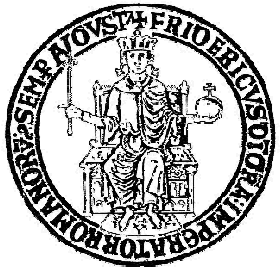


3° Training school on “Application of computer models for advancement of X-ray breast imaging techniques”

Napoli, 17 - 19 September 2018

Implementation of interference effects in coherent X-ray scattering in Geant4

G. Paternò

INFN - Ferrara

MaXIMA

Three dimensional breast cancer models for X-ray imaging research

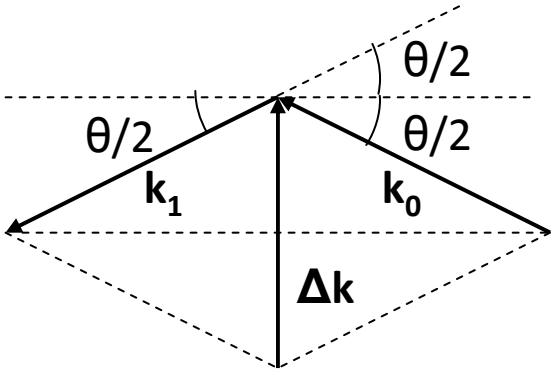
HORIZON 2020
European Union funding
for Research & Innovation

Outline

- Theoretical background
- Implementation in Geant4
- Case studies

Theoretical background: Coherent Scattering

In **Rayleigh (Coherent) Scattering**, photons are scattered by **bound atomic electrons** without excitation of the target atom, i. e., the energy of incident and scattered photons is the same.



$$\frac{d\sigma_{Ra}}{d\Omega} = \frac{d\sigma_{Th}}{d\Omega}\left|F(q,Z) + f' + if''\right|^2 \approx r_e^2 \frac{1+\cos^2\theta}{2}\left|F(q,Z)\right|^2$$

Dispersion correction, negligible for materials and energies of medical interest (above K absorption edge)

momentum transfer

$$q = \hbar\,|\,k_1 - k_0\,| = 2k\hbar\sin(\theta/2) = \frac{4\pi\hbar}{\lambda}\sin(\theta/2) = 2\frac{E}{c}\sin(\theta/2)$$

Parameters used in the literature and MC codes

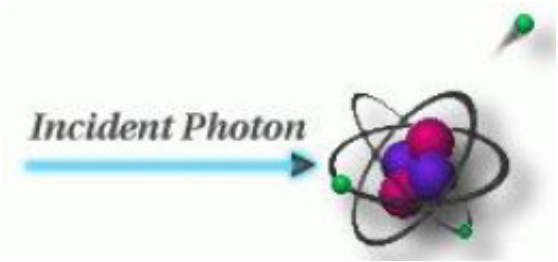
$$x = \frac{q}{2h} = \frac{1}{\lambda}\sin(\theta/2) \quad [\text{nm}^{-1}] \qquad \tilde{q} = \frac{q}{m_e c} \quad [\text{adimensional}]$$

$$\sigma_{Ra} = \int \frac{d\sigma_{Ra}}{d\Omega}\,d\Omega = \pi r_e^2 \int_0^{\pi} (1+\cos^2\theta)\left|F(q,Z)\right|^2 \sin\theta\, d\theta$$

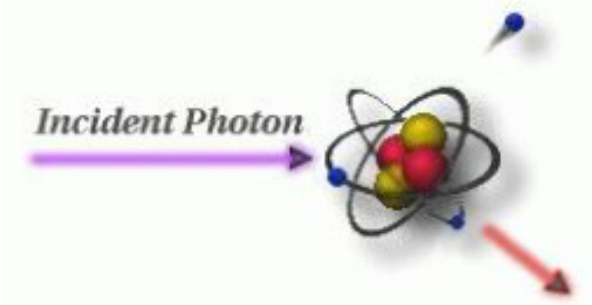
For low photon energies: $\sigma_{Ra} \approx \sigma_{Th} = 8/3\pi r_e^2 Z^2$

For high photon energies (E>Z/2 MeV): $\sigma_{Ra} \sim E^{-2}$

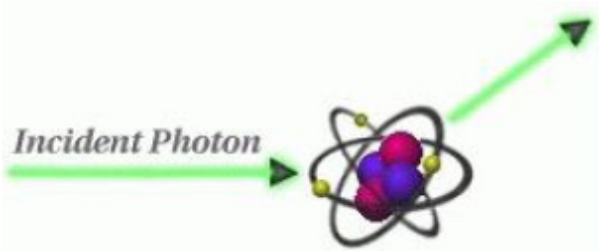
Theoretical background: X-ray interactions with matter at diagnostic energies



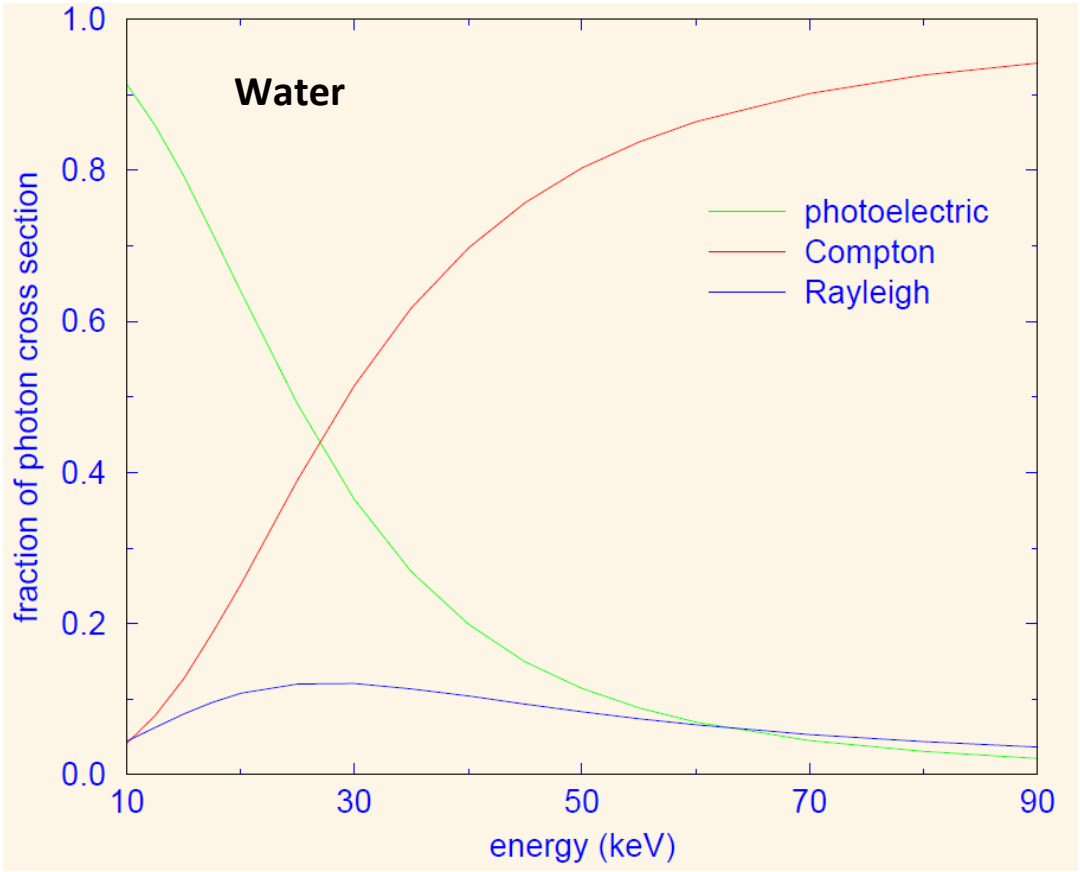
Photoelectric effect



Compton scattering



Rayleigh scattering



Theoretical background: Atomic form factor

$$\frac{d\sigma_{Ra}}{d\Omega} = r_e^2 \frac{1+\cos^2\theta}{2}\left|F(q,Z)\right|^2$$

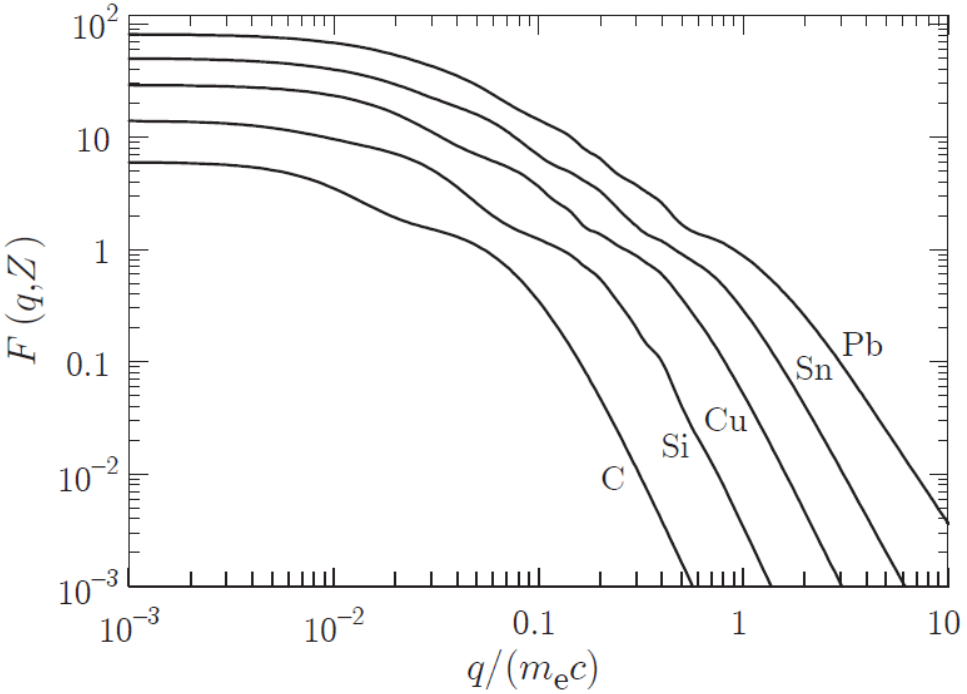
The atomic form factor, F(q,Z) is the Fourier transform of the atomic electron density ρ(r).

For spherically symmetric atoms

$$F(q,Z) = \int \rho(\vec{r}) e^{-i\vec{q}\cdot\vec{r}}\, dV = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr/\hbar)}{qr/\hbar} r^2 dr$$

F(q,Z) is a **monotonically decreasing** function of q that varies from **F(0,Z) = Z to F(∞,Z) = 0,** thus resulting **in a forward peaked scatter distribution**.

The most accurate form factors are those obtained from **non-relativistic Hartree-Fock calculations** (see, **Hubbell et al., 1975)** on which is based **EPDL97** of **LLNL**).



Atomic form factors of neutral atoms of the indicated elements, taken from the EPDL (Cullen et al., 1997).

Theoretical background: Differential linear scattering coefficient

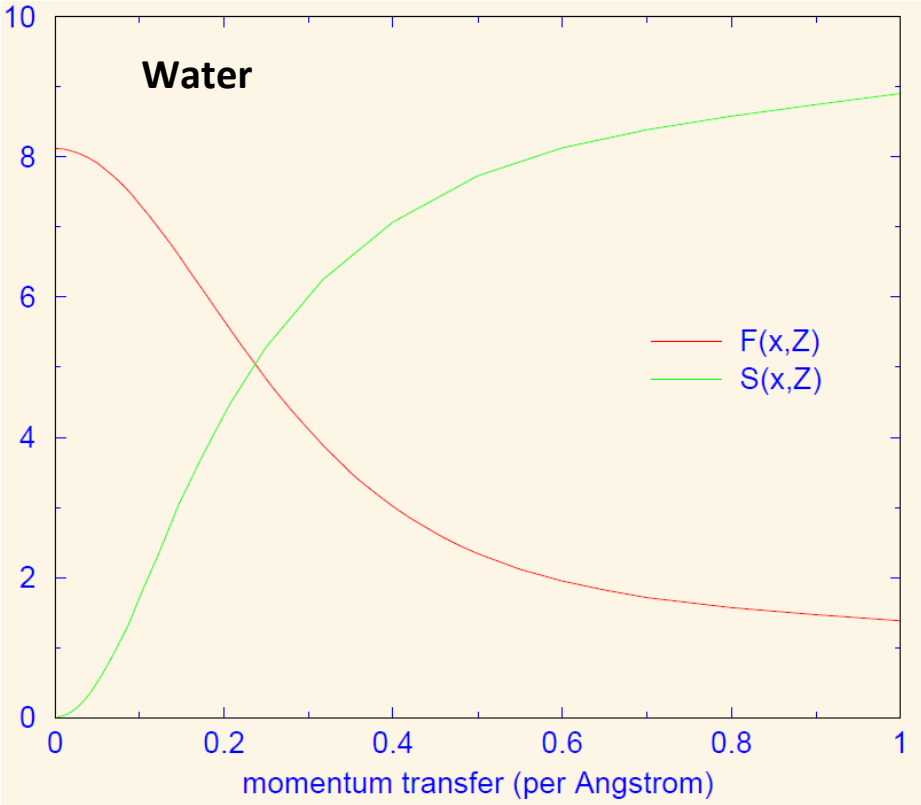
$$\mu_S = \frac{N_A \rho}{M}\left[\frac{d\sigma_T(\theta)}{d\Omega}F^2(x,Z) + \frac{d\sigma_{KN}(\theta)}{d\Omega}S(x,Z)\right]$$

[cm^-1 sr^-1]

$$\frac{d\sigma_{KN}}{d\Omega} = \frac{r_e^2}{2}\left(\frac{K}{K_0}\right)^2\left(\frac{K}{K_0} + \frac{K_0}{K} + \cos^2\theta - 1\right)$$

$$\frac{K}{K_0} = \frac{1}{1+\gamma(1-\cos\theta)} \qquad \gamma = \frac{E}{m_e c^2}$$

$$F^2(x,Z) + S(x,Z) \cong 1$$



Theoretical background: Molecular form factor

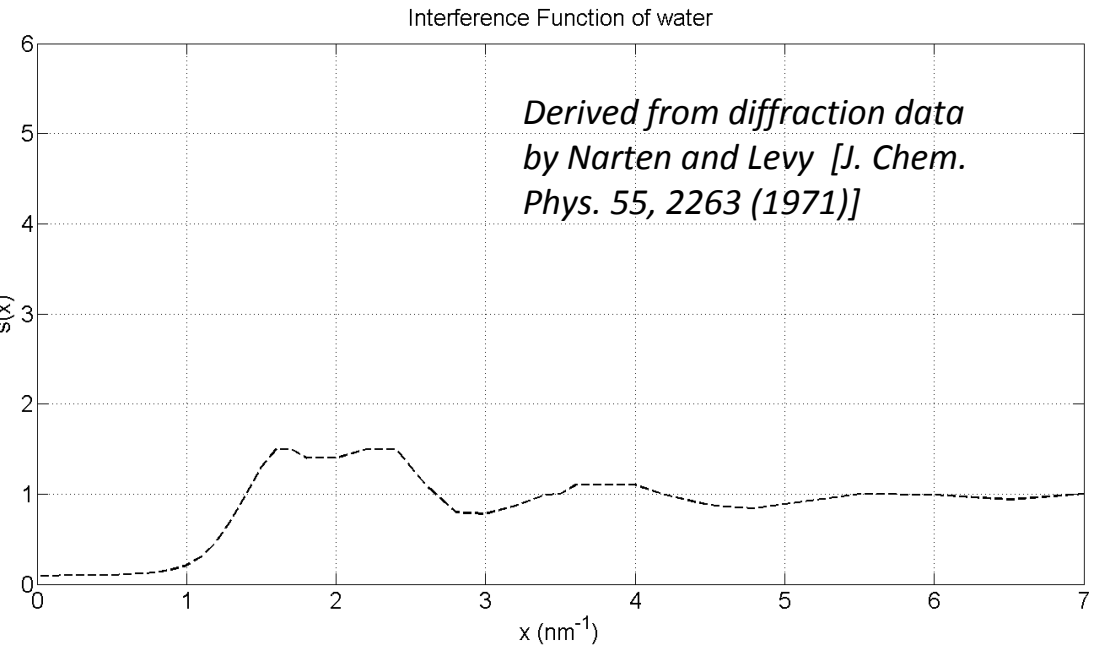
$$F^2_{mol,IAM}(q) = W\sum_i \frac{w_i}{A_i} F^2(q, Z_i)$$

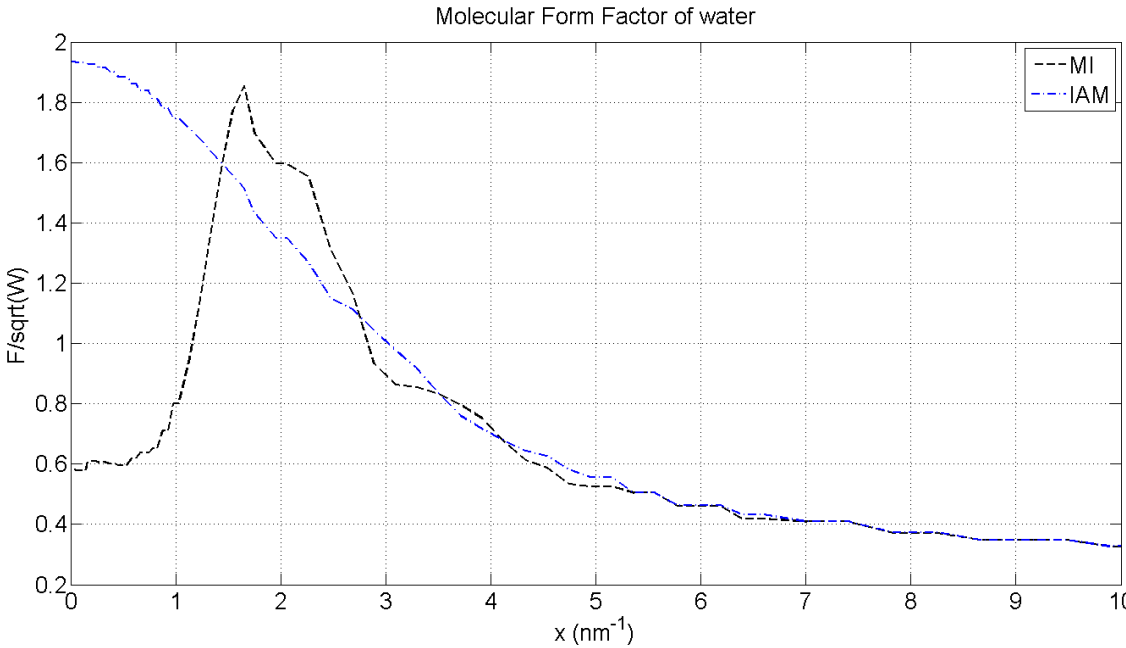
$$F^2_{mol}(q) = F^2_{mol,IAM}(q)\cdot s(q)$$

Independent-Atoms Model (IAM)

Molecular Interference (MI) effects appear in **liquid** and **amorphous solids** (not only in crystals) due to **short-rang (A) order (d=1/(2x))**.
The peaks of F_{mol} are characteristic of the material

$$2d\sin(\theta/2) = \lambda$$





The fraction of coherent scattering interactions is about 10% for materials and energies of medical interest but, due to MI, coherent radiation is not forward peaked and is distinguishable from primary radiation.

Theoretical background: Molecular Form Factor

Why is it important to evaluate as accurately as possible coherent scattering?

- It can be used to **correct** absorption-based images

(Johns & Yaffe, "Coherent scatter in diagnostic radiology" Med. Phys., 1983)

- It can exploited for **tissue characterization** (in particular for breast)

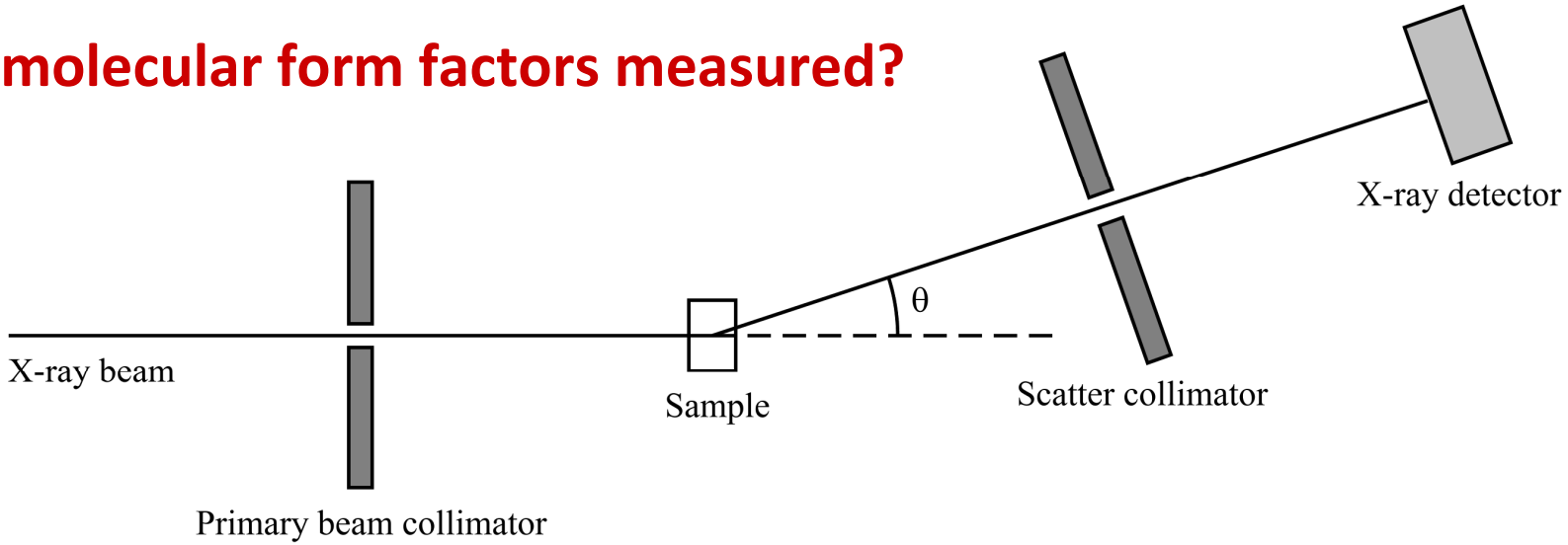
(Harding & Co., "X-ray diffraction computed tomography", Med. Phys., 1987)

- At very small-angle, it can be used to characterize **ordered structure at a larger scale** [nm - tens of nm] in biological samples, such as **collagen**.

(Fernandez & Co., "Small-angle x-ray scattering studies of human breast tissue samples", Phys. Med. Biol. 47 (2002) 577–592)

X-ray diffraction (XRD) experiments

How are molecular form factors measured?



ADXRD

- Scattering signal acquired as a function of θ
- Monochromatic X-ray beam
- Low photon flux
- Higher resolution (Δx/x) achievable

EDXRD

- Scattering signal acquired at fixed angle θ
- Polychromatic X-ray beam
- Require a spectroscopic detector
- Faster

It is possible to combine these methods to improve the sensitivity *(see, for instance, Marticke et al., NIM A 867 (2017) 20-31)*

X-ray diffraction (XRD) experiments

$$\mu_S(\theta) = \frac{N_A \rho}{M}\left[\frac{d\sigma_T(\theta)}{d\Omega}F^2(x) + \frac{d\sigma_{KN}(\theta)}{d\Omega}S(x)\right] \quad \text{[cm^-1 sr^-1]}$$

Measured intensity I(θ) must be corrected in order to extract the form factor of the material

$$\mu_S = K\{I(\theta) - [B(\theta) + MS(\theta)]\}M(\theta)A(\theta)$$

- B(θ) -> Background
- MS(θ) -> Multiple Scattering
- M(θ) -> Polychromatic beam
- A(θ) -> Self-attenuation and geometric effects
- K -> normalization factor obtained from IAM for large x (3 – 6 nm^-1)

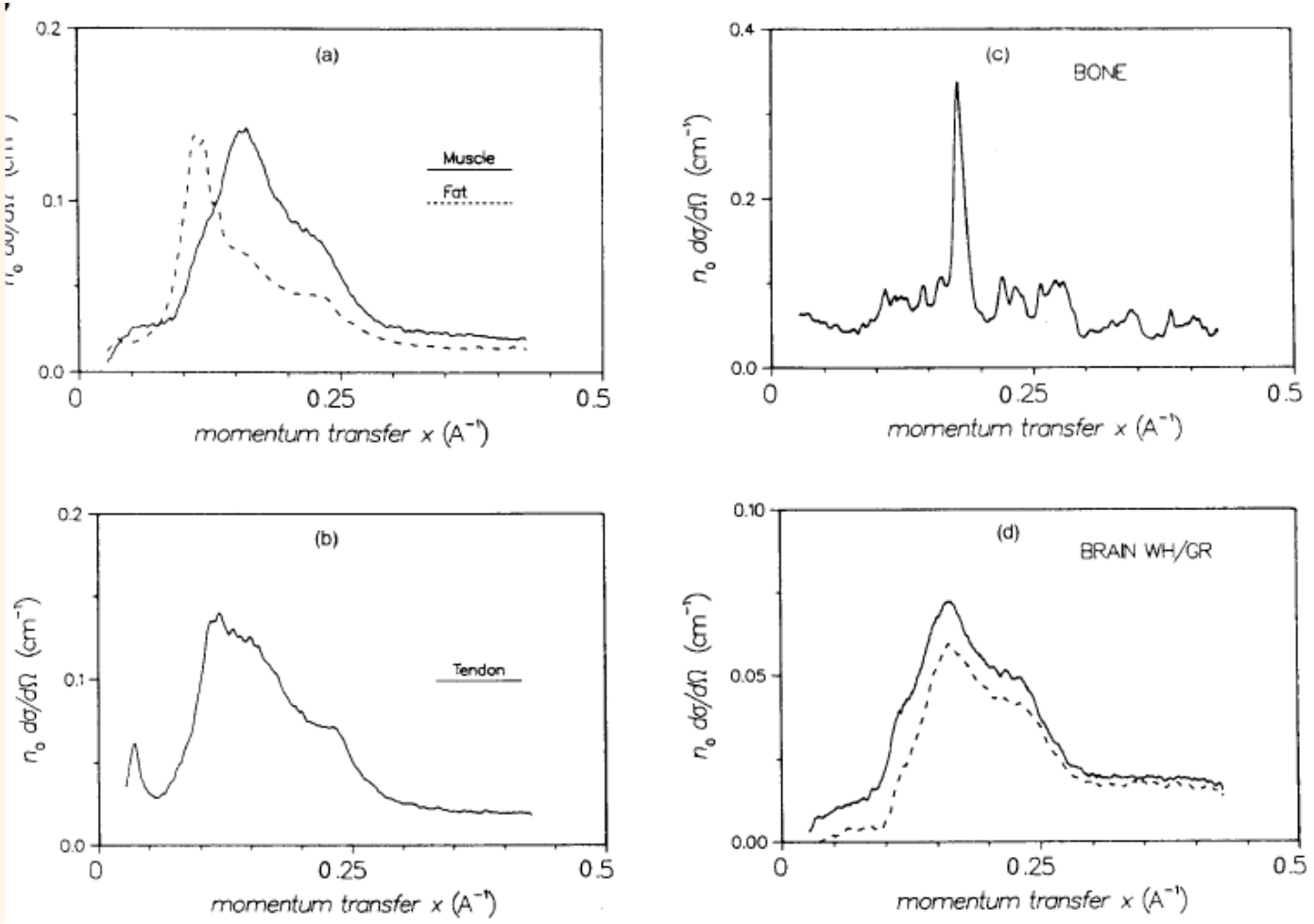
Measured form factors

Various research groups have measured form factors for biological tissues and plastic materials. A short list is

- Kosanetzky & Co.
- Kidane & Co.
- Peplow & Verghese
- Tartari, Taibi & Co.
- Leclair & Co.
- Poletti & Co.
- Chaparian & Co.
- King & Johns

However **there is not a coherent database of form factors**, and data slightly differ from each other.

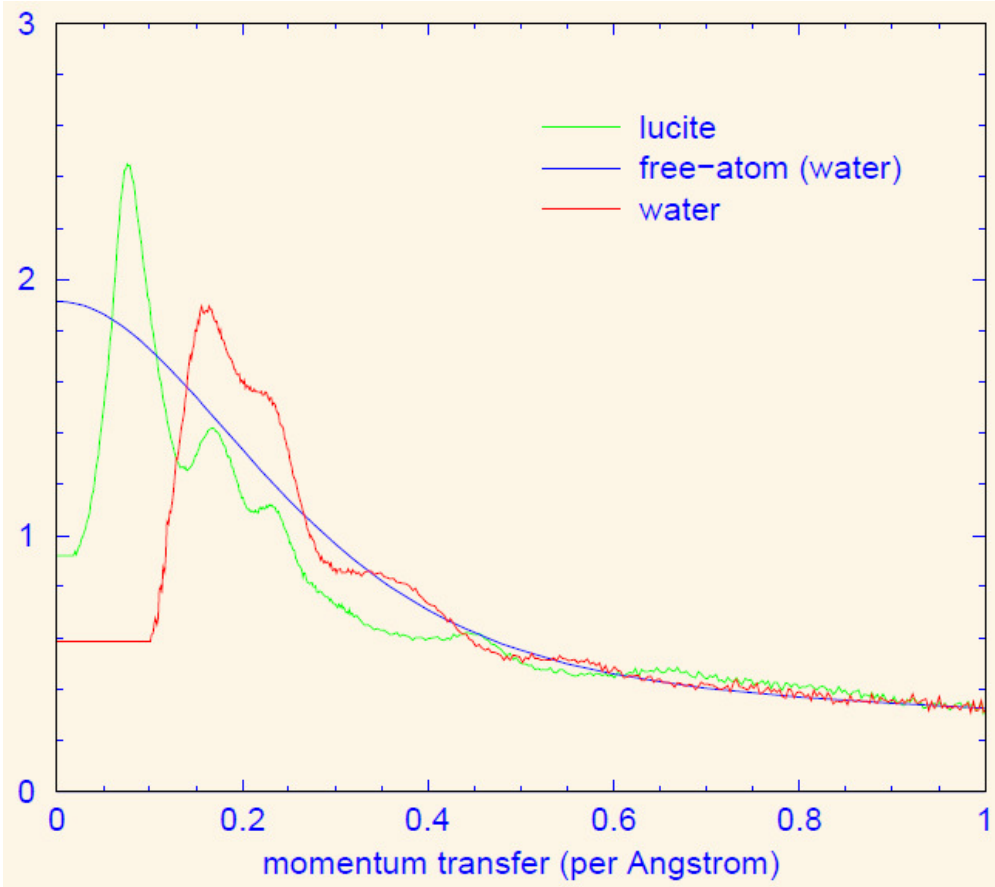
Examples of form factors

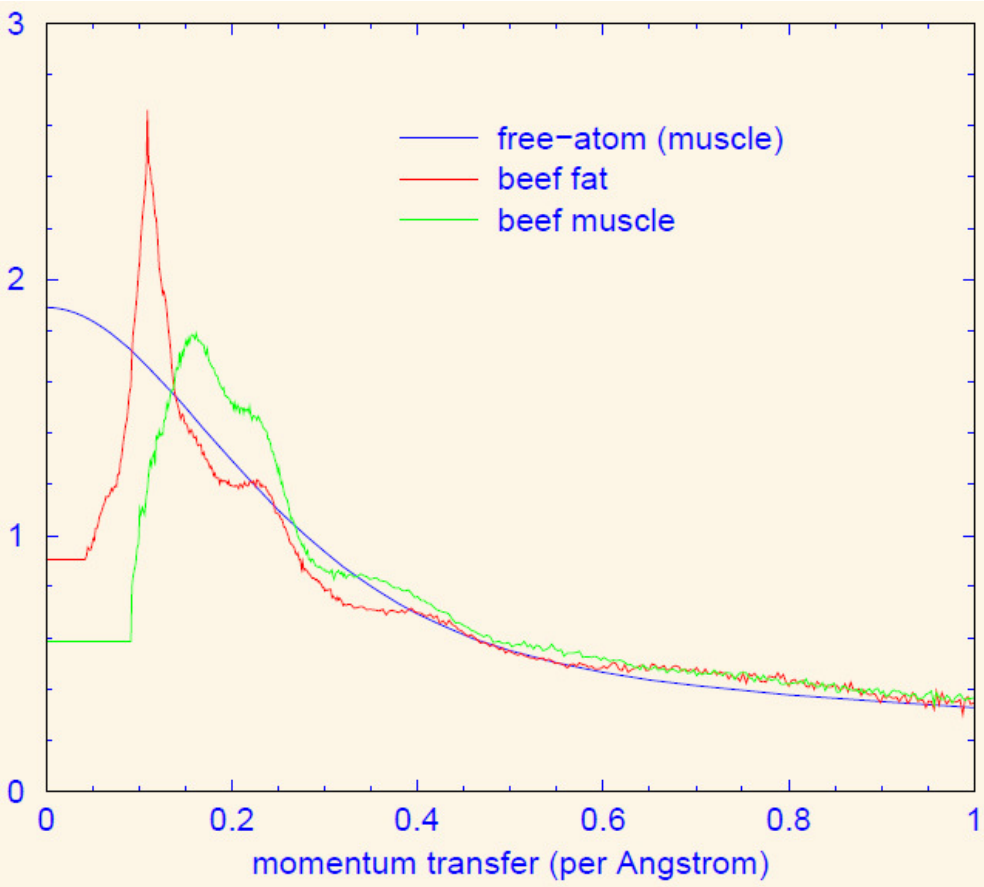


Kosanetzky & Co., "X-ray diffraction measurement of some plastic material and body tissues", Med. Phys., 14 (4), 1987

ADXRD with a diffractometer

Examples of form factors





Peplow & Verghese., "Measured molecular coherent scattering form factors of animal tissues, plastics and human breast tissue", Phys. Med. Biol. 43 (1998) 2431–2452

National Synchrotron Light Source at Brookhaven National Laboratory

Simulation of MI in coherent scattering

The most used **particle tracking codes** do not natively consider molecular interference in coherent scattering.

For some of them, interested users have developed **custom models of Rayleigh scattering** that include MI. See, for example:

PENELOPE: *Ghammraoui et al., Proc SPIE 2014;9033:90334N*
EGS4: *Taibi et al., IEEE Trans Nucl Sci 2000;47:1581–6*

Geant4 simulation toolkit

Geant4 is a **open-source C++ based object-oriented** Monte Carlo toolkit for particle transport in matter. It is routinely used in **many scientific disciplines** included medical science. It provides:

- advanced geometry modeling,
- high quality physics models,
- advanced tracking algorithms,
- interactive facilities for visualization and execution.

For each physical process various models are available (specialized for particle type and energy scope). **Electromagnetic** physics foresees **Standard** and **Low Energy** packages.

In **Standard models**, the energy of the particles > 1 keV, the atom nucleus is free, the atomic electrons are quasi-free, and matter is described as homogeneous, isotropic, amorphous.

The **Low Energy package** extends the coverage of electromagnetic interactions down to 250/100 eV, it includes processes based on **detailed models** (atom shell structure, precise angular distributions, polarization, etc).

The **coherent scattering models** current implemented in the official release **do not take into account the influence of molecular interference.**

Electromagnetic physics in Geant4

EM processes → **Low Energy** →

in **two "flavors" of models**:
- based on the Livermore Library
- à la Penelope

- Multiple scattering
- Bremsstrahlung
- Ionization
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh scattering
- e+e- pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Scintillation
- Refraction (opticlal ph)
- Reflection (opticlal ph)
- Absorption (opticlal ph)
- Fluorescence
- Auger

Livermore

- Based on evaluated data libraries from LLNL (**mixture of experiments and theories for electrons and photons**):
  - EADL *(Evaluated Atomic Data Library)*
  - EEDL *(Evaluated Electrons Data Library)*
  - EPDL97 *(Evaluated Photons Data Library)*

  especially formatted for Geant4 distribution *(courtesy of D. Cullen, LLNL)*
- Validity range: 250 eV - 100 GeV
- Elements Z=1 to Z=100

Penelope

- The whole physics of Penelope code has been re-engineered into Geant4 (it benefit from OO power)
- Physics models by F. Salvat et al. (**version 2008**)
- **Mixed approach**: analytical, parameterized & data-driven (down to 100 eV)
- **Great care of atomic effects, fluorescence, Doppler broadening, etc**
- **Manages positrons**

Simulation of coherent scattering events: Penelope algorithm

First, the occurrence of a coh. scatt. event is determined from σ_{Ra}, then the angular deflection is sampled

$$P_{Ra}(\cos\theta) = \frac{1+\cos^2\theta}{2} F^2(q) \qquad 0 \le q \le q_{\max} = 2E/c = 2m_e c\kappa$$

$$P_{Ra}(\cos\theta) = g(\cos\theta)\pi(q^2) \qquad g(\cos\theta) = \frac{1+\cos^2\theta}{2} \qquad \pi(q^2) = F^2(q)$$

rejection method

1. Using the **RITA algorithm**, sample a random value of q^2 from the distribution $\pi(q^2)$, restricted to the interval $[0, q_{max}^2]$.
2. Set $\cos\theta = 1 - 1/2 * q^2/k^2$ ($k = E/m_e c^2$). *(it comes from the definition of $q = 2E/c[\sin(\theta/2)] = (E/c[2(1-\cos\theta)]^{1/2})$*
3. Generate a new random number ξ (uniformly distributed in the interval [0,1]).
4. If $\xi > g(\cos\theta)$, go to step 3. *(note that **g is a valid rejection function** since $0 < g \le 1$)*
5. Deliver $\cos\theta$.

Sampling efficiency higher than 66%

MI effect implementation in Geant4

- **Penelope model of Rayleigh scattering** (*G4PenelopeRayleighModel* class – 10.3.1 version) was modified in order to take into account MI effect by **reading custom molecular form factors** (through the new method: *ReadMolInterferenceData()*).

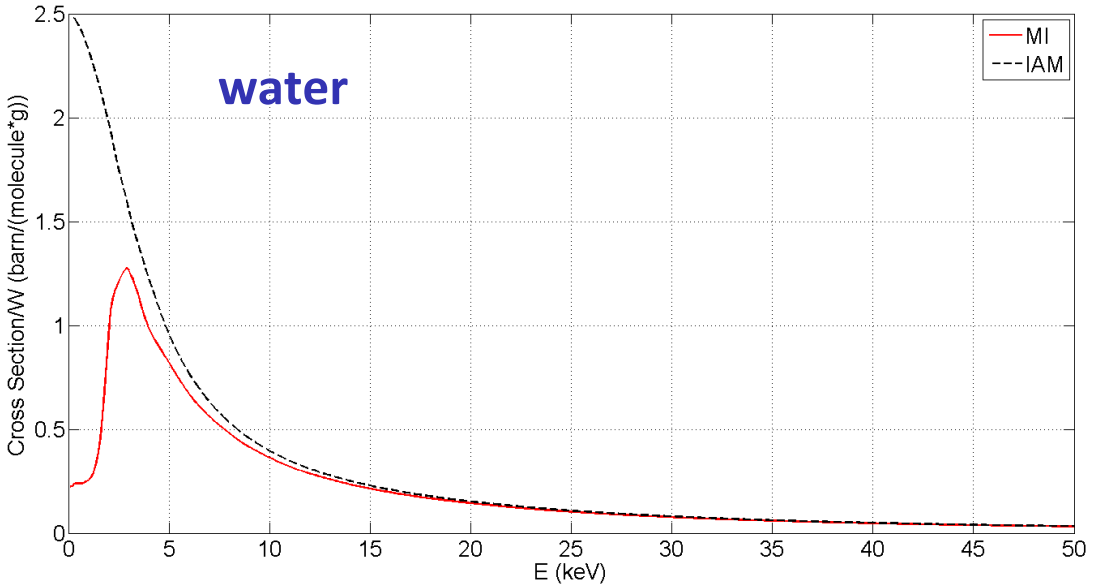
- **A database of form factors for a set of material of medical interest** (various tissues and plastics) was prepared. The files were positioned inside the directory "MIFF" located at the low energy data path:

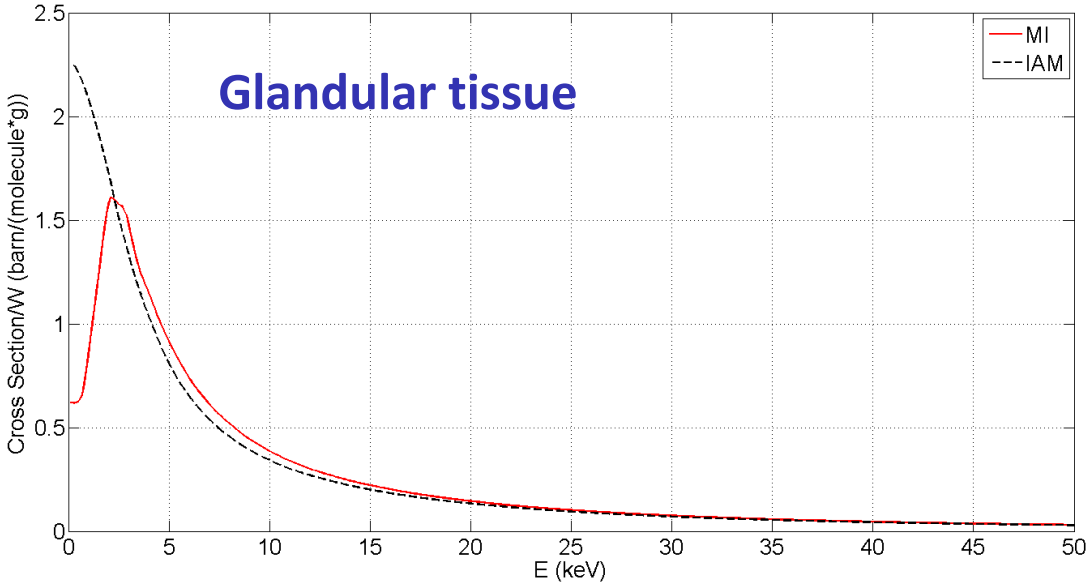
  Geant4_installation_path/share/Geant4-10.3.1/data/G4EMLOW6.50/penelope/rayleigh/

- Molecular form factors including MI can be accessed by **assigning proper names to the materials** used in the simulation.

MI effect implementation in Geant4

Since coherent scattering total cross-section for compounds is managed by a separate class ad it remains approximately the same with and without MI for energies of medical interest (see the figure), **the modified form factors is used only for sampling the photon angular deflection**.





List of implemented Molecular Form Factors

A total of 24 Molecular Form Factors have been included

Tartari et al., Phys. Med. Biol. 47 (2002), 163-175

- fat
- water
- collagen (bone matrix)
- hydroxyapatite (mineral)
- PMMA

Peplow and Verghese, Phys. Med. Biol. 43, No. 9 (1998), 2431-2452

- lucite, lexan, kapton, water
- pork heart, kidney, liver, muscle
- beef blood
- human breast

Kidane et al., Phys. Med. Biol. 44 (1999), 1791-1802

- carcinoma tissue

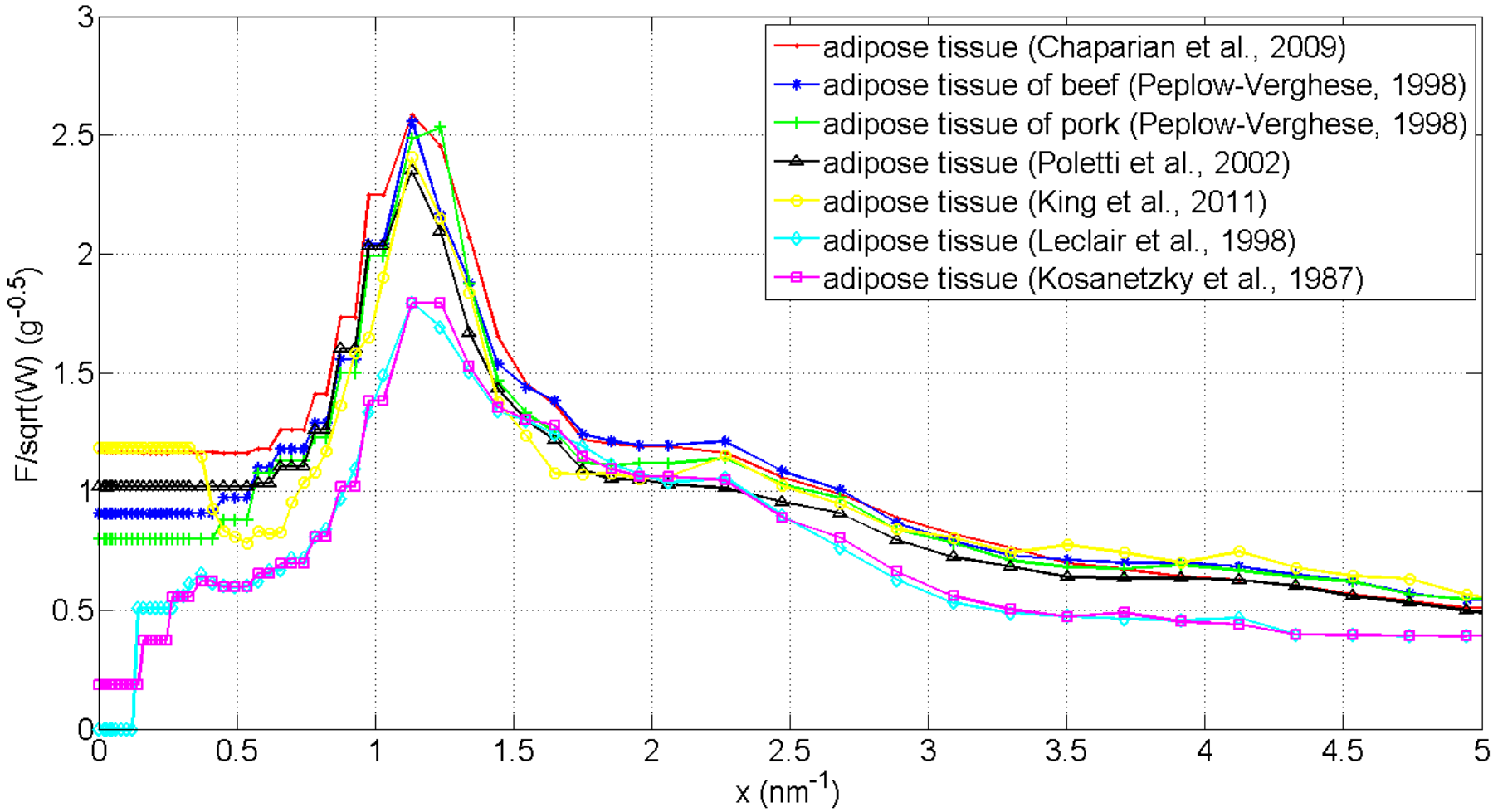
Chaparian et al., Iran. J. Radiat. Res., 2009; 7 (2): 113-117

- adipose
- glandular
- breast tissue (50% water - 50% lipid)
- water

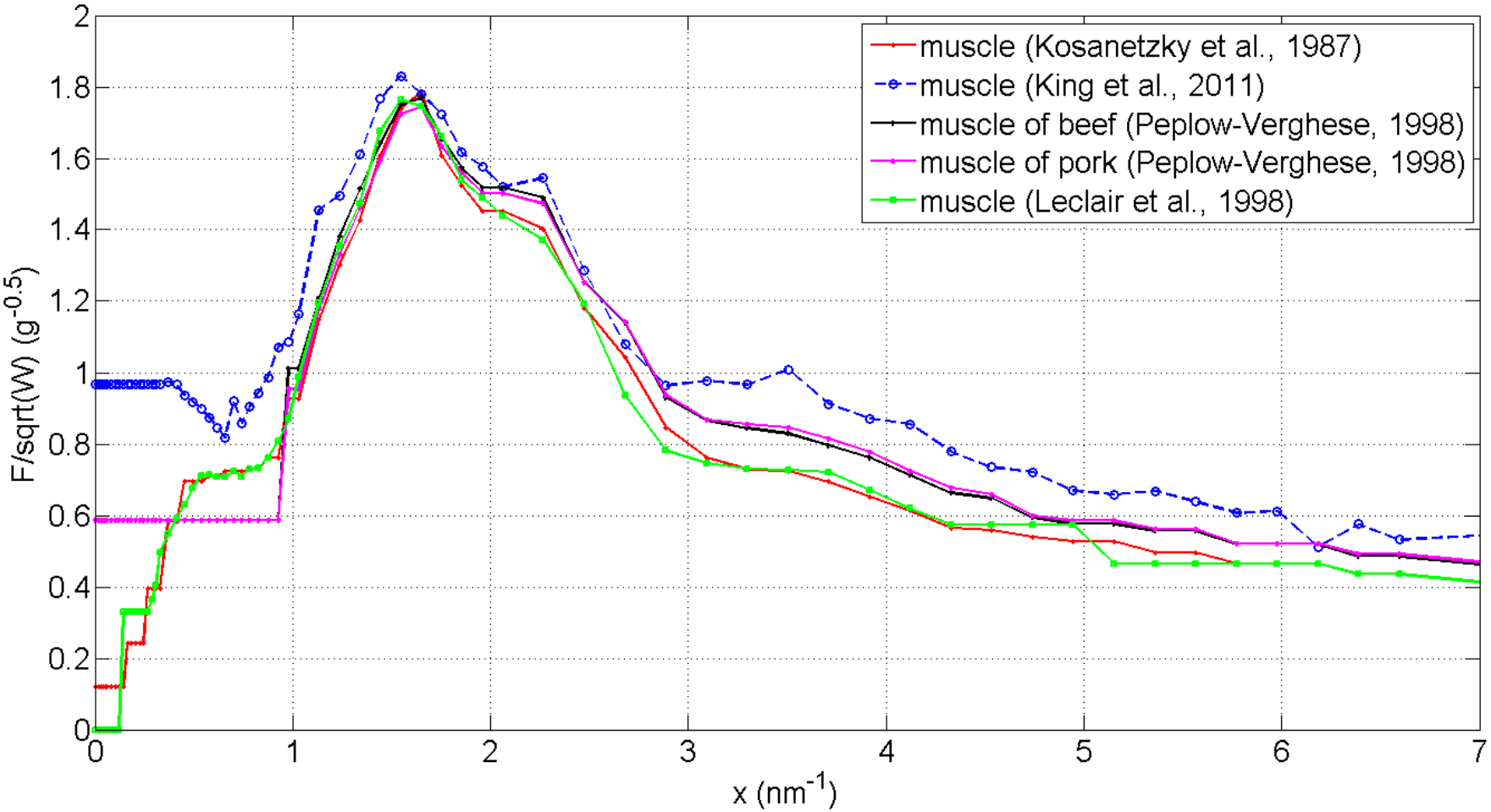
Kosanetzky et al., Med. Phys. 14 (4) 1987, 527-532

- nylon
- polyethylene
- polystyrene
- gray matter

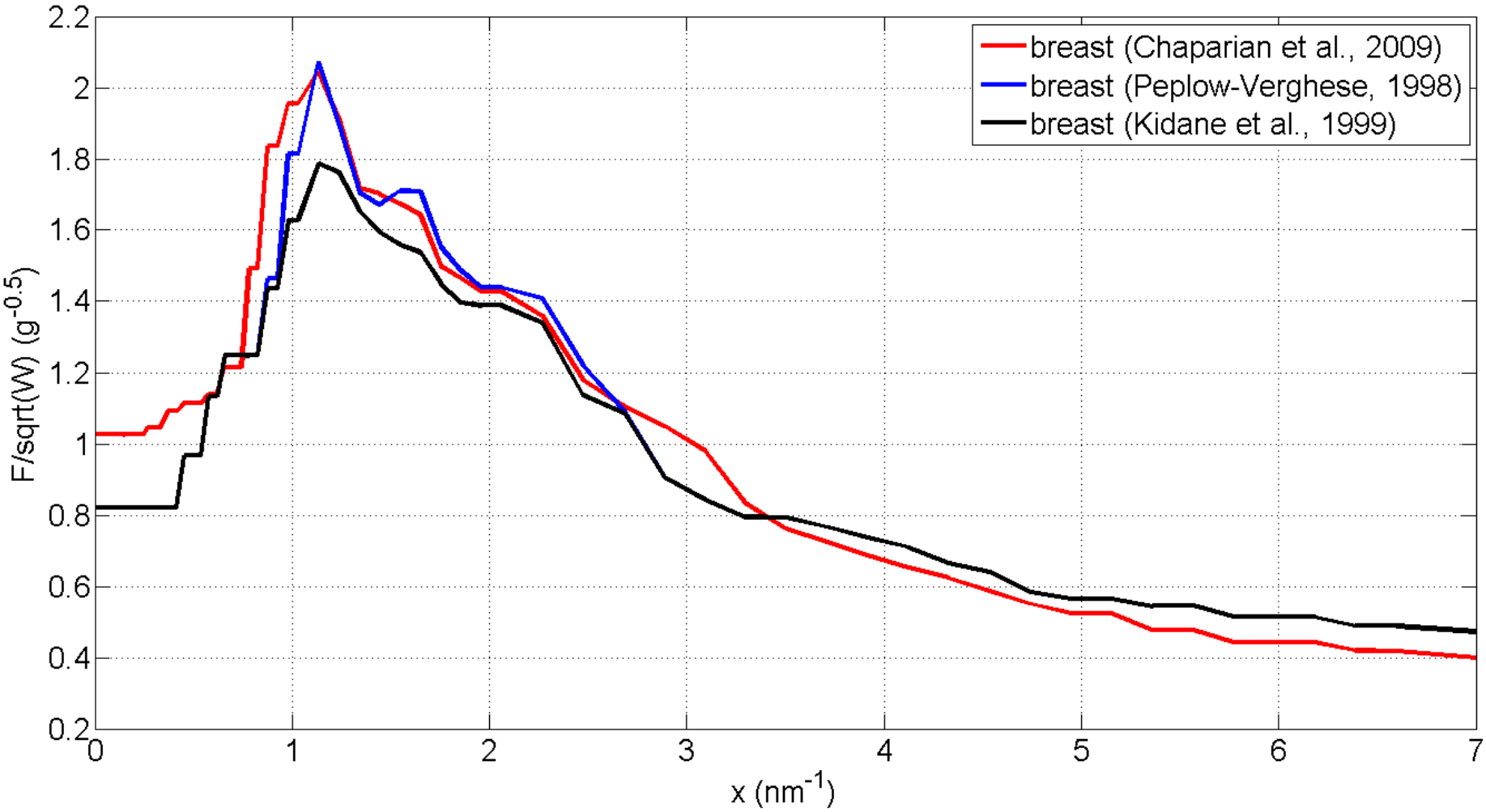
Examples of Molecular Form Factors



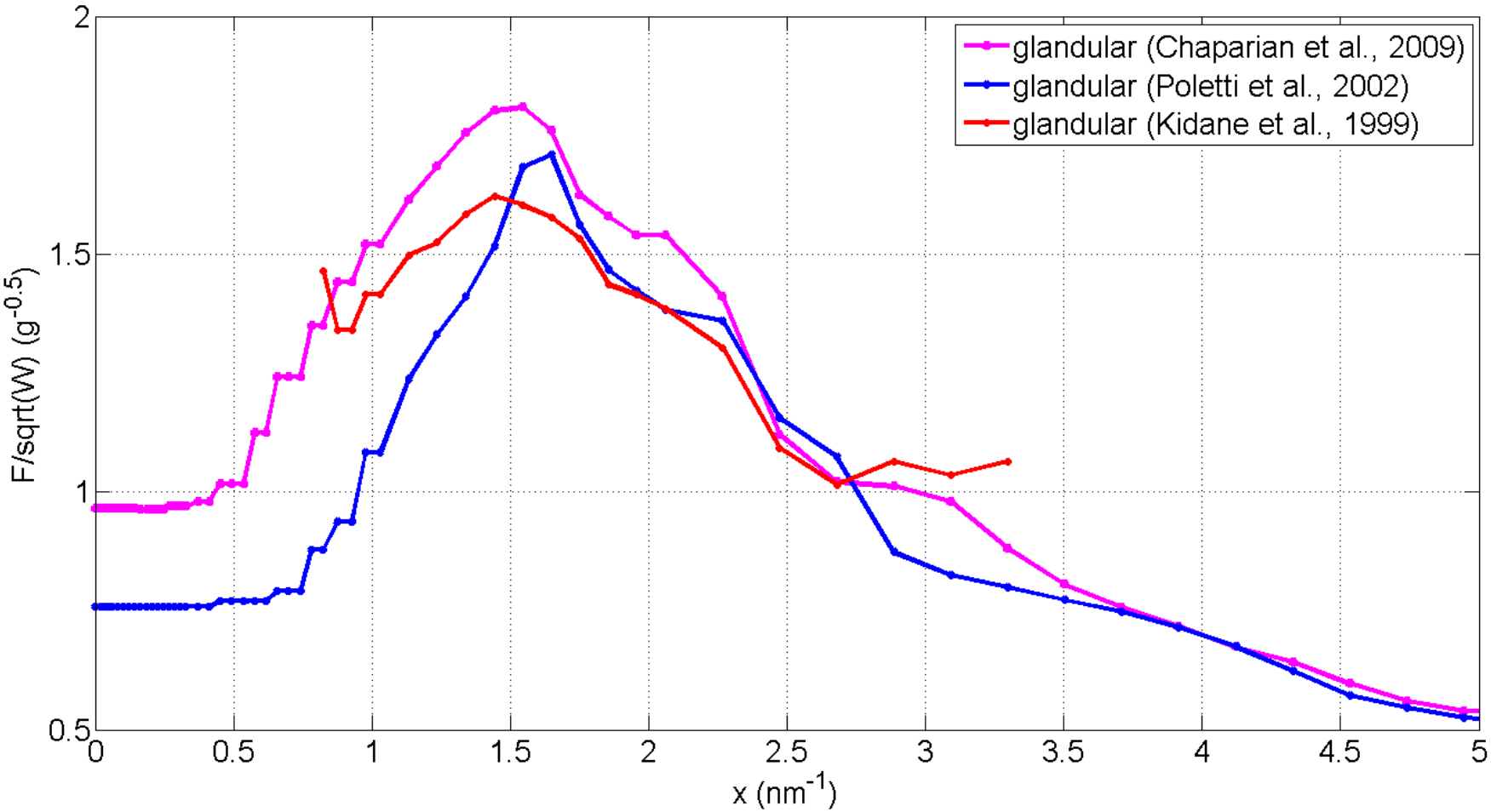
Examples of Molecular Form Factors



Examples of Molecular Form Factors



Examples of Molecular Form Factors



List of implemented Molecular Form Factors

tissue → { soft tissue (fat, water); bone tissue → { dry bone (mineral, non-mineral); red and yellow marrow (soft issue) }

A set of four components, namely **fat**, **water**, **bone matrix (BM)** and **hydroxyapatite (HA)**, **can represent a basis for the composition of the human tissues**. Once the basis is defined, **one can simulate a given tissue by linear combination**.

$$F^2_{tissue}(q) = a_1 F^2_{fat}(q) + a_2 F^2_{water}(q) + a_3 F^2_{BM}(q) + a_4 F^2_{HA}(q)$$

Elemental composition by mass of the four basis materials

Substance	H	C	N	O	p	Ca	Density (g/cm^3)
water	0.1119			0.8881			1.00
fat	0.1190	0.7720		0.1090			0.923
bone matrix (collagen)	0.0344	0.7140	0.1827	0.0689			-
hydroxyapatite (mineral)	0.0020			0.4140	0.1850	0.3990	2.74

This approach was proposed in:

.*Taibi et al., Proceedings of the Monte Carlo 2000 Conference , Lisbon, 23–26 October 2000.*

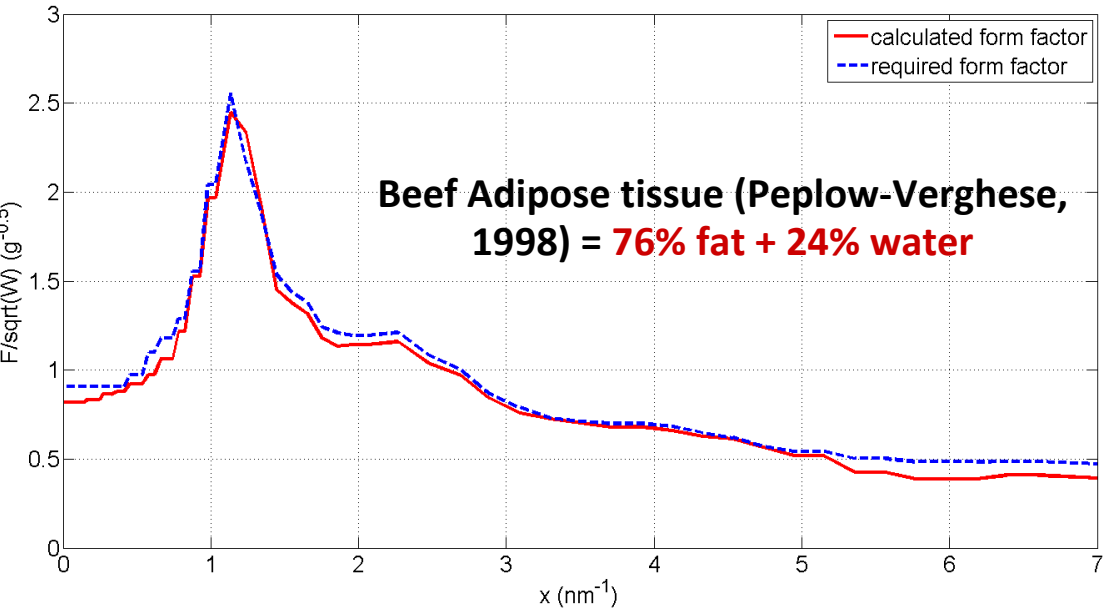
.*Tartari et al., Radiation Physics and Chemistry 61 (2001) 631–632.*

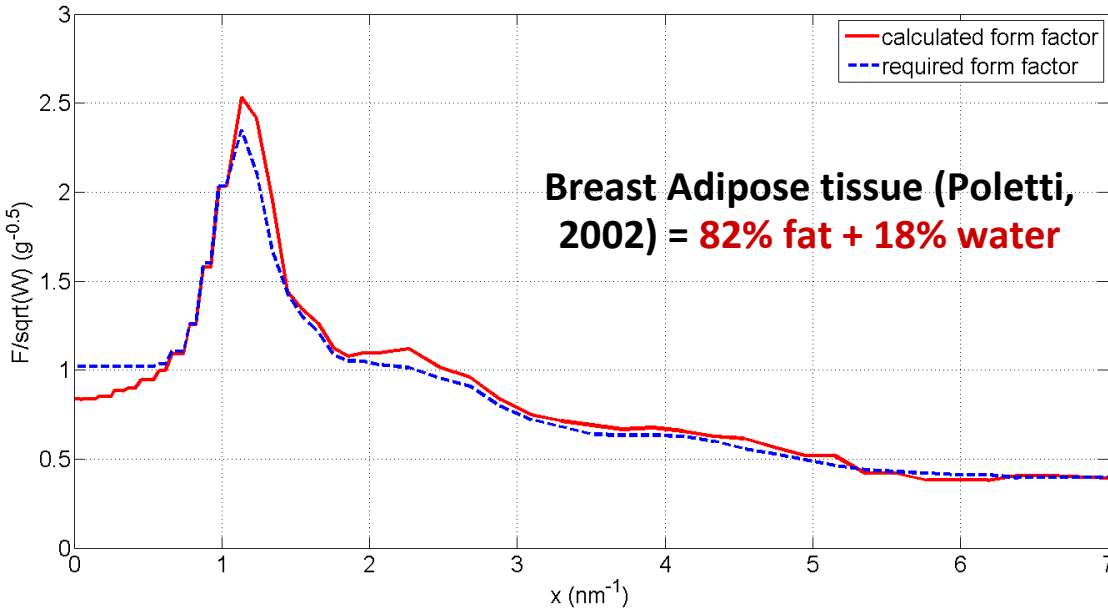
.*Tartari et al., Phys. Med. Biol. 47 (2002), 163-175.*

List of implemented Molecular Form Factors

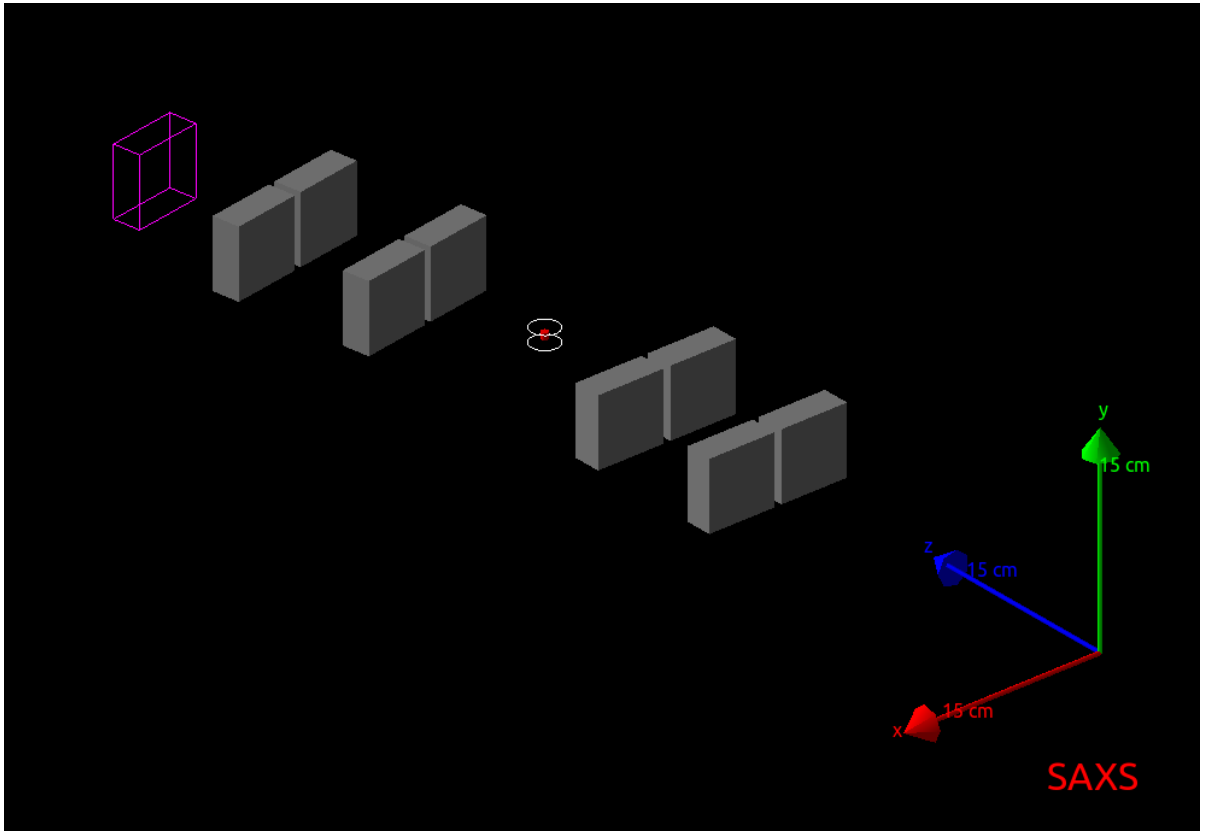
This approach permit us to model unclassified tissues in term of a proper linear combination of the 4 basis materials.

a_j coefficient can be obtained by a multivariate approach (method of least squares)





Validation: the SAXS application



A **dedicated tool** has been developed in Geant4 to test the molecular interference implementation.

- **Geometry, materials, physics and X-ray source** configuration through **custom commands** (to be used in a macro file)
- **Material management** (the "**basis approach**" is foreseen and can be activated by codifying the material composition in its name, e. g., "*MedMat_0.25_0.36_0.13_0.36*")
- **Scoring** through *SteppingAction* and *SensitiveDetector* (simple scoring screen or Ge detector) -> a number of **root scripts** available for data analysis
- Calculation of **Dose** delivered to phantom/detail

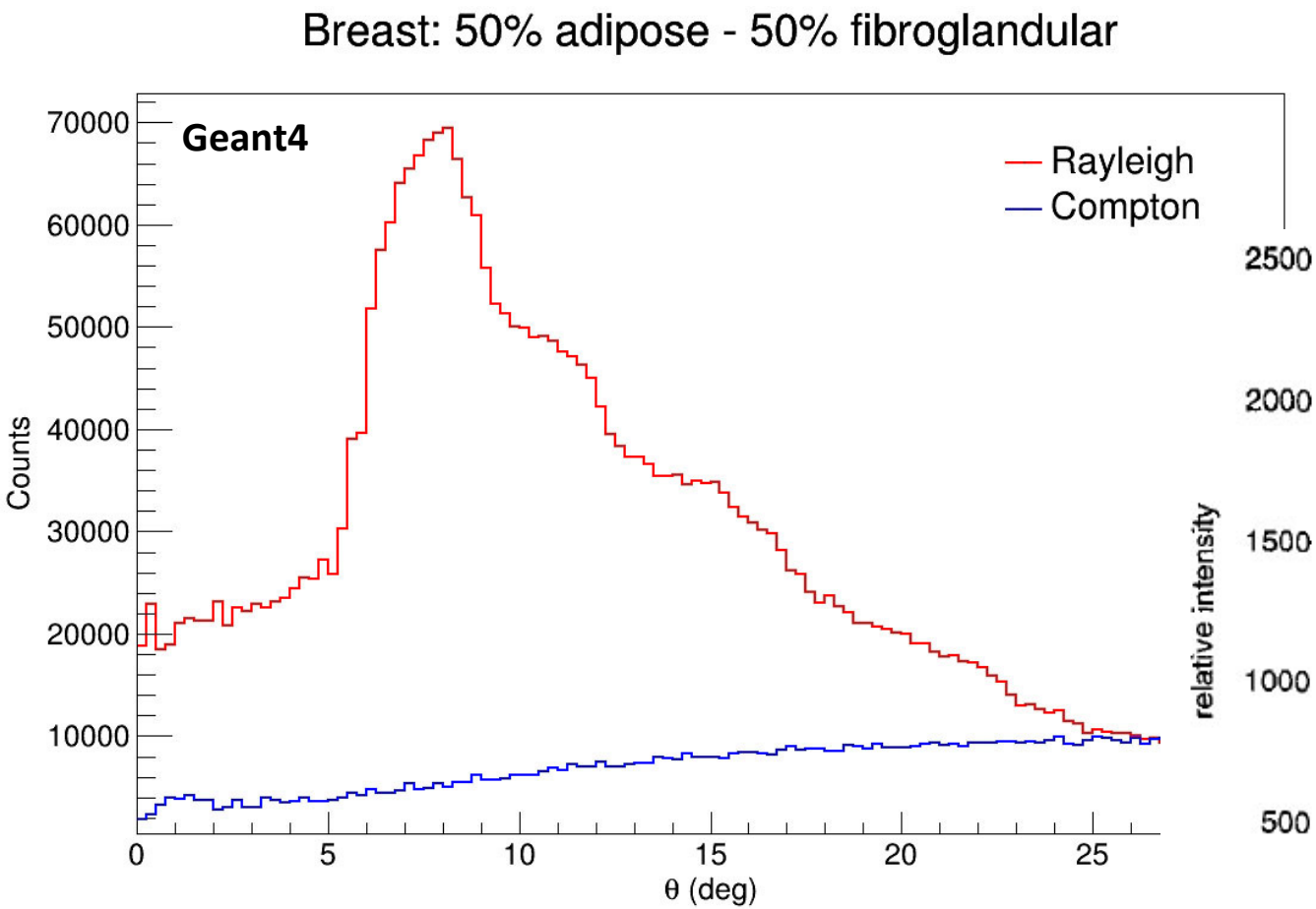
Validation: example of input macro (run.mac)

```
/det/setComp0 0.00
det/setComp1 0.00
det/setComp2 0.00
/det/setComp3 1.00

/det/setPhantomType 1
/det/setPhantomRotation 1
/det/setPhantomZ 100. mm
/det/setPhantomMaterial 2
/det/setPhantomDiameter 50. mm
/det/setPhantomThickness 5. mm

/det/setDetailMaterial 2
/det/setDetailDiameter 10. mm
/det/setDetailThickness 1. mm
/det/setDetailPosition 0. 0. 0. mm
```

```
/det/setThetaSetup 0.


/det/setSlitThickness 20. mm
/det/setSlit1SampleDistance 200. mm
/det/setSlit2SampleDistance 100. mm
/det/setSlit3SampleDistance 100. mm
/det/setSlit4SampleDistance 200. mm
/det/setSlit1Aperture 5. mm
/det/setSlit2Aperture 5. mm
/det/setSlit3Aperture 5. mm
/det/setSlit4Aperture 5. mm

#/det/setWindowThickness 2. mm
#/det/setWindowSampleDistance 1500. mm

/det/setThetaSetup 0.
```

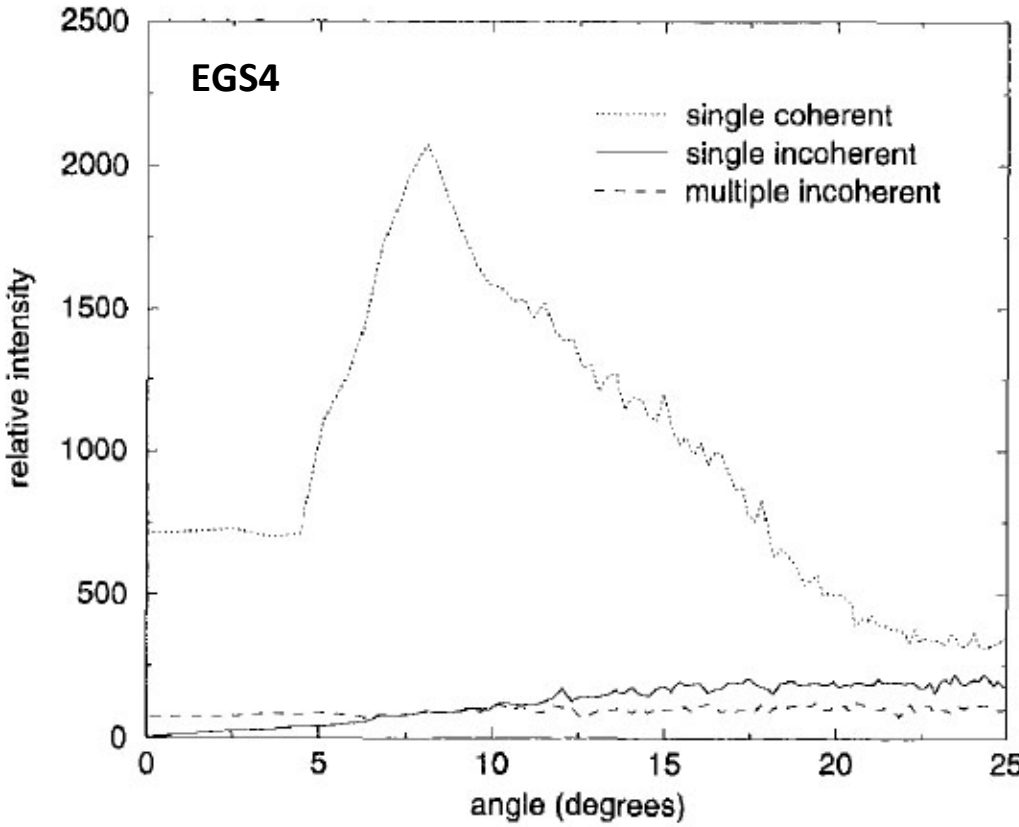
```
det/setDetectorSize 200. mm
/det/setDetectorSampleDistance 400. mm

/det/setMI 1
/det/setScoringIndex 1

/phys/SelectPhysicsList penelope
/phys/setCuts 0.001 mm
/run/initialize
/sd/setEdep true

/run/setfilenamesave output/output

/control/execute input/beam.mac

/run/printProgress 1000000
/run/beamOn 100000000
```

Validation: comparison with previous simulations

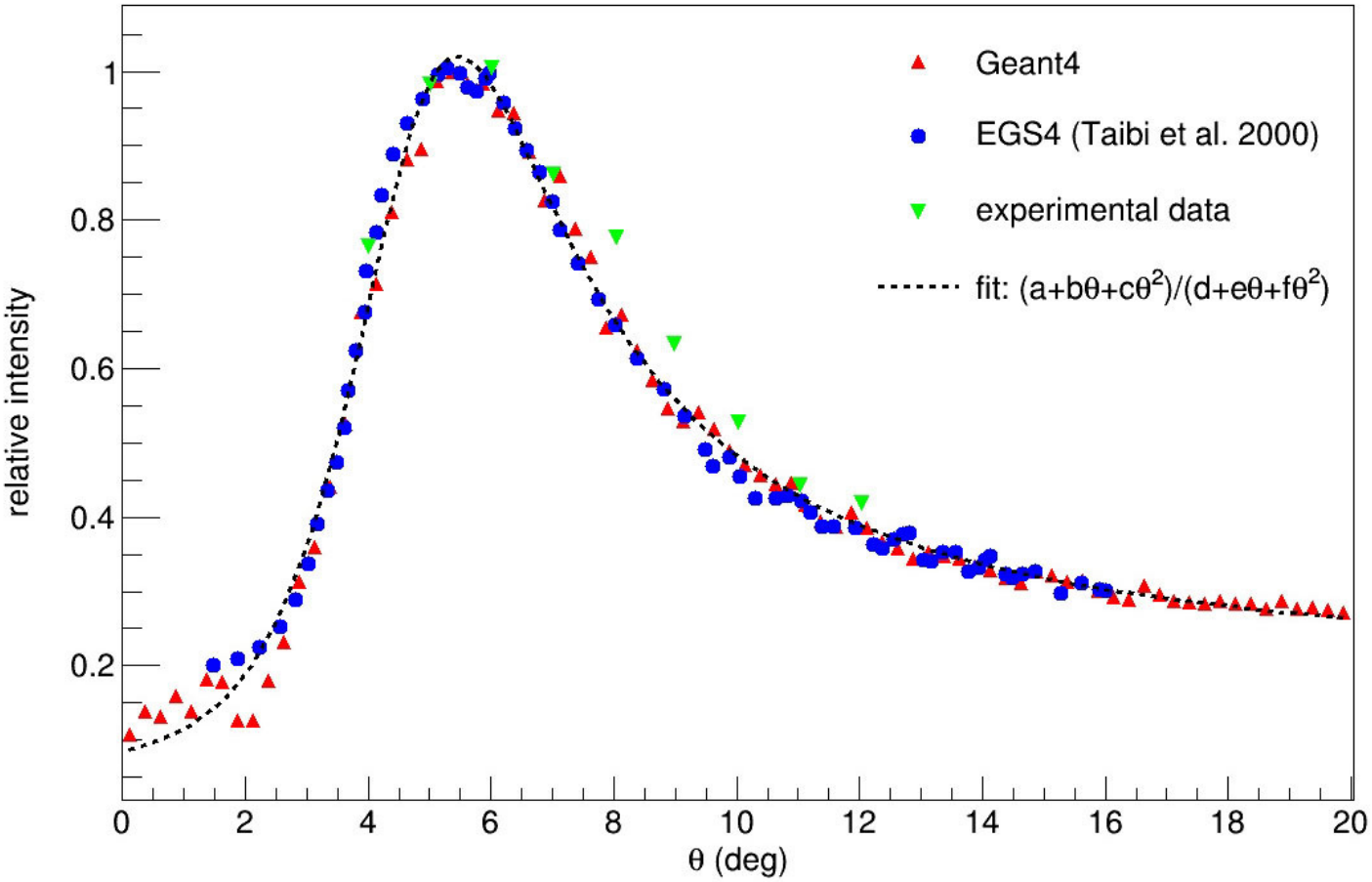


Scatter profiles of **20 keV** photons impinging on a **5 cm-thick human breast sample.**

Taibi et al., IEEE trans. on nuclear science, vol 47 n. 4, 2000, 1581-1586.



Validation: comparison with experiments

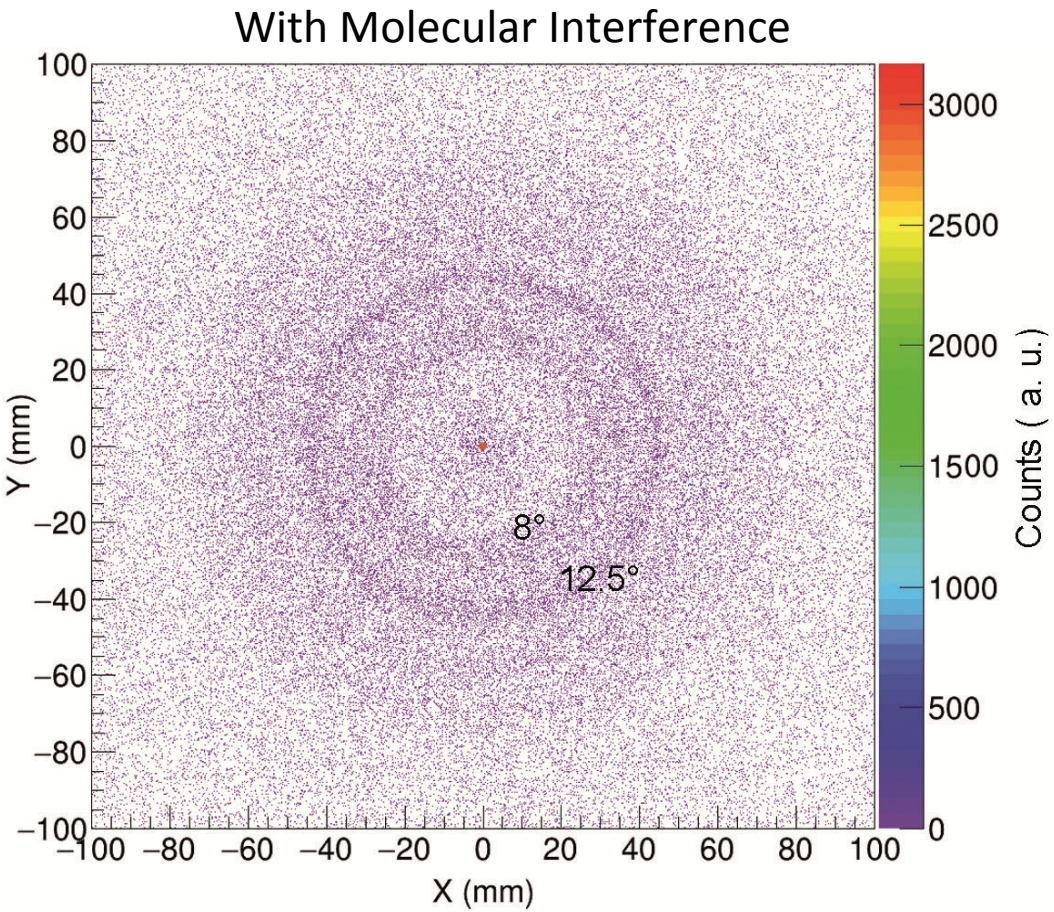


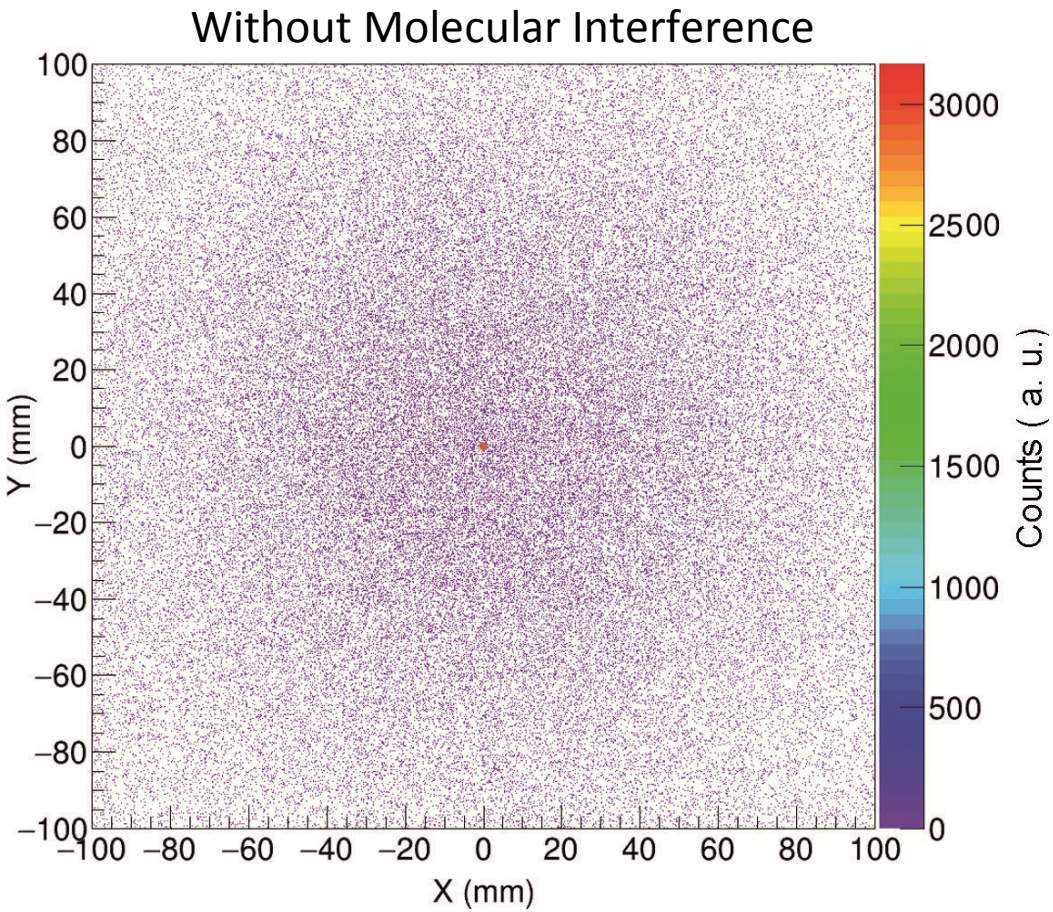
Simulation of the experiment by Evans et al., 1991: Scattering of **polychromatic X-rays** (60 kVp and filtration of 0.5 mm Cu) **from a 5 mm-thick carcinoma sample.**

Simulations are in agreement with the experiment.

G. Paternò et al., Physica Medica 51 (2018) 64 -70

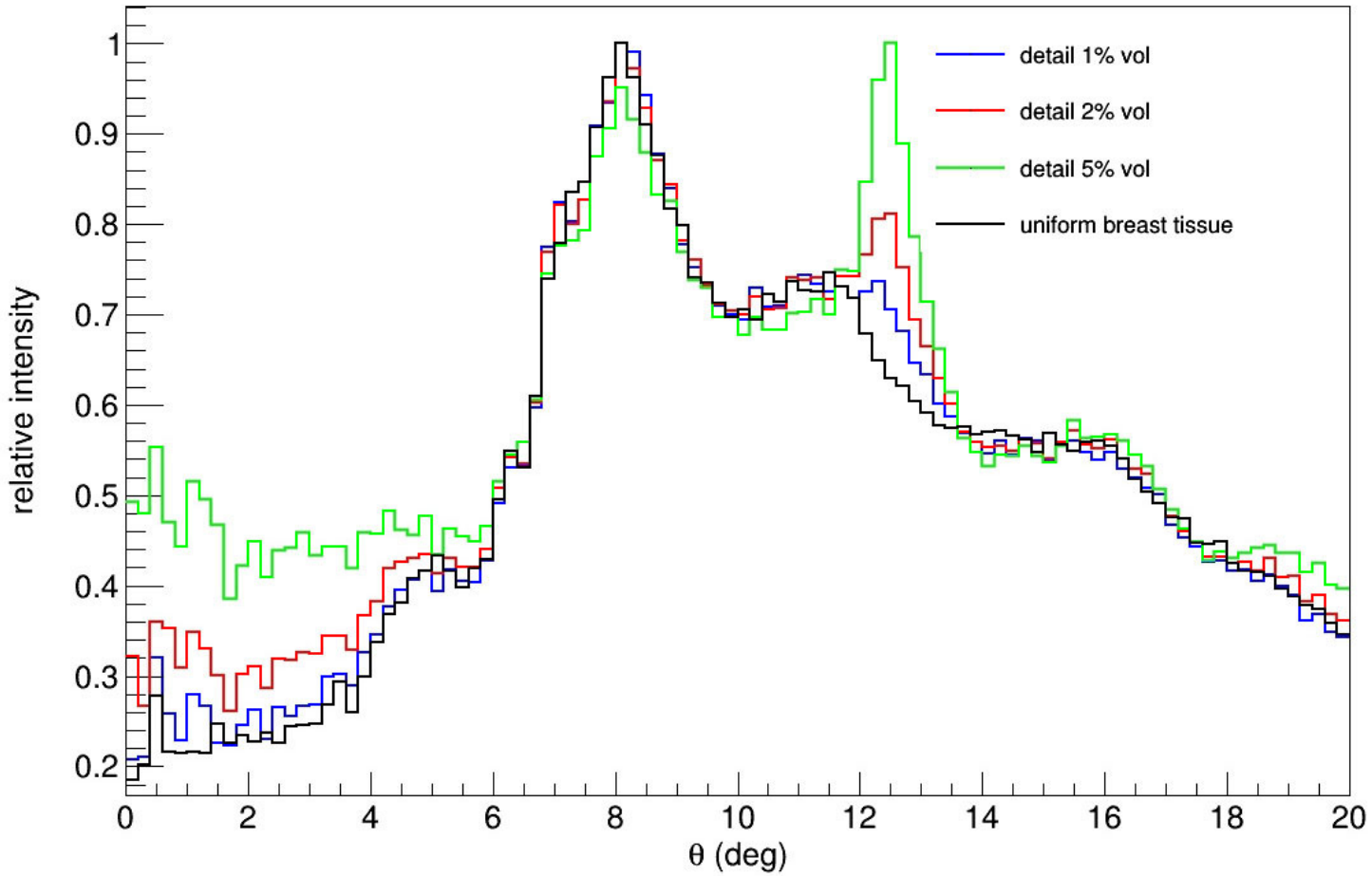
Application: more realistic evaluation of scattering





Scattering of a **20 keV pencil photon beam** impinging on a **5 cm-thick human breast** sample with a **1 mm-thick hydroxyapatite detail** embedded (simulating a calcification).

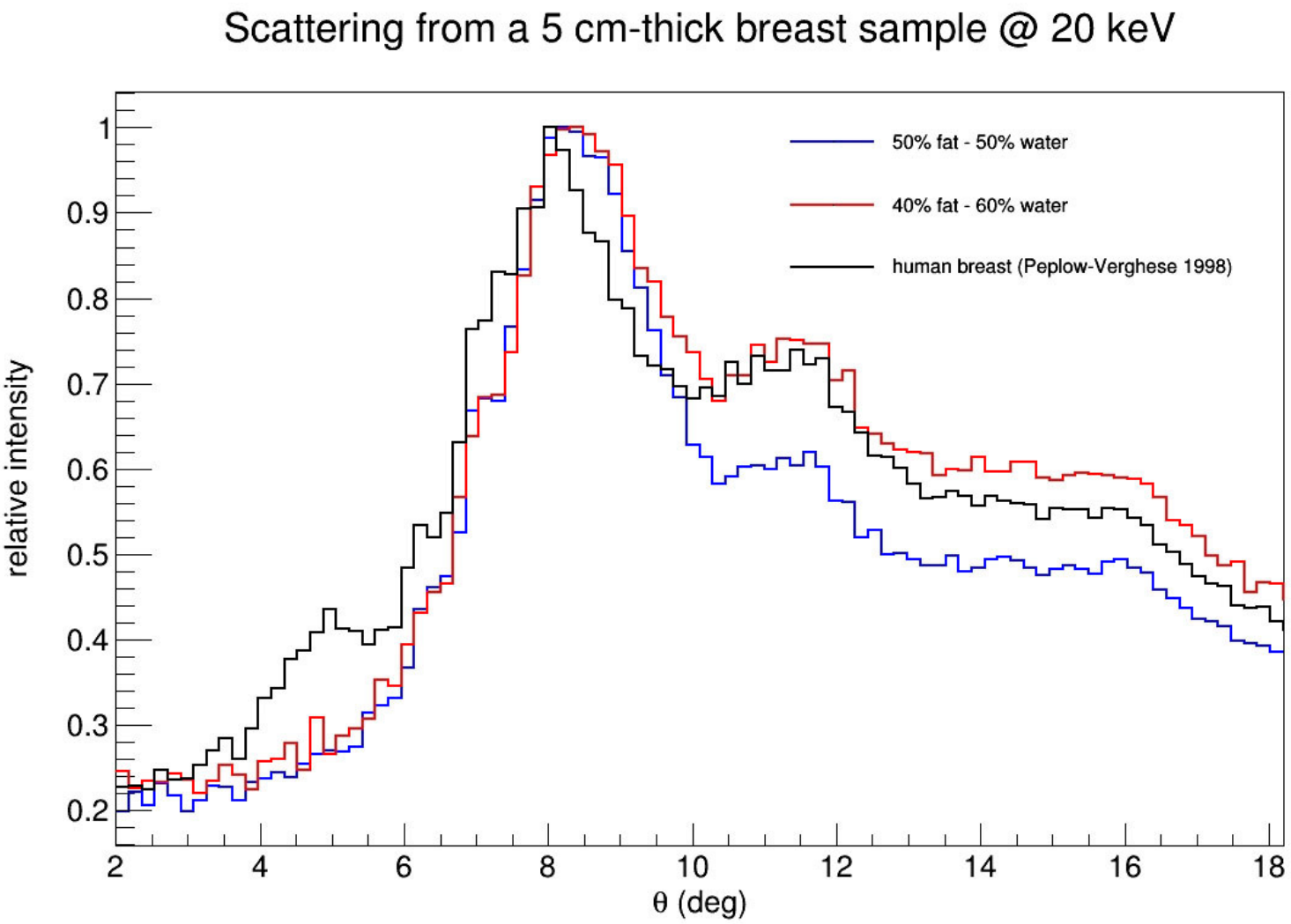
Application: identification of tissues



Through simulations it can be possible to determine the tissue composition that better agrees with the measures.

Scattering of a **20 keV pencil photon beam** incident on a **5 cm-thick human breast** sample with a **hydroxyapatite detail of various size** embedded (simulating a calcification).

Application: identification of tissues

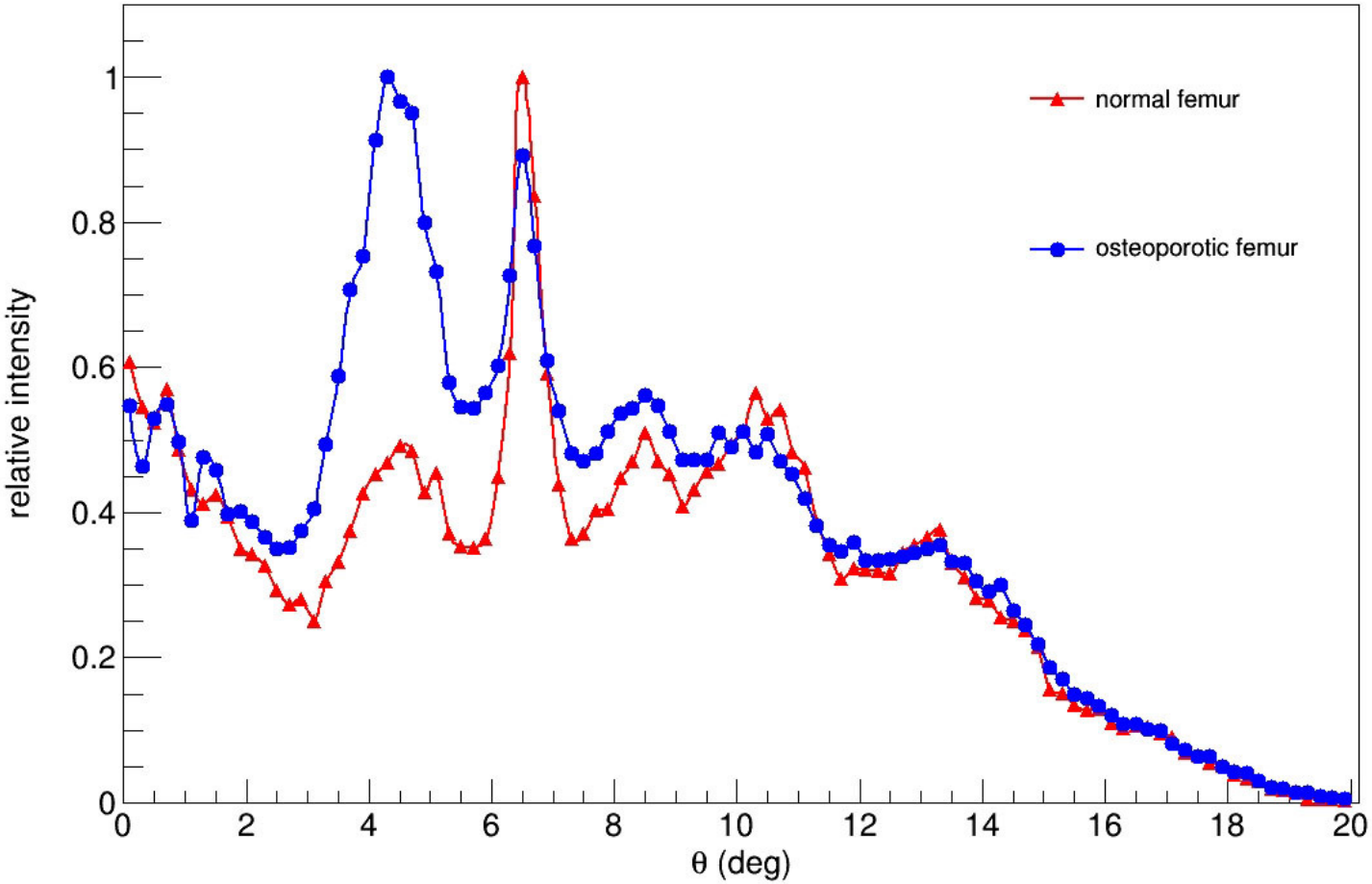


The relative quantity of adipose and glandular tissue in a woman breast is variable and depends also on the age.

Measurements on unclassified tissues are useless for simulation of clinical applications

A more rigorous approach requires the **decomposition in basis materials**

Application: identification of tissues



Scattering of a **38 keV pencil photon beam** incident on two **5 cm-thick samples of human femoral bone (trabecular tissue)**

Normal = 36% fat + 15% water + 13% collagen + 36% HA

Osteoporotic = 55% fat + 25% water + 05% collagen + 15% HA

Identification of osteoporotic state:
proposed by Royle & Speller (1995) and subsequently by Allday & Farquharson (2001) and Hussein et al. (2004).

Form factors at very low momentum transfer

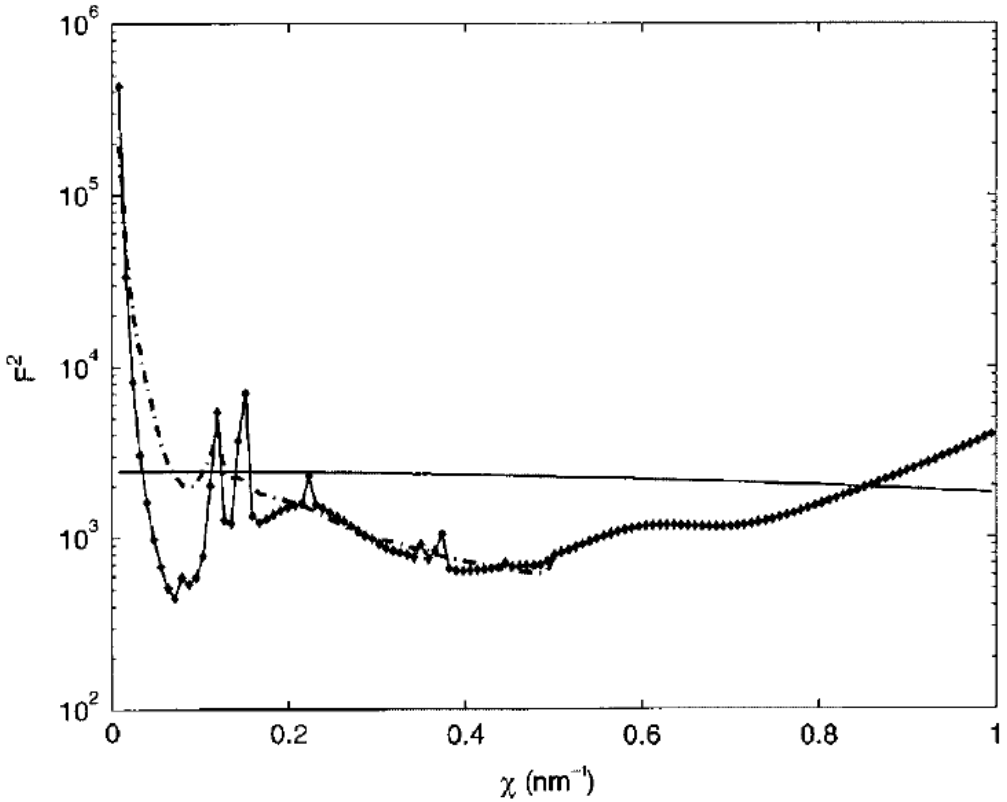


Figure 3. SAXS experimental data, $\chi < 0.5$ nm, for adipose tissue, (♦) and filtered fat: - - - -, ———, corresponding IAM results.

Tartari et al. X-Ray Spectrom. 2005; ***34****: 421–425.*

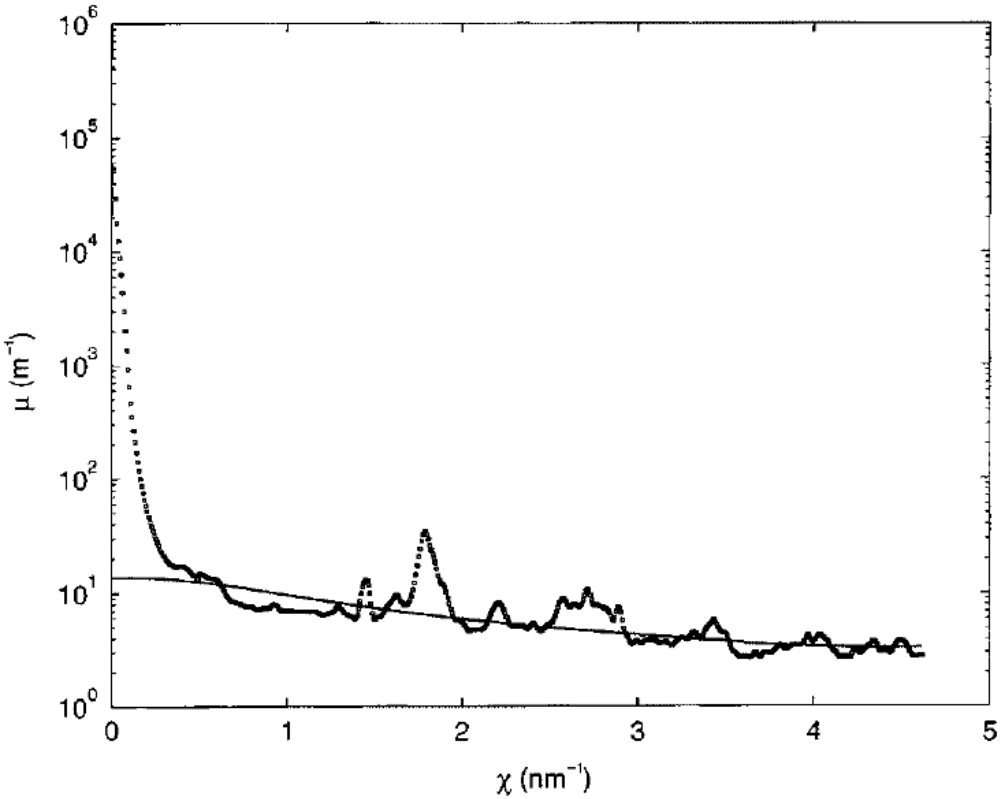
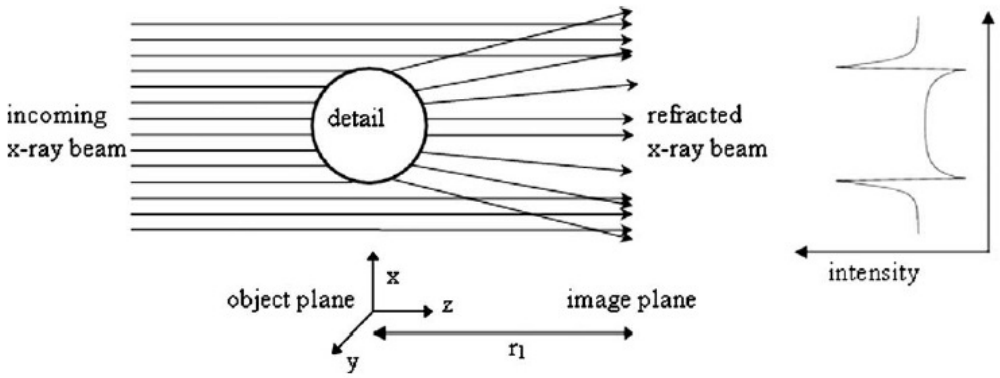


Figure 2. SAXS data, $\chi < 0.5$ nm, together with the WAXS data for dry bone sample. □, experimental; ———, IAM results.

The drastic divergence at low angle was associated with the fractal properties of material large-scale arrangement

Toward the simulation of Phase-Contrast Imaging in Geant4

Propagation-based PCI



$$I(x,y) \cong I_0 e^{-2B(x,y)}\left(1-\frac{\lambda r_1}{2\pi M}\nabla_\perp^2\Phi(x,y)\right)$$

$$\Phi(x) = -\frac{2\pi}{\lambda}\int_O dz\,\delta(x,y,z)$$

$$B(x,y) = \frac{2\pi}{\lambda}\int_O dz\,\beta(x,y,z)$$

$$n = 1 - N\frac{r_e\lambda^2}{2\pi}f = 1 - N\frac{r_e\lambda^2}{2\pi}(f'+if'') = 1-\delta+i\beta$$

$$\delta = \frac{Nr_e\lambda^2}{2\pi}f' \qquad \beta = \frac{Nr_e\lambda^2}{2\pi}f'' = \mu\frac{\lambda}{4\pi}$$

The main approach to include phase effects in general purpose particle tracking codes is to **implement X-ray refraction** (Snell's law). This **ray-optical approach**, instead of the more rigorous Fresnel-Kirchhoff diffraction theory, holds if

$$\frac{\pi\lambda r_1 M}{[2F_g]^2} << 1$$

Peterzol et al., Med. Phys. 32 (12), 2005

FLUKA: *Cipiccia et al. (Opt Express. 2014, 22(19):23480-8)*

GEANT4: *Wang et al., 2009 IEEE Nuclear Science Symposium Conference Record*

Improved form factors with small-angle data should lead to a more accurate calculation of the refractive index

Conclusions

• Molecular **interference effect** in coherent scattering has been implemented in Geant4 for a variety of materials.

• The implementation has been **validated** comparing Geant4 simulations with previous results obtained through a different MC code and experimental data.

• The proposed extension will allow the user to **evaluate more rigorously the scatter profile** and **simulate SAXS experiments for tissue characterization**.

• Future development: FF including SAXS data, **implementation of X-ray refraction for phase-contrast imaging simulation,** implementation of X-ray diffraction from crystalline materials.

Back-up slides

Simulation of coherent scattering events

```
291 //....oooO0000ooo........oooO0000ooo........oooO0000ooo........oooO0000ooo....
292 namespace { G4Mutex  PenelopeRayleighModelMutex = G4MUTEX_INITIALIZER; }
293 G4double G4PenelopeRayleighModel::ComputeCrossSectionPerAtom(const G4ParticleDefinition*,
294                                 G4double energy,
295                                 G4double Z,
296                                 G4double,
297                                 G4double,
298                                 G4double)
299 {
300   // Cross section of Rayleigh scattering in Penelope v2008 is calculated by the EPDL97
301   // tabulation, Cuellen et al. (1997), with non-relativistic form factors from Hubbel
302   // et al. J. Phys. Chem. Ref. Data 4 (1975) 471; Erratum ibid. 6 (1977) 615.
303
304    if (verboseLevel > 3)
305     G4cout << "Calling CrossSectionPerAtom() of G4PenelopeRayleighModel" << G4endl;
306
307    G4int iZ = (G4int) Z;
308
309    //Either Initialize() was not called, or we are in a slave and InitializeLocal() was
310    //not invoked
311    if (!logAtomicCrossSection)
312      {
313        //create a **thread-local** version of the table. Used only for G4EmCalculator and
314        //Unit Tests
315        fLocalTable = true;
316        logAtomicCrossSection = new std::map<G4int,G4PhysicsFreeVector*>;
317      }
318    //now it should be ok
319    if (!logAtomicCrossSection->count(iZ))
320      {
321        //If we are here, it means that Initialize() was inkoved, but the MaterialTable was
322        //not filled up. This can happen in a UnitTest or via G4EmCalculator
323        if (verboseLevel > 0)
324     {
325        //Issue a G4Exception (warning) only in verbose mode
326        G4ExceptionDescription ed;
327        ed << "Unable to retrieve the cross section table for Z=" << iZ << G4endl;
328        ed << "This can happen only in Unit Tests or via G4EmCalculator" << G4endl;
329        G4Exception("G4PenelopeRayleighModel::ComputeCrossSectionPerAtom()",
330                "em2040",JustWarning,ed);
331     }
332        //protect file reading via autolock
```

C++ ▾ Tab Width: 4 ▾ Ln 305, Col 31 INS

Simulation of coherent scattering events

```
664 //....oooOOOOOooo........oooOOOOOooo........oooOOOOOooo........oooOOOOOooo....
665
666 void G4PenelopeRayleighModel::SampleSecondaries(std::vector<G4DynamicParticle*>* ,
667                         const G4MaterialCutsCouple* couple,
668                         const G4DynamicParticle* aDynamicGamma,
669                         G4double,
670                         G4double)
671 {
672   // Sampling of the Rayleigh final state (namely, scattering angle of the photon)
673   // from the Penelope2008 model. The scattering angle is sampled from the atomic
674   // cross section dOmega/d(cosTheta) from Born ("Atomic Phyisics", 1969), disregarding
675   // anomalous scattering effects. The Form Factor F(Q) function which appears in the
676   // analytical cross section is retrieved via the method GetFSquared(); atomic data
677   // are tabulated for F(Q). Form factor for compounds is calculated according to
678   // the additivity rule. The sampling from the F(Q) is made via a Rational Inverse
679   // Transform with Aliasing (RITA) algorithm; RITA parameters are calculated once
680   // for each material and managed by G4PenelopeSamplingData objects.
681   // The sampling algorithm (rejection method) has efficiency 67% at low energy, and
682   // increases with energy. For E=100 keV the efficiency is 100% and 86% for
683   // hydrogen and uranium, respectively.
684
685   if (verboseLevel > 3)
686     G4cout << "Calling SamplingSecondaries() of G4PenelopeRayleighModel" << G4endl;
687
688   G4double photonEnergy0 = aDynamicGamma->GetKineticEnergy();
689
690   if (photonEnergy0 <= fIntrinsicLowEnergyLimit)
691     {
692       fParticleChange->ProposeTrackStatus(fStopAndKill);
693       fParticleChange->SetProposedKineticEnergy(0.);
694       fParticleChange->ProposeLocalEnergyDeposit(photonEnergy0);
695       return ;
696     }
697
698   G4ParticleMomentum photonDirection0 = aDynamicGamma->GetMomentumDirection();
699
700   const G4Material* theMat = couple->GetMaterial();
701
702
703   //1) Verify if tables are ready
704   //Either Initialize() was not called, or we are in a slave and InitializeLocal() was
705   //not invoked
706   if (!pMaxTable || !samplingTable || !logAtomicCrossSection || !atomicFormFactor ||
707       !logFormFactorTable)
708     {
```

C++ ▾ Tab Width: 4 ▾ Ln 666, Col 31 INS

Implementation

DetectorConstruction.cc × G4PenelopeRayleighModel.cc ×

```
179         matname = "BoneMatrix";
180     } else {
181         matname = "BoneMatrix_noint";
182     }
183     BoneMatrix = new G4Material(matname, d_BoneMatrix, nel);
184     BoneMatrix->AddElement(elH, 0.0344);
185     BoneMatrix->AddElement(elC, 0.7140);
186     BoneMatrix->AddElement(elN, 0.1827);
187     BoneMatrix->AddElement(elO, 0.0689);
188
189     //Mineral (Hydroxyapatite)
190     G4double d_Mineral = 2.74*g/cm3;
191     nel = 4;
192     if (IWantMI) {
193         matname = "Mineral";
194     } else {
195         matname = "Mineral_noint";
196     }
197     Mineral = new G4Material(matname, d_Mineral, nel);
198     Mineral->AddElement(elH, 0.002);
199     Mineral->AddElement(elO, 0.414);
200     Mineral->AddElement(elP, 0.185);
201     Mineral->AddElement(elCa, 0.399);
202
203     //Medical Material
204     G4double comp[] = {Comp0, Comp1, Comp2, Comp3}; //enter the material composition
205     G4double d_MedMat = d_Fat*d_Water*d_BoneMatrix*d_Mineral/(comp[0]*d_Fat*d_BoneMatrix*d_Mineral+comp[1]*d_Water*d_BoneMatrix*d_Mineral+comp
    [2]*d_Fat*d_Water*d_Mineral+comp[3]*d_Fat*d_Water*d_BoneMatrix);
206     G4cout << "### MedMat density: " << d_MedMat/(g/cm3) << " ###" << G4endl;
207     G4int n_MedMat = 0;
208     for (size_t i=0; i<4; i++) {
209         if (comp[i]>0) n_MedMat++;
210         if (comp[i]<0 || comp[i]>1) {
211             G4String excep = "Error in Medical Material composition: comp[i]<0 or comp[i]>1";
212             G4Exception("DetectorConstuction::DefineMaterials()",
213             "em0001",FatalException,excep);
214             return;
215         }
216     }
217     std::stringstream ss0,ss1,ss2,ss3;
218     ss0 << comp[0];
219     ss1 << comp[1];
220     ss2 << comp[2];
221     ss3 << comp[3];
```

C++ ▾ Tab Width: 4 ▾

Implementation

DetectorConstruction.cc × G4PenelopeRayleighM Copy the selection

```
438  G4PhysicsFreeVector* graymatterFF = MolInterferenceData->find(24)->second;
439
440  G4String matname = material->GetName();
441
442  //medical material: composition of fat, water, bonematrix, mineral
443  if (matname.find("MedMat") != std::string::npos) {
444    G4cout << "MIFF: MedMat" << G4endl;
445
446    //get the material composition from its name
447    G4int ki, kf=6, ktot=19;
448    G4double comp[4];
449    G4String compstring = matname.substr(kf+1, ktot);
450    for (size_t j=0; j<4; j++) {
451        ki = kf+1;
452        kf = ki+4;
453        compstring = matname.substr(ki, 4);
454        comp[j] = atof(compstring.c_str());
455        G4cout << "MedMat comp[" << j+1 << "]: "  << comp[j] << G4endl;
456    }
457
458    //get and combine the molecular form factors with interference effect
459    for (size_t k=0;k<logQSquareGrid.size();k++) {
460        G4double ff2 = 0;
461        G4double ffat = (*fatFF)[k];
462        G4double fwater = (*waterFF)[k];
463        G4double fbonematrix = (*bonematrixFF)[k];
464        G4double fmineral = (*mineralFF)[k];
465        ff2 = comp[0]*ffat*ffat+comp[1]*fwater*fwater+comp[2]*fbonematrix*fbonematrix+comp[3]*fmineral*fmineral;
466        if (ff2) theFFVec->PutValue(k,logQSquareGrid[k],std::log(ff2));
467    }
468  }
469
470  //other materials with interference function
471  else if (matname == "PMMA") {
472    G4cout << "MIFF: PMMA" << G4endl;
473    for (size_t k=0;k<logQSquareGrid.size();k++) {
474        G4double ff2 = 0;
475        G4double f = (*PMMAFF)[k];
476        ff2 = f*f;
477        if (ff2) theFFVec->PutValue(k,logQSquareGrid[k],std::log(ff2));
478    }
479  } else if (matname == "Adipose") {
480    G4cout << "MIFF: Adipose" << G4endl;
481    for (size_t k=0;k<logQSquareGrid.size();k++) {
```

Application: identification of cancer signatures