

Recent developments and validation of Geant4 PIXE

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Goal of the project

Develop a new library, called here **G4-ANSTO**, modelling PIXE

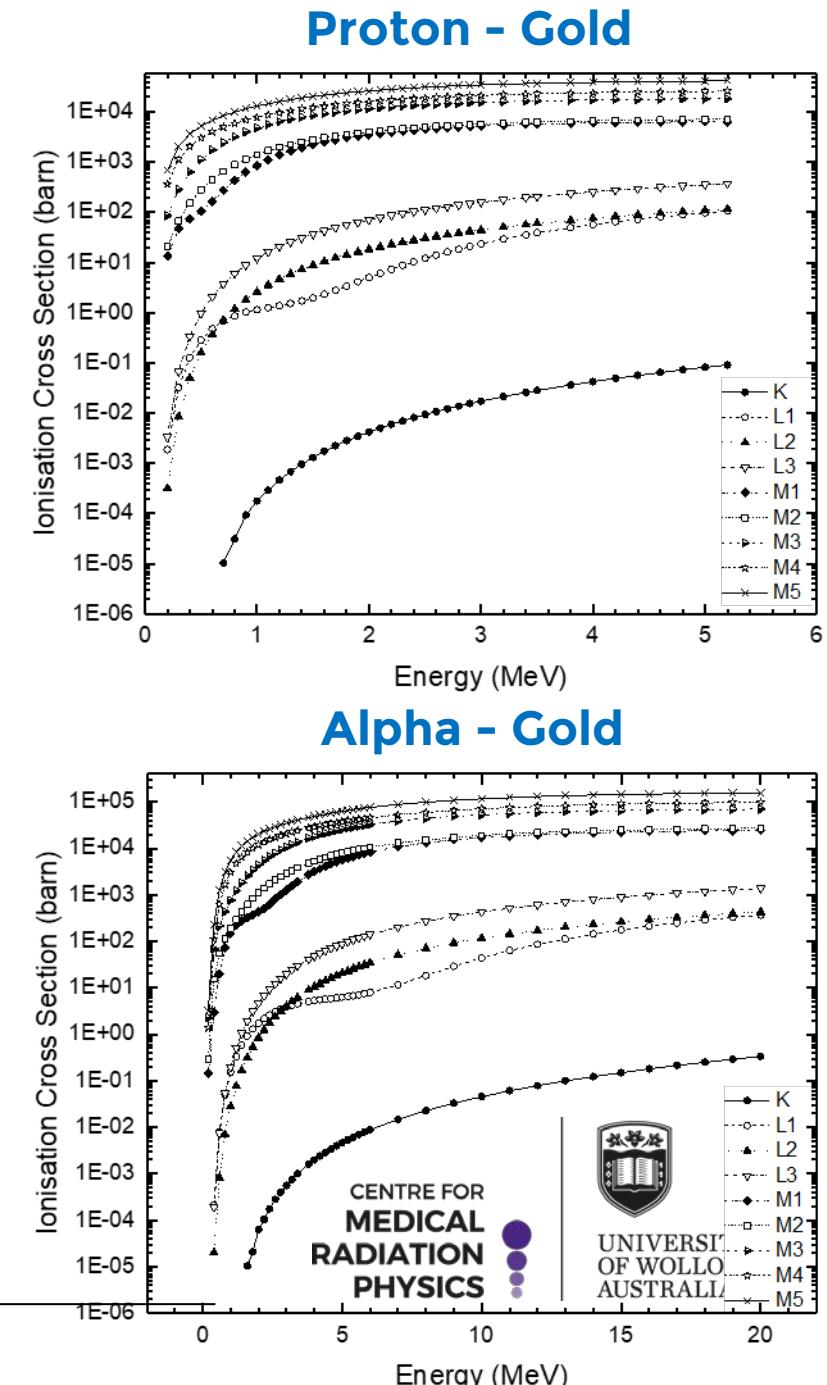
- p and α ionisation cross sections ($< 5 \text{ MeV/u}$)
- fluorescence yields
- described in D. D. Cohen, et al., NIM B, vol. 363, pp. 7–18, 2015
- thoroughly validated against experimental measurements performed at ANSTO
- alternative to the existing Geant4 PIXE and fluorescence data libraries
- available since Geant4 11.0, G4EMLOW 8.0
- extended example TestEm5 shows how to activate the new data libraries via UI commands

PIXE Ionisation cross sections

- **ECPSSR theory in ANSTO model**
 - 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.

Table (1). Kinetic energy and elements ranges of the ANSTO ECPSSR cross-sections for incident protons and alpha particles

	Kinetic energy	Target elements		
	K, L, M	K	L	M
Proton	0.2-5.2 MeV			
Alpha	0.2-20.2 MeV	6-92	25-92	60-92

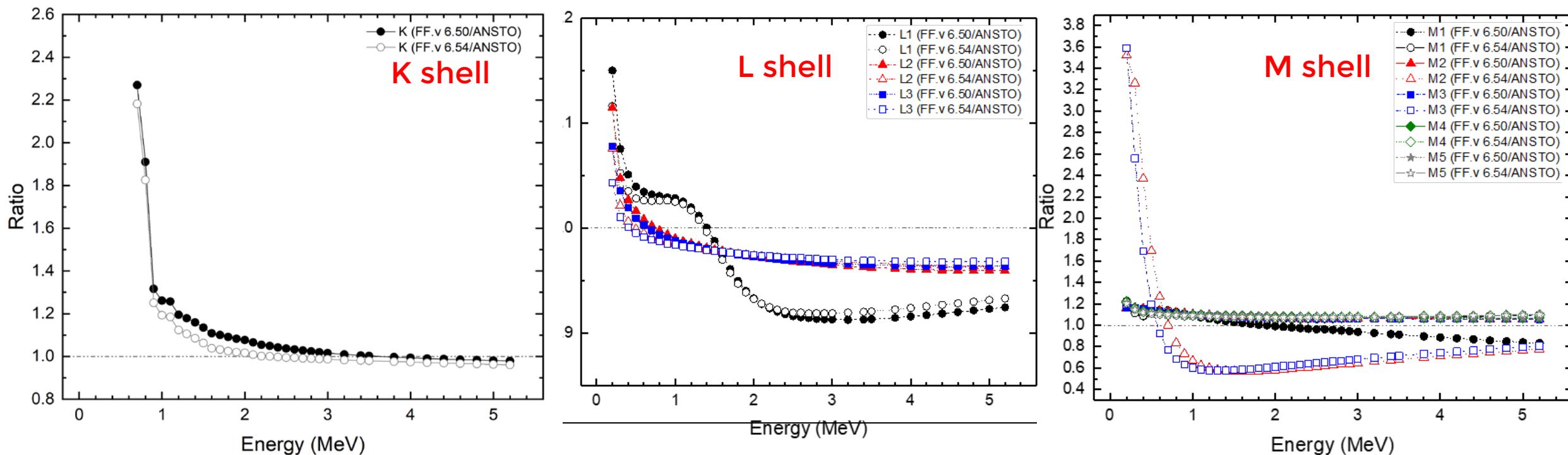


Comparison to the Geant4 ECPSSR Form Factor (1)

Comparison with ECPSSR Form Factor cross sections, based on a polynomial approximation of the ionisation cross sections of K, L and a selection of M shells calculated by Taborda et al (Incerti, Barberet et al. 2015)

Example: protons incident on gold

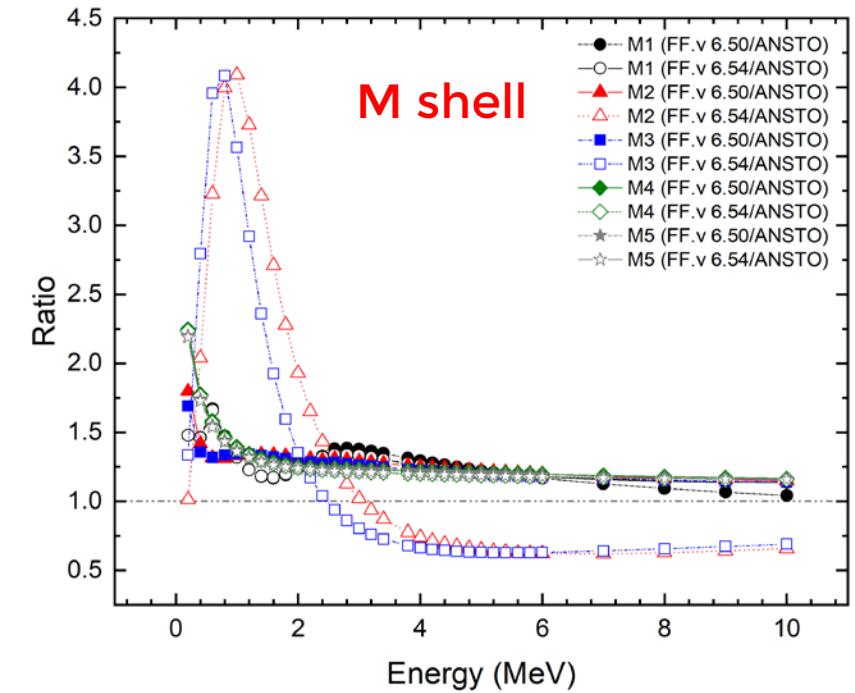
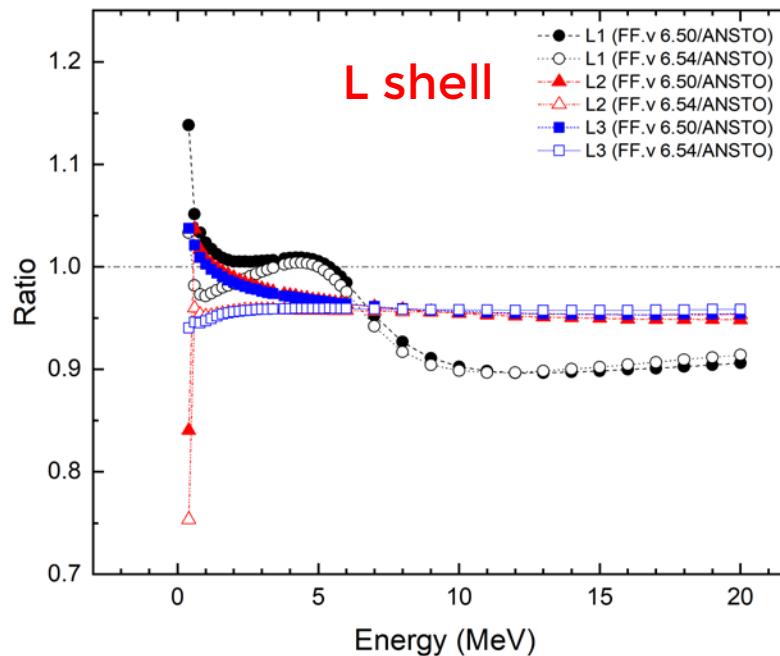
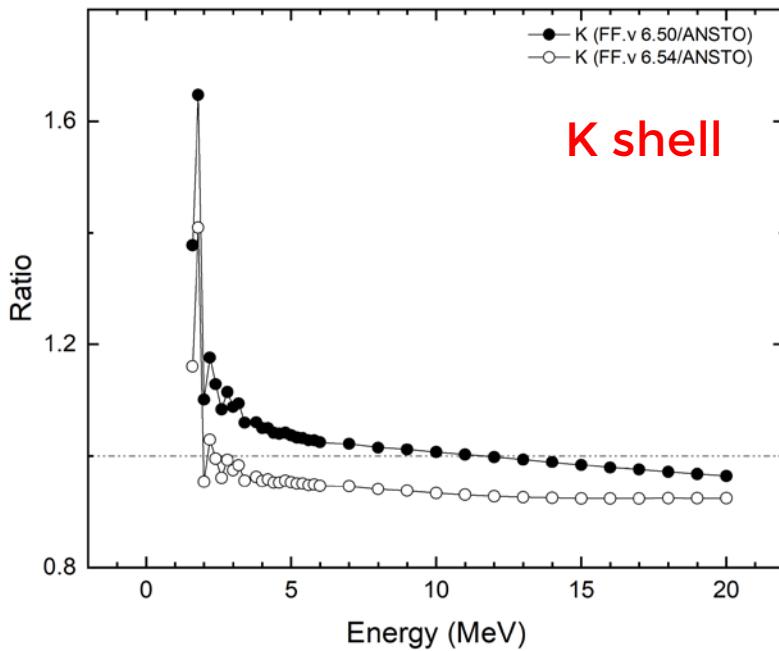
$$R = \frac{\sigma_{ECPSSR_Form_Factor}}{\sigma_{ECPSSR_ANSTO}}$$



Comparison to the Geant4 ECPSSR Form Factor (2)

Example: alpha particles incident on gold

$$R = \frac{\sigma_{ECPSSR_Form_Factor}}{\sigma_{ECPSSR_ANSTO}}$$



For heavier ions:

$$\sigma_h(E) = Q^2 \cdot \sigma_p\left(E \cdot \frac{M_p}{M_h}\right)$$



New X-ray fluorescence data library

- D. D. Cohen, J. Crawford, and R. Siegele, “K, L, and M shell datasets for PIXE spectrum fitting and analysis,” NIM B, vol. 363, pp. 7–18, 2015.
- Data library of ANSTO with the same format of EADL
- The same binding energies of EADL are adopted
- The radiative transition probabilities reported in the EADL were calculated according to Hartree Slater (HS) methods, however [Cohen et al 2015] recommends the Hartree-Fock approach for M shell

Comparisons

Ionisation cross-sections:

- Based on Form Factor (Taborda K, L, M 2011-2013)
- ANSTO PIXE cross section

Transition probabilities:

- EADL, G4EMLOW7.7
- ANSTO-fluo

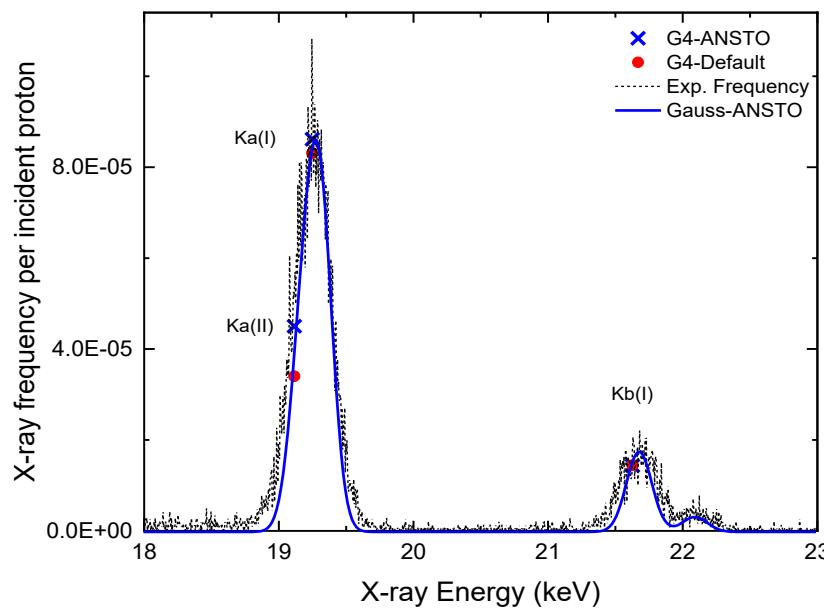
Against experimental measurements

Methodology

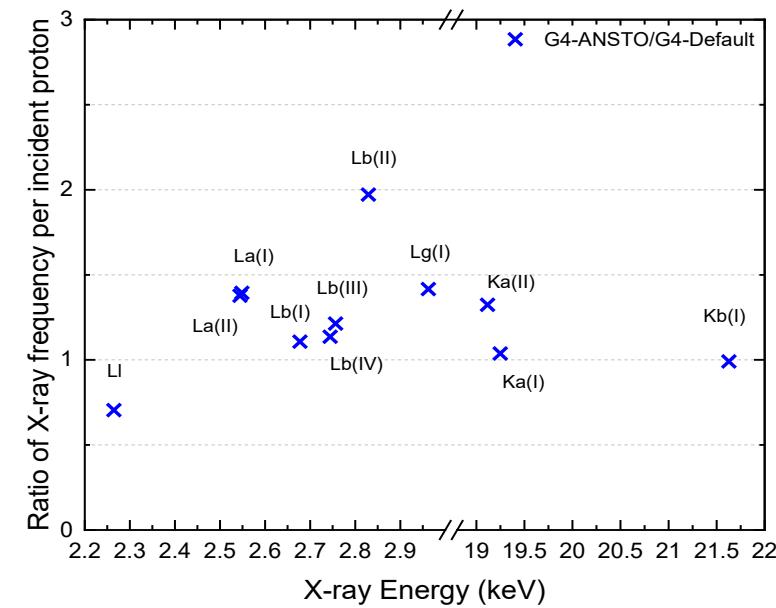
- **Geant4 TestEm5 extended example (Geant4 10.05.p01)**
 - Monochromatic beams of proton, alpha particles and carbon ions are incident on 25 μm thick targets (50 μm lateral sizes)
 - G4-ANSTO and EADL has been compared in terms of fluorescence X-ray yields per incident particle
 - Validation against experimental data
 - For low, medium and high Z
 - Protons, alpha particles and carbon ions
 - For few projectile kinetic energies

Comparison against experimental measurements performed at ANSTO: protons

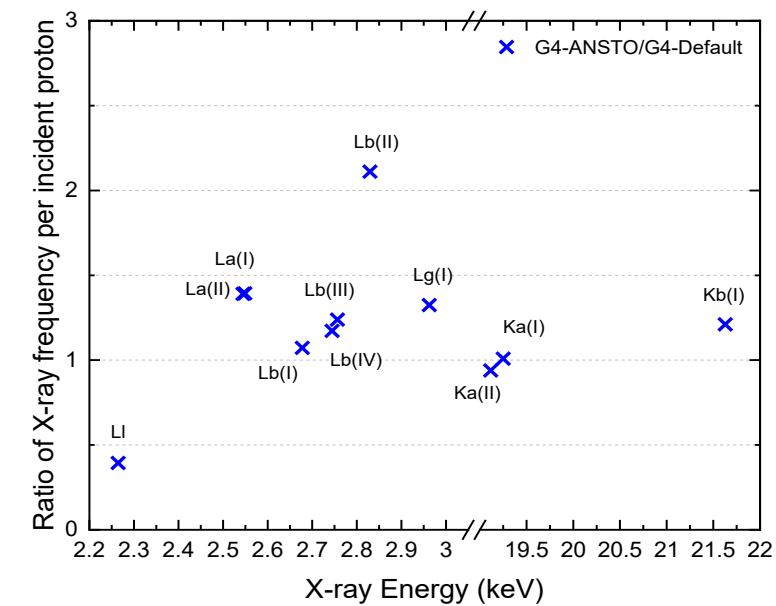
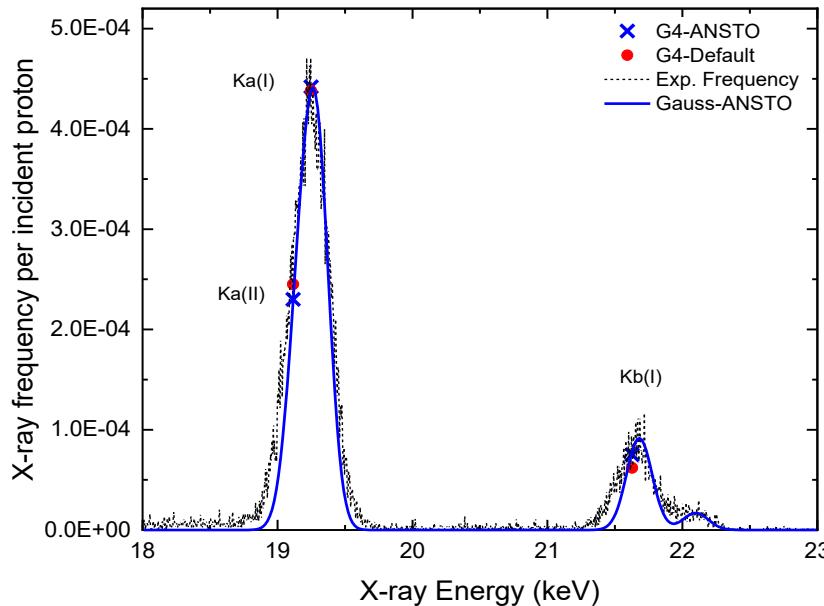
2 MeV proton Ru, Z=44



Ru, Z=44

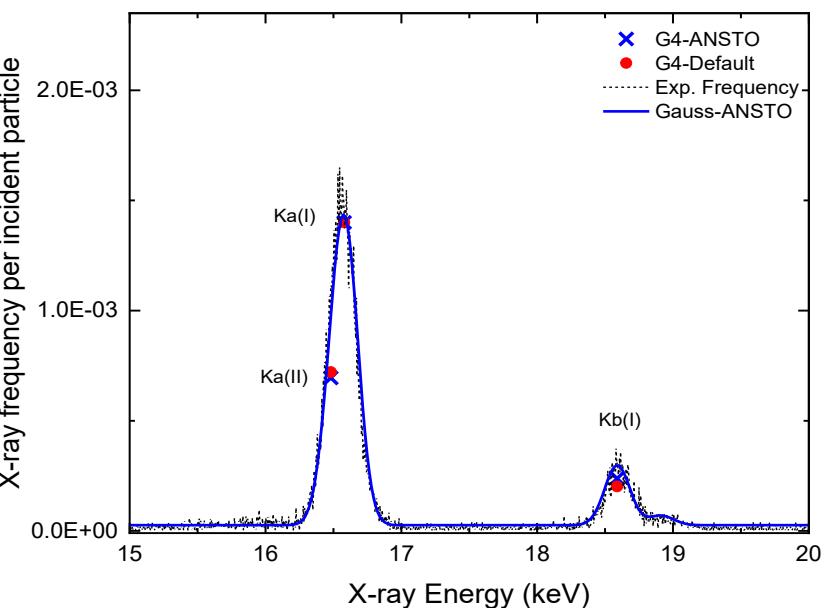


3 MeV proton

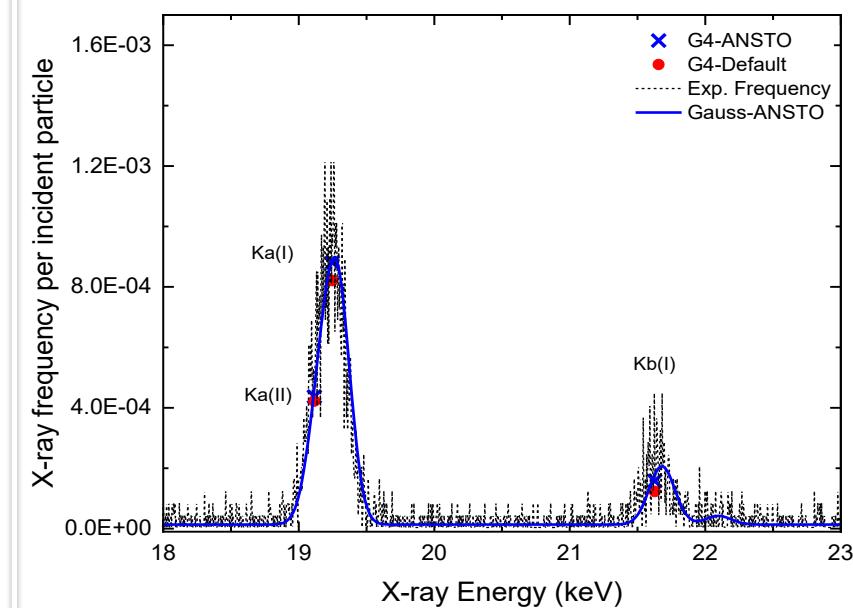


Comparison against experimental measurements performed at ANSTO: Alpha particles

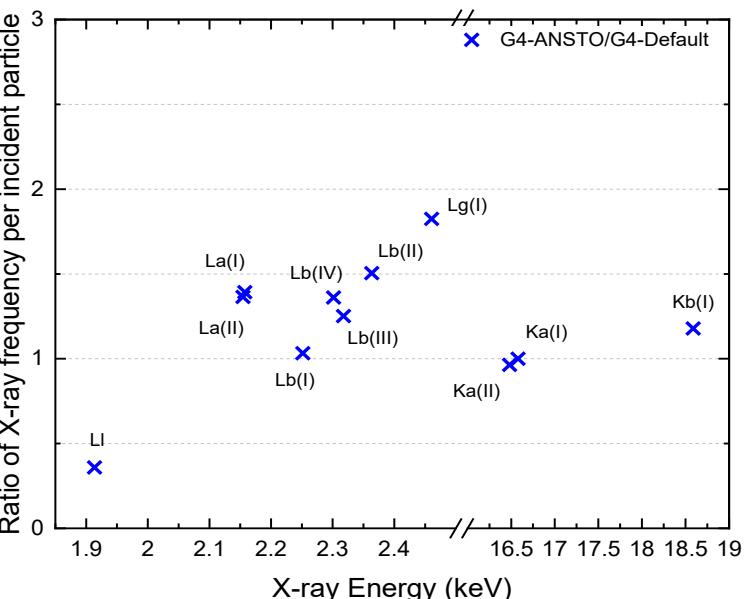
2.5 MeV/u alpha Nb, Z=41



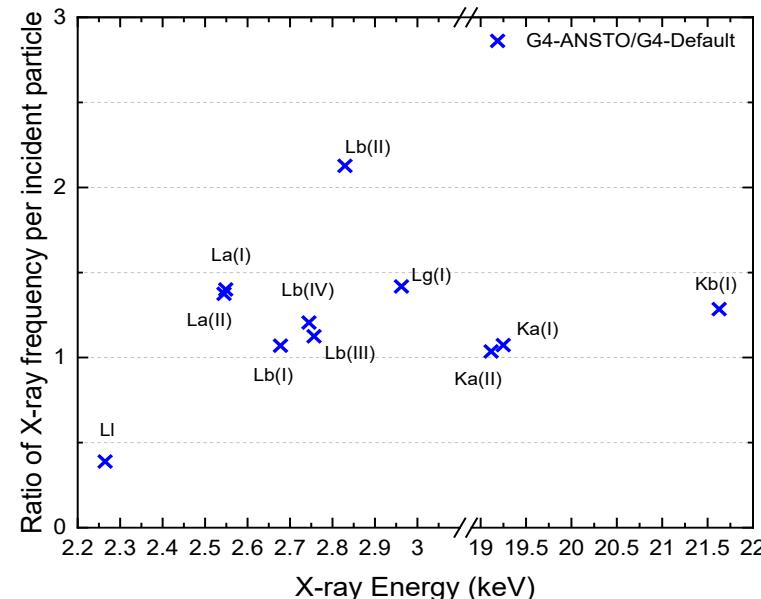
Ru, Z=44



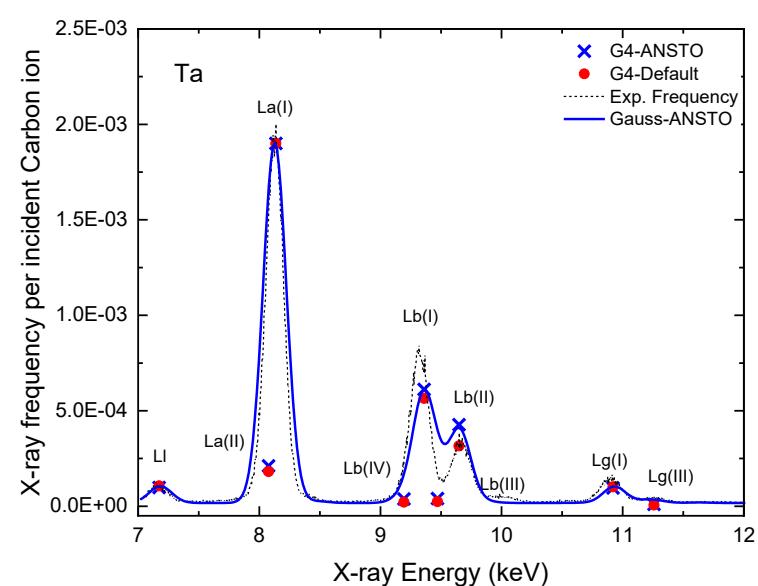
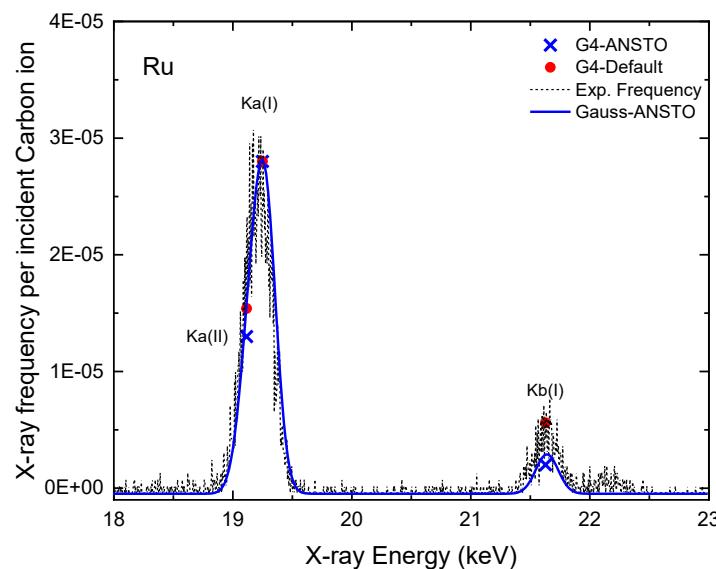
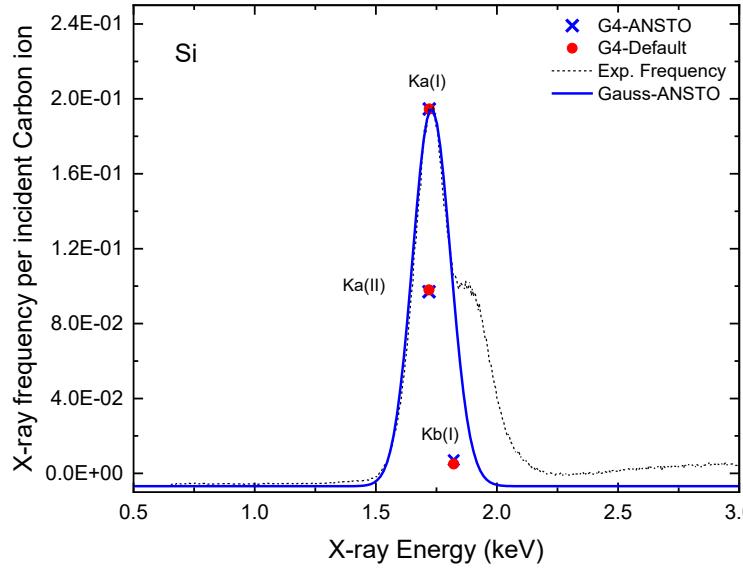
Nb, Z=41



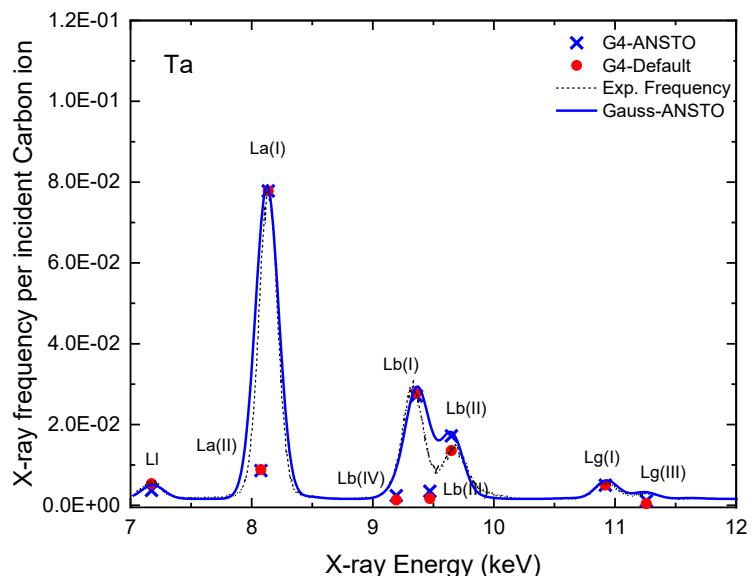
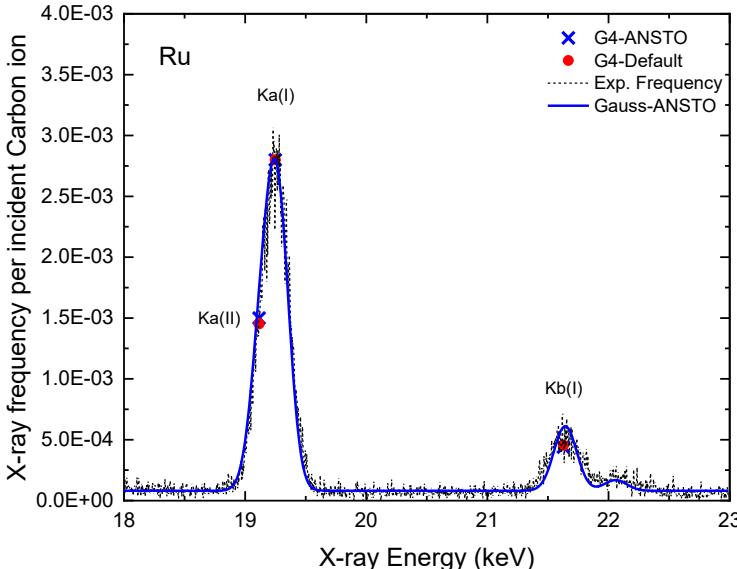
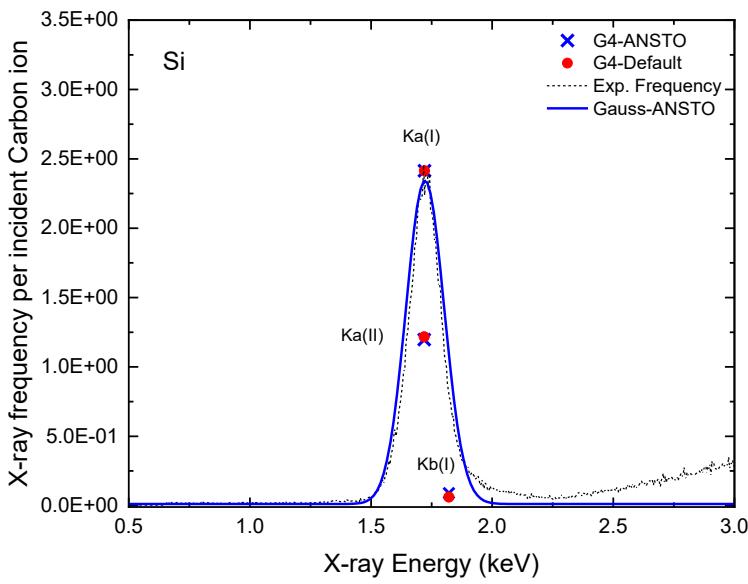
Ru, Z=44



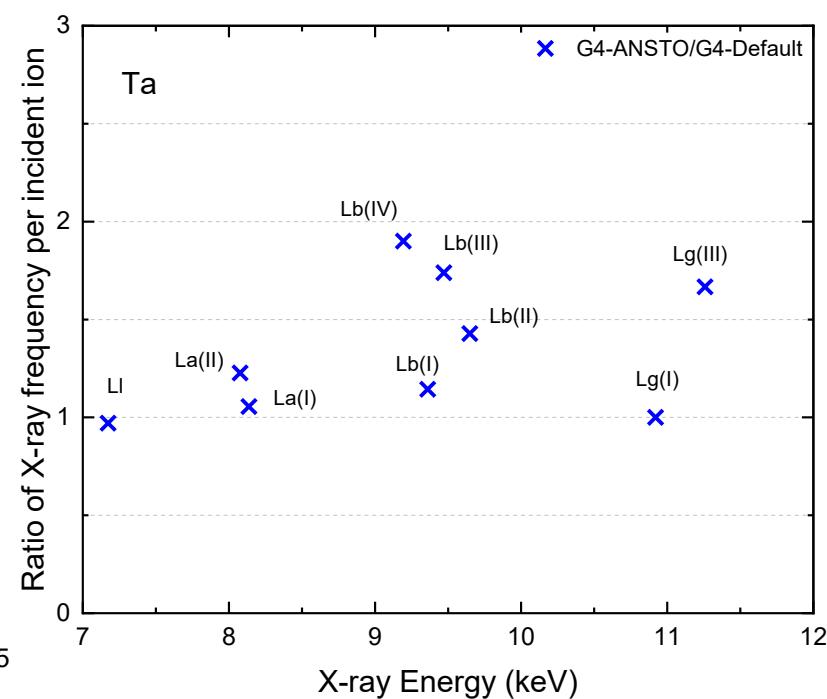
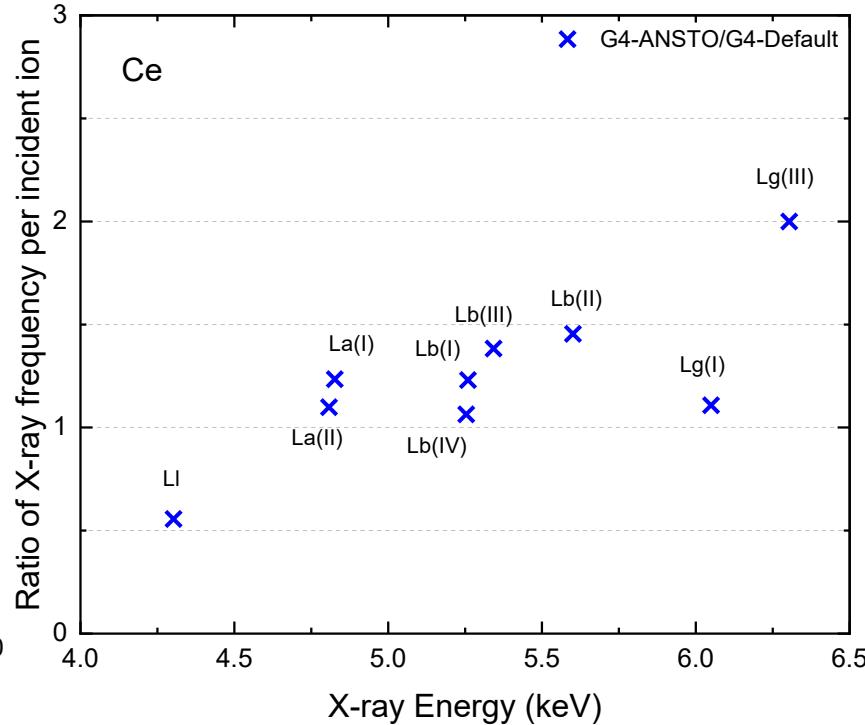
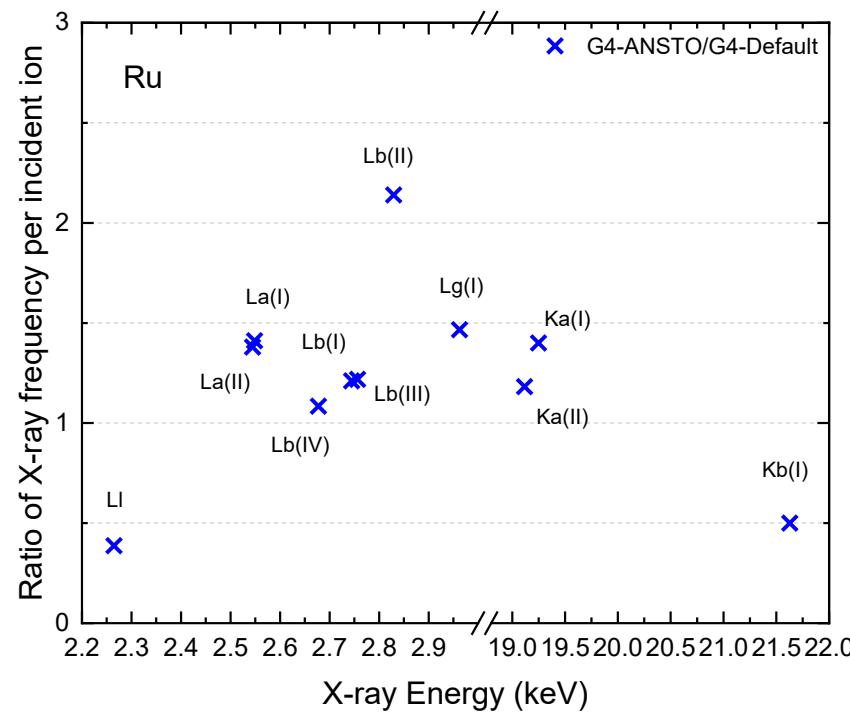
1 MeV/u ^{12}C



3 MeV/u ^{12}C



Carbon ions



“ANSTO” data libraries predict similar or usually higher X-ray emissions



Conclusions

- New PIXE/X-ray fluorescence library implemented in Geant4.
- Emission X-ray spectra using the ANSTO approach provide similar or higher X-ray emission rates, depending on the energy of the incident particle and target material.
- It would be excellent to find other applications domains to test the novel data libraries
- First time validation of Geant4 for PIXE applications with carbon ions
 - Good agreement with experimental data.
- Work documented in:
 - Bakr, S., et al (2021) Geant4 X-ray fluorescence with updated libraries, NIM B, 507: 11-19
 - Bakr, S. , et al (2018) Latest Geant4 developments for PIXE applications, NIM B, 436: 285-291
 - Bakr, S., et al, Validation of the Geant4 PIXE component for incident carbon ions, NIM B, *accepted with minor revisions*

EXTRA INFORMATION

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Implement recommended approach for X-ray emission

Recommended in Cohen DD, Crawford J, Siegele R. K, L, and M shell datasets for PIXE spectrum fitting and analysis. NIM B. 2015, 363, pp. 7-18.

W_K: Krause(1979), based on experimental measurements

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

$$^1\sigma_{L_p}^X = \sigma_1^I \omega_1 \frac{\Gamma_{L_p}}{\Gamma_{L_1}}$$

$$^2\sigma_{L_p}^X = (\sigma_1^I f_{12} + \sigma_2^I) \omega_2 \frac{\Gamma_{L_p}}{\Gamma_{L_2}}$$

$$^3\sigma_{L_p}^X = (\sigma_1^I (f_{12}f_{23} + f_{13} + f'_{13}) + \sigma_2^I f_{23} + \sigma_3^I) \omega_3 \frac{\Gamma_{L_p}}{\Gamma_{L_3}}$$

