MC-INFN project

Refinement and extension of photon coherent interaction models with matter

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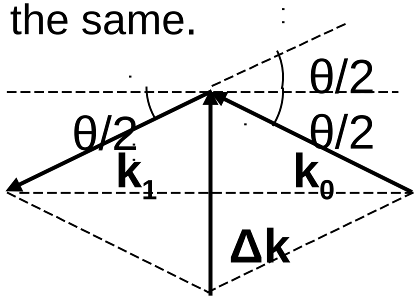
MC-INFN/GEANT4 meeting, June 12, 2020

TASKS

- Development of interference effects in coherent X-ray scattering model.
- Development of diffraction process in polycrystalline materials.
- Development of refraction/reflection of X-rays (milestone 31/12/2020).

Development of interference effects in coherent X-ray scattering model

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.



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

Differential cross-section

Momentum transfer

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

$$x = \frac{q}{2h} = \frac{1}{\lambda}\sin(\theta/2) \quad [\mathrm{nm}^{-1}]$$

Total cross-section

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

Common MC approach for molecules: IAM

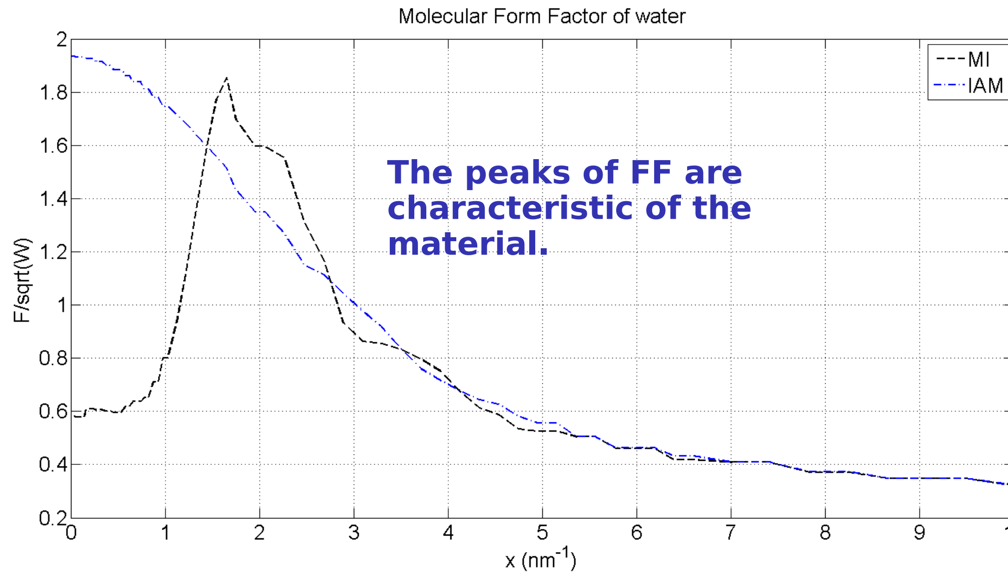
$$F^2_{mol,IAM}(q) = W \sum_i \frac{w_i}{A_i} F^2(q,Z_i)$$

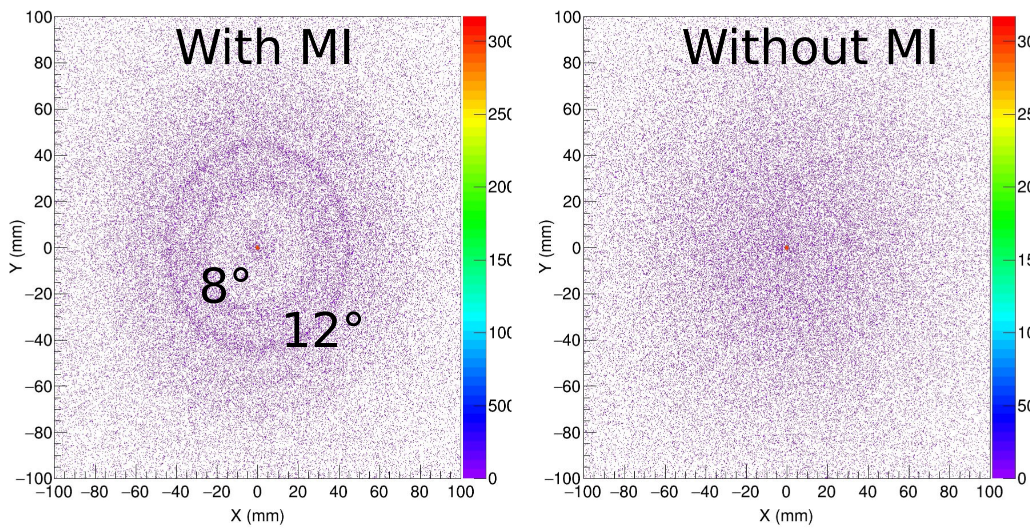
→ **No interference effects**

For each material a proper Form Factor including interference effects is required

Development of interference effects in coherent X-ray scattering model

- The **Penelope model has been modified** to read molecular form factors (FF) with interference effects [*G. Paterno et al, Physica Medica 51 (2018) 64–70*]. The cross-section is re-calculated.
- A **library of 70 FFs** is made available.
- Every **biological tissue** can be **segmented in basis components** [*paper under review for publication on PMB*].
- The user can introduce **custom form factors** with interference (using G4ExtendedMaterial).
- The code allows the user to:
  - account for phase effects,
  - remove scatter from images,
  - simulate WAXS/SAXS exp.,
  - classify tissues.





Scattering of a **20 keV photon beam** in a **human breast** sample

Development of diffraction process in polycrystalline materials

The **cross-section for Bragg diffraction** from a **crystalline powder** sample is given by:

$$\sigma_B = \frac{r_e{}^2\lambda^2}{2NV}\sum_{i=hkl}\left(\frac{1+cos^2\theta}{2}\right)m_i d_i|F_i|^2 \qquad (1)$$

Bragg's law states that scattering can only occur when 2dsin(θ/2)=λ and being x=1/λsin(θ/2), it follows that **d=1/(2x).** Therefore:

$$\sigma_B = \frac{r_e{}^2}{4}\frac{(1+cos^2\theta)sin^2(\theta/2)}{2}|F_B(x)|^2 \qquad (2)$$

$$|F_B(x)|^2 = \frac{1}{NV}\sum_{i=hkl}\frac{m_i|F_i|^2}{x^3}\delta(x-x_i) \qquad (3)$$

The scattering angle $\theta=2\theta_B$ is determined by sampling x from the **Bragg form factor F_B**, which contains all of the material-dependent terms (**$F_i=f_i*G_i*DW_i$**). The middle term in equation (2) depends only on angle and is used as the rejection function applied to the sampled x values.

Development of diffraction process in polycrystalline materials

The **atomic form factor f** can be calculated using the Cromer-Mann coefficients (a_i,b_i,c):

$$f(x) = c + \sum_{i=1}^{4} a_i e^{(-b_i x^2)}$$

The **geometric factor G** depends on the crystal structure

$$G = \sum_j e^{-\overrightarrow{G_m} \cdot \overrightarrow{\rho_j}}$$

Where G_m is the **reciprocal lattice vector** and ρ_j is the position of the j-th atom in the **unit cell**.

The **Debye-Waller factor DW**, due to the atom vibration, depends also on crystal structure. There are semi-empirical formulas that allow one to estimate it.

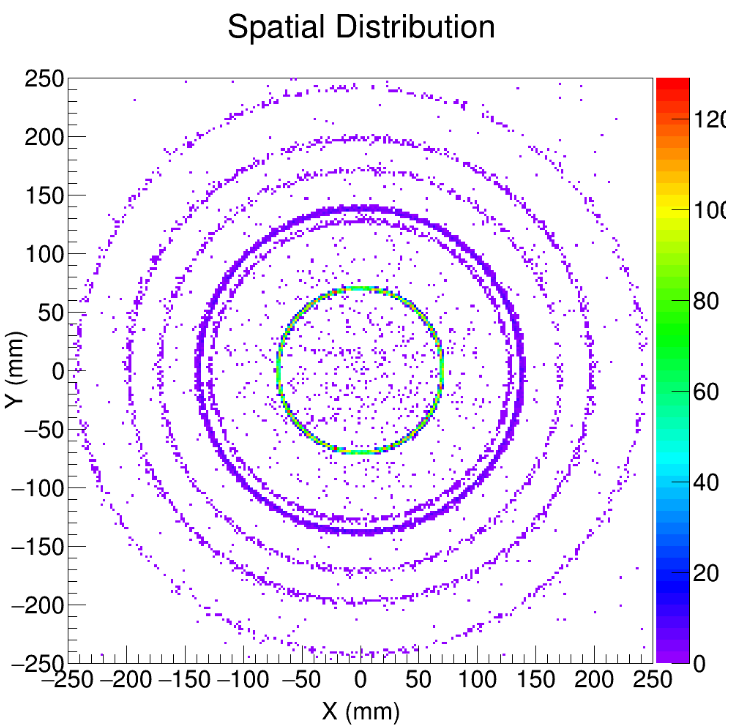
Peak broadening (FWHM): $W_i = \dfrac{K\lambda}{L_G \cos\theta_B}$

Development of diffraction process in polycrystalline materials

- Development, from scratch, of a **specific physical process**, which implements the theory seen before exploiting the **G4CrystalExtension** (unit cell management, plane spacing and structure factor calculation).
- Development of **ExtraCrystalData** class, extension of G4Material, to add further properties to crystalline materials, such as, structure type, Debye temperature, crystallite size L_G, Scherrer GrainShape Factor K.
- **Automatic calculation** of diffraction multiplicity, main diffraction lines and Debye temperature for a given crystal structure **has yet to be implemented** (by extending G4CrystalExtension).

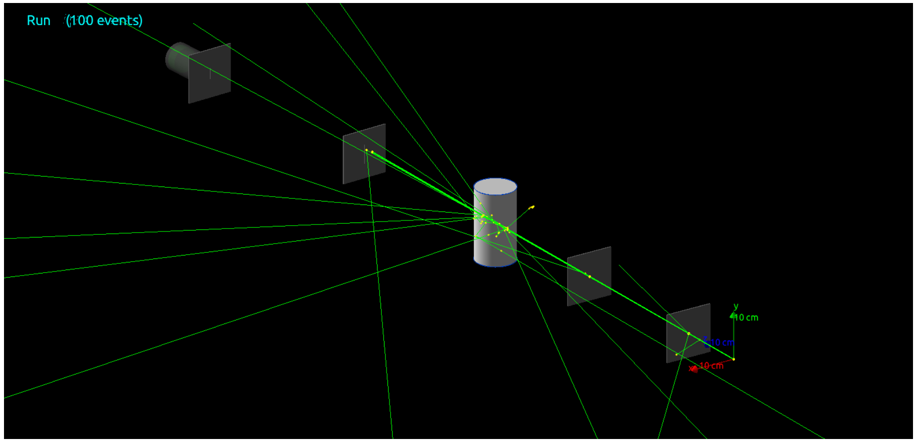
Development of diffraction process in polycrystalline materials

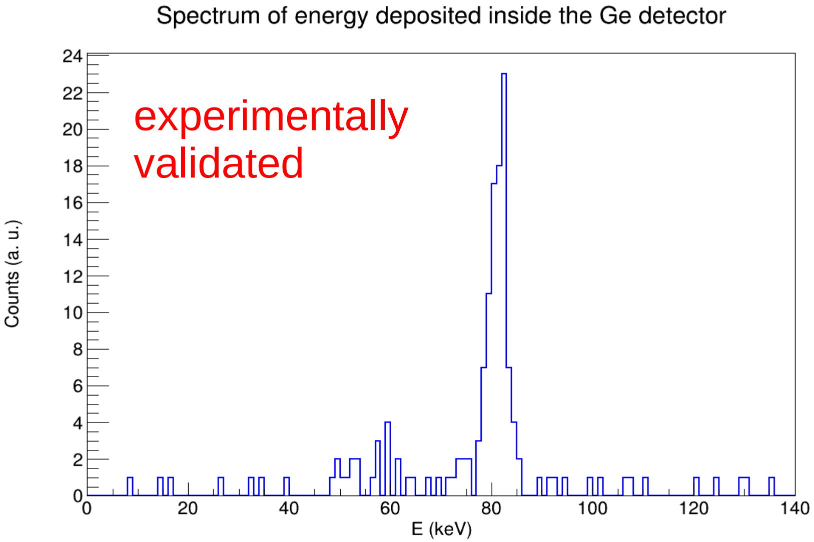
Simple test: diffraction of a **8 keV** X-ray beam from a thin "slab" of a **graphite powder**.



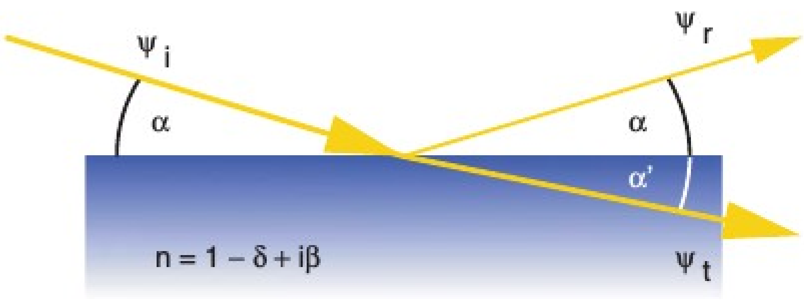
Line position, width and relative intensity in agreement with analytical calculation.

Advanced test: diffraction of a **polychromatic** X-ray beam from a cylinder of **graphite powder**. The set-up is conceived to select the most intense line.





Development of refraction/reflection of X-rays



$$n = 1 - \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_i(0),$$

complex refraction index

$$\boxed{\cos\alpha = n\cos\alpha'}$$

Snell's law

$$\alpha_c = \sqrt{2\delta}$$

Total external reflection for $\alpha \leq \alpha_c$

$$\boxed{r \equiv \frac{a_R}{a_I} = \frac{\alpha - \alpha'}{\alpha + \alpha'}\,; \quad t \equiv \frac{a_T}{a_I} = \frac{2\alpha}{\alpha + \alpha'}}$$

$$r = \frac{\sin\alpha - (n^2 - \cos^2\alpha)^{1/2}}{\sin\alpha + (n^2 - \cos^2\alpha)^{1/2}}$$

Fresnel equations for perfect surfaces (In this form, they are exact for s-pol and approx for p-pol)

$$R_r = R_f \cdot \exp\left[-(2k\alpha\sigma)^2\right]$$

$R=|r|^2$ reflectivity. Fresnel equations for rough surfaces (σ = roughness)

Development of refraction/reflection of X-rays

- ***STATUS***:
  - Defined the main algorithms and new classes to be implemented.
  - Identified a database for index of refraction (CXRO).
  - Concrete implementation has yet to be done (milestone 31-12-2020).

- A bibliographic research highlighted that these effects were already implemented in Geant4/Gate by different groups [1,2,3,4], with different levels of accuracy and subsequent application. These works can be used as **benchmarks**.

[1] Langer M. et al, Towards Monte Carlo simulation of X-ray phase contrast using GATE, Optics Express 28, 2020.

[2] Sanctorum J. et al, X-ray phase-contrast simulations of fibrous phantoms using GATE, 2018 IEEE Nuclear Science Symposium and Medical Imaging Conference Proceedings.

[3] Buis E.J, G. Vacanti, X-ray tracing using Geant4, NIM-A 599 (2009) (code freely download-able).

[4] Wang Z. et al, Implement X-ray refraction effect in Geant4 for phase contrast imaging, 2009 IEEE Nuclear Science Symposium Conference Record.

Activity foreseen for 2021

- Experimental validation of implemented X-ray refraction/reflection and phase-contrast effects due to simple objects.

- Simulation of phase-contrast imaging with proper mammographic phantoms, which can be voxelized (in collaboration with AGATA project).