

How to simulate ?

Atomic deexcitation (fluorescence, Auger electron emission, including Auger cascades since release 10.2 and PIXE) can be activated for processes producing vacancies in atomic shells. Currently these processes are the photoelectric effect, ionization and Compton scattering. This new feature is available for **Livermore**, **Penelope**, **Standard electromagnetic**, and **Geant4-DNA** processes.

In the recent MT releases of Geant4, the activation of atomic deexcitation in **Geant4 physics lists** (and "physics constructors") can be easily done directly via **UI commands**:

```
/process/em/fluo true
/process/em/auger true
/process/em/augerCascade true
/process/em/pixe true
```

These UI commands should be put **BEFORE** the UI command:

```
/run/initialize
```

Note that **fluorescence is activated by default in G4EmLivermorePhysics, G4EmLivermorePolarizedPhysics and G4EmPenelopePhysics physics constructors** while Auger production and PIXE are not.

Important note on

Remember that production cuts for secondaries can be specified as range cuts, which are converted at initialisation time into energy thresholds for secondary gamma, electron, positron and proton production.

A **range cut** value is set by default to 0.7 mm in Geant4 reference physics lists. This value can be specified in the optional SetCuts() method of the user physics list or via **UI commands**, for eg. to set a range cut of 10 micrometers, one can use:

```
/run/setCut 0.01 mm
```

or, for a given particle type (for e.g. electron),

```
/run/setCutForAGivenParticle e- 0.01 mm
```

If a range cut equivalent to an energy lower than 990 eV is specified, **the energy cut is still set to 990 eV**. In order to **decrease this value** (for eg. down to 250 eV, to see low energy emission lines of the fluorescence spectrum), one can use the **UI command**:

```
/cuts/setLowEdge 250 eV
```

or alternatively directly in the user **physics list**, in the optional SetCuts() method, using:

```
G4ProductionCutsTable::GetProductionCutsTable()->SetEnergyRange(250*eV, 1*GeV);
```

These 3 UI commands should be put **BEFORE** the UI command:

```
/run/initialize
```

Note that a command is also available in order to disable usage of production threshold for fluorescence and Auger electron production:

```
/process/em/deexcitationIgnoreCut true
```

Important note on

Since Geant4 10.2 release, in all ionization processes which simulate energy loss along step, a lowest energy limit is introduced which forces full energy deposition of electrons and positrons at a step independently on material. This value may be changed via a dedicated UI command or through the interface class G4EmParameters. The default value is **1 keV**, but for the G4EmstandardPhysics_option3, G4EmstandardPhysics_option4, G4EmLivermorePhysics and G4EmPenelopePhysics constructors, this energy limit is set at **100 eV**.

A different value (eg. X eV) can be specified using the UI command:

```
/process/em/lowestElectronEnergy X eV
```

A similar command is available for muons and hadrons, see Geant4 documentation.

How to change ionisation cross section models ?

The user can also select which cross section model to use in order to calculate shell ionisation cross sections for generating PIXE.

When using the **Geant4 physics lists** (and "physics constructors"), the following UI command is available:

```
/process/em/pixeXSmodel value
```

where **value** is equal to **Empirical** or **ECPSSR_FormFactor** or **ECPSSR_Analytical**.

Shell cross sections models are available for K, L and selected M shells:

- the **Empirical** models are from Paul "reference values" (for protons and alphas for K-Shell) and Orlic empirical model for L shells (only for protons and ions with $Z > 2$);
- the **ECPSSR_FormFactor** models derive from A. Taborda et al. calculations (see A. Taborda et al., X-Ray Spec. 40 (2011) 127-134 and A. Taborda et al., X-Ray Spec. 42 (2013) 177-182) of ECPSSR values directly form Form Factors and it covers K, L shells in the range 0.1-100 MeV and M shells in the range 0.1-100 MeV;
- the **ECPSSR_Analytical** models derive from an in-house analytical calculation of the ECPSSR theory (see A. Mantero et al., X-Ray Spec. 40 (2011) 135-140);

The **Empirical** models are the models used by default. Out of the energy boundaries of these models, the "ECPSSR_Analytical" models are used. We recommend to use default settings if not sure what to use.

Note that shell cross section selection is also available for **electrons** via the following **UI command** (needed only for simulations which make use of continuous ionisation process, like the low energy G4EmLivermorePhysics or G4EmPenelopePhysics constructors):

```
/process/em/pixeElecXSmodel Livermore
```

or

```
/process/em/pixeElecXSmodel Penelope
```

How to change the fluorescence lines data set ?

The alternative set of data by Bearden (1967) for the modelling of fluorescence lines had been added to the G4LEDATA archive, kindly provided by Stéphane Paltani, Geneva U., Switzerland. This set can be selected in any physics list with:

```
G4AtomicTransitionManager::Instance()->SetFluoDirectory("/fluor_Bearden");
```

or using UI command:

```
/process/em/fluoBearden true
```

Example

As an example on how to simulate atomic deexcitation, please refer to the **electromagnetic extended example TestEm5** and the **pixe.mac** macro.

Publications

For further details on **atomic deexcitation**, please refer to:

- Simulation of Auger electron emission from nanometer-size gold targets using the Geant4 Monte Carlo simulation toolkit [↗](#), S. Incerti, B. Suerfu, J. Xu, V. Ivantchenko, A. Mantero, J.M.C. Brown, M.A. Bernal, Z. Francis, M. Karamitros, H.N. Tran, **Nucl. Instrum. Meth. B 372 (2016) 91-101**
- Validation of a Geant4 model of the X-ray fluorescence microprobe at the Australian Synchrotron [↗](#), M. R. Dimmock, M. D. de Jonge, D. L. Howard, S. A. James, R. Kirkham, D. M. Paganin, D. J. Paterson, G. Ruben, C. G. Ryan and J. M. C. Brown, **Journal of synchrotron radiation 22 (2) (2015) 354-365**
- Comparison of experimental proton-induced fluorescence spectra for a selection of thin high-Z samples with Geant4 Monte Carlo simulations [↗](#), S. Incerti, Ph. Barberet, G. Dévès, C. Michelet, Z. Francis, V. Ivantchenko, A. Mantero, Z. El Bitar, M. A. Bernal, H. N. Tran, M. Karamitros, H. Sez nec, **Nucl. Instrum. Meth. B 358 (2015) 210-222**
- A comparison between Geant4 PIXE simulations and experimental data for standard reference samples [↗](#), Z. Francis, M. El Bast, R. El Haddad, A. Mantero, S. Incerti, V. Ivanchenko, Z. El Bitar, C. Champion, M.A. Bernal, M. Roumie, **Nucl. Instrum. and Meth. B 316 (2013) 1-5**
- Geant4 electromagnetic physics: improving simulation performance and accuracy [↗](#), V. N. Ivanchenko, S. Incerti, J. Allison, A. Bagulya, J. M. C. Brown, C. Champion, S. Elles, Z. Francis, V. Grichine, A. Ivantchenko, J. Jacquemier, M. Karamitros, M. Maire, A. Mantero, J. P. Marques, L. Pandola, M. Raine, M. A. Reis, G. Santin, D. Sawkey, A. Schaelicke, M. Schenk, A. Taborda, L. Urban and T. Yamashita, **Proceedings of the Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)**, La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013
- Polynomial approximation to universal M-shell ionisation cross-sections induced by H+ and He2+ ions [↗](#), A. Taborda, P. C. Chaves, M. L. Carvalho, M. A. Reis, **X-Ray Spec. 42 (2013) 177-182**
- Polynomial approximation to universal ionisation cross-sections of K and L shells induced by H and He ion beams [↗](#), A. Taborda, P. C. Chaves, M. A. Reis, **X-Ray Spec. 40 (2011) 127-134**
- PIXE simulation in Geant4 [↗](#), A. Mantero, H. Ben Abdelouahed, C. Champion, Z. El Bitar, Z. Francis, P. Guèye, S. Incerti, V. Ivanchenko, M. Maire, **X-Ray Spec. 40 (2011) 135-140**
- New Geant4 cross section models for PIXE simulation [↗](#), H. Ben Abdelouahed, S. Incerti, A. Mantero, **Nucl. Instrum. and Meth. B 267 (2009) 37-44**

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