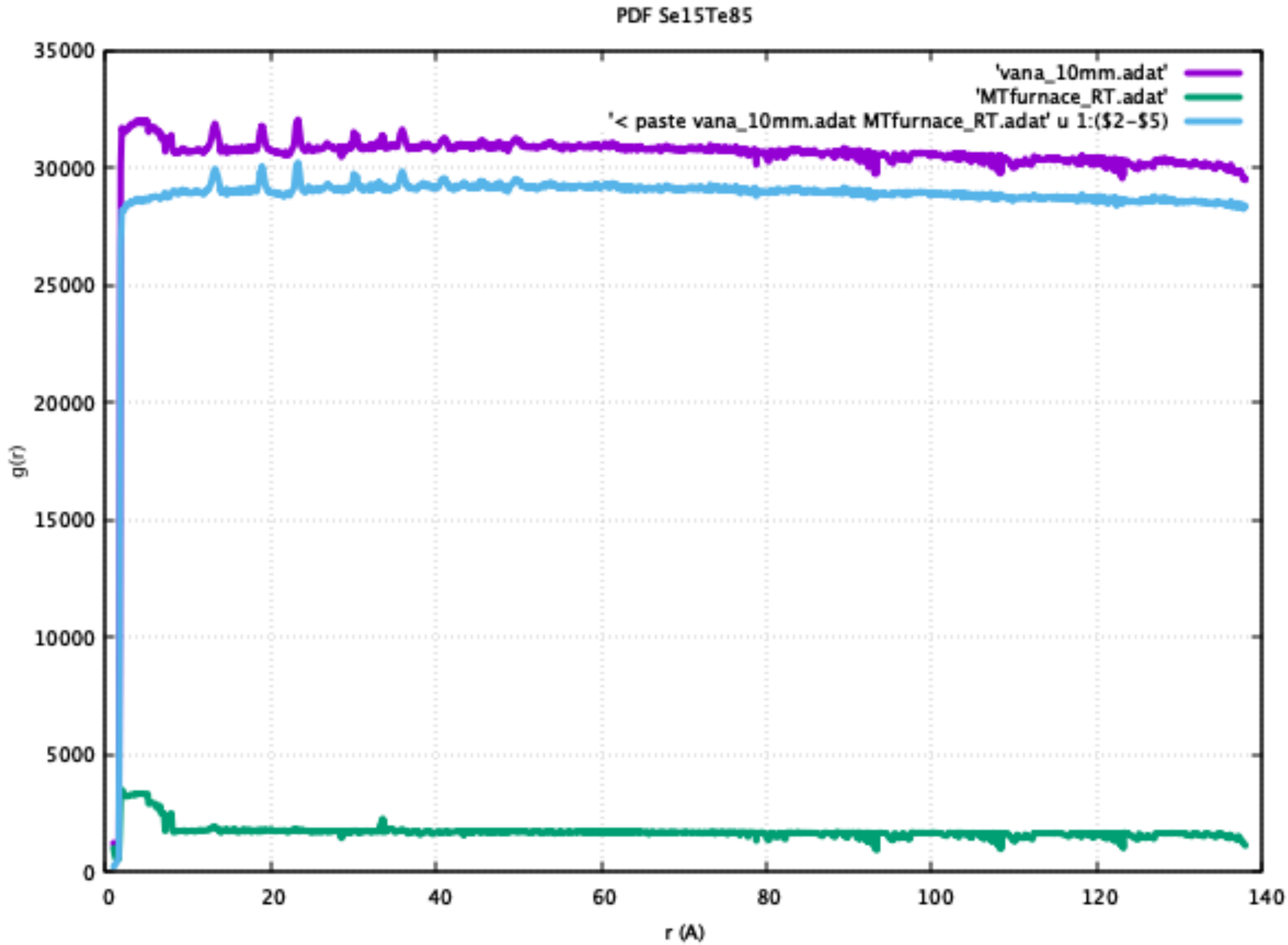
Raw data

$Se_{25}Te_{75}$ @ 400 C



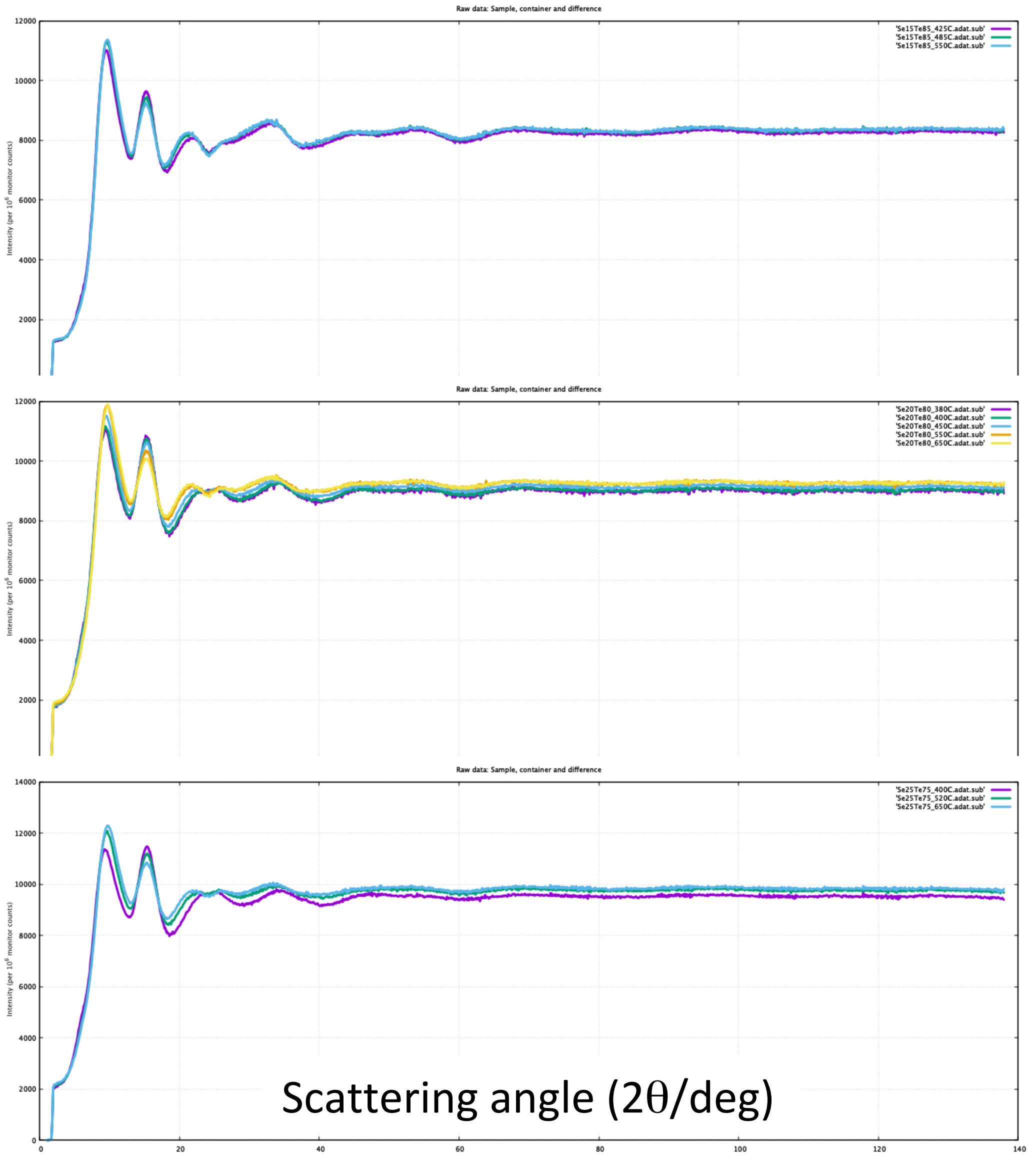
Sample = (Sample+container) − Container

Raw data


PDF Se15Te85
'vana_10mm.adat'
'MTfurnace_RT.adat'
'< paste vana_10mm.adat MTfurnace_RT.adat' u 1:($2-$5)
g(r)
r (A)
0
5000
10000
15000
20000
25000
30000
35000
0
20
40
60
80
100
120
140

Raw data

Intensity (10^6 monitor counts)



$Se_{15}Te_{85}$

$Se_{20}Te_{80}$

$Se_{25}Te_{75}$

Data reduction

$$I(2\theta,\omega) = C\,\Phi_0\,N\,\frac{k'}{k}\,\frac{\sigma}{4\pi}\,S(\vec{Q},\omega)\,\epsilon(k')$$

$$I(2\theta) = C\,\Phi_0\,N\,\frac{\sigma}{4\pi}\int_{\substack{-\infty \\ \text{constant } 2\theta}}^{E_{\max}} \mathrm{d}\omega\,\frac{k'}{k}\,S(\vec{Q},\omega)\,\epsilon(k')$$

Formal aspects

- Elastic scattering (diffraction) – Bragg's law (for *Q*); Integration limits ($\pm\infty$)
- Stationary beam
- Constant efficiency detector
- One interaction processes (single scattering)

$$I(2\theta) = C\,\Phi_0\,N/4\pi\,\left(\sigma_{coh}\,S(Q) + \sigma_{inc}\right)\,\varepsilon(k)$$

Practical aspects

- Monochromatic beam
- No background
- No attenuation
- Single scattering

$\Rightarrow$

No beam
No container
No sample
No environment
No detector

$\Rightarrow$ No problem!

Experimental corrections

Instrumental effects

- Background
- Detector efficiency
- Detector dead-time
- Instrumental resolution

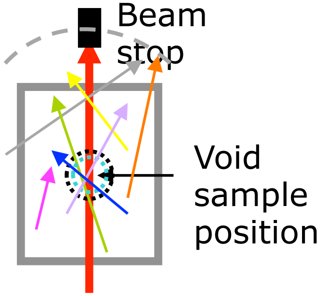
Sample effects

- Inelasticity
- Attenuation (container)
- Multiple scattering
- Normalisation

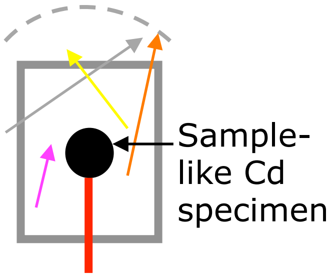
Background noise

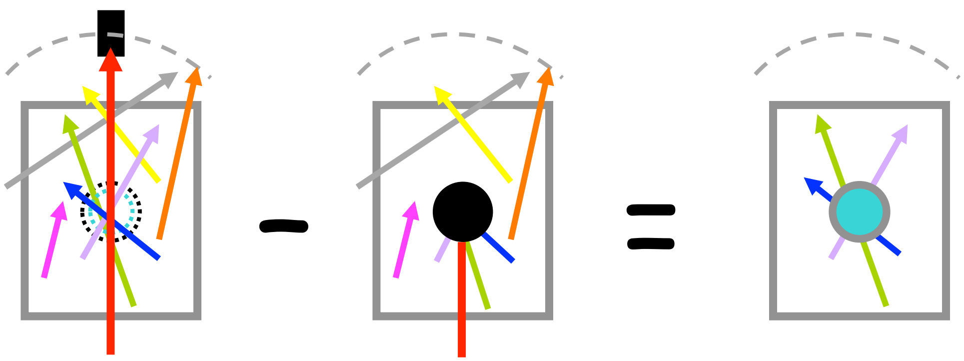
Requires two measurements:

- Empty beam
  (no sample, no container)



- Sample-like Cd specimen





$T = \exp\{- n\, \sigma_T(E)\, d\}$

Inelasticity effects

1

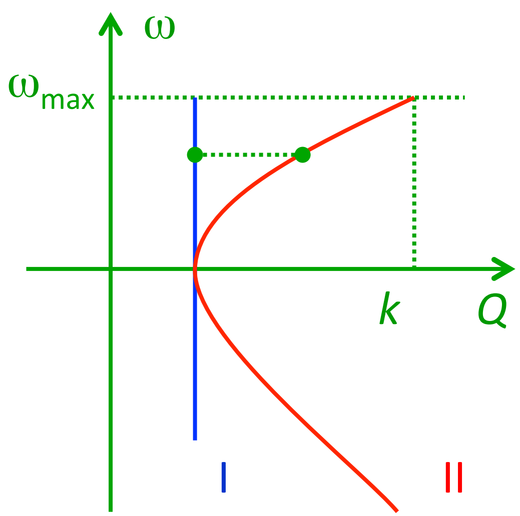
ε(*k*)

∞

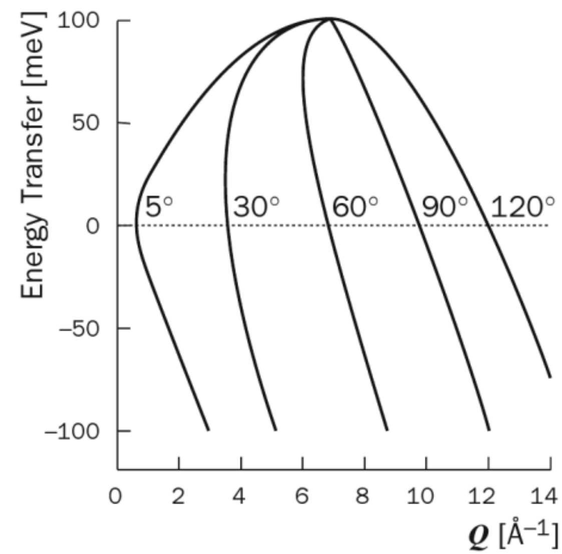
$$I(2\theta) = C\;\Phi_0\;N\;\frac{\sigma}{4\pi}\int_{-\infty}^{E_{\max}} \frac{k'}{k}\,S(\vec{Q},\omega)\,\epsilon(k')\,\mathrm{d}\omega$$

Constant 2θ

Constant 2Θ



$$\frac{\hbar^2 Q^2}{2m} = 2E + \hbar\omega - 2\sqrt{E^2 + \hbar\omega E}\;\cos 2\theta$$



Placzek's correction

These effects are closely associated
to the detector efficiency

Placzeck's corrections

Efficiency

- Black detector, $\varepsilon(E) = 1$
- $1/v$ detector, $\varepsilon(E) \propto E^{-1/2}$
- Exponential detector, $\varepsilon(E) = 1 - \exp\{-\alpha\ (E/E')^{1/2}\}$

- Taylor expansion of $S(Q_{|},\omega)$ around $(Q_{|},\omega) \longrightarrow S(Q_{||},\omega)$
- Expansion of $Q_{||}^2 - Q_{|}^2$, $\varepsilon(k)$ and k'/k in powers of ω/ω_{max}
- Energy integration

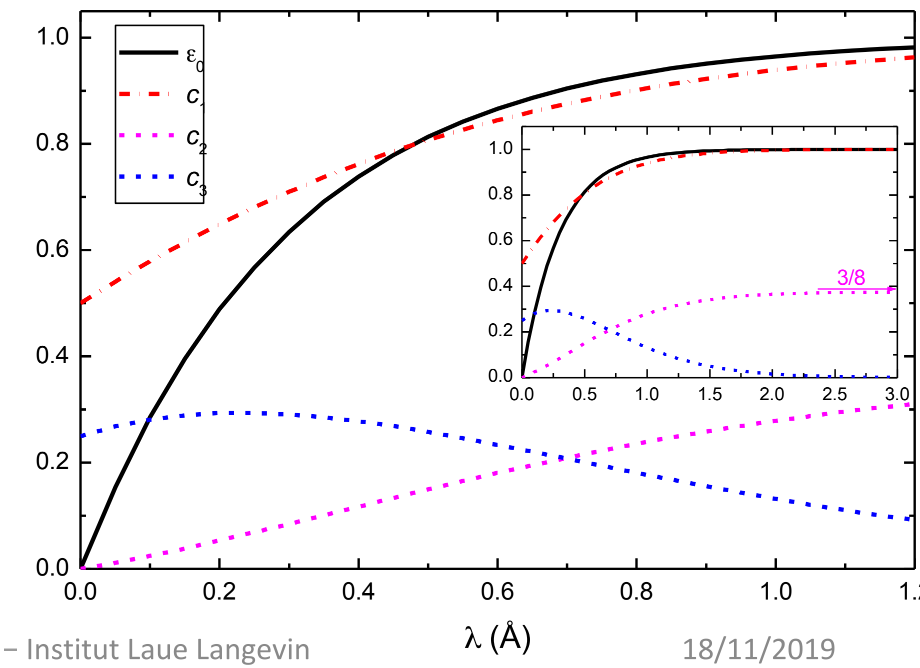
$$S(Q) = \frac{1}{\epsilon_0}\,\frac{1}{b_{\rm coh}^2}\,\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\rm corr} + \left(1 + \frac{b_{\rm inc}^2}{b_{\rm coh}^2}\right)\left(C_1\delta - C_2\delta^2 + C_3\delta\gamma - \frac{m}{2M}\,(\delta+\gamma)\right) - \frac{b_{\rm inc}^2}{b_{\rm coh}^2}$$

For an exponential detector

$$C_1 = 1 - \frac{\alpha/2}{e^{\alpha} - 1}$$

$$C_2 = \frac{3}{8} - \frac{\alpha\,(\alpha+3)}{8\,(e^{\alpha}-1)}$$

$$C_3 = \frac{\alpha(\alpha+1)}{4\,(e^{\alpha}-1)}$$



Sample related corrections

Attenuation

Multiple Scattering

Sample
+
Container

Minimisation by choosing an adequate sample geometry

$$I_{\mathrm{S}}^{\mathrm{corr}}(2\theta) = \frac{1}{\alpha_{\mathrm{S,SC}}(2\theta)}\left(I_{\mathrm{S}}(2\theta) - I_{\mathrm{S}}^{\mathrm{B}}(2\theta) - \frac{\alpha_{\mathrm{C,SC}}(2\theta)}{\alpha_{\mathrm{C,C}}(2\theta)}\left(I_{\mathrm{C}}(2\theta) - I_{\mathrm{C}}^{\mathrm{B}}(2\theta)\right)\right) - \Delta$$

Paalman & Pings' coefficients

Cylindrical geometry

Blech & Averbach's correction

Complete knowledge of $S(\boldsymbol{Q},\omega)$
Numerical simulation

Normalisation

Absolute scale
Vanadium diffractogram

Correction programs

Required data

CORRECT, Gudrun, etc. etc.

- Sample + container : as many as (sample,*T*) pairs.
- Container : enough to be able to interpolate.
- Empty instrument : the sample chamber and the sample environment.
- Absorber : a sample-like absorber

  (Cd for thermal neutrons and B for hot neutrons).
- Vanadium rod : a sample-like vanadium.
- Crystalline powder sample : for wavelength and zero-angle (Ni).
- A good description of the geometry.

Output: Differential cross section in barns/sterad./scatt. unit

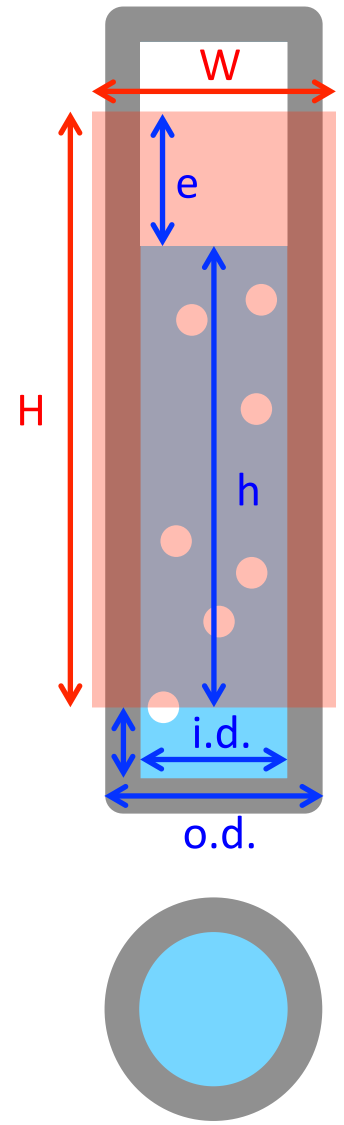
$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{corr}}$$

Input file for CORRECT

```
! Se15Te85_425C.com
!
inst D4
!
sample "Se15Te85_425C.adat" 0.45 /temperature=698.0 /density=0.026857 /packing=0.95668
! ds/dO_coh_self per atom = avr(bcoh^2)  :  0.38122 barns/sr
! total sample composition in relative fractions (integer number of atoms/10)
component 1.5 Se
component 8.5 Te
!
! Container quartz o.d.= 11 mm, i.d.= 9 mm. Wall thickness = 1 mm
container "quartz_425C_110.adat" 0.55
!
! The background id the empty furnace
background "MTfurnace_RT.adat"
!
! 6mm08 vanadium with mtfurnace background
vanadium "vana_10mm.adat" 0.5 /smoothing=1
background /vanadium "MTfurnace_RT.adat"
!
wavelength 0.4989
! zeroangle = -0.090 already subtracted
zeroangle 0.0
! Beam dimensions in cm (height x width)
beam 5.0 1.2
! Placzek correction (inelasticity)
placzek SERIES_EXPANSION
!
! The output file is the coherent differential cross section
! corrected by inelasticity, multiple scattering, attenuation
! and properly normalised by vanadium
xout q
output "Se15Te85_425C.corr.q”
spectrum 1
execute/nopause
!
quit
```

/packing=ρ_{eff}/ρ

/fullness=h/H



Output CORRECT (1)

Check the input data

```
CORRECT version ILL 3.20 (3 July 17)
CORRECT> @Se15Te85_425C
CORRECT> ! Se15Te85_425C.com
CORRECT> !
CORRECT> inst D4
CORRECT> !
CORRECT> sample "Se15Te85_425C.adat" 0.45 /temperature=698.0 /density=0.026857 /packing=0.95668
CORRECT> ! ds/dO_coh_self per atom = avr(bcoh^2)  :  0.38122 barns/sr
CORRECT> ! total sample composition in relative fractions:
CORRECT> component 0.15 Se
CORRECT> component 0.85 Te
CORRECT> container "quartz_425C_110.adat" 0.55
CORRECT> background "MTfurnace_RT.adat"
CORRECT> !
CORRECT> ! 6mm08 vanadium with mtfurnace background
CORRECT> vanadium "vana_10mm.adat" 0.5 /smoothing=1
CORRECT> background /vanadium "MTfurnace_RT.adat"
CORRECT> !
CORRECT> wavelength 0.4989
CORRECT> ! zeroangle = -0.090 already subtracted
CORRECT> zeroangle 0.0
CORRECT> beam 5.0 1.2
CORRECT> placzek SERIES_EXPANSION
CORRECT> !
CORRECT> !xout angle
CORRECT> !output aa_1212.corr
CORRECT> !title "filename.corr (after correct)"
CORRECT> !spectrum 1
CORRECT> !execute/nopause
CORRECT> !
CORRECT> xout q
CORRECT> output "Se15Te85_425C.corr.q”
CORRECT> spectrum 1
CORRECT> execute/nopause
```

Output CORRECT (2)

General information

```
CORRECT
=======

Correcting data from 2-AXIS diffractometer D4


Sample data is read from file Se15Te85_425C.adat
with background from file MTfurnace_RT.adat

Container data is read from file quartz_425C_110.adat
with background from file MTfurnace_RT.adat

Vanadium data is read from file vana_10mm.adat
with background from file MTfurnace_RT.adat
Vanadium smoothing with polynomial order 0

Output will be to file Se15Te85_425C.corr.q


Can absorption c/s (at 2200m/s) :  5.080 barns
Can scattering c/s              :  4.950 barns
Can number density              : 0.0722 per cu. Angstrom
V absorption c/s (at 2200m/s)   :  5.080 barns
Vanadium scattering c/s         :  4.950 barns
Vanadium number density         : 0.0722 per cu. Angstrom
Sample intrinsic number density : 0.0269 per cu. Angstrom
Sample packing fraction         : 0.9567
Sample fullness                 : 1.0000
Sample temperature              :  698.0 K
Sample new title                : filename.corr.q (after correct)
```

```
Sample geometry is CYLINDRICAL
 Sample radius                    : 0.4500 cm
 Can outer radius                 : 0.5500 cm
 Vanadium radius                  : 0.5000 cm


 The sample consists of  2 species:

 at.num  symbol  rel.conc.  at.weight    bcoh    scatt.c-s  incoh.c-s  abs.c-s
  34     Se       0.15000    78.9600    7.9700    8.3000     0.3177    11.7000
  52     Te       0.85000   127.6000    5.8000    4.3200     0.0927     4.7000


 Beam height                      : 5.0000 cm
 Beam width                       : 1.2000 cm

 Placzek correction will be SERIES_EXPANSION

 Incident wavelength              : 0.4989 Angstroms
 2theta zeroangle                 :   0.0000 Degrees


  1 spectra will be corrected:

     Spectrum  1

 For the vanadium at wavelength  0.49890 AA :

    mu_scat = scattering attenuation constant :   0.35739 cm-1
    mu_abs = absorption attenuation constant  :   0.10177 cm-1
    mu_tot = total attenuation constant       :   0.45916 cm-1
 And using an effective pathlength = sqrt(pi)*r*0.85 of  0.75329 cm :
    scattering of beam (w/o absorption)       :  0.23602
    true absorption of beam (w/o scattering)  :  0.07380
    transmission (i.e. 1 - total_attenuation) :  0.70760
```

Output CORRECT (3)

```
  Some differential cross sections, etc, for the sample:

  ds/dO_self per atom = avr(b^2)          :  0.39128 barns/sr
  ds/dO_coh_self per atom = avr(bcoh^2)  :  0.38122 barns/sr
  ds/dO_incoh per atom = avr(bincoh^2)   :  0.01006 barns/sr
  --> fraction incoh/self :  0.02571
  Yarnell ds/dO_self/atom=avr(b^2)        :  0.39161 barns/sr
  Yarnell ds/dO_coh_self/atom=avr(bcoh^2):  0.38154 barns/sr
  Yarnell ds/dO_incoh/atom=avr(bincoh^2) :  0.01007 barns/sr
  --> Yarnell fraction incoh/self :  0.02571

  b_coh = avr(b) over all isotopes in sample :  6.12550 fm
  (avr(b))^2 over all isotopes in sample :  0.37522 barns/sr
And taking into account the imaginary part of b_coh:
  b_coh = sample's avr(b) =  6.12550 fm  +  i *  0.00160 fm
  |avr(b)|^2 over all isotopes in sample :  0.37522 barns/sr

  avr(atwgt) over all isotopes in sample : 120.30400 a.u.
  --> intrinsic mass density :   5.36444 g/cm**3



For the sample at wavelength  0.49890 AA :

   mu_scat = scattering attenuation constant :   0.12634 cm-1
   mu_abs = absorption attenuation constant  :   0.04099 cm-1
   mu_tot = total attenuation constant       :   0.16733 cm-1
And using an effective pathlength = sqrt(pi)*r*0.85 of  0.67796 cm :
   scattering of beam (w/o absorption)       :  0.08209
   true absorption of beam (w/o scattering)  :  0.02741
   transmission (i.e. 1 - total_attenuation) :  0.89276
```

Cross sections

```
Sample bkg to be subtracted with coeff of  0.89276
which should correspond to the coefficient multiplying
the MTcontainer scan in the background subtraction of the
do_sample script file and should be roughly equal to the
ratio Acsch/Acch evaluated at an intermediate angle.

Container bkg to be subtracted with coeff of  1.00000
which should correspond to ( 1 - the coefficient multiplying
the e.g. MTbelljar scan in the background subtraction of the
do_sample script file ) and should be roughly equal to the
Acch coefficient evaluated at an intermediate angle.

Furnace bkg to be subtracted with coeff of  1.00000
Vanadium bkg to be subtracted with coeff of  0.70760
which should correspond to the coefficient multiplying the
e.g. MT_belljar scan in the background subtraction of the
do_vanadium script file and should be slightly more than
the Avvch coefficient evaluated at an intermediate angle.
```

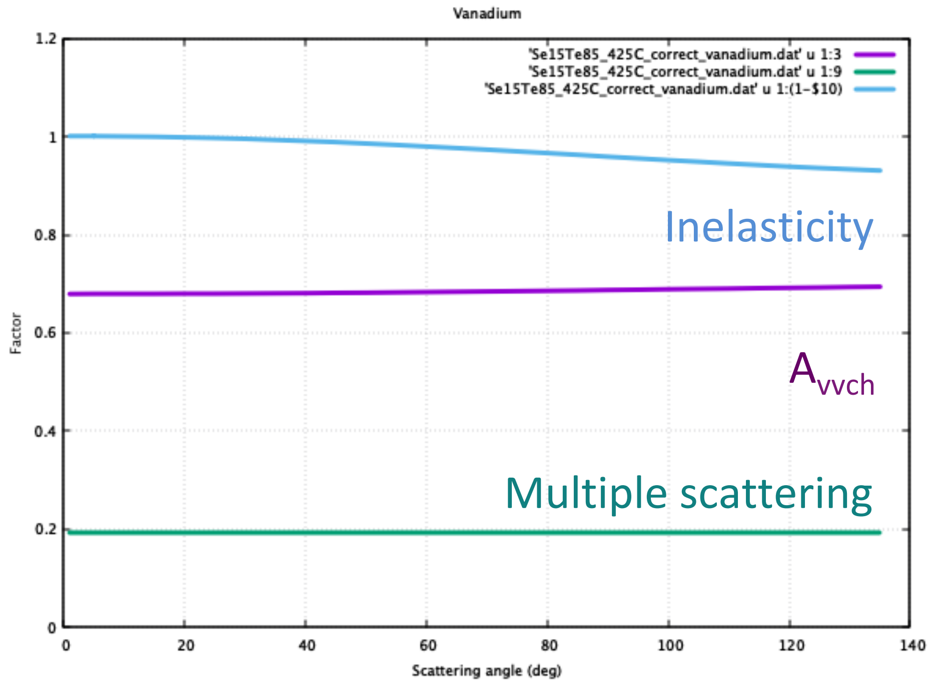
Output CORRECT (4)

Vanadium absorption, multiple scattering and Placzek corrections:

Linear attenuation coefficient (mu_tot) * radius = 0.22958

Angle	Q	Avvch	Acvch	Acch	Ahvch	Ahch	Ahh	m.s.	Placzek
1.06	0.23	0.67941	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	-0.00094
5.06	1.11	0.67944	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	-0.00078
10.06	2.21	0.67952	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	-0.00029
15.01	3.29	0.67964	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00051
20.01	4.38	0.67982	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00164
25.01	5.45	0.68004	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00306
30.01	6.52	0.68032	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00478
35.11	7.60	0.68065	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00682
40.11	8.64	0.68102	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.00908
45.00	9.64	0.68144	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.01152
50.00	10.64	0.68191	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.01424
55.00	11.63	0.68243	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.01716
60.00	12.59	0.68300	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.02024
65.05	13.54	0.68361	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.02351
70.05	14.46	0.68426	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.02687
75.05	15.34	0.68494	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.03033
80.08	16.20	0.68566	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.03387
85.08	17.03	0.68640	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.03743
90.08	17.82	0.68716	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.04100
95.11	18.59	0.68794	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.04458
100.11	19.31	0.68872	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.04810
105.05	19.99	0.68950	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.05151
110.05	20.64	0.69029	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.05486
115.05	21.25	0.69106	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.05810
120.05	21.82	0.69181	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.06120
125.06	22.35	0.69253	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.06413
130.06	22.83	0.69322	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.06688
135.06	23.28	0.69386	1.00000	1.00000	1.00000	1.00000	1.00000	0.19384	0.06943

Vanadium



- Paalman & Pings' coefficients
- Multiple scattering (Blech & Averbach)
- Inelasticity (Placzek)

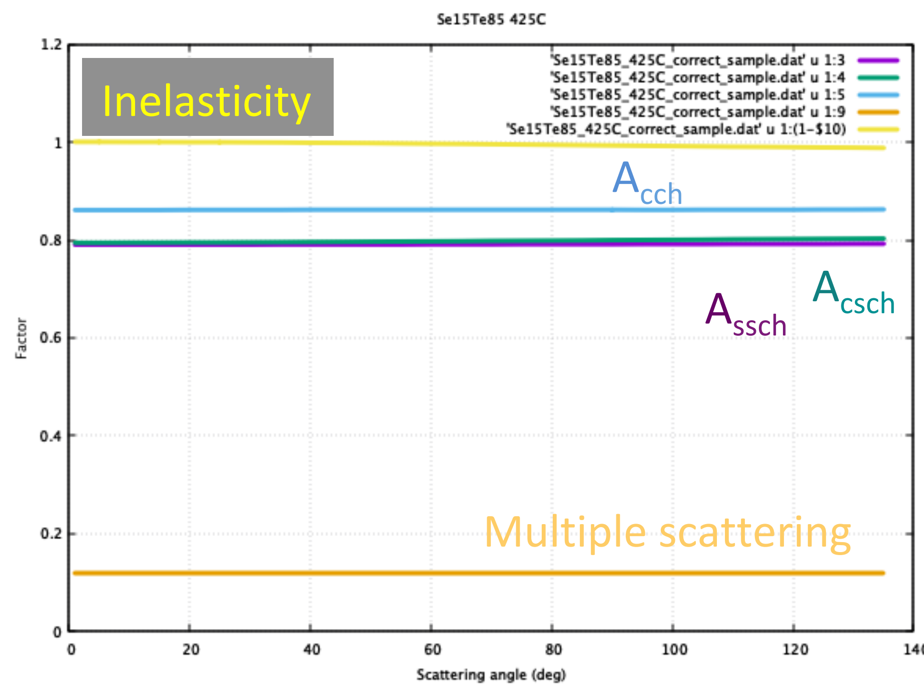
Output CORRECT (4)

```
Sample absorption, multiple scattering and Placzek corrections:

Linear attenuation coefficient (mu_tot) * radius =  0.07530

 Angle  Q    Assch   Acsch   Acch    Ahsch   Ahch    Ahh       m.s.     Placzek
  1.06  0.23 0.79040 0.79431 0.86102 1.00000 1.00000 1.00000  0.12060 -0.00037
  5.06  1.11 0.79040 0.79435 0.86110 1.00000 1.00000 1.00000  0.12060 -0.00034
 10.06  2.21 0.79041 0.79444 0.86119 1.00000 1.00000 1.00000  0.12060 -0.00025
 15.01  3.29 0.79043 0.79458 0.86129 1.00000 1.00000 1.00000  0.12060 -0.00012
 20.01  4.38 0.79045 0.79476 0.86138 1.00000 1.00000 1.00000  0.12060  0.00008
 25.01  5.45 0.79049 0.79497 0.86146 1.00000 1.00000 1.00000  0.12060  0.00032
 30.01  6.52 0.79054 0.79522 0.86154 1.00000 1.00000 1.00000  0.12060  0.00061
 35.11  7.60 0.79059 0.79550 0.86160 1.00000 1.00000 1.00000  0.12060  0.00096
 40.11  8.64 0.79066 0.79581 0.86165 1.00000 1.00000 1.00000  0.12060  0.00135
 45.00  9.64 0.79072 0.79612 0.86169 1.00000 1.00000 1.00000  0.12060  0.00177
 50.00 10.64 0.79080 0.79647 0.86172 1.00000 1.00000 1.00000  0.12060  0.00224
 55.00 11.63 0.79087 0.79683 0.86173 1.00000 1.00000 1.00000  0.12060  0.00274
 60.00 12.59 0.79096 0.79720 0.86174 1.00000 1.00000 1.00000  0.12060  0.00327
 65.05 13.54 0.79104 0.79759 0.86174 1.00000 1.00000 1.00000  0.12060  0.00384
 70.05 14.46 0.79113 0.79798 0.86173 1.00000 1.00000 1.00000  0.12060  0.00442
 75.05 15.34 0.79122 0.79838 0.86171 1.00000 1.00000 1.00000  0.12060  0.00502
 80.08 16.20 0.79132 0.79878 0.86169 1.00000 1.00000 1.00000  0.12060  0.00564
 85.08 17.03 0.79141 0.79918 0.86167 1.00000 1.00000 1.00000  0.12060  0.00626
 90.08 17.82 0.79151 0.79959 0.86165 1.00000 1.00000 1.00000  0.12060  0.00689
 95.11 18.59 0.79160 0.79999 0.86164 1.00000 1.00000 1.00000  0.12060  0.00752
100.11 19.31 0.79170 0.80039 0.86164 1.00000 1.00000 1.00000  0.12060  0.00813
105.05 19.99 0.79179 0.80078 0.86165 1.00000 1.00000 1.00000  0.12060  0.00873
110.05 20.64 0.79188 0.80117 0.86169 1.00000 1.00000 1.00000  0.12060  0.00933
115.05 21.25 0.79197 0.80155 0.86175 1.00000 1.00000 1.00000  0.12060  0.00990
120.05 21.82 0.79206 0.80193 0.86184 1.00000 1.00000 1.00000  0.12060  0.01045
125.06 22.35 0.79214 0.80230 0.86197 1.00000 1.00000 1.00000  0.12060  0.01097
130.06 22.83 0.79223 0.80267 0.86214 1.00000 1.00000 1.00000  0.12060  0.01146
135.06 23.28 0.79230 0.80302 0.86237 1.00000 1.00000 1.00000  0.12060  0.01191
 correct_2axis executed
CORRECT> !
CORRECT> quit
```

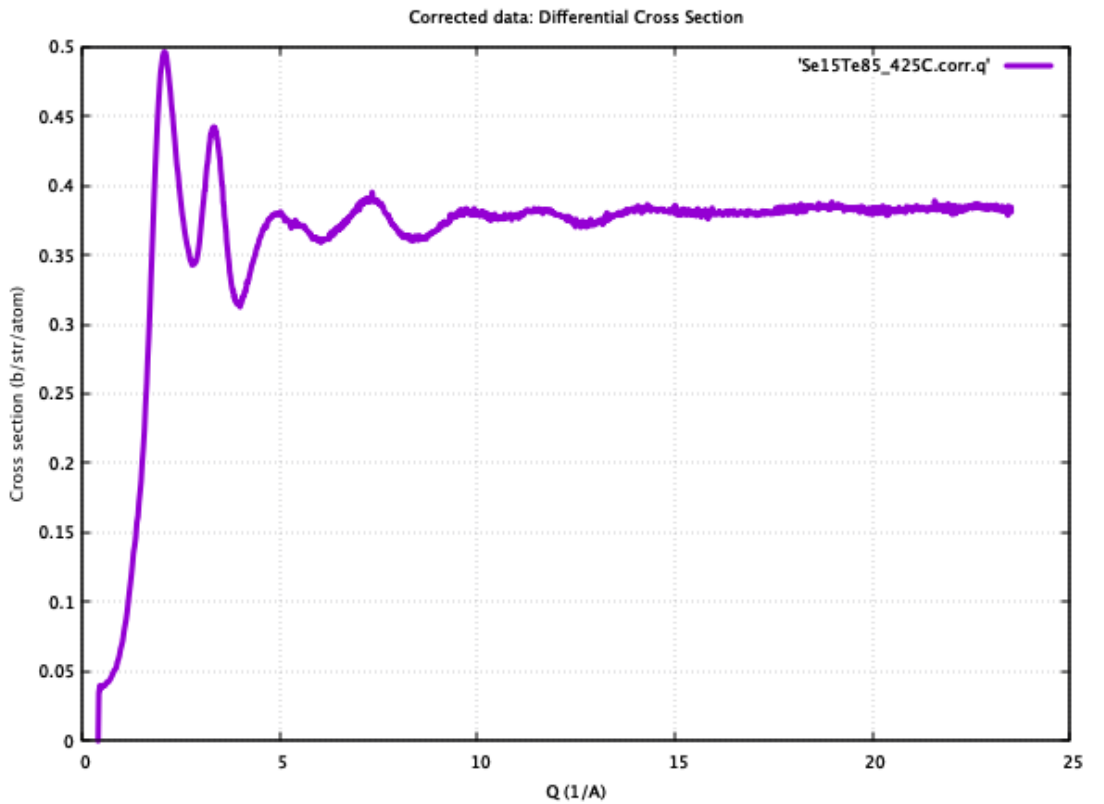
Sample



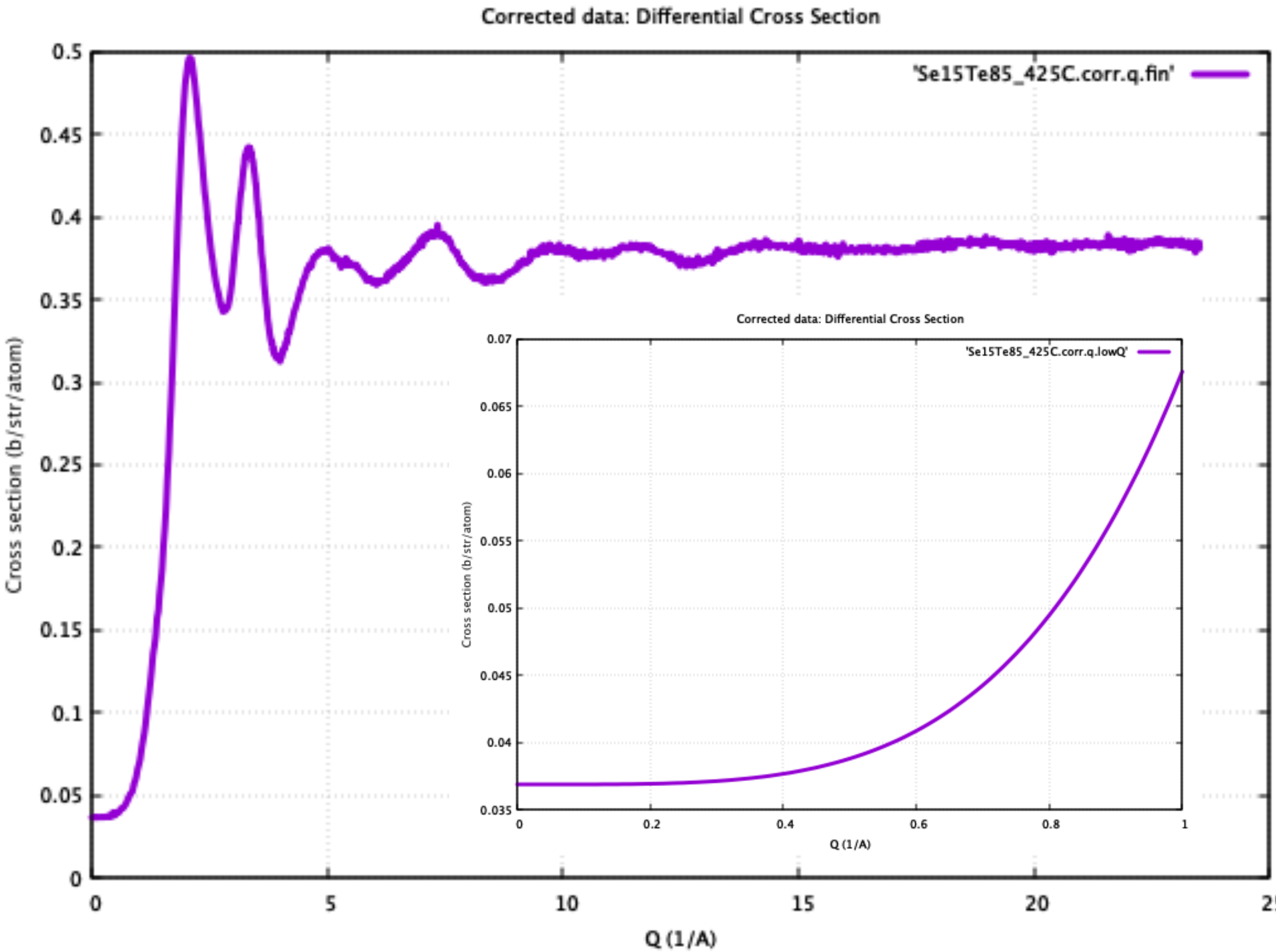
- Paalman & Pings' coefficients
- Multiple scattering (Blech & Averk
- Inelasticity (Placzek)

Output file CORRECT

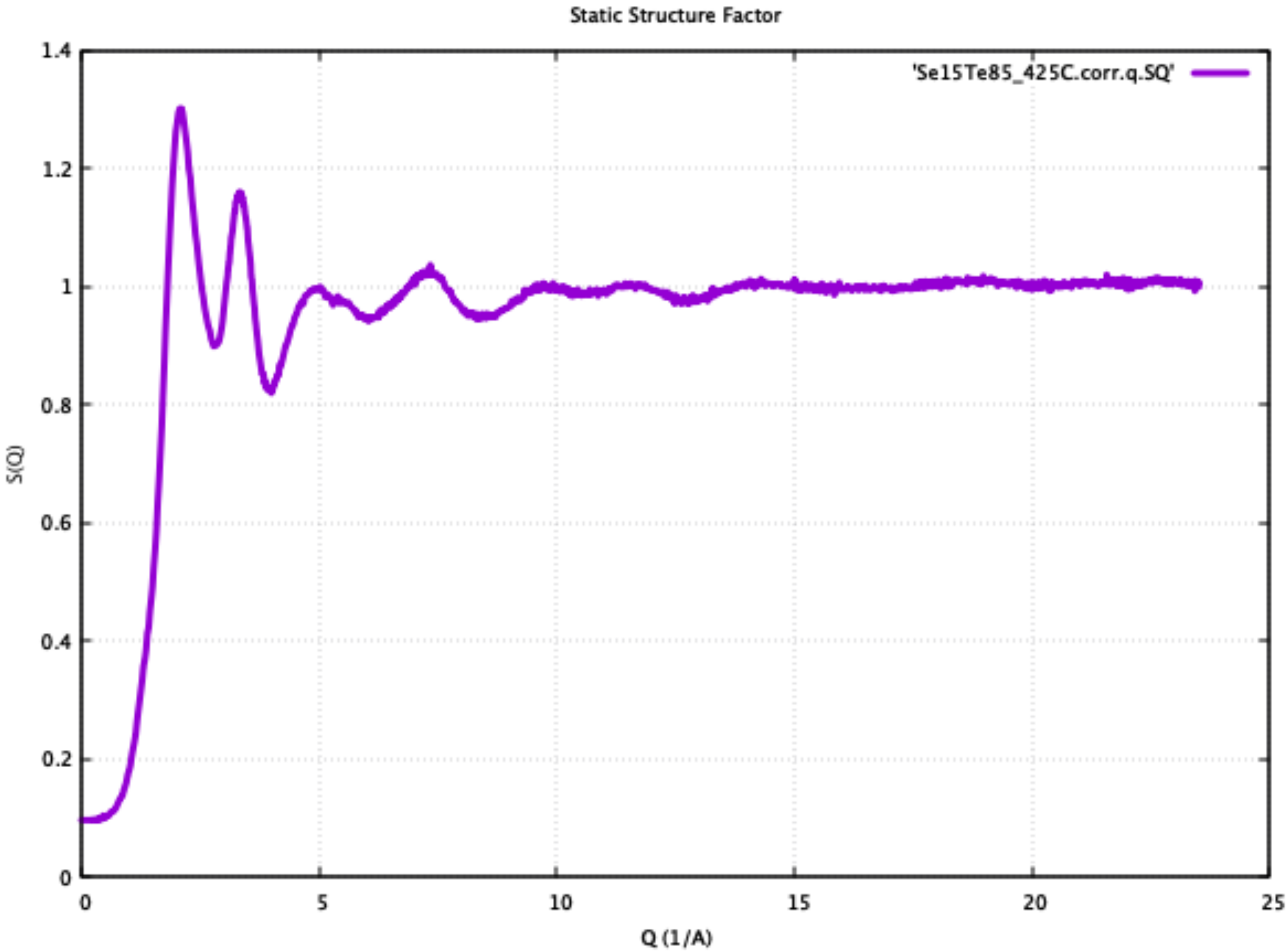
```
# filename.corr.q (after correct)
#Block  1
#========
#
#Instrument: D4
#User      : cuello (/net/serdon/illdata/processed/163/d4/
exp_6-03-419/processed)
#Run number:           1
#Spectrum  :           1
#Title     : filename.corr.q (after correct)
#Run date  : Mon Jan 30 14:34:39 2017
#X caption : Momentum transfer (A**-1)
#Y caption : Cross-section
#Histogram :           F
#Points    :        1448
  0.232993290      -4.62648682E-02   3.51537281E-04
  0.261566997      -4.64400165E-02   3.06130416E-04
  0.287942380      -4.63275239E-02   2.72539881E-04
  0.316515416      -4.66136783E-02   2.61351408E-04
  0.342890084      -4.60411571E-02   2.60503730E-04
  0.371462286      -4.54884954E-02   2.68991600E-04
  0.397836119      -1.95801519E-02   4.88558842E-04
  0.426407456       3.49235497E-02   7.47496902E-04
  0.452780336       3.98697816E-02   7.62447249E-04
  0.481350482       3.80599499E-02   7.57011061E-04
  0.507722378       3.90205234E-02   7.52640422E-04
  0.536291301       3.93197648E-02   7.49911123E-04
  0.562662005       3.99930254E-02   7.50510953E-04
  0.591229618       4.01250273E-02   7.55647954E-04
  0.617598951       4.20581698E-02   7.60504045E-04
  0.646165073       4.25601229E-02   7.65911187E-04
  0.672532976       4.25573699E-02   7.71594932E-04
  0.701097429       4.38850597E-02   7.76210974E-04
  0.727463782       4.49257679E-02   7.81205890E-04
  0.756026447       4.70207781E-02   7.87560362E-04
  0.782391071       4.85052131E-02   7.92242179E-04
```



Extrapolation to low-Q

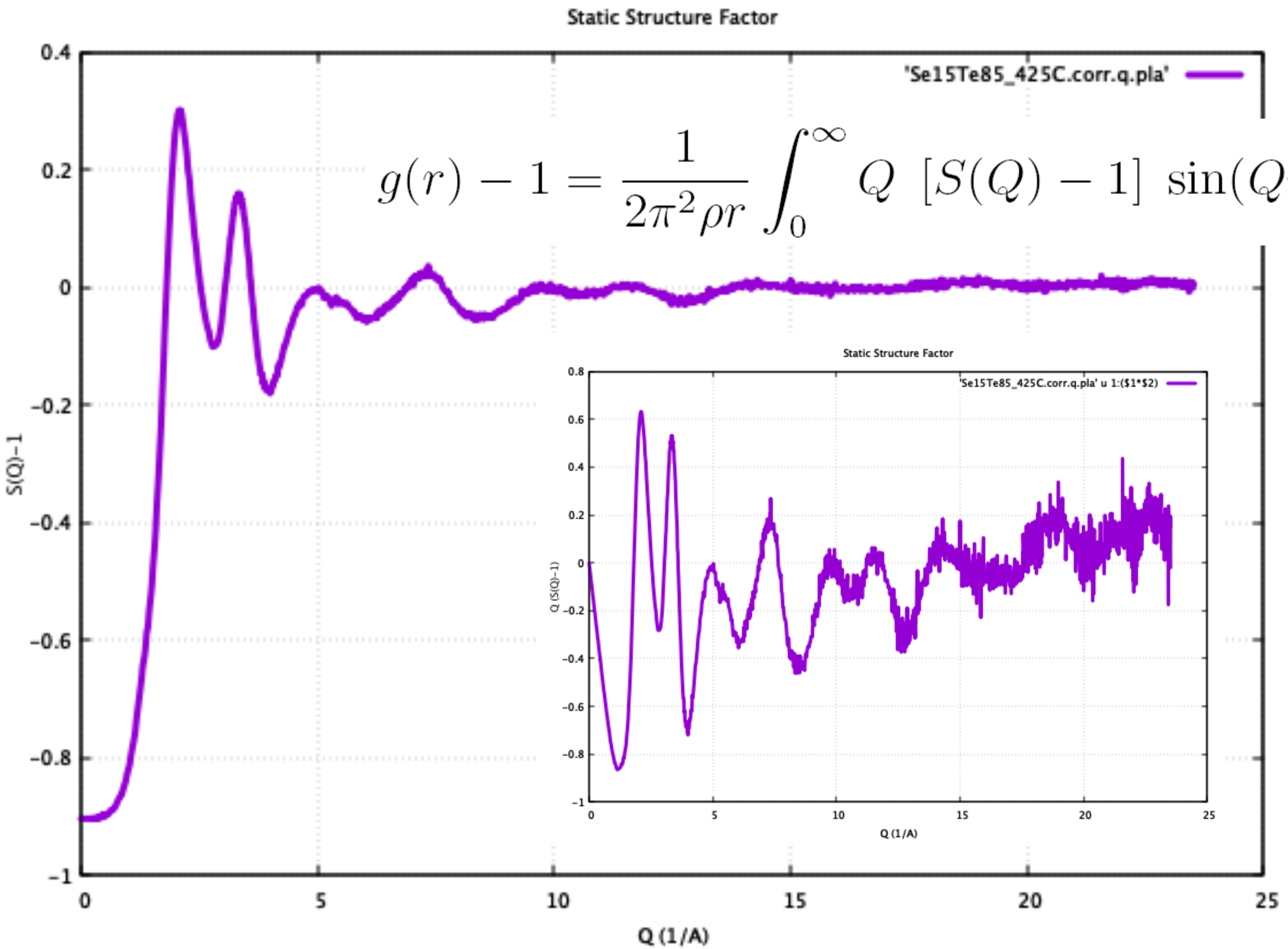


Static Structure factor $S(Q)$



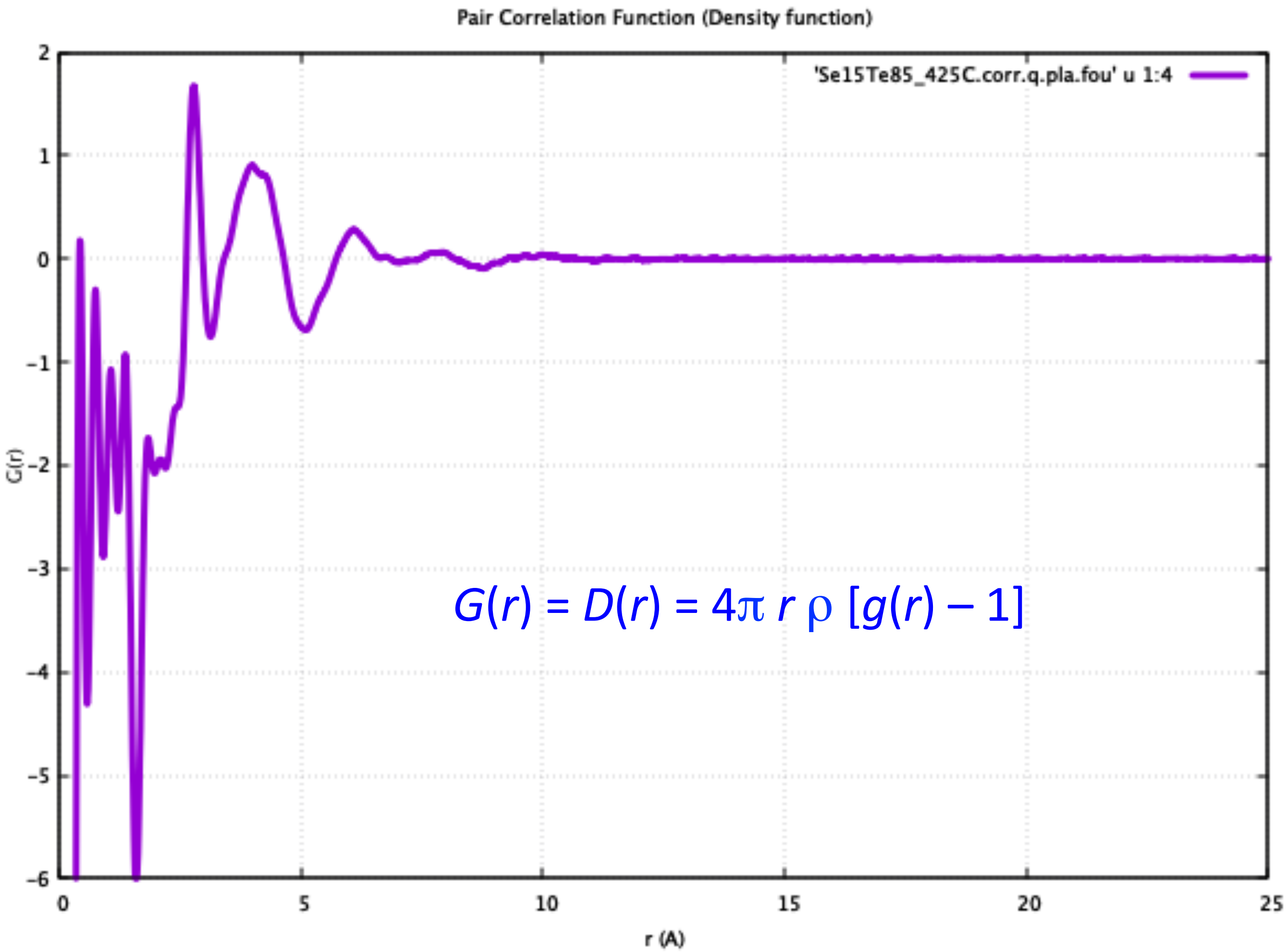
$F(Q) = S(Q) - 1$

$$g(r) - 1 = \frac{1}{2\pi^2 \rho r} \int_0^\infty Q\ [S(Q) - 1]\ \sin(Qr)\ \mathrm{d}Q$$



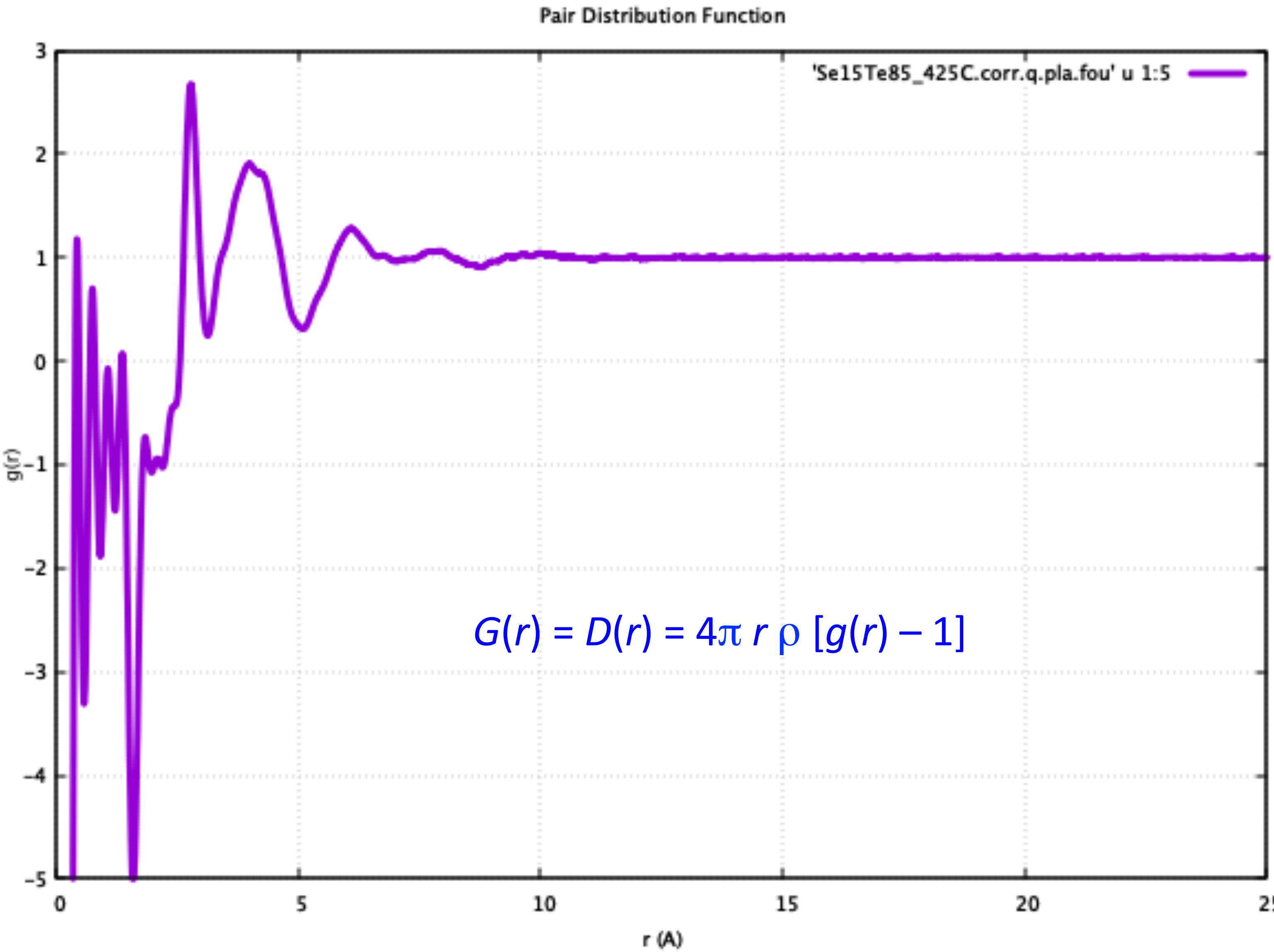
Sinus FT: Pair Correlation Function

$$g(r) - 1 = \frac{1}{2\pi^2 \rho r} \int_0^\infty Q \; [S(Q) - 1] \; \sin(Qr) \, \mathrm{d}Q$$

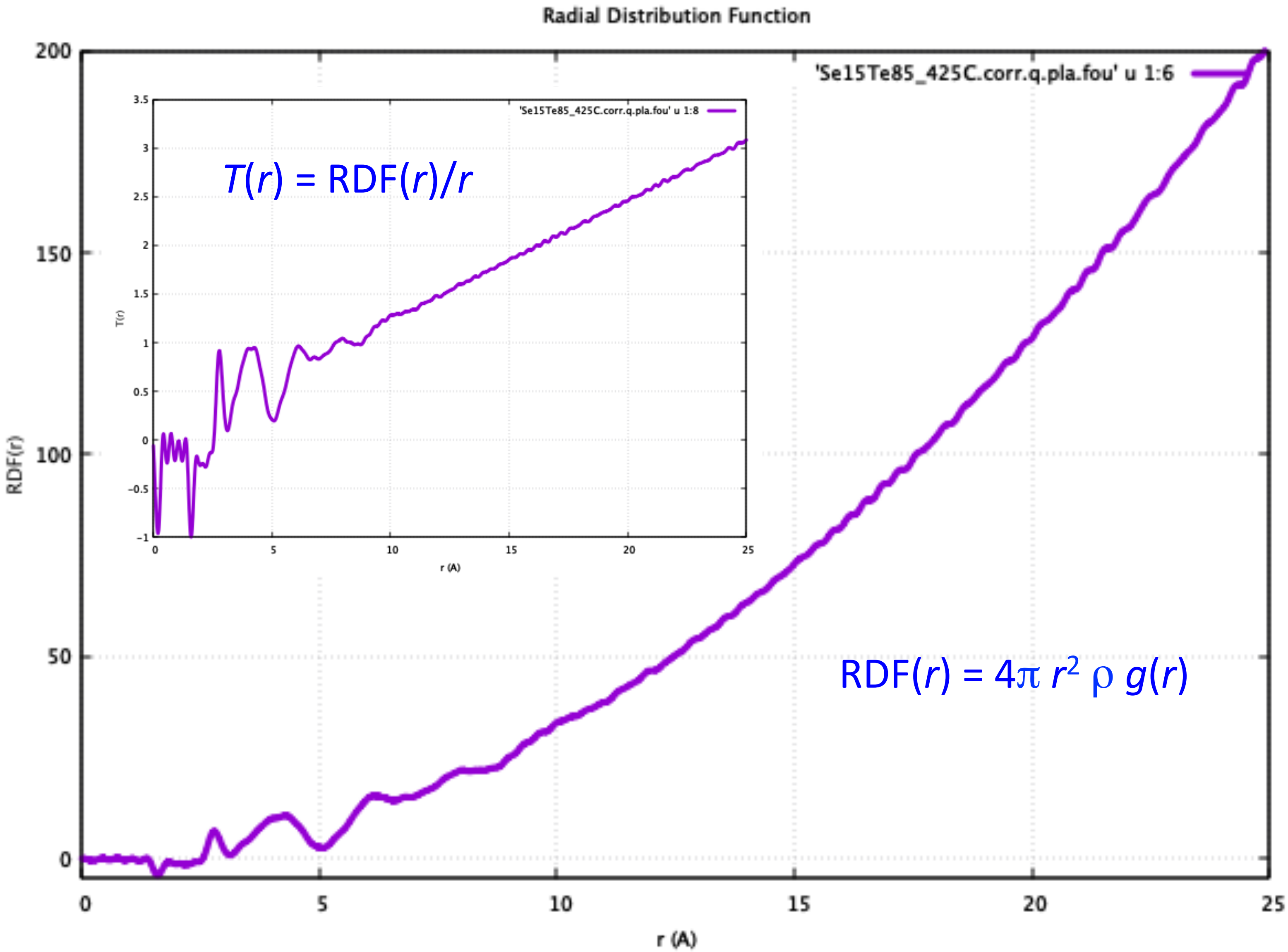


$G(r) = D(r) = 4\pi \, r \, \rho \, [g(r) - 1]$

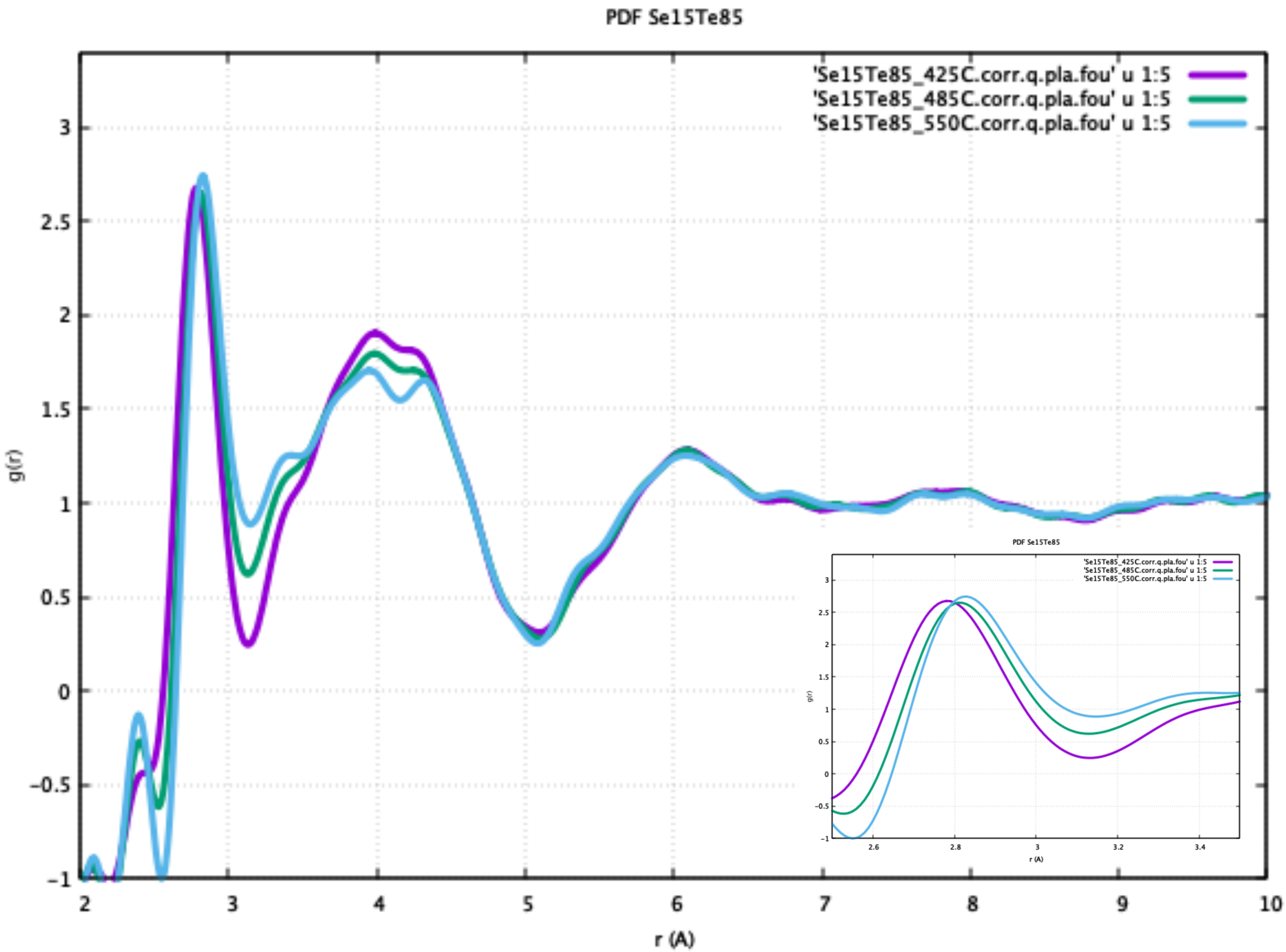
Pair Distribution Function (PDF)



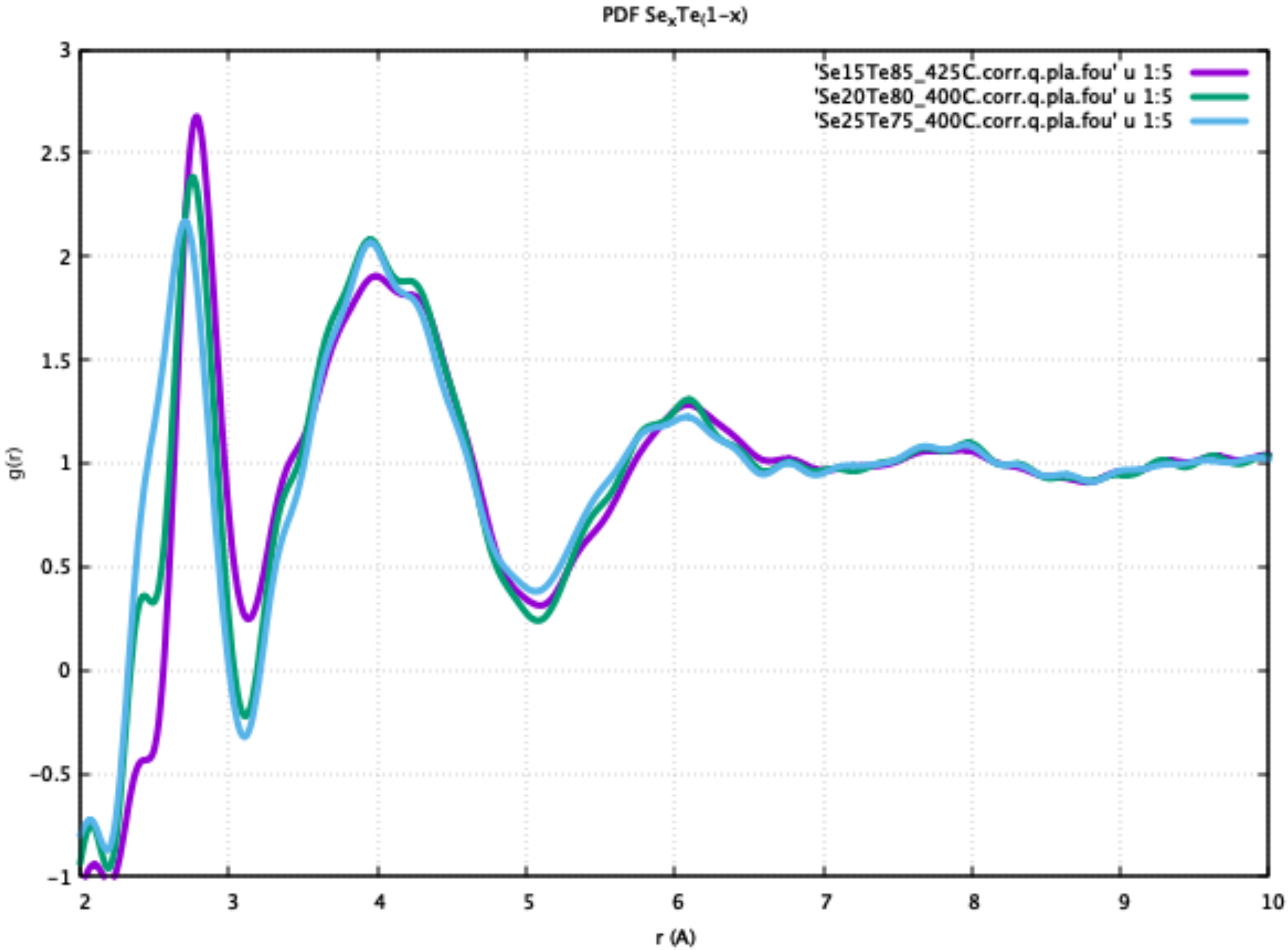
Radial Distribution Function



PDF $Se_{15}Te_{85}$



PDF Se_xTe_{1-x}



PDF Se$_x$Te$_{(}$1−x)
'Se15Te85_425C.corr.q.pla.fou' u 1:5
'Se20Te80_400C.corr.q.pla.fou' u 1:5
'Se25Te75_400C.corr.q.pla.fou' u 1:5
g(r)
r (A)
3
2.5
2
1.5
1
0.5
0
−0.5
−1
2
3
4
5
6
7
8
9
10

Questions?

Presentation and tutorial available at the School website

cuello@ill.fr