Validation of proton interaction models with liquid water above 100 MeV for Geant4-DNA

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Outline

- Motivation and goal
- RPWBA theory
- Model database and implementation
- Validation
- Conclusions

Motivation and goal

http://geant4-dna.org/

Max. energy Limit → 100 MeV

Max. energy of clinical proton therapy beams → ≈250 MeV

Range in liquid water → ≈ 39 cm

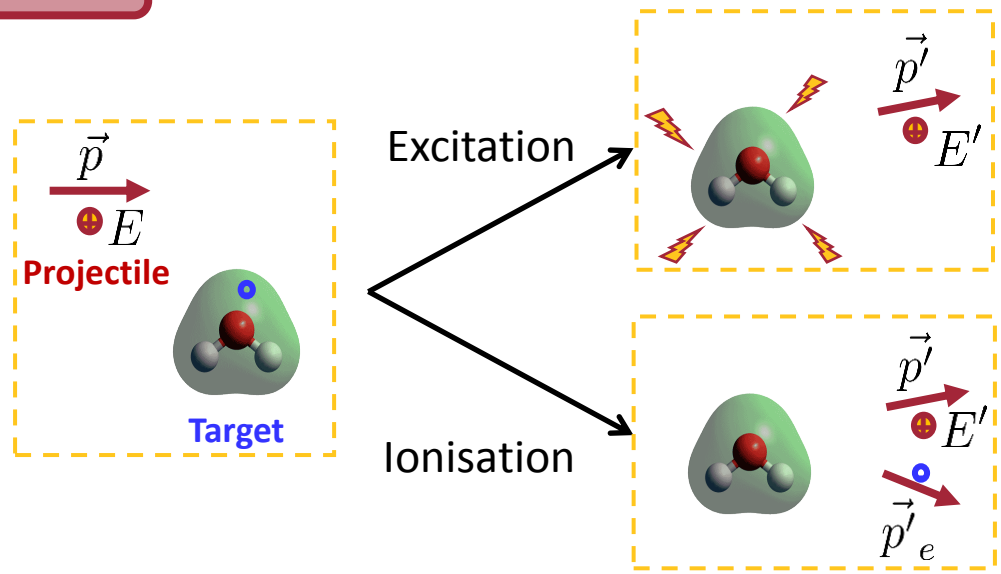
- **Proton interactions** **Liquid water**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill (5)	Type
nuclear scattering (5)	G4DNAElastic	G4DNAIonElasticModel	100 eV	1 MeV	100 eV	interpolated
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	10 eV	500 keV	-	analytical
electronic excitation	G4DNAExcitation	G4DNABornExcitationModel	500 keV	100 MeV	-	interpolated
ionisation	G4DNAIonisation	G4DNARuddIonisationModel (G4DNARuddIonisationExtendedModel is also usable)	0 eV	500 keV	100 eV	interpolated
ionisation	G4DNAIonisation	G4DNABornIonisationModel	500 keV	100 MeV	-	interpolated
electron capture	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	100 eV	100 MeV	-	analytical

(5) indicates the tracking cut applied by the corresponding model.

RPWBA theory

RPWBA **Relativistic Plane Wave Born Approximation**



Individual inelastic collisions

In terms of

Energy loss $W = E - E'$

Momentum transfer $\vec{q} = \vec{p} - \vec{p'}$

Recoil energy Q

DDCS **Doubly differential cross section**

$$\frac{d^2\sigma}{dW\,dQ} = \frac{2\pi Z_P^2 e^4}{m_e c^2 \beta^2}\left\{\frac{2m_e c^2}{WQ(Q+2m_e c^2)} + \frac{2m_e c^2}{[Q(Q+2m_e c^2) - W^2]^2}\left[\beta^2 - \frac{W^2}{Q(Q+2m_e c^2}\right]\right\}\frac{df(Q,W)}{dW}$$

Generalized oscillator strength (GOS)

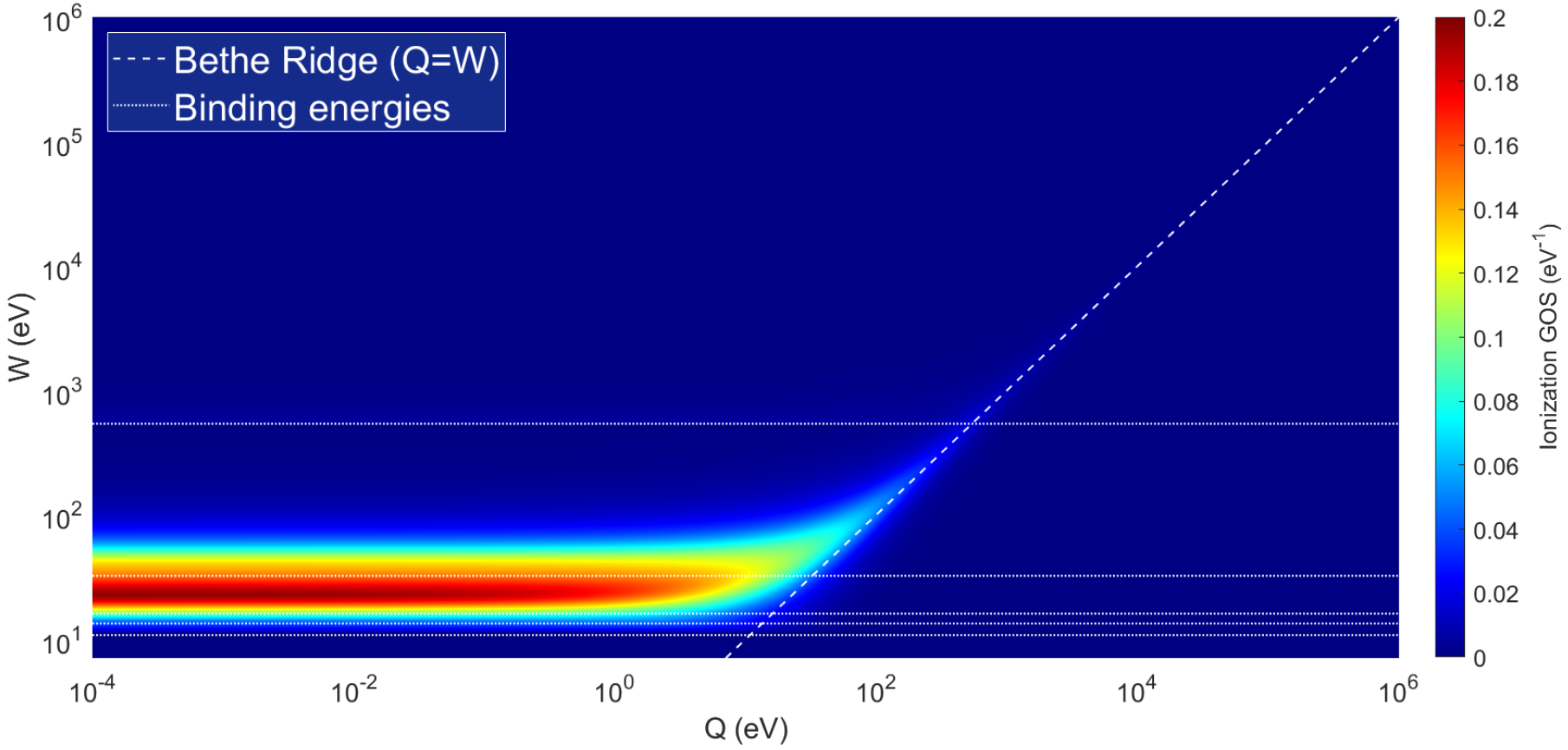
Response of the material $\frac{df(Q,W)}{dW}$

Model database

Parameters values taken from [D. Emfietzoglou / *Radiation Research 164 (2005) 202–211]*

Ionisation GOS

$$\frac{df(Q,W)}{dW}$$



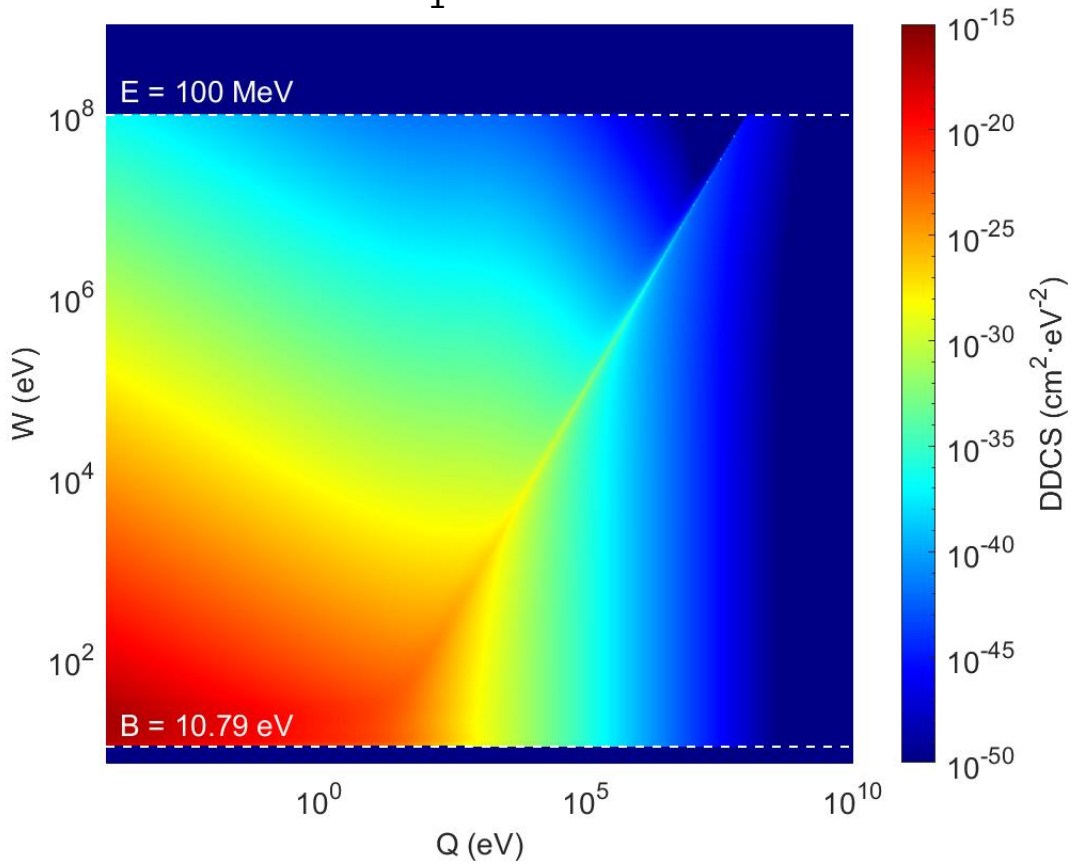
Sum of ionization GOS for each shell

Shell	Binding energy (eV)
($1b_1$)	10.79
($3a_1$)	13.39
($1b_2$)	16.05
($2a_1$)	32.30
(K shell)	539

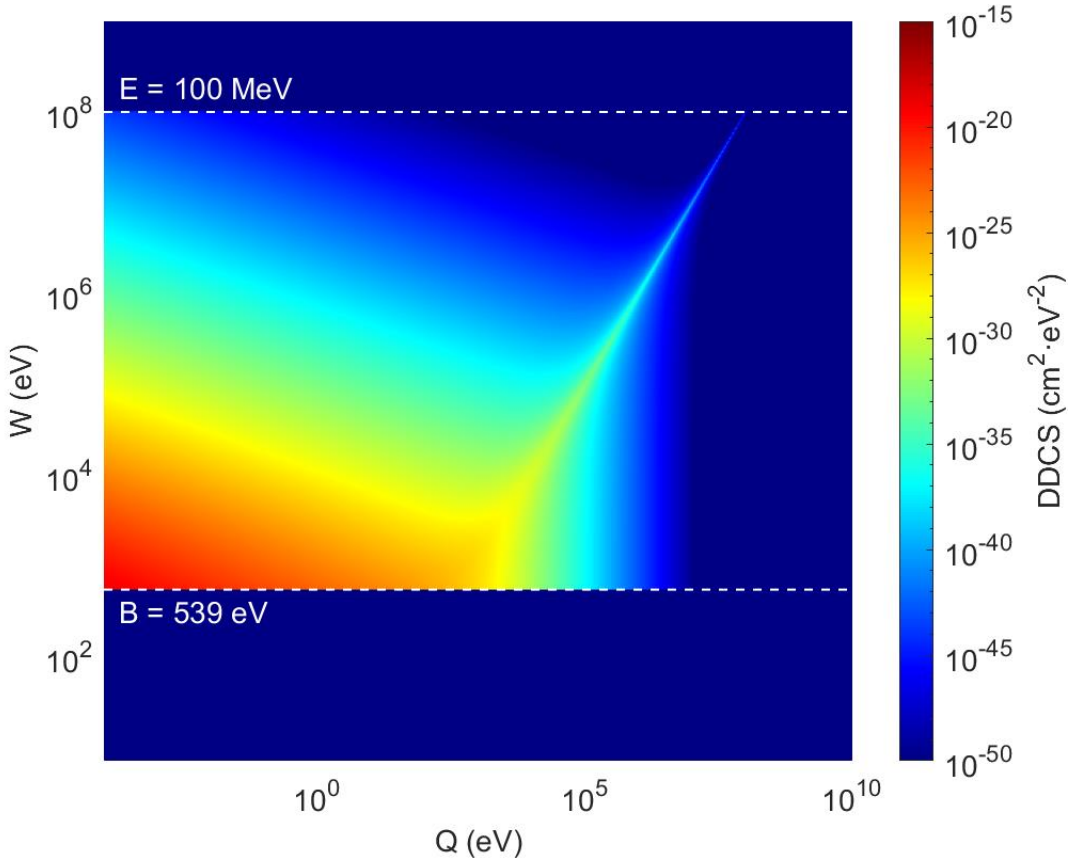
Model database

Ionisation DDCS

$1b_1$ - shell



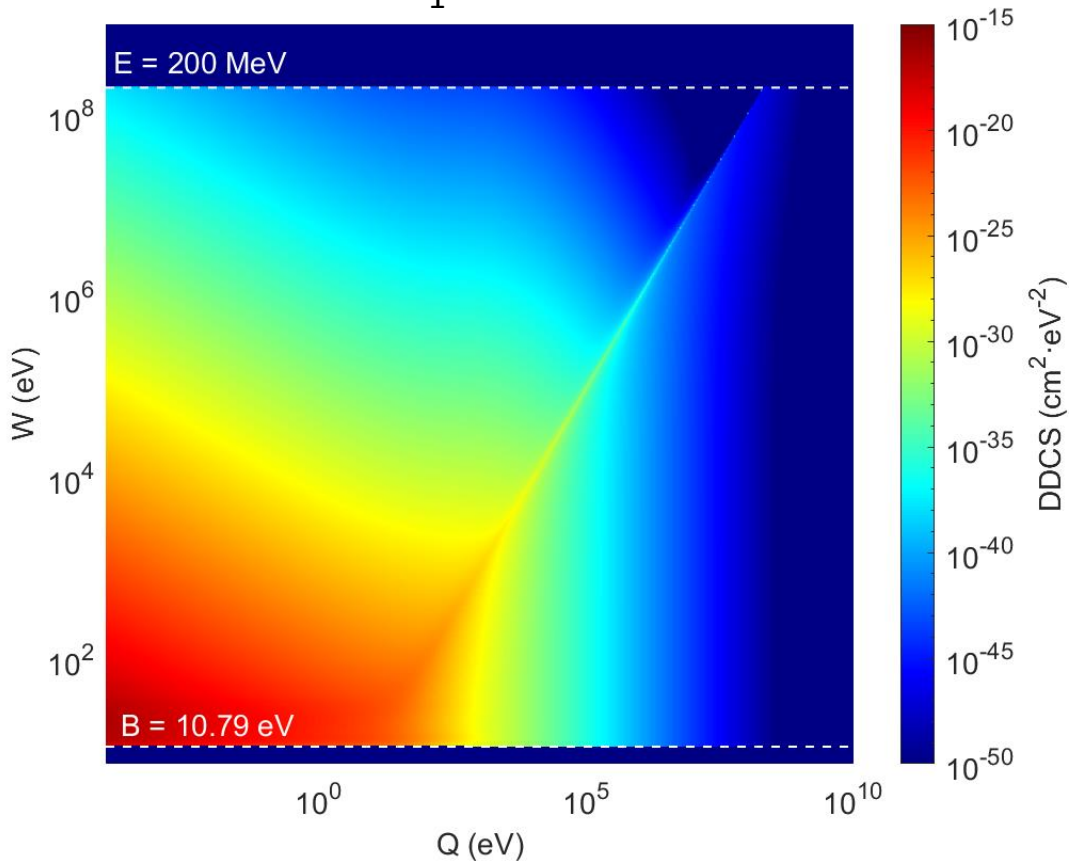
K - shell



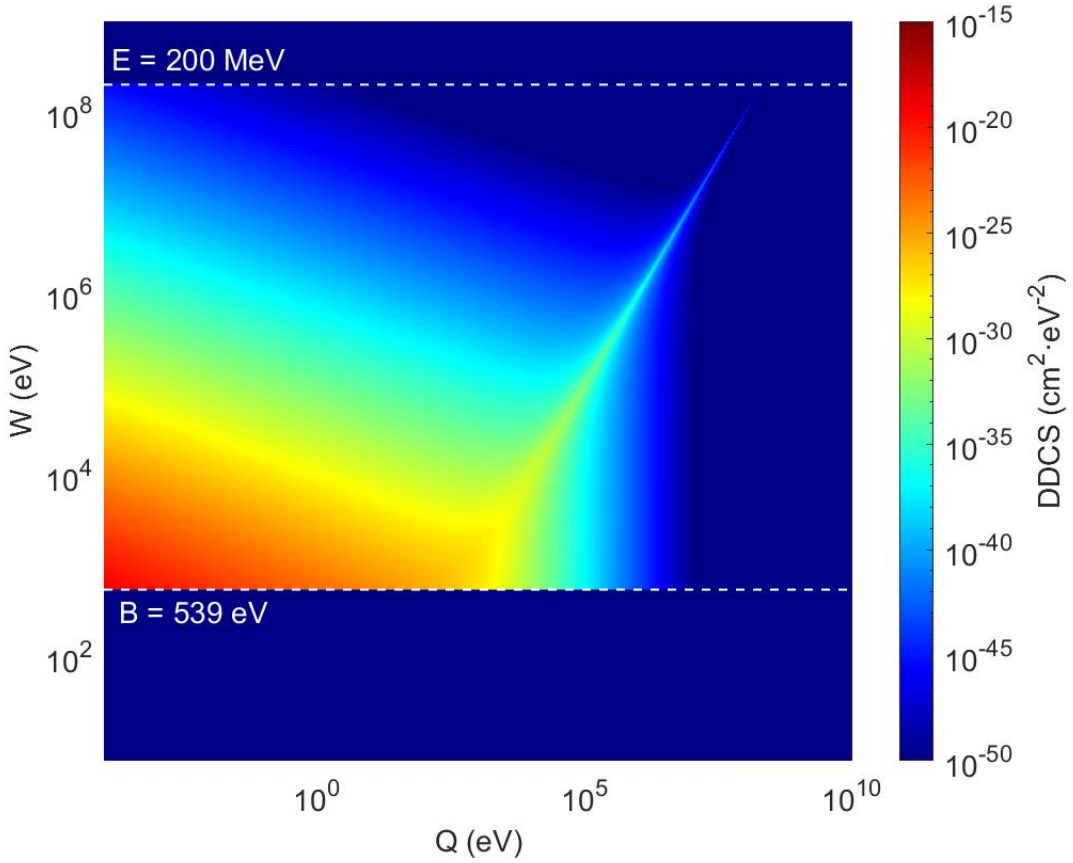
Model database

Ionisation DDCS

$1b_1$ - shell



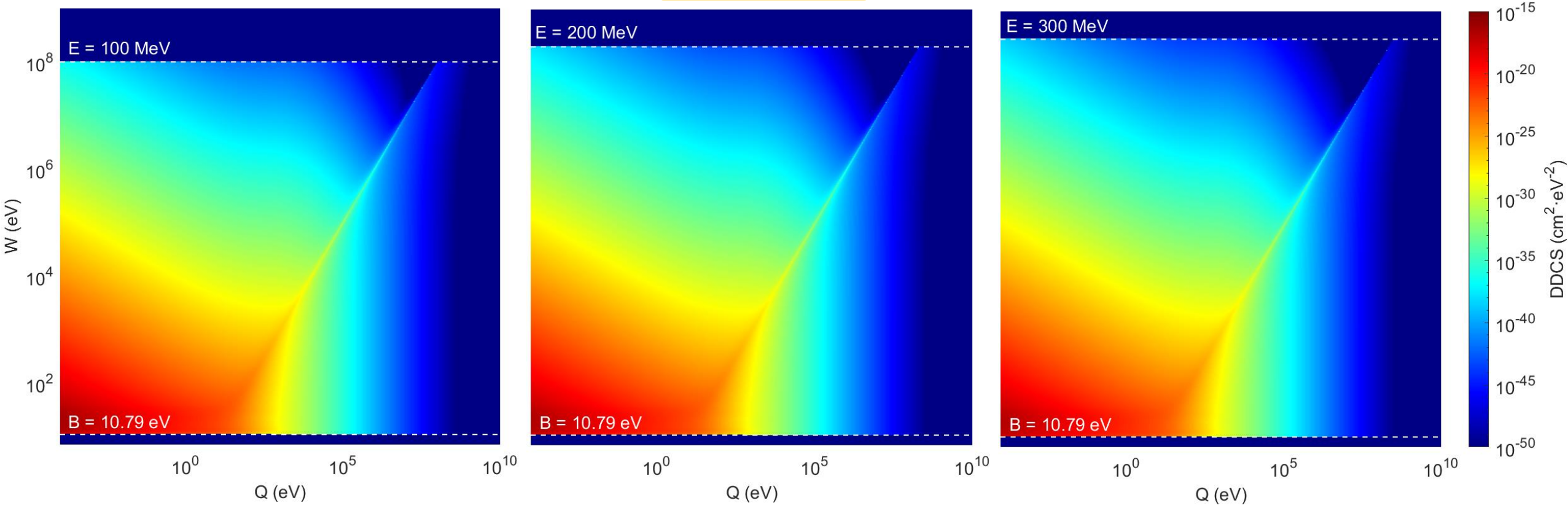
K - shell



Model database

Ionisation DDCS

$1b_1$ - shell

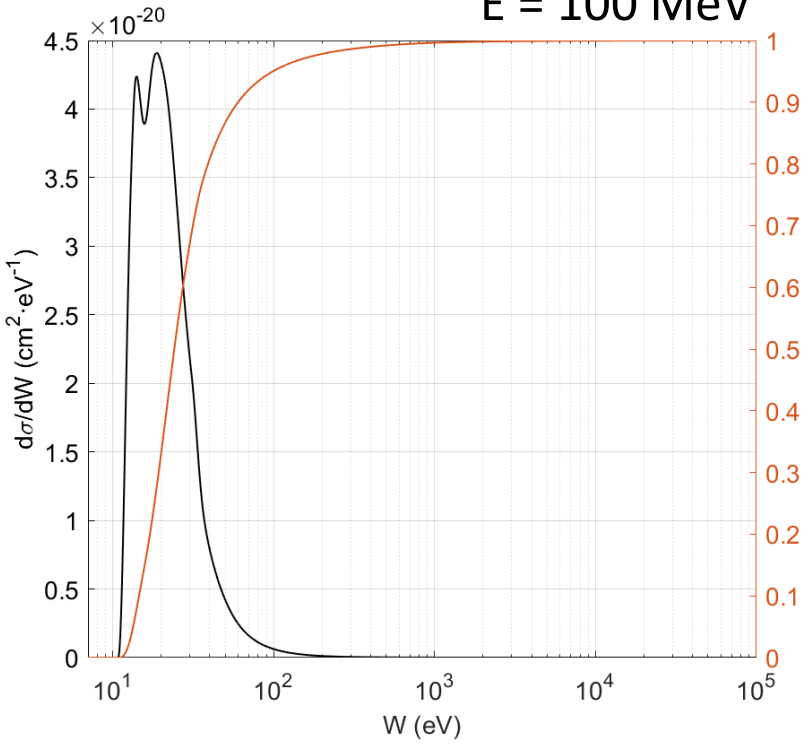


Model database

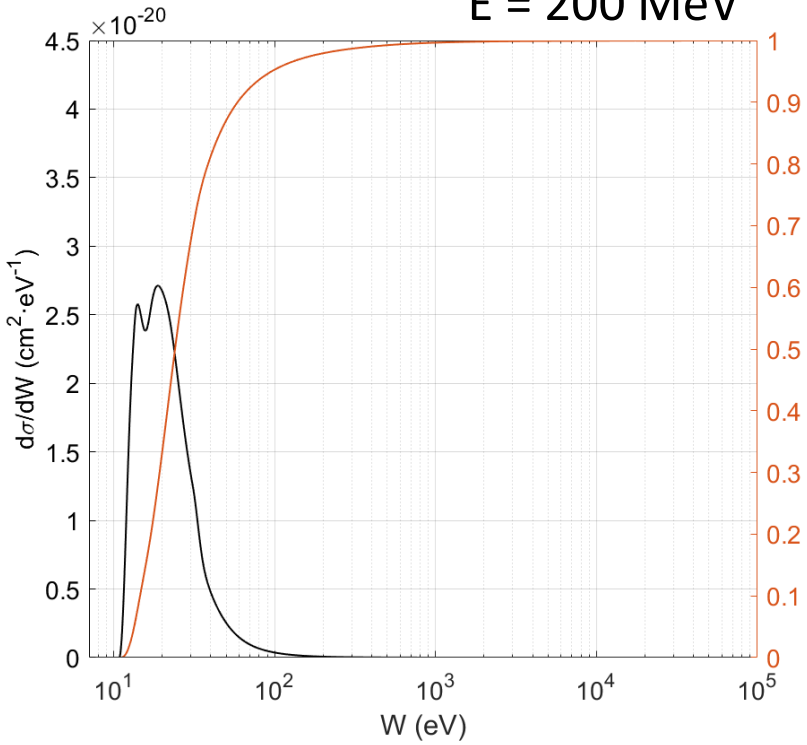
Ionisation DCS

$1b_1$ - shell

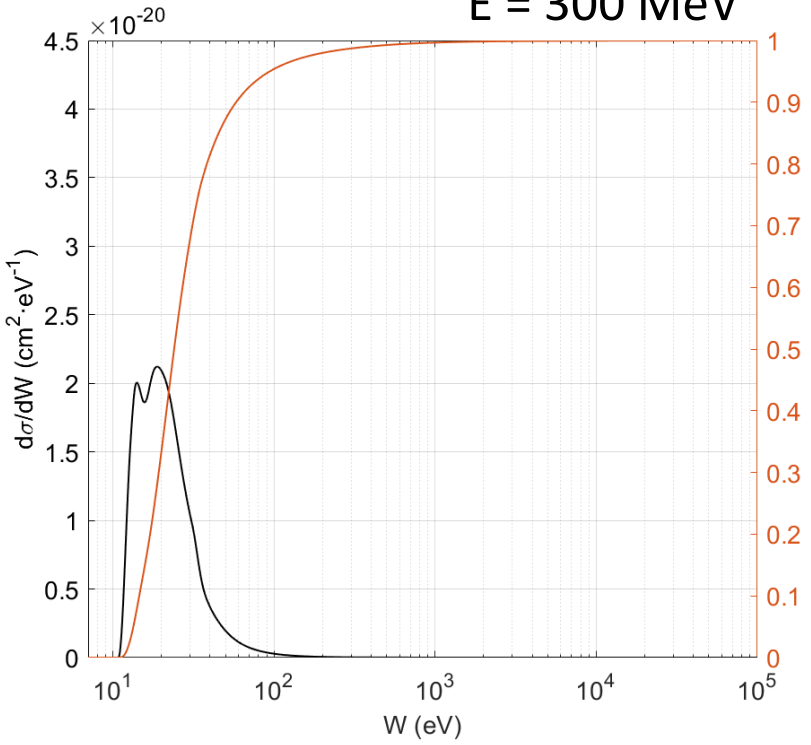
E = 100 MeV



E = 200 MeV



E = 300 MeV

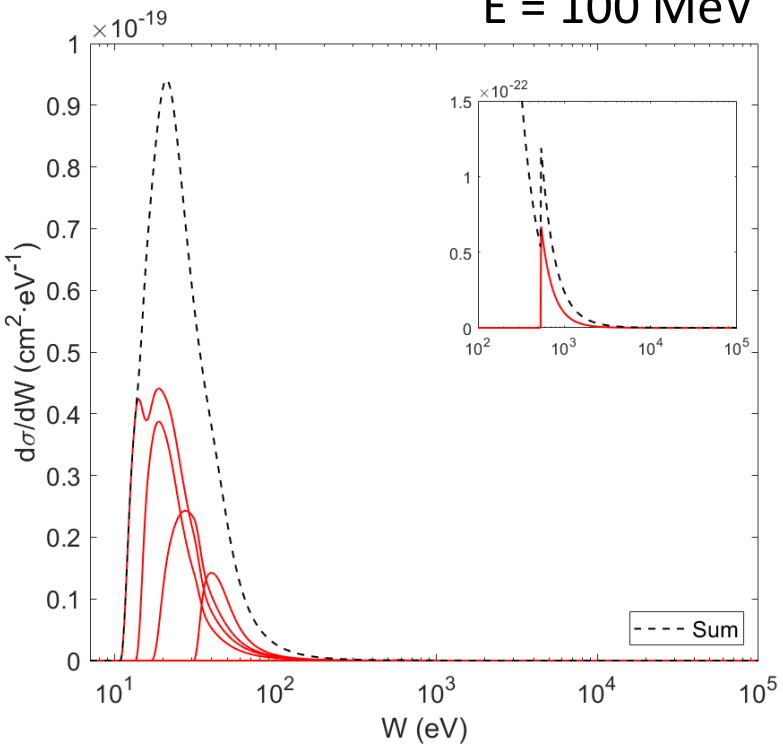


Cumulated distribution

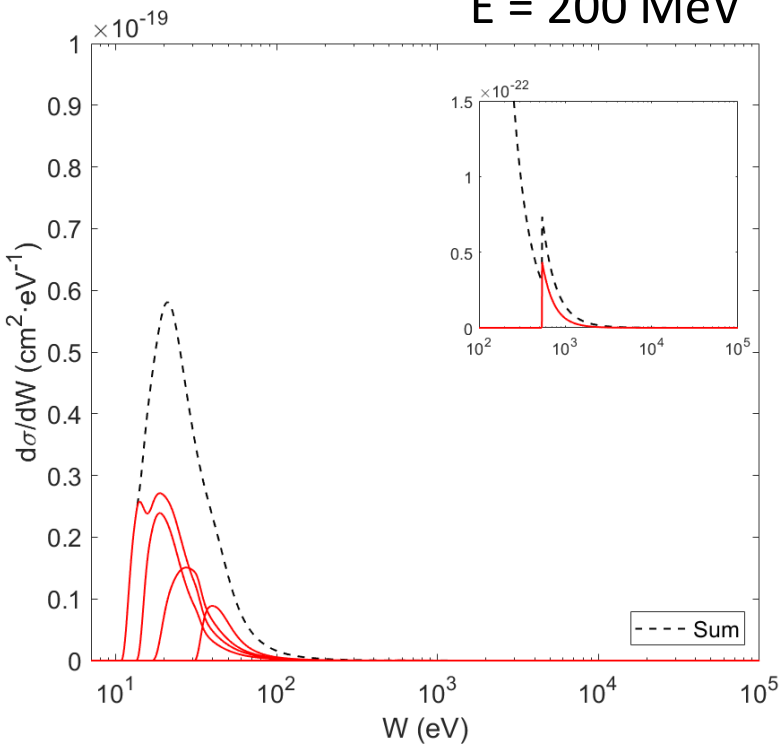
Model database

Ionisation DCS

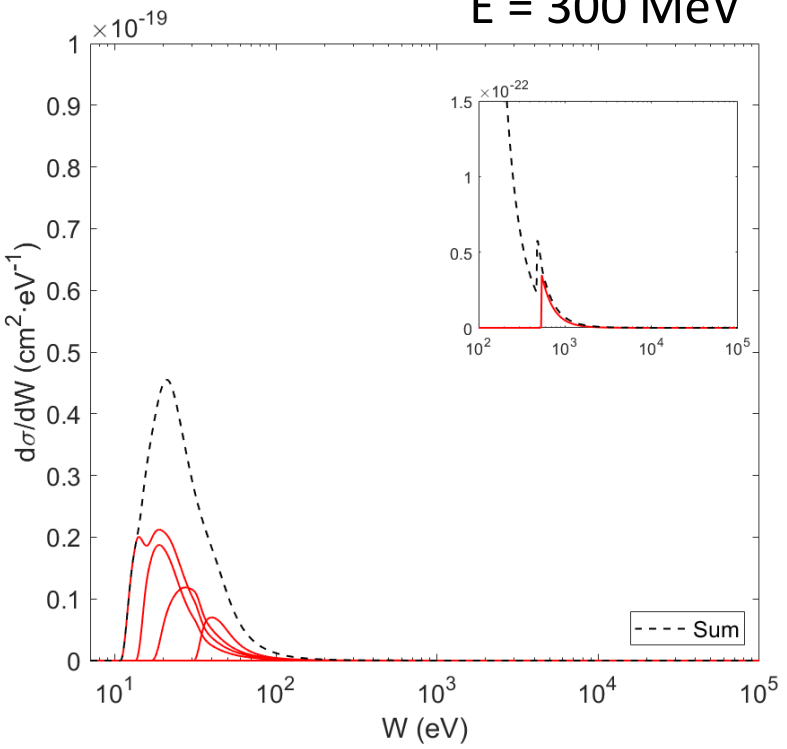
E = 100 MeV



E = 200 MeV



E = 300 MeV

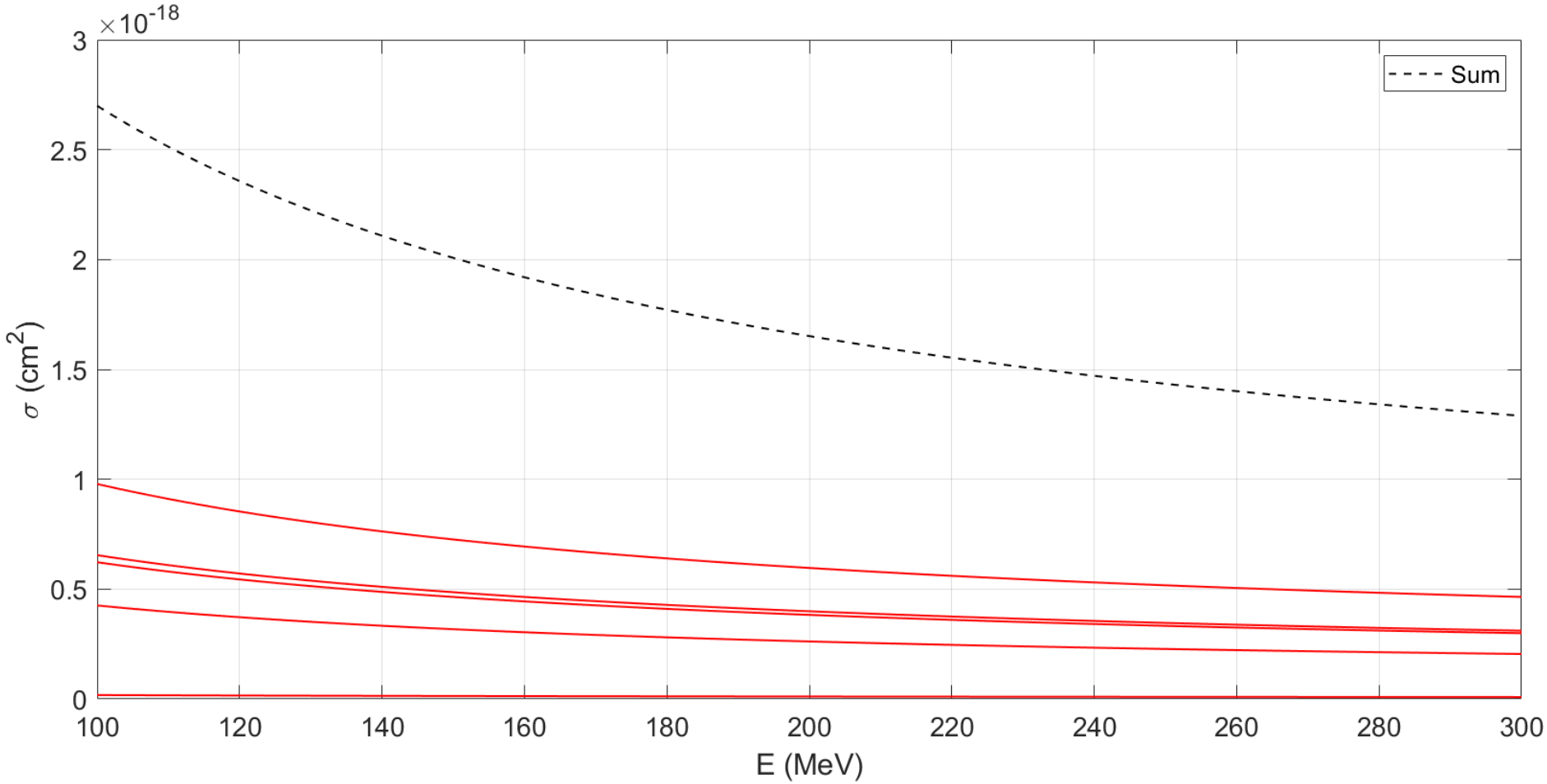


New data files!! sigmadiff_ionisation_p_RPWBA sigmadiff_cumulated_ionisation_p_RPWBA

Model database

Ionisation CS

New data file!! sigma_ionisation_p_RPWBA

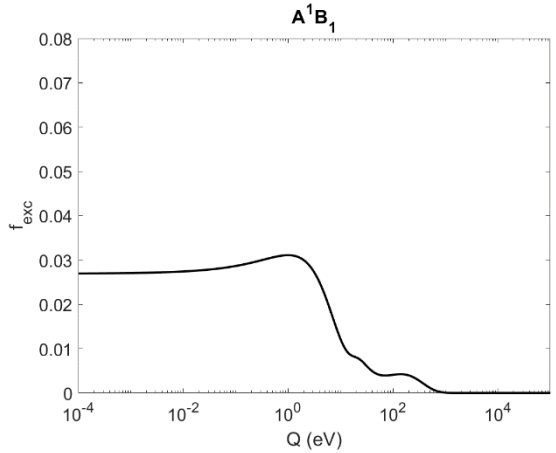


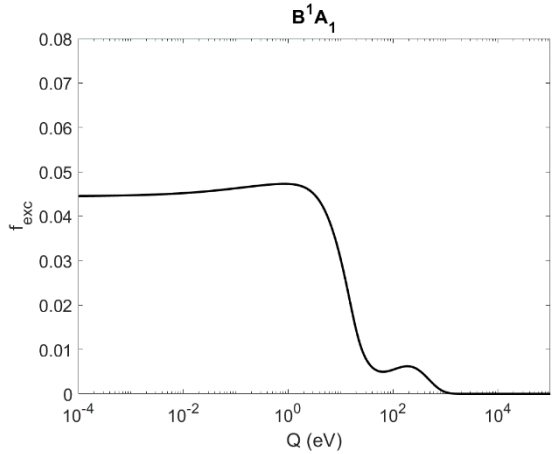
Model database

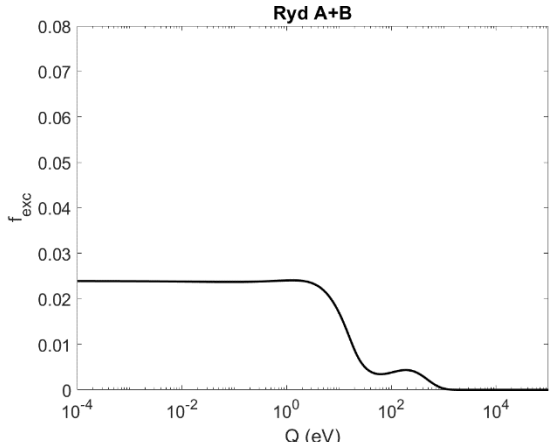
Parameters values taken from [D. Emfietzoglou / *Radiation Research 164 (2005) 202–211]*

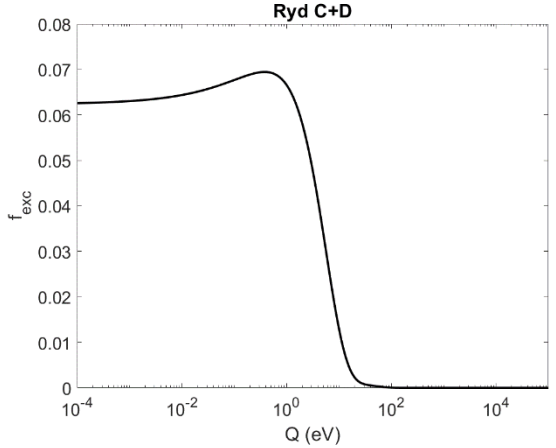
Excitation GOS

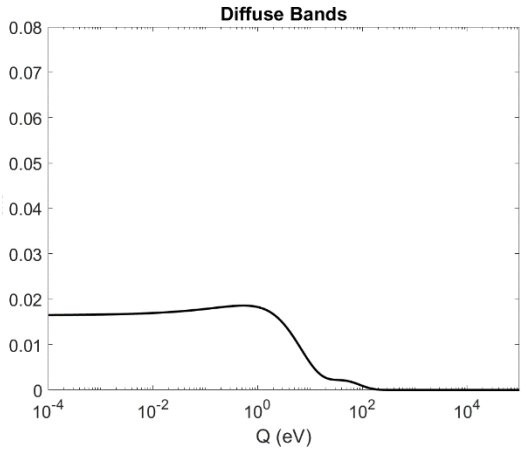
$$\frac{df_{\mathrm{exc}}(Q,W)}{dW} = f_{\mathrm{exc}}(Q)\delta(W - W_{\mathrm{exc}})$$











Excitation GOS for **discrete** transitions

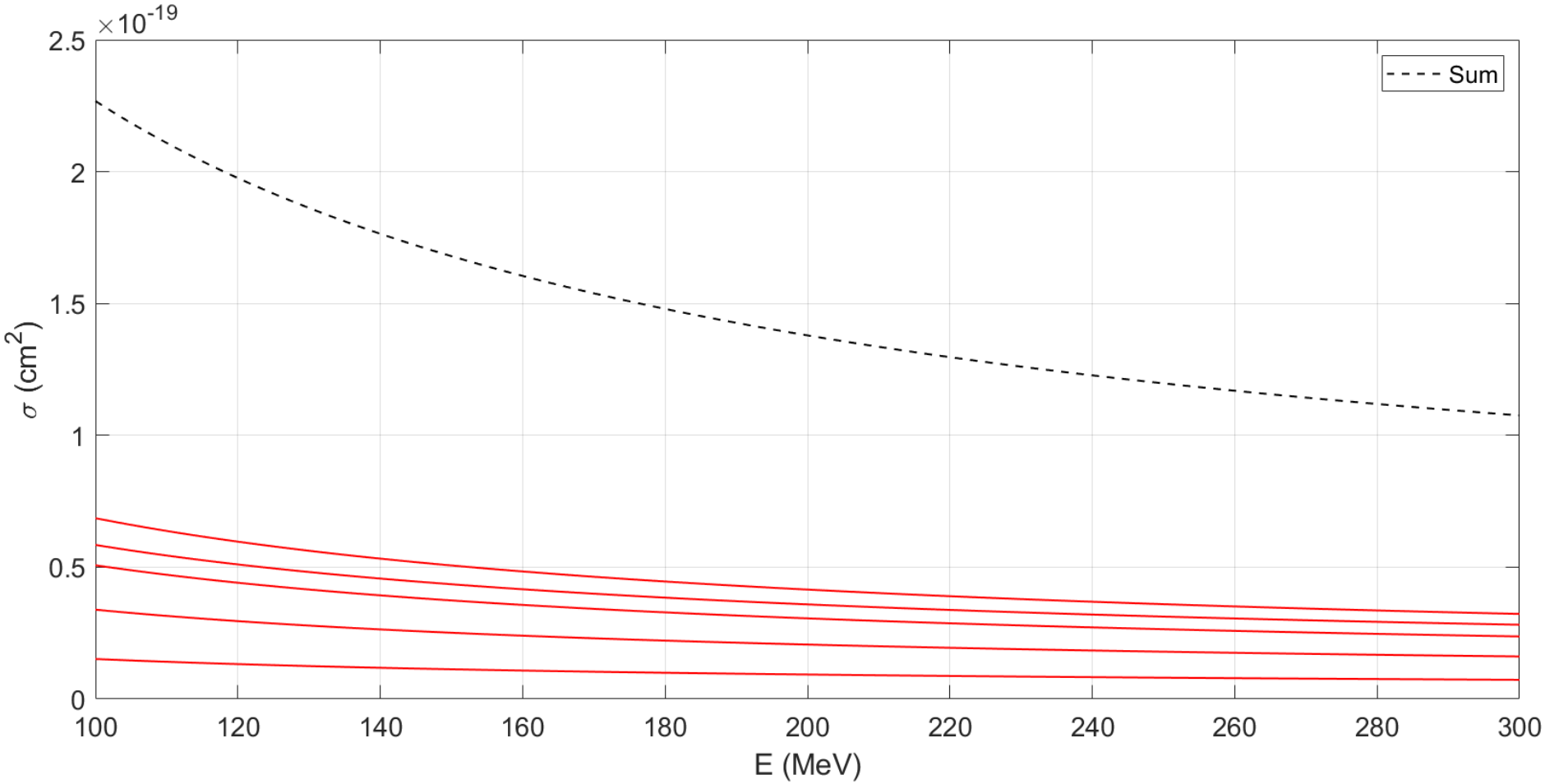
Transition	Discrete energy (eV)
(A^1B_1)	8.10
(B^1A_1)	10.10
(Ryd A+B)	12.00
(Ryd C+D)	13.51
(Diffuse bands)	14.41

Model database

Excitation CS

New data file!!

sigma_excitation_p_RPWBA



Model implementation

G4DNARPWBAIonisationModel.cc

Models

G4DNARPWBAExcitationModel.cc

Processes

G4DNAIonisation.cc

```
else if(name == "proton")
{
  if(!EmModel(0)) // MK: Is this a correct test ?
  {
    G4DNAMillerGreenExcitationModel* miller =
        new G4DNAMillerGreenExcitationModel();
    SetEmModel(miller);
    miller->SetLowEnergyLimit(10 * eV);
    miller->SetHighEnergyLimit(500 * keV);

    G4DNABornExcitationModel* born = new G4DNABornExcitationModel();
    SetEmModel(born);
    born->SetLowEnergyLimit(500 * keV);
    born->SetHighEnergyLimit(100 * MeV);

    G4DNARPWBAExcitationModel* RPWBA = new G4DNARPWBAExcitationModel();
    SetEmModel(RPWBA);
    RPWBA->SetLowEnergyLimit(100 * MeV);
    RPWBA->SetHighEnergyLimit(300 * MeV);
  }
```

G4DNAExcitation.cc

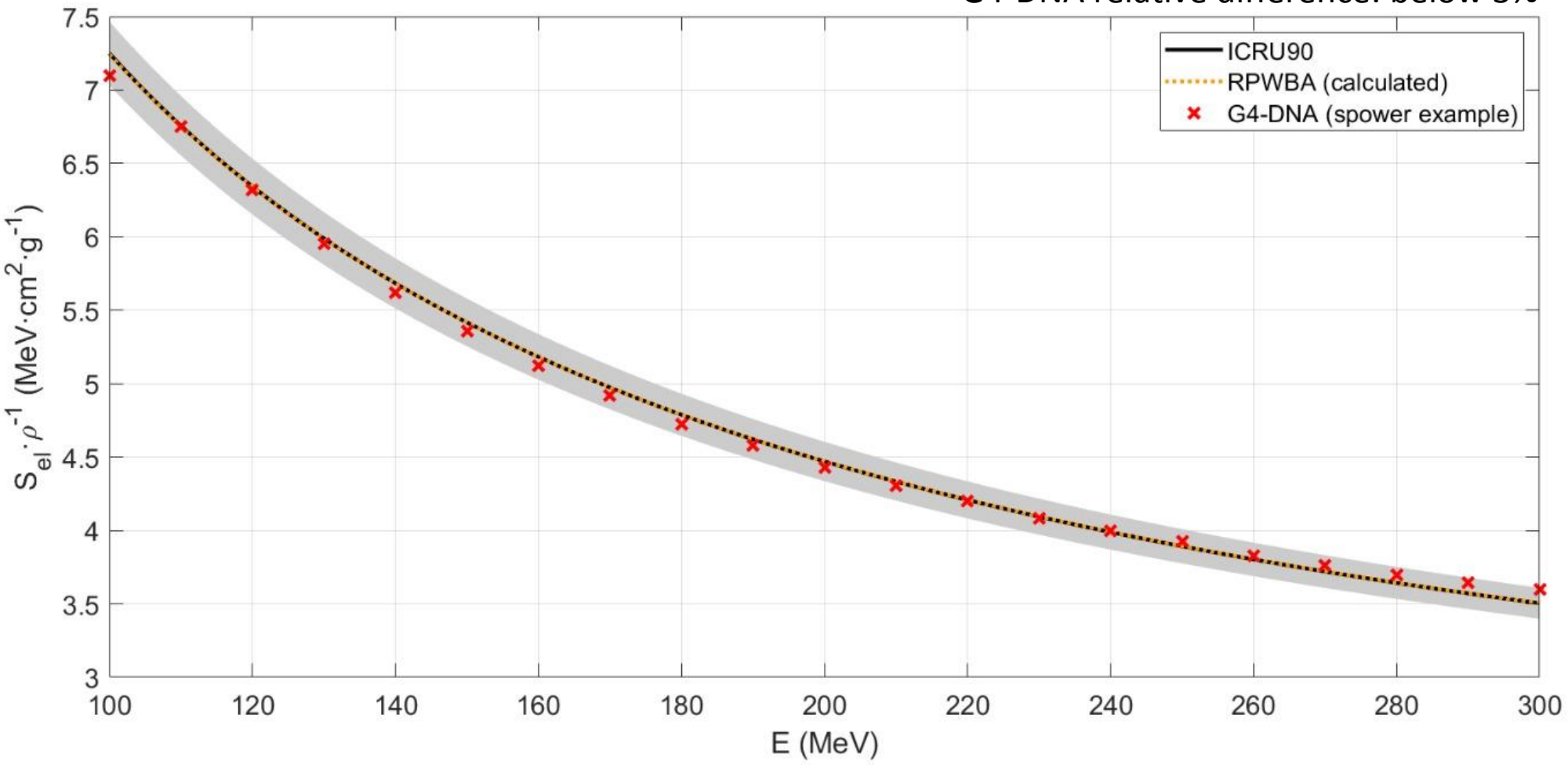
```
else if(name == "proton")
{
  if(!EmModel(0)) // MK: Is this a correct test ?
  {
    G4DNAMillerGreenExcitationModel* miller =
        new G4DNAMillerGreenExcitationModel();
    SetEmModel(miller);
    miller->SetLowEnergyLimit(10 * eV);
    miller->SetHighEnergyLimit(500 * keV);

    G4DNABornExcitationModel* born = new G4DNABornExcitationModel();
    SetEmModel(born);
    born->SetLowEnergyLimit(500 * keV);
    born->SetHighEnergyLimit(100 * MeV);

    G4DNARPWBAExcitationModel* RPWBA = new G4DNARPWBAExcitationModel();
    SetEmModel(RPWBA);
    RPWBA->SetLowEnergyLimit(100 * MeV);
    RPWBA->SetHighEnergyLimit(300 * MeV);
  }
```

Validation

Stopping power

Reference data: ICRU90

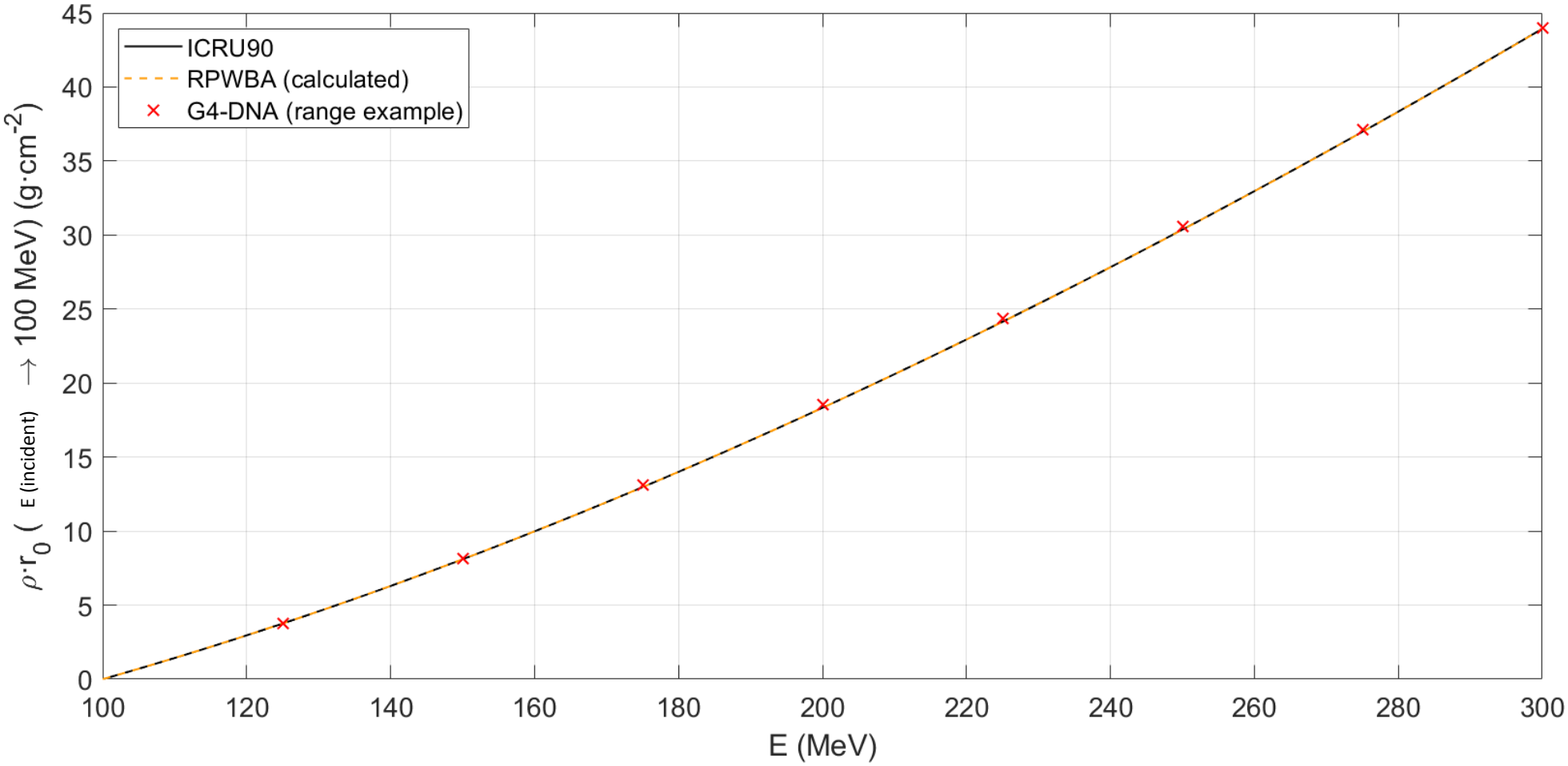
ICRU90 data uncertainty: 3% (shaded region)
RPWBA relative difference: below 0.1%
G4-DNA relative difference: below 3%



Validation

Range

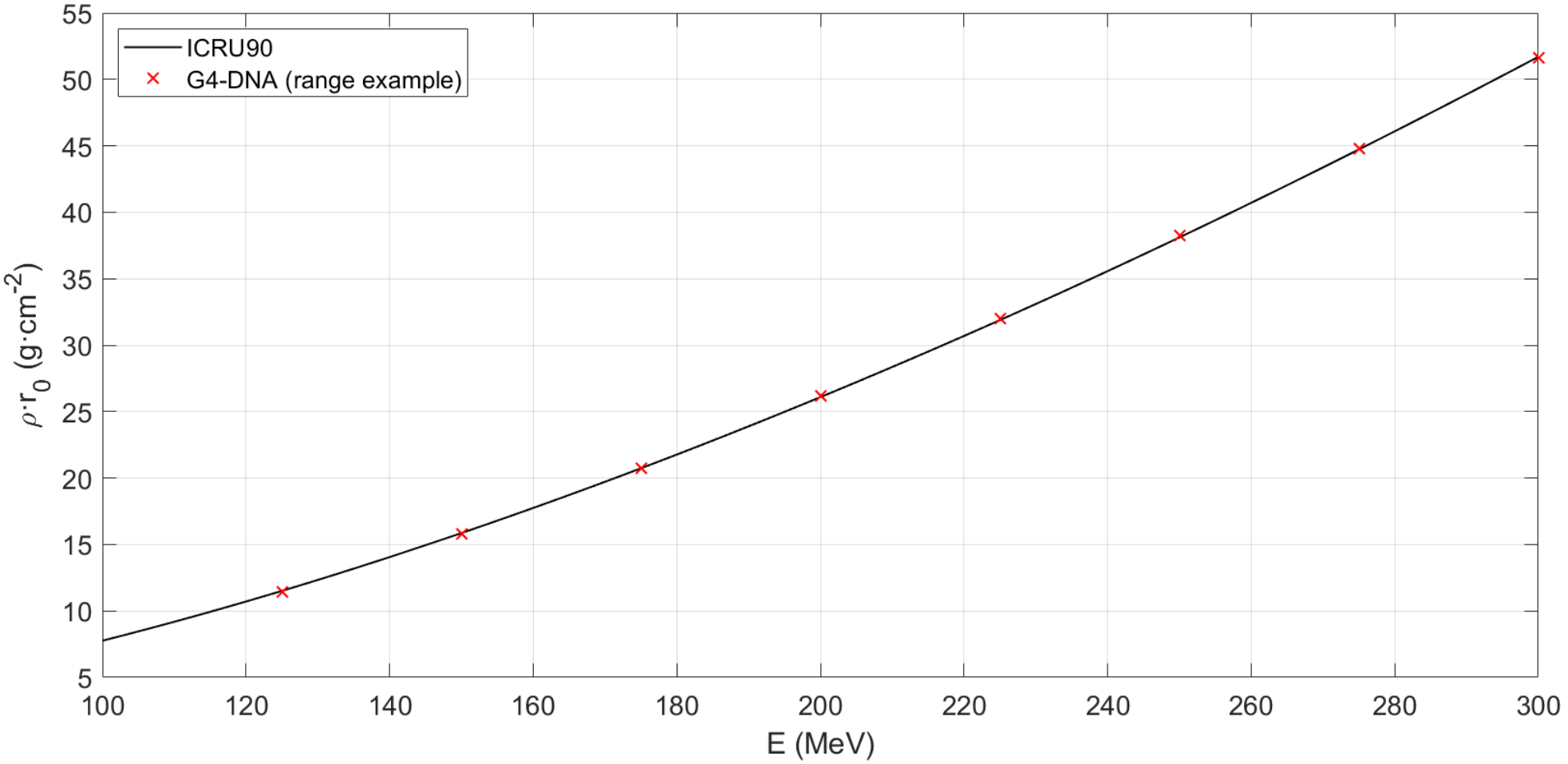
Reference data: ICRU90



Validation

Range

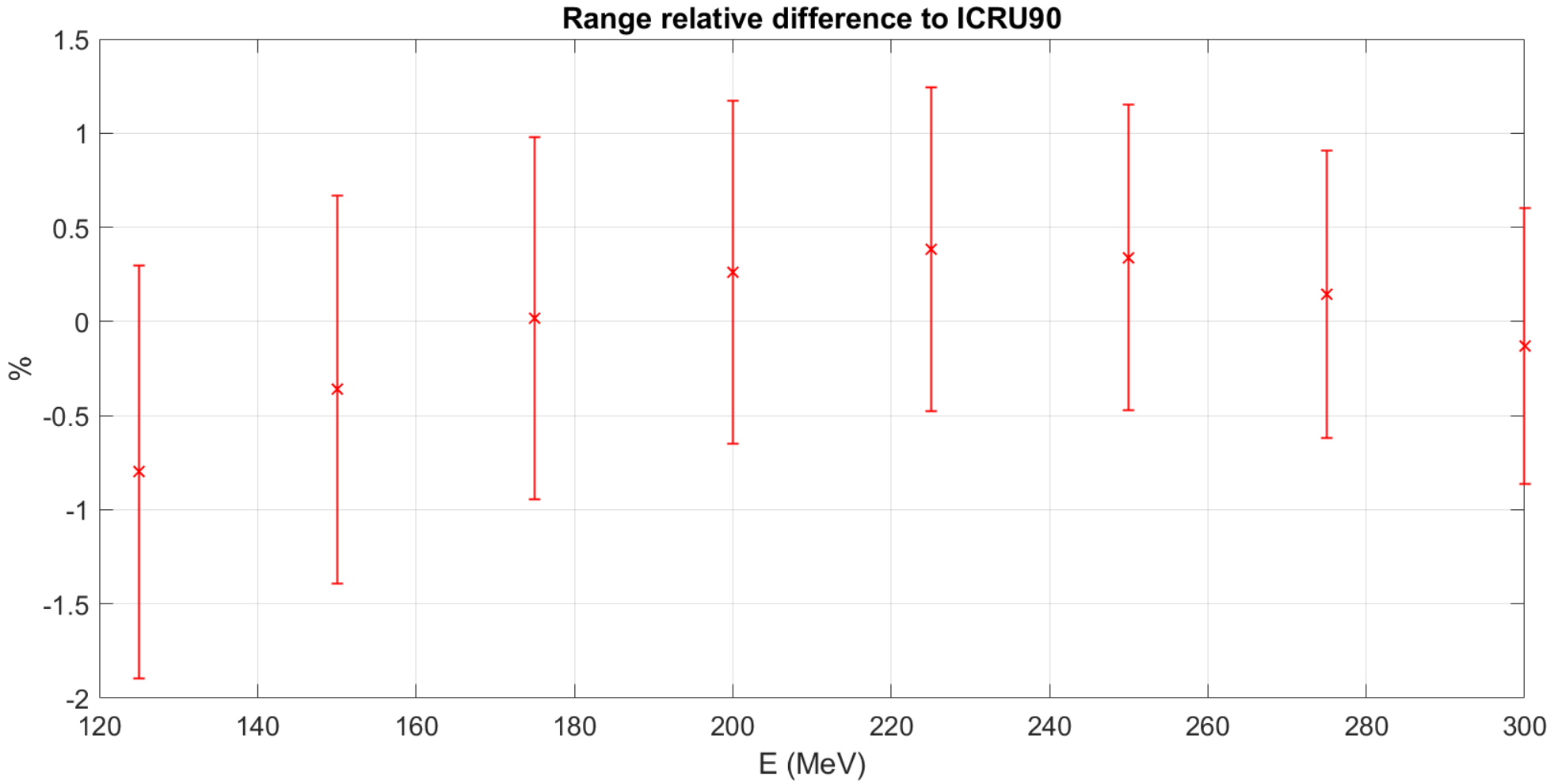
Reference data: ICRU90



Validation

Range

Reference data: ICRU90



Conclusions

- RPWBA theory separates projectile and target contributions to DDCS.
- GOS characterizes the response of the material. Liquid water GOS model used contains 5 excitation levels and 5 ionization shells.
- Database for proton ionization and excitation is obtained integrating the doubly-differential cross section for each shell/level contained in water liquid GOS.
- Two new model classes, one for ionization and other for excitation, are created and included in the corresponding processes between 100 MeV and 300 MeV.
- Validation of the model and the implementation is made comparing with stopping power and range data of ICRU90. Results are in good agreement.