The ANSTO evaluated PIXE Model

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Geant4 EM Low Energy Activity

ANSTO Evaluated PIXE data library

- By J. Crawford, D. Cohen, R. Siegele, G. Doherty, A. Atanacio
- Up to 5 MeV proton energy
- Data available also for deuterium and helium as incident particles
- Targets with Z between 6 and 92
- Data provided within a self-consistent database

Evaluated data libraries

W_k: Krause(1979)

W_L: Campbell (2003) and (2009)

W_M: Dirac Fock theoretical data

K and L shell emission rates: Salem (1974)

M shell emission rate: Dirac Fock theoretical data set. Compilation of Chauhan and Puri – At. Data nucl. Data Tables 94(2008) 38-49

C-K transitions: Chauhan and Puri – At. Data nucl. Data Tables 94(2008) 38-49

Ionisation cross sections

- **ECPSSR theory**
  - Plane wave Born Approx, with corrections for energy loss, Coulomb deflection of the projectile, perturbed stationary states of the target atoms, relativistic nature of the inner electrons
  - Tabulated in Cohen & Harrigan, At. Data Nucl. Data Tables 33 (1985) 255.
  - Agreement with experimental data
    - Few % for k-shell
    - 5-15% for L-shell
    - 10-50% for M- shell

K, L and Mshell X-ray production cross sections

- $\sigma_{k\_\alpha}{}^{X} = \sigma_k{}^{I}\omega_k \frac{\Gamma_{k\_\alpha}}{\Gamma_k}$
- $\sigma_{k\_\beta}{}^{X} = \sigma_k{}^{I}\omega_k \frac{\Gamma_{k\_\beta}}{\Gamma_k}$
- ${}^{1}\sigma_{L\_p}{}^{X} = \sigma_1{}^{I}\omega_1 \frac{\Gamma_{L\_p}}{\Gamma_{L\_1}}$
- ${}^{2}\sigma_{L\_p}{}^{X} = (\sigma_1{}^{I}f_{12} + \sigma_2{}^{I})\omega_2 \frac{\Gamma_{L\_p}}{\Gamma_{L\_2}}$
- ${}^{3}\sigma_{L\_p}{}^{X} = (\sigma_1{}^{I}(f_{12}f_{23} + f_{13} + f_{13}{}') + \sigma^{I}{}_2 f_{23} + \sigma^{I}{}_3)\omega_3 \frac{\Gamma_{L\_p}}{\Gamma_{L\_3}}$
- ${}^{1}\sigma_{M\_p}{}^{X} = \sigma_1{}^{I}\omega_1 \frac{\Gamma_{M\_p}}{\Gamma_{M\_1}}$
- ${}^{2}\sigma_{M\_p}{}^{X} = (\sigma_1{}^{I}f_{12} + \sigma_2{}^{I})\omega_2 \frac{\Gamma_{M\_p}}{\Gamma_{M\_2}}$
- ${}^{3}\sigma_{M\_p}{}^{X} = (\sigma_1{}^{I}(f_{12}f_{23} + f_{13} + f_{13}{}') + \sigma^{I}{}_2 f_{23} + \sigma^{I}{}_3)\omega_3 \frac{\Gamma_{M\_p}}{\Gamma_{M\_3}}$
- ${}^{4}\sigma_{M\_p}{}^{X} = (\sigma_1{}^{I}(f_{14} + f_{12}f_{24} + f_{13}f_{34} + f_{12}f_{23}f_{34}) + \sigma^{I}{}_2(f_{24} + f_{23}f_{34}) + \sigma^{I}{}_3 f_{34} + \sigma^{I}{}_4)\omega_4 \frac{\Gamma_{M\_p}}{\Gamma_{M\_4}}$
- ${}^{5}\sigma_{M\_p}{}^{X} = (\sigma_1{}^{I}(f_{15} + f_{12}f_{25} + f_{13}f_{35} + f_{14}f_{45} + f_{12}f_{23}f_{35} + f_{12}f_{24}f_{45} + f_{12}f_{23}f_{34}f_{45}) + \sigma^{I}{}_2(f_{25} + f_{24}f_{45} + f_{23}f_{34}f_{45}) + \sigma^{I}{}_3(f_{35} + f_{34}f_{45}) + \sigma^{I}{}_4 f_{45} + \sigma^{I}{}_5)\omega_5 \frac{\Gamma_{M\_p}}{\Gamma_{M\_5}}$

X-ray emission line cross sections

Cross section of each X-ray emission line for each incident proton energy and Z :

- $K\alpha_1$, $K\alpha_2$, $K\alpha_{3,}$ $K\beta_1$, $K\beta_2$, $K\beta_3$, $K\beta_4$, $K\beta_5$
- Ll, $L\alpha_1$, $L\alpha_2$, $L\eta$, $L\beta_1$, $L\beta_{215}$, $L\beta_3$, $L\beta_4$, $L\beta_5$, $L\beta_6$, $L\gamma_1$, $L\gamma_2$, $L\gamma_{3,}$ $L\gamma_{44,}$ $L\gamma_{5,}$ $L\gamma_6$, Lb_{910}
- M5-N3, M5-N7, M5-N6, M5-O3, M4-N2, M4-N3/Md, M4-N6/Mb, M4-O3, M4-O2, M3-N1, M3-N2, M3-O1, M3-O45, M3-N5, M3-N4/Mg, M3-N67/Mm1, M2-N1/Mz, M2-O1/Mm2, M2-O4, M2-N4, M1-N23, M1-O23, Total, F-M1, F-M2, F-M3, F-M4, F-M5

X-ray spectra

- Tabulated for Z=6-92
- K- L- shell X-ray spectra from GEOPIXE and Kaye & Laby (NPL)
- The M shell X-ray energies have been calculated from the electron binding energies (obtained from the Lawrence Berkeley National Labs)

Workflow

1) Implement the ANSTO PIXE model in Geant4

Using the current software design

2) Verify that the implementation is correct against the original ANSTO PIXE database

3) Validate against experimental measurements

4) Compare the alternative Geant4 PIXE models to experimental data

The collaboration with ANSTO started in July 2016

Implement the ANSTO PIXE evaluated library in Geant4

1. Investigate the database coherence
2. Develop a Geant4 “ANSTO-Deexcitation” model:
    1. ECPSSR ionisation cross sections
    2. Radiation yields
    3. Koster-Kronig transitions
    4. X-Ray emission rates
    5. X-Ray Energies
    6. ECPSSR for ions (t.b.v. with ANSTO)

Validation of the Geant4-ANSTO Pixe model

- Against experimental data
  - ANSTO micro-PIXE beam
- Compare the alternative Geant4 PIXE models against experimental measurements

Limitations of the ANSTO PIXE model

- De-excitation cascade?
  - To be checked
- Multiple vacancies from high energy ions not modelled
- Chemical effects not modelles: outer e- can influence light atoms inner shells vacancies

Future

- Current approach is to "adapt" ANSTO PIXE model to Geant4 software design

- For the future:
  - Maybe a "Fluorescence" process:

  Proton has ionisation -> get directly the X-ray emission line calculated based only on the X-ray emission cross section (and not on ionisation cross section, fluorescence yield, etc)