MC-INFN project

Activity of 2nd semester of 2020: Introduction of interference effects in the official Penelope X-ray coherent scatter model of Geant4

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Introducing 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.

Differential cross-section

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

Momentum transfer [nm^{-1}]

$$x = \frac{q}{2h} = \frac{1}{\lambda}\sin(\theta/2)$$

Common MC approach for molecules: IAM

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

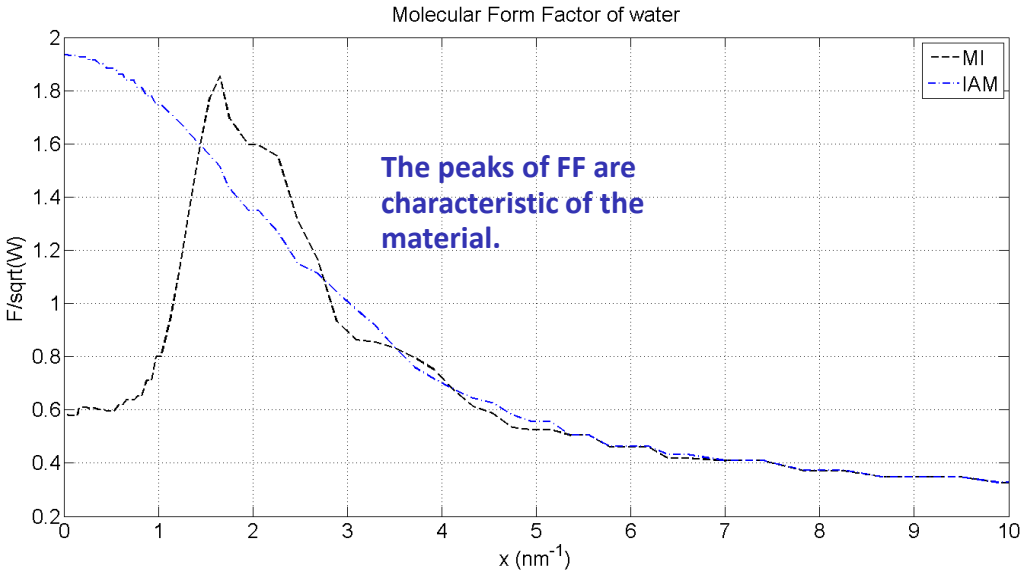
→ **No interference effects**

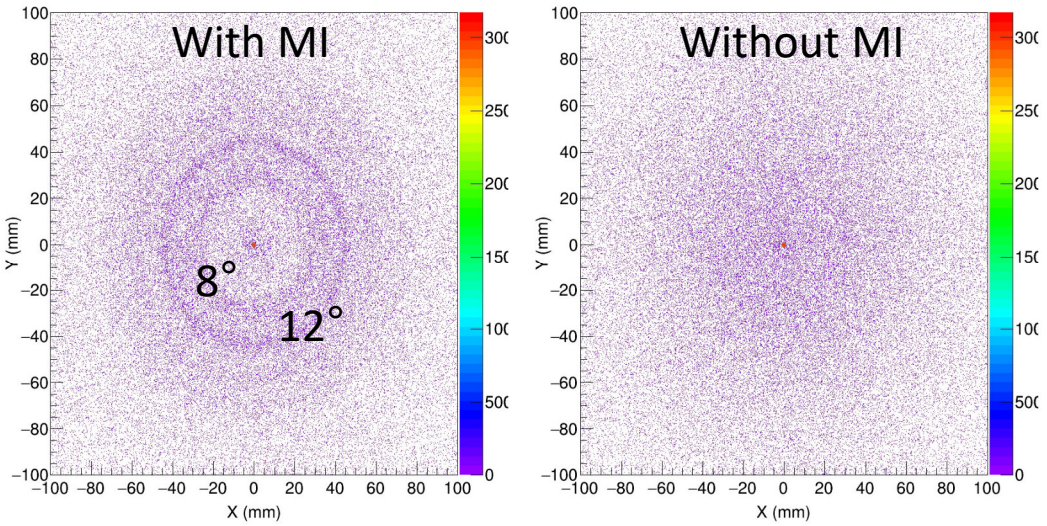
For each material **a proper Form Factor including interference effects** is required

Introducing interference effects in coherent X-ray scattering model

Effect of Molecular Interference (MI)

Coherent scattering **dominates** Compton scattering at low angles and it is **distinguishable** from primary beam.





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

Introducing interference effects in coherent X-ray scattering model

- The Penelope model was extended **(G4PenelopeRayleighModelMI)** to **read molecular form factors (FF) with interference effects** *[G. Paterno et al, Physica Medica 51 (2018) 64–70]*.
- **G4PenelopeRayleighModelMI** class coexists with the "standar" **G4PenelopeRayleighModel** class and it can be selected instead in the user **PhysicsList** to activate MI.
- A **library of 32 FFs** is made available. The database was **rationalized** avoiding redundance and fully **validated** with respect to previous implementation.
- Every **biological tissue** can be **segmented in 4 basis components** *[G. Paterno et al, Physics in Medicine and Biology Vol. 65(2020), 245002]*.
- The user can introduce **custom form factors** with interference (using the support of **G4ExtendedMaterial**).
- **The cross-section is re-calculated integrating the DCS**.
- A significant amount of work was done to make the developed code **compliant** with the **Geant4 official guidelines** and **avoid** any possible **bug** and **memory waste**.

Introducing interference effects in coherent X-ray scattering model

Read the Form Factors with Molecular Interference (MIFF)

A new method of G4PenelopeRayleighModelMI: **ReadMolInterferenceData(const G4String&,const G4String& filename="NULL")** is used to read the form factor (FF) with molecular interference (MI) of a **selected variety of materials**, according to a well-defined association "matname" → "MIFF".

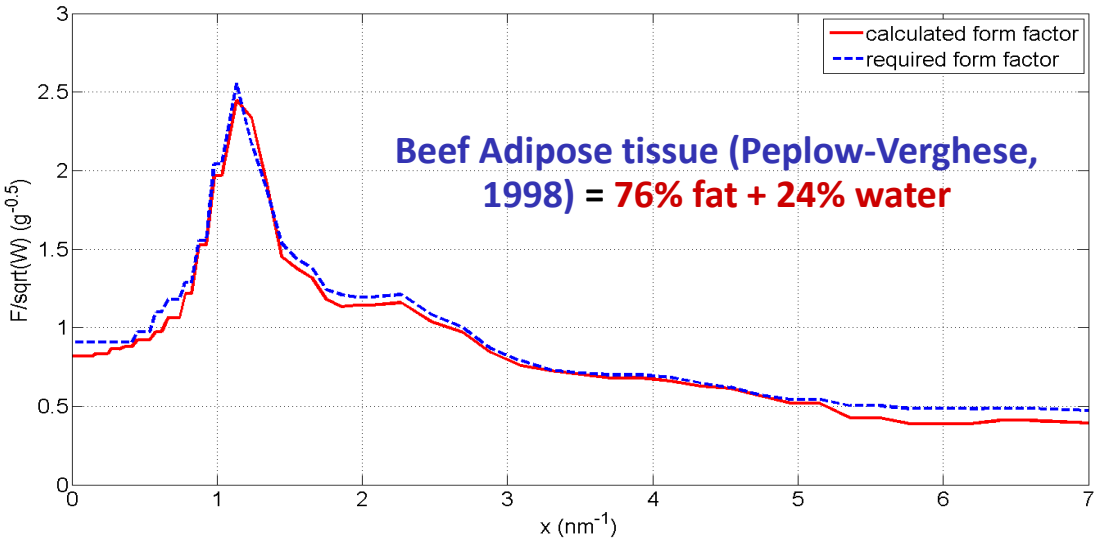
```
fKnownMaterials->insert(std::pair<G4String,G4String>("Fat_MI","FF_fat_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("Water_MI","FF_water_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("BoneMatrix_MI","FF_bonematrix_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("Mineral_MI","FF_mineral_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("adipose_MI","FF_adipose_Poletti2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("glandular_MI","FF_glandular_Poletti2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("breast5050_MI","FF_human_breast_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("carcinoma_MI","FF_carcinoma_Kidane1999.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("muscle_MI","FF_pork_muscle_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("kidney_MI","FF_pork_kidney_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("liver_MI","FF_pork_liver_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("heart_MI","FF_pork_heart_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("blood_MI","FF_beef_blood_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("grayMatter_MI","FF_gbrain_DeFelici2008.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("whiteMatter_MI","FF_wbrain_DeFelici2008.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("bone_MI","FF_bone_King2011.dat"));
```

MIFF then are stored in a dedicated map (matname is the key):
std::map<G4String,G4PhysicsFreeVector*> ***MolInterferenceData**;
This map is recalled in **BuildFormFactorTable(const G4Material*)** method.

For materials with MIFF, the cross-section is calculated by integrating the DCS (overriding of **ComputeCrossSectionPerVolume(const G4Material*)** of G4VEmModel). If a coherent scattering event occurs, the scattering angle is sampled according to RITA algorithm, which was not modified).

Introducing interference effects in coherent X-ray scattering model

Decomposition of tissues in basis components



$$\frac{F^2}{W} = \sum_{i=1}^{4} a_i \frac{F_i^2}{W_i}$$

i=fat, water, collagen, hydroxyapatite

Avoid to use unclassified tissues

No extension needed, simply define a material and label it as "**MedMat_a1_a2_a3_a4**", where **ai are the weight fractions of the 4 basis materials** (example: "MedMat_0.80_0.20_0.00_0.00").

In the **BuildFormFactorTable(const G4Material*)** method, the basis FFs are mixed accordingly.

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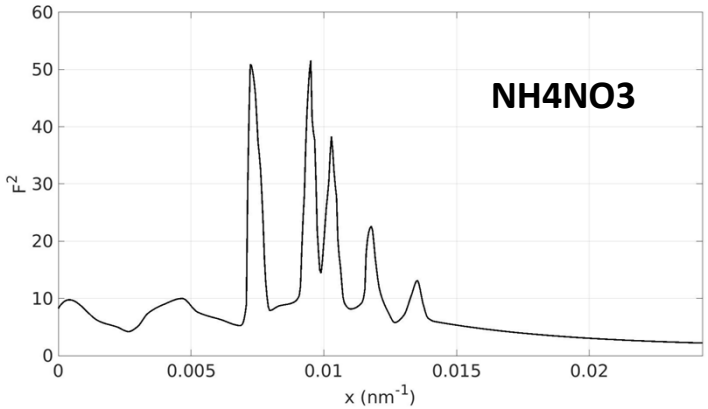
Form factor defined by the user



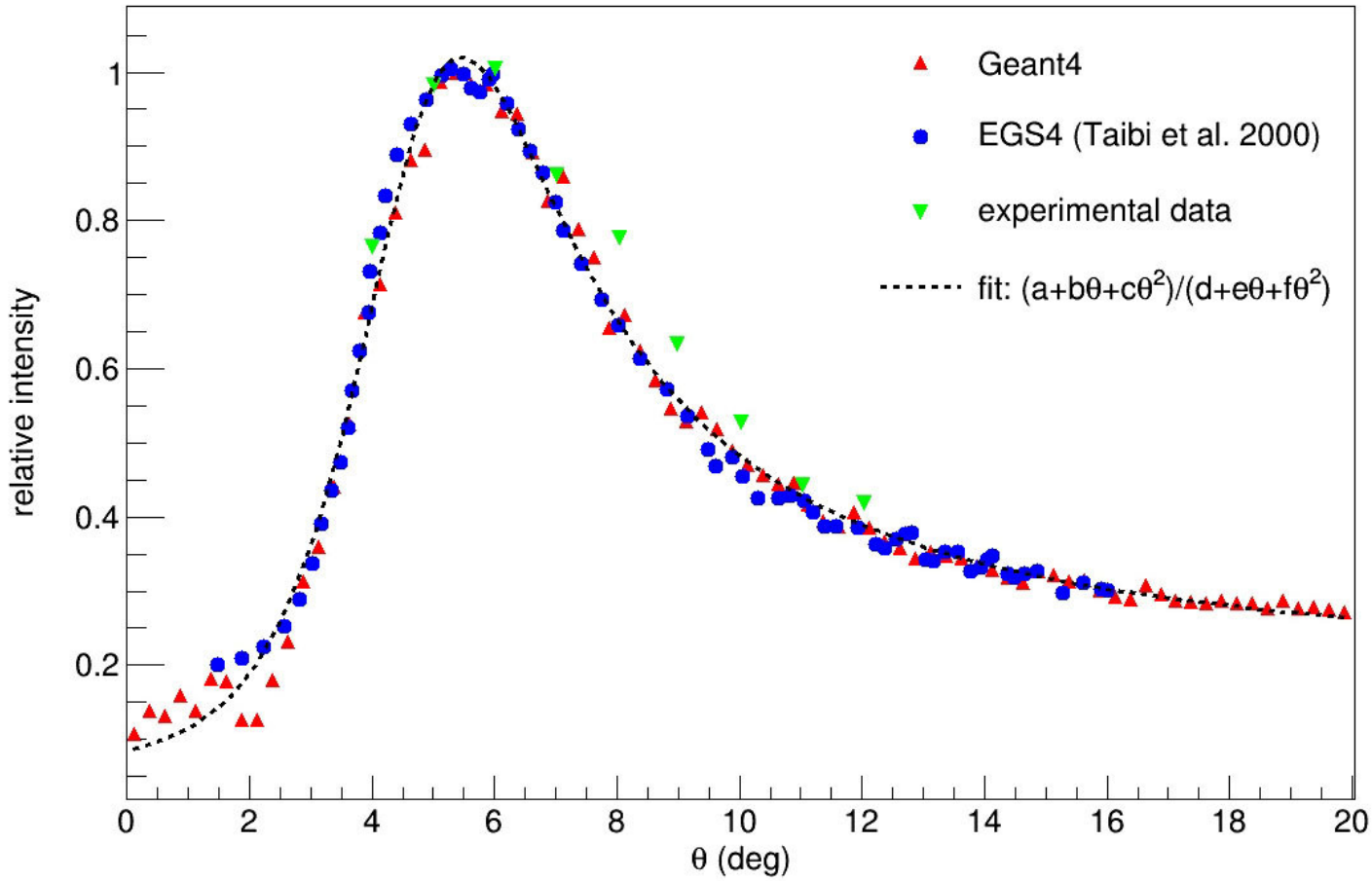
Useful for materials with partial crystalline behavior

In the **DetectorConstrucion.cc**, use the new **G4MIdata** extension to provide the path of the FF file of the material (through **setFilenameFF(G4String)** method).

```
d = CustomMatDensity*g/cm3;
matname = "CustomMat";
CustomMat = new G4ExtendedMaterial(matname, d, nel);
if (CustomMatHmassfract) CustomMat->AddElement(elH, CustomMatHmassfract);
if (CustomMatCmassfract) CustomMat->AddElement(elC, CustomMatCmassfract);
if (CustomMatNmassfract) CustomMat->AddElement(elN, CustomMatNmassfract);
if (CustomMatOmassfract) CustomMat->AddElement(elO, CustomMatOmassfract);
if (CustomMatNamassfract) CustomMat->AddElement(elNa, CustomMatNamassfract);
if (CustomMatPmassfract) CustomMat->AddElement(elP, CustomMatPmassfract);
if (CustomMatSmassfract) CustomMat->AddElement(elS, CustomMatSmassfract);
if (CustomMatClmassfract) CustomMat->AddElement(elCl, CustomMatClmassfract);
if (CustomMatKmassfract) CustomMat->AddElement(elK, CustomMatKmassfract);
if (CustomMatCamassfract) CustomMat->AddElement(elCa, CustomMatCamassfract);
//Extend the material
CustomMat->RegisterExtension(std::unique_ptr<MIdata>(new MIdata("MI")));
MIdata* dataMICustomMat = (MIdata*)CustomMat->RetrieveExtension("MI");
dataMICustomMat->SetFilenameFF(fCustomMatFF);
```

It will be used in the **BuildFormFactorTable**(const G4Material*) method.

Introducing interference effects in coherent X-ray scattering model: **Validation**

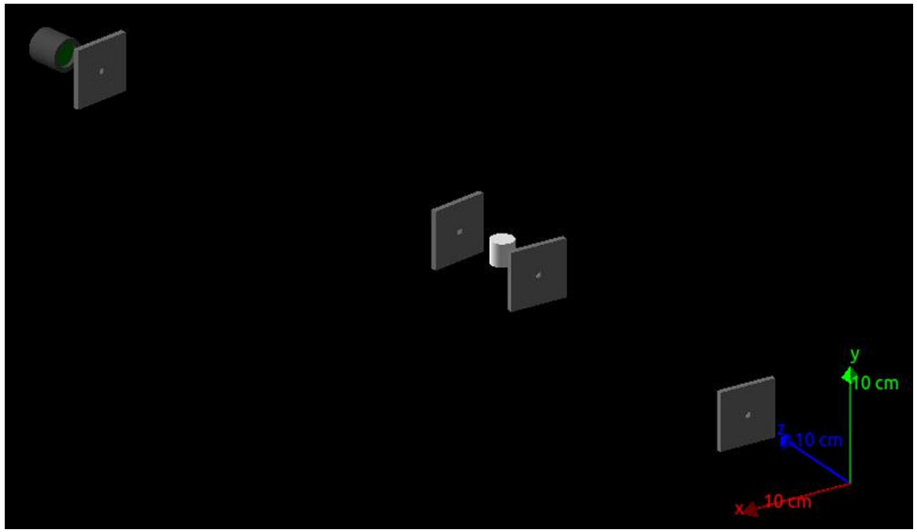


Simulation of the experiment by Evans et al., 1991: Scattering of **polychromatic X-rays** (60 kVp and filtration of 0.5 mm Cu) **from a 5 mm-thick carcinoma sample.**

Simulations agree with the experiment.

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

Introducing interference effects in coherent X-ray scattering model: **saxs** example



A **dedicated (extended) example** was developed to show the use of how molecular interference implementation.

- **Geometry, materials and X-ray source** can be set 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 *SensitiveDetecto*r (simple scoring screen or Ge detector) -> **root scripts** are provided for data analysis

Introducing interference effects in coherent X-ray scattering model: **saxs** example

saxs.in

```
/det/setComp0 0.80
det/setComp1 0.20
det/setComp2 0.00
/det/setComp3 0.00

/det/setPhantomMaterial 2
/det/setPhantomDiameter 10. mm
/det/setPhantomHeight 10. mm
/det/setPhantomZ 500. 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/setDetectorSize 200. mm
/det/setDetectorThickness 20. mm
/det/setDetectorSampleDistance 400. mm

/phys/SelectPhysicsList penelopeMI

/phys/setCuts 0.1 mm

/run/initialize
/run/setfilenamesave output
/control/execute beam.mac
/run/printProgress 100000
/run/beamOn 1000000
```

Introducing interference effects in coherent X-ray scattering model: **saxs** example

saxs README

```
 ============================================================
 Geant4 - an Object-Oriented Toolkit for Simulation in HEP
 ============================================================

                      Extended Example saxs
                      ---------------------

The example saxs implements the typical setup of a Small Angle X-ray
Scattering (SAXS) experiment. It is meant to illustrate the
usage of molecular interference (MI) of Rayleigh (coherent) scattering
of photons inside the matter, which is implemented in the
G4PenelopeRayleighModelMI model.

1- GEOMETRY

 The setup consists of a phantom/sample under investigation, slits
 to collimate the photon beam and a shielded detector to collect
 the photons scattered by the phantom (see SAXSDetectorConstruction).

 The geometry is scalable through the interactive commands defined
 in the SAXSDetectorConstructionMessenger class. All the significant
 quantities, such as the setup (scattering) rotation angle, the position
 and size of all the volumes, as well as the phantom material can be
 set via macro commands.

 Two macro files come with this example: saxs.in and saxs_slits.in.

 In the saxs.in macro, the phantom is a cylinder with a diameter and
 a height of 10 mm made of a mixture of 80% fat and 20% water.
 In general, if the argument of /det/setPhantomMaterial command is 2,
 as in this case, the material is a biological tissue ("MedMat")
 defined as a mixture of fat, water, collagen and hydroxyapatite.
 The weight fraction of the mixture components can be set through commands
 /det/setComp0, /det/setComp1, /det/setComp2, /det/setComp3, respectively.
 The tissue form factor (including MI) is automatically calculated as a
 weighed sum of the form factors of the basis components.
 In this case, no slits are foreseen and the sensitive detector
 positioned 400 mm downstream of the phantom collects all the photons
```

Introducing interference effects in coherent X-ray scattering model: **documentation**

https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsReferenceManual/html/electromagnetic/gamma_incident/elastic/penelope_rayleigh.html

Geant4 Homepage

Physics Reference Manual

10.7 (doc Rev5.0)

Search docs

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General Information

Particle Decay

Electromagnetic Interactions

Electromagnetic Physics in GEANT4

Gamma incident

Introduction to Gamma Processes

Elastic Scattering

Penelope Model

Livermore Model

JAEA Elastic Scattering Model

CIRS30-70	CIRS30-70_MI
CIRS50-50	CIRS50-50_MI
CIRS70-30	CIRS70-30_MI
RMI454	RMI454_MI

Due to the tissue variability, the measured diffraction patterns of two samples of the same tissue type may differ significantly. To overcome this problem, a generic tissue can be decomposed in simpler basis materials with well-defined elemental composition. In particular, each tissue is considered as a composition of four components, namely fat, water, collagen or bone matrix, and hydroxyapatite (see [PaternoCC+18], [PaternoCGT20]). The form factor of a generic tissue can be then expressed through the mixture rule using tissues (molecules or supramolecules) instead of atoms as:

$$\frac{F^2(q)}{W} = \sum_{i=1}^{4} \frac{a_i F_i^2(q)}{W_i}, \tag{3}$$

where a_i is the mass fraction of i-th basis component.

In order to enable this functionality, the user has to create the mixture of basis materials (whose composition and density are defined in [PaternoCGT20] and label the material as *MedMat_a1_a2_a3_a4*, where *ai* are three digit numbers representing the mass fraction of the basis components. Then, the form factor of the material is automatically calculated according to Eq.(3).

In order to gain generality, the user has the faculty of providing the form factor of the materials he wants to consider. This is obtained by defining a material as *G4ExtendedMaterial* and registering *G4MIData* extension. The *SetFilenameFF()* method of this class allows to specify the path of the file with the form factor of the material. This functionality is particularly suited for modeling materials with partial crystalline beahviour, such as powder and polycrystals, which are characterize by a large number of sharp diffraction peaks.

Conclusions

- The development of **interference effects in coherent X-ray scattering model** is completed and it was introduced in the official Geant4 release (from 10.7). A dedicated example was also implemented and made available to users as an official extended example. All the documentation describing the developed code was also produced.
- **The code developed allows** the user to:

  - remove scatter from images,

  - simulate WAXS/SAXS experiments,

  - classify unknown tissues.

- The development of **refraction/reflection of X-rays**, which was foreseen to be completed by the end of 2020, has been postponed and we foresee to complete it and validate the code within this year.