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Accelerator Physics Center

Modified Moliere's Screening Parameter and its Impact on Calculation of Radiation Damage

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OUTLINE

- Models of elastic Coulomb scattering
- Screening parameter in Hartree-Fock model
- Correction to Born approximation
- Comparison with other calculations
- Conclusion

Models of Elastic Coulomb scattering

- At energies below 10 MeV, Coulomb interactions dominate the production of displaced atoms from their lattice sites
- For protons classical mechanics approach can be used at energies $< Z/10$ MeV
- Quantum-mechanical description of elastic scattering including a relativistic treatment is also available
- Classical and quantum mechanics provide similar results at energies $> Z/10$ MeV where relativistic and spin effects do not matter

Models of Elastic Coulomb scattering-II

- IOTA code (Konobeyev et al), NASA SEE and SET programs (Jun et al) - energy-transfer differential cross section based on Lindhard, Nielsen, Scharff "Approximation method in classical scattering by screened coulomb field". This approach was applied to Tomas-Fermi potential. Reduced scattering cross section was obtained as a function of a single scattering parameter.
- At large momentum transfer this cross section has same behavior as Rutherford cross section - cross section for scattering on unscreened Coulomb potential

Models of Elastic Coulomb scattering-III

- G4 code (Boschini et al) - Wentzel-Moliere treatment of single scattering

$$\frac{d\sigma^{WM}}{dT} = 2\pi \left(\frac{zZe^2}{\beta} \right)^2 \frac{1}{(T + p^2 \chi_a^2 / (2M))^2}$$

χ_a^2 - Moliere screening parameter. T, Z and M energy, charge and mass of recoil nuclei. z, p and β - charge, momentum and velocity of projectile

Models of Elastic Coulomb scattering-IV

MARS code - Wentzel-Moliere formula with spin correction and nuclear screening

$$\frac{d\sigma}{dT} = \frac{d\sigma^{WM}}{dT} R_M(T) F_n(q)$$

R_M - Mott spin correction. F_n - nuclear form factor squared, q - momentum transfer.

Screening parameter in Hartree-Fock model

Moliere calculated the screening angle using Thomas-Fermi model. Since the Thomas-Fermi model is statistical, for light element it cannot provide a high accuracy of calculation. More precise results can be obtained within the Hartree-Fock approach. It takes into account individual properties of atoms—in particular, their shell structure. Salvat et al propose a simple analytical approximation for atomic screening function depending on five parameters which are determined from the results of Dirac-Hartree-Fock-Slater calculations

Screening parameter in Hartree-Fock model

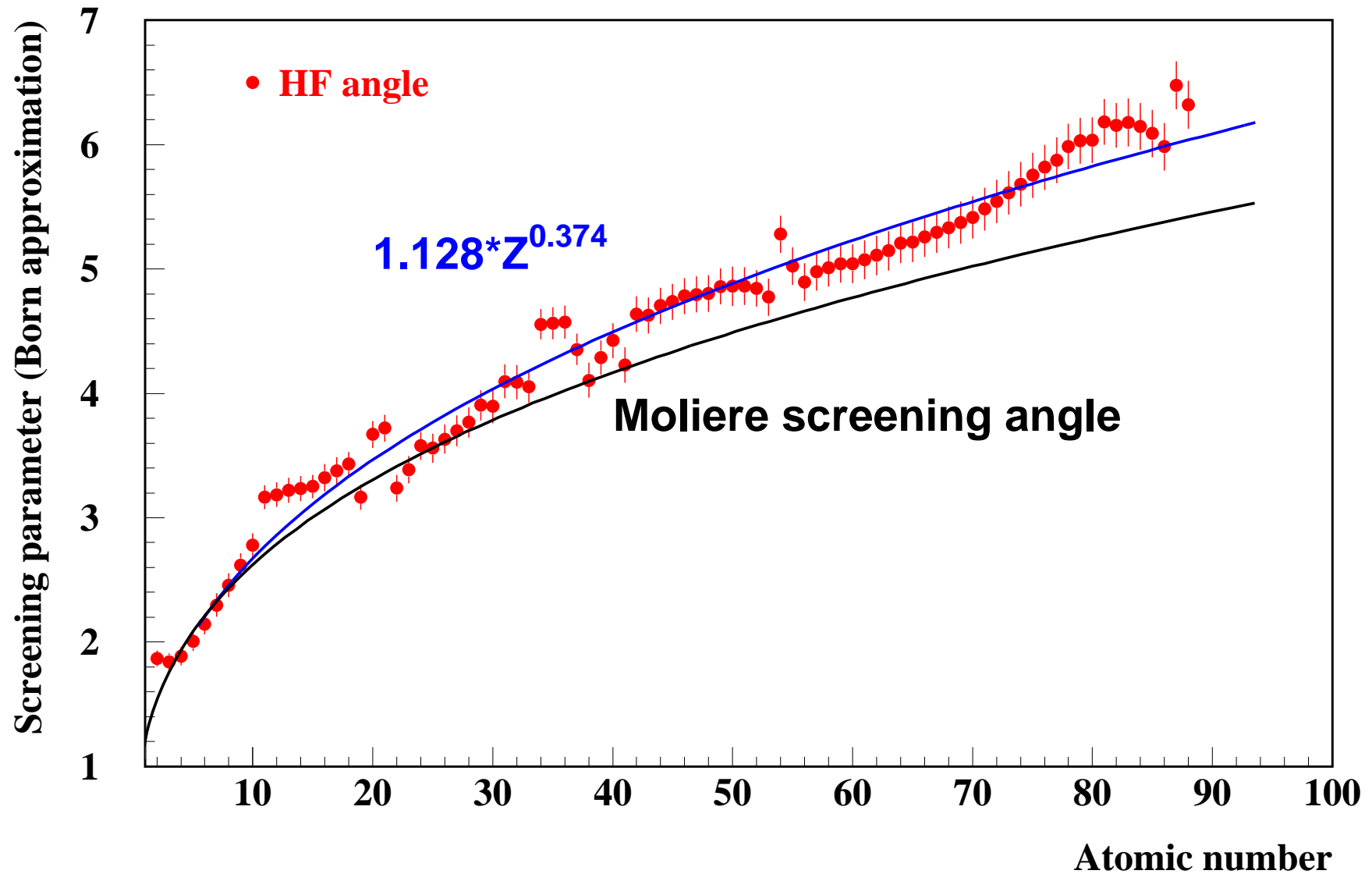
Salvat et al has approximated Hartree-Fock atomic form factor as

$$F_a(q) = \sum_{i=1}^3 A_i \alpha_i^2 / (\alpha_i^2 + q^2)$$

In Born approximation Moliere "screening angle" reads

$$\ln \chi_a = \ln(m_e \alpha / p) + \sum_{i=1}^3 A_i^2 (\ln \alpha_i - 0.5) + 2A_1 A_2 (\alpha_2^2 \ln \alpha_2 - \alpha_1^2 \ln \alpha_1) / (\alpha_2^2 - \alpha_1^2) + 2A_1 A_3 (\alpha_3^2 \ln \alpha_3 - \alpha_1^2 \ln \alpha_1) / (\alpha_3^2 - \alpha_1^2) + 2A_2 A_3 (\alpha_2^2 \ln \alpha_2 - \alpha_3^2 \ln \alpha_3) / (\alpha_2^2 - \alpha_3^2) - 0.5$$

Screening parameter in Hartree-Fock model



Correction to Born approximation

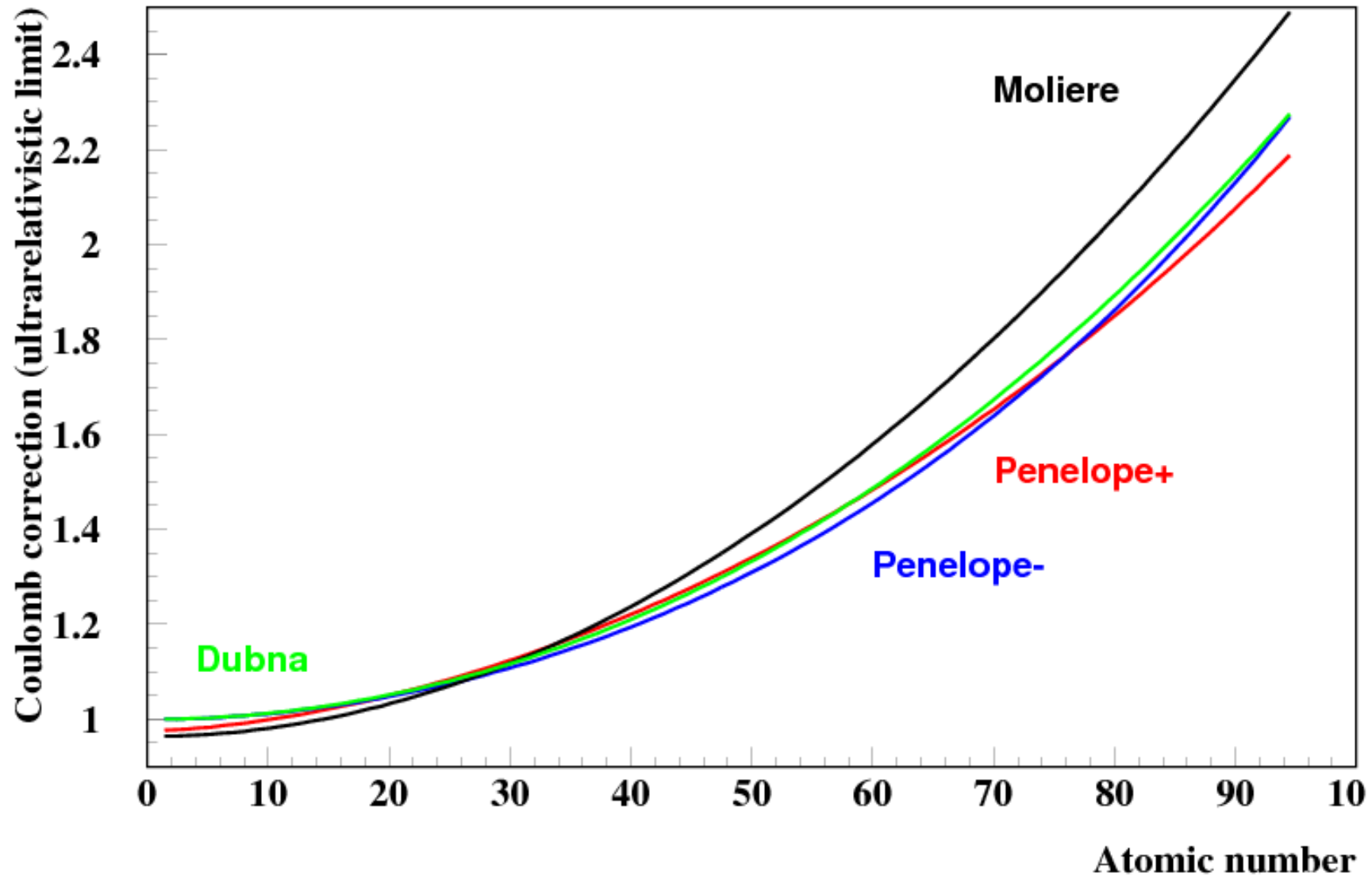
Coulomb correction is the difference between the values of parameters calculated in the eikonal approximation and in Born approximation. An exact formula for the differential cross section in terms of an integral is given in Moliere's paper, but his final evaluation of integral is numerical and only approximate. Recently, Kuraev et al (JINR, Dubna) have found exact solution in the ultra relativistic limit. Their result reveals significant deviation from Moliere's approximation for sufficiently heavy elements.

Correction to Born approximation - II

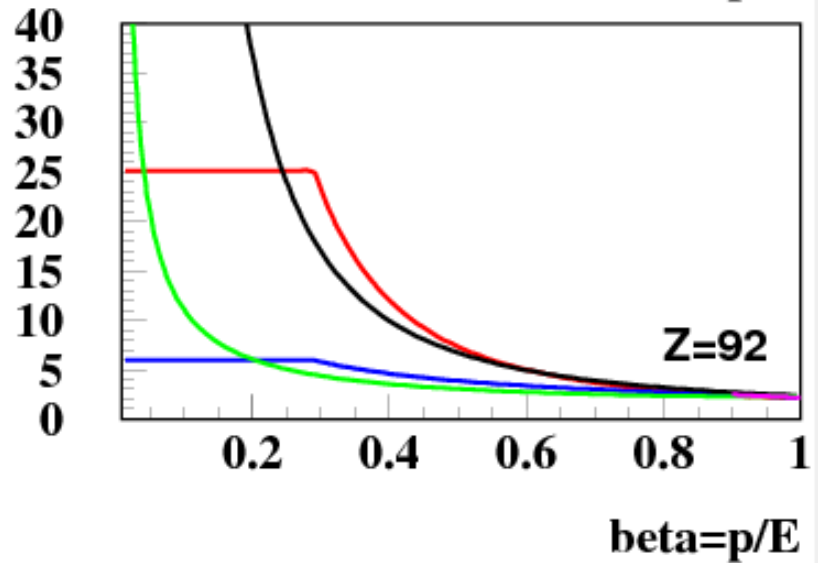
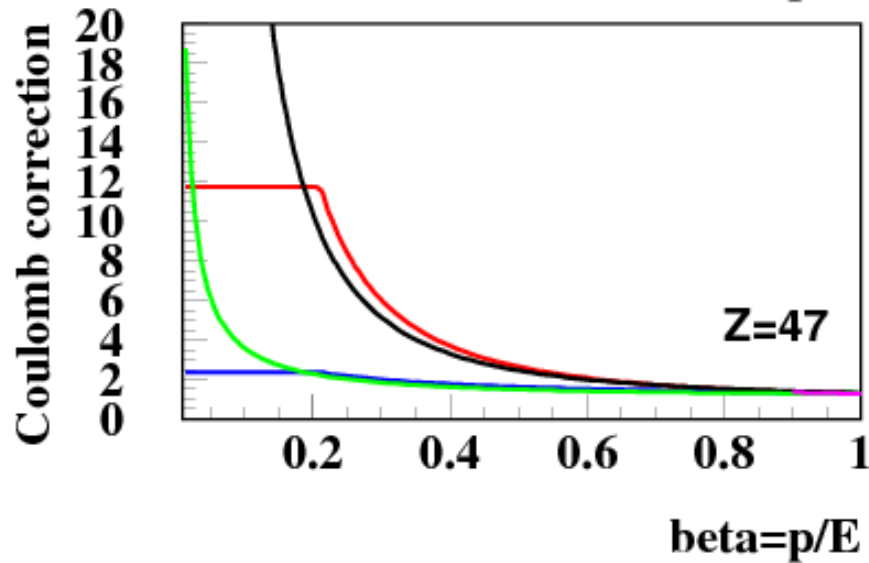
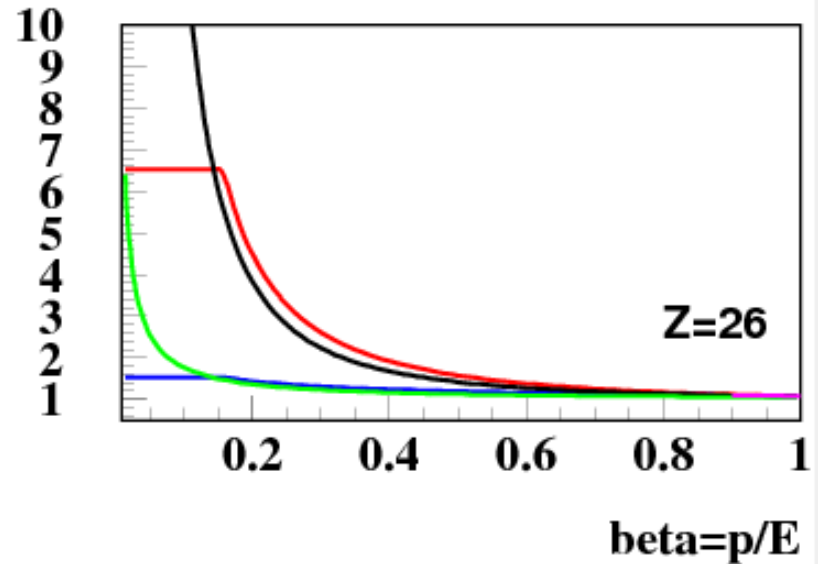
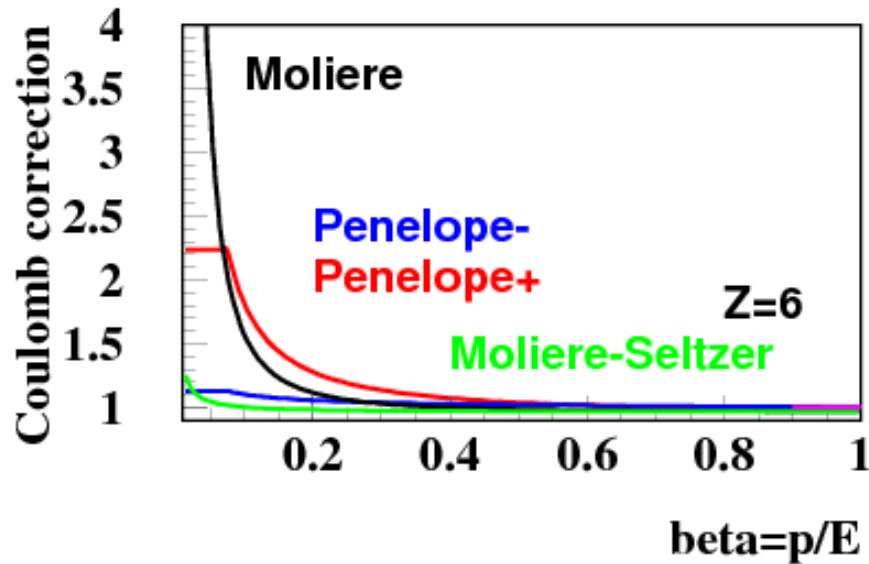
Fernandez-Varea et al proposed a precise form for elastic Coulomb scattering cross section based on Hartree-Fock atomic form factor for electron with energy $> Z$ keV correction. They introduced correction parameter to improve agreement with precise partial wave calculation. This cross section is used in popular PENELOPE code for simulation of multiple Coulomb scattering. We can use this parameter as another way of "practical estimate" of Coulomb correction.

For electron energies less than Z keV, accuracy of correction progressively deteriorates. Correction parameter still yields accurate results if kinetic energy $E_c = 0.25Z$ keV is used, when $E < E_c$

Correction to Born approximation: ultrarelativistic case



Correction to Born approximation: energy dependence

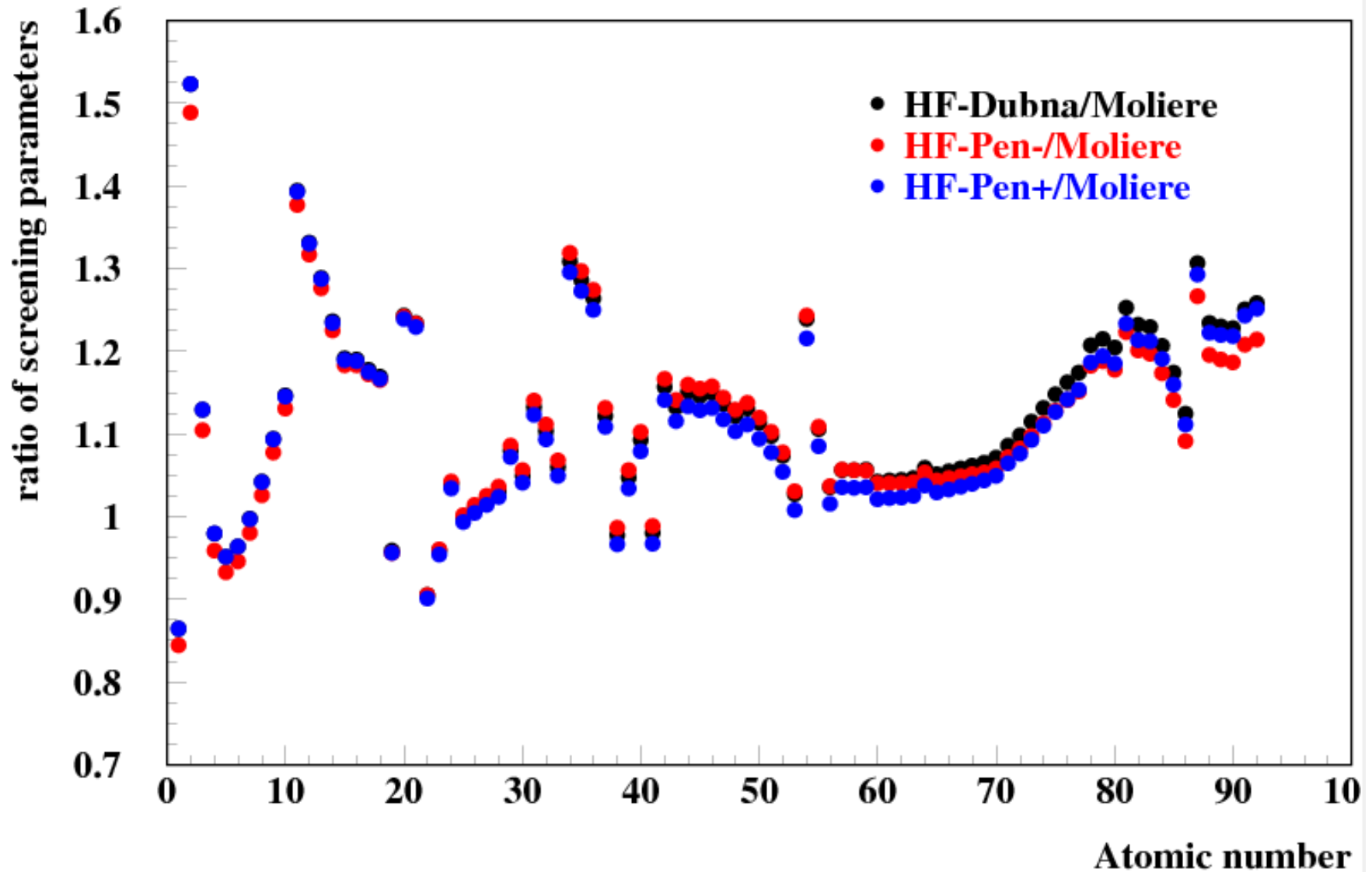


Correction to Born approximation

Recently, Salvat presented computer code for calculation Coulomb elastic scattering of protons with energies 10 keV-10 GeV. Elastic collisions are described in terms of numerical differential cross sections, calculated from eikonal approximation with Dirac-Hartree-Fock-Slater atomic potential (NIM B316 (2013) 144-159).

So, we'll obtain soon tool to check energy dependence of screening based on rigorous calculation.

Screening parameters: ultrarelativistic case



Comparison with other calculation

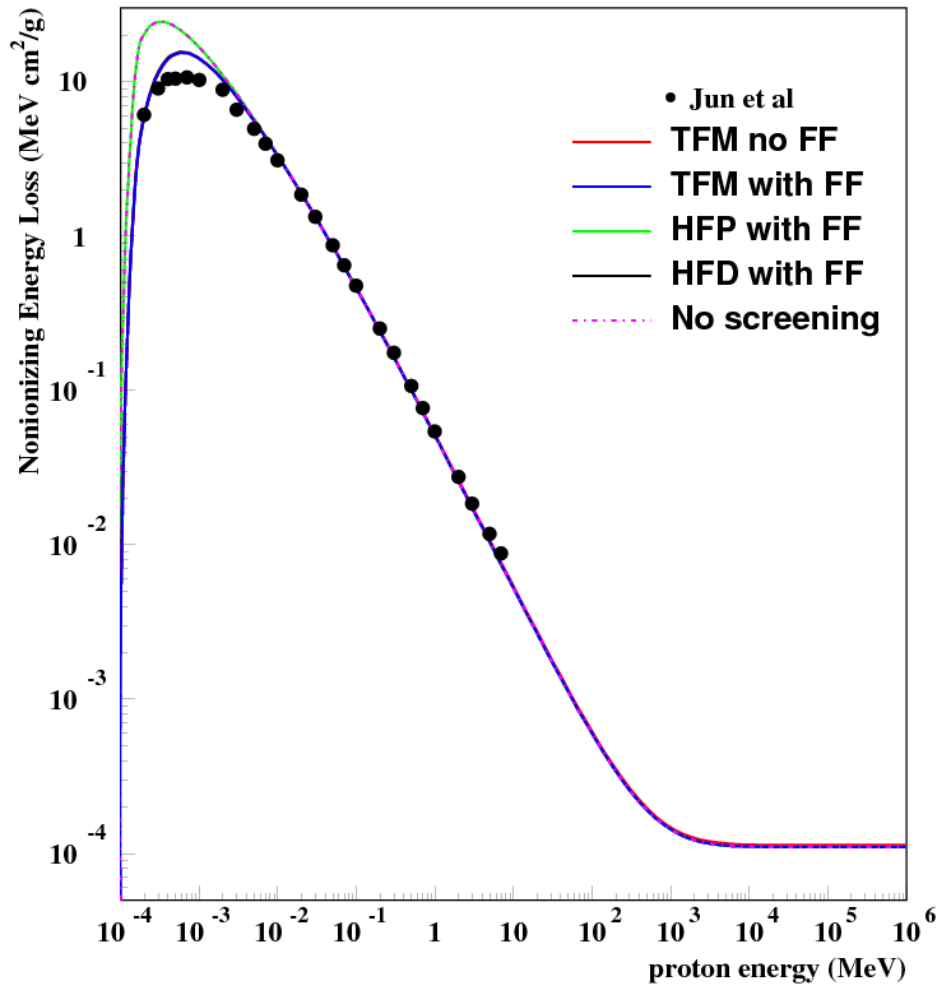
We are going to compare calculation Non-Ionizing Energy-Loss (NIEL) and dpa using:

- classical approach: NASA team - Jun et al and IOTA code - Konobeyev et al
- quantum-mechanics Tomas-Fermi-Moliere approach - G4 team - Boschini et al

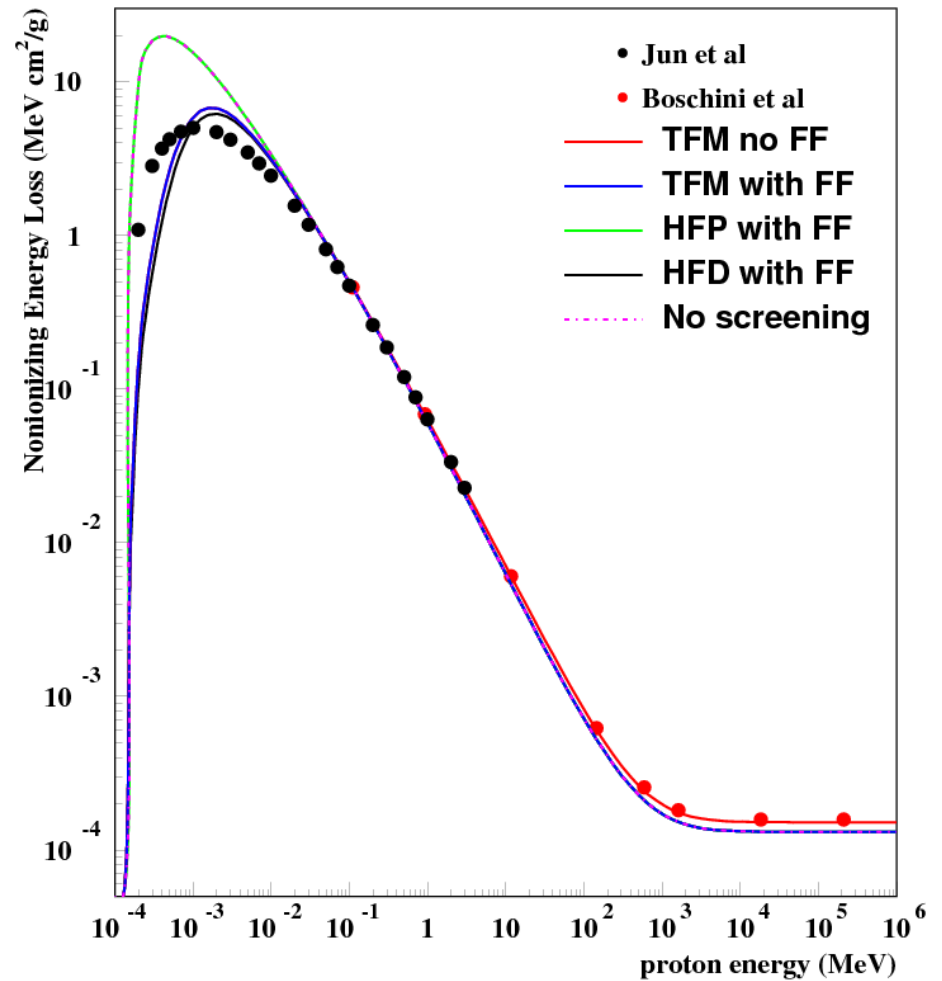
With our quantum-mechanics calculation:

- Tomas-Fermi-Moliere-Mott + nuclear screening - **TFM**: Moliere screening parameter
- Hartree-Fock-Penelope-Mott + nuclear screening - **HFP**: Hartree-Fock screening parameter in Born approximation. Penelopa "practical correction" at low energies
- Hartree-Fock-Moliere-Dubna-Mott + nuclear screening - **HFD**: Hartree-Fock screening parameter in Born approximation. Dubna Coulomb correction at ultrarelativistic energies. Moliere Coulomb correction at low energies.

Comparison with other calculation: NIEL

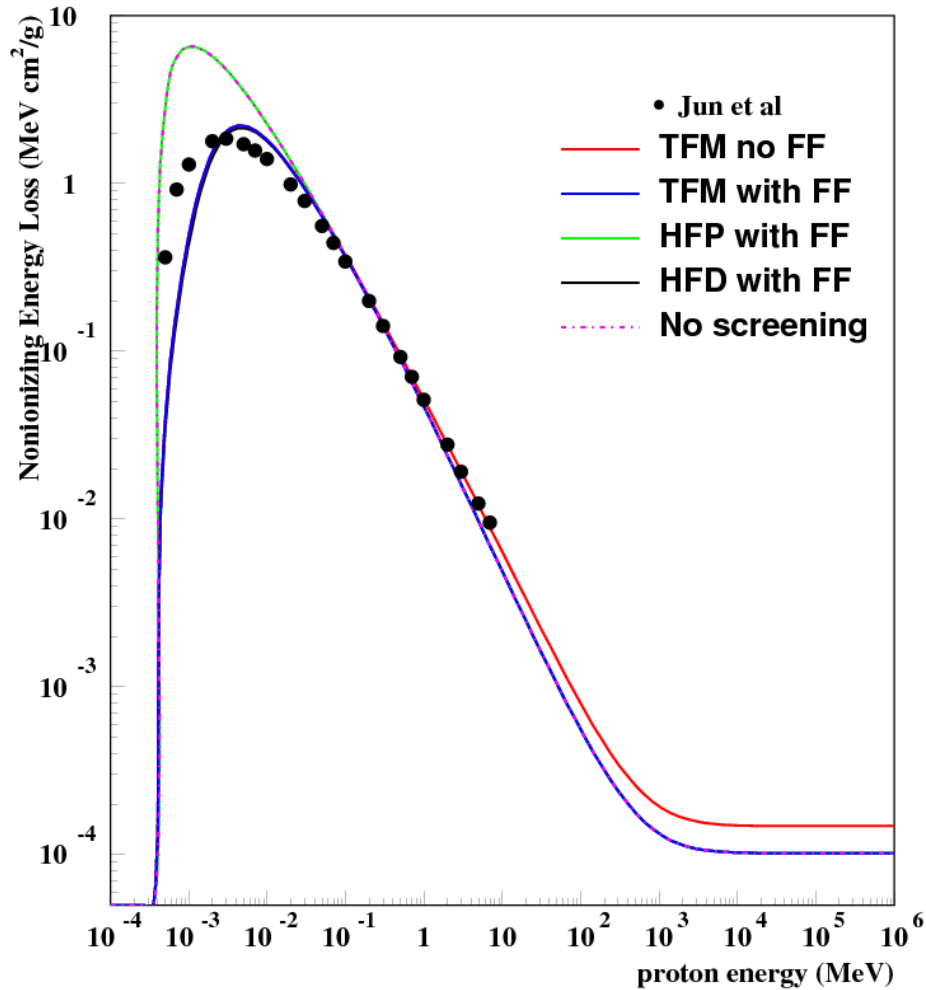


Proton NIEL for carbon due the Coulomb scattering

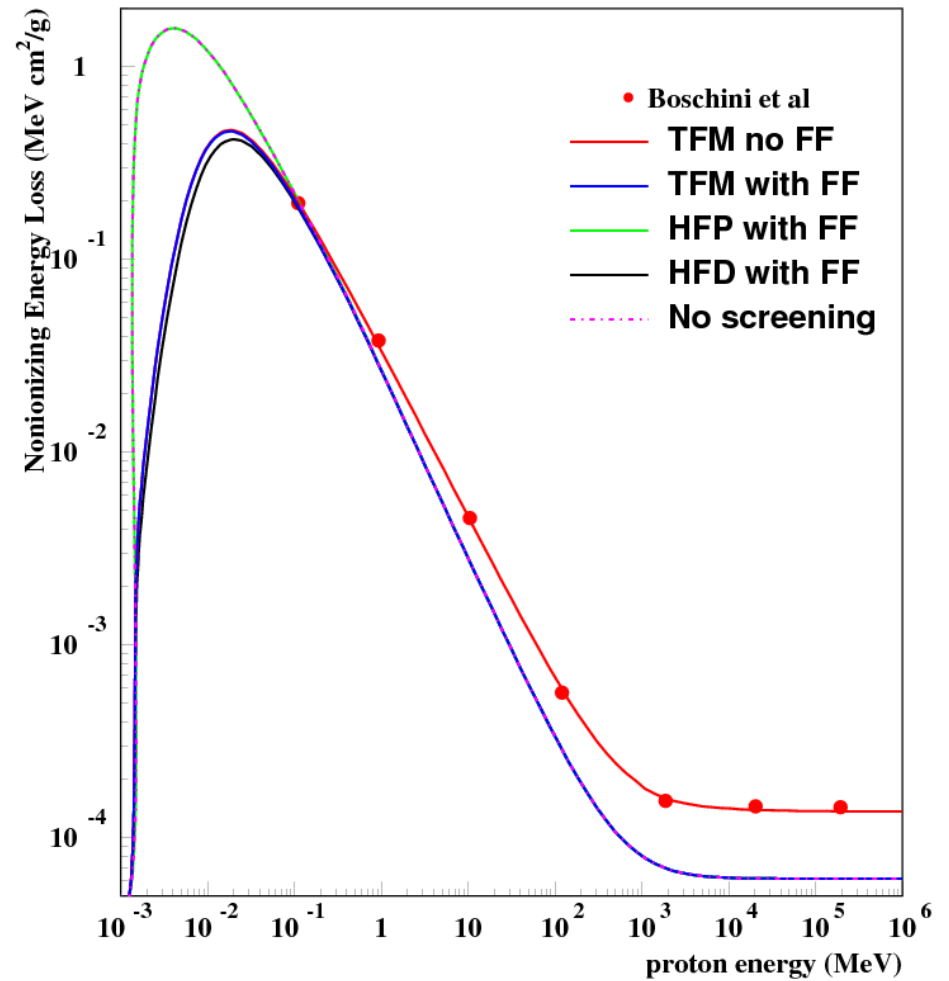


Proton NIEL for silicon due the Coulomb scattering

Comparison with other calculation: NIEL

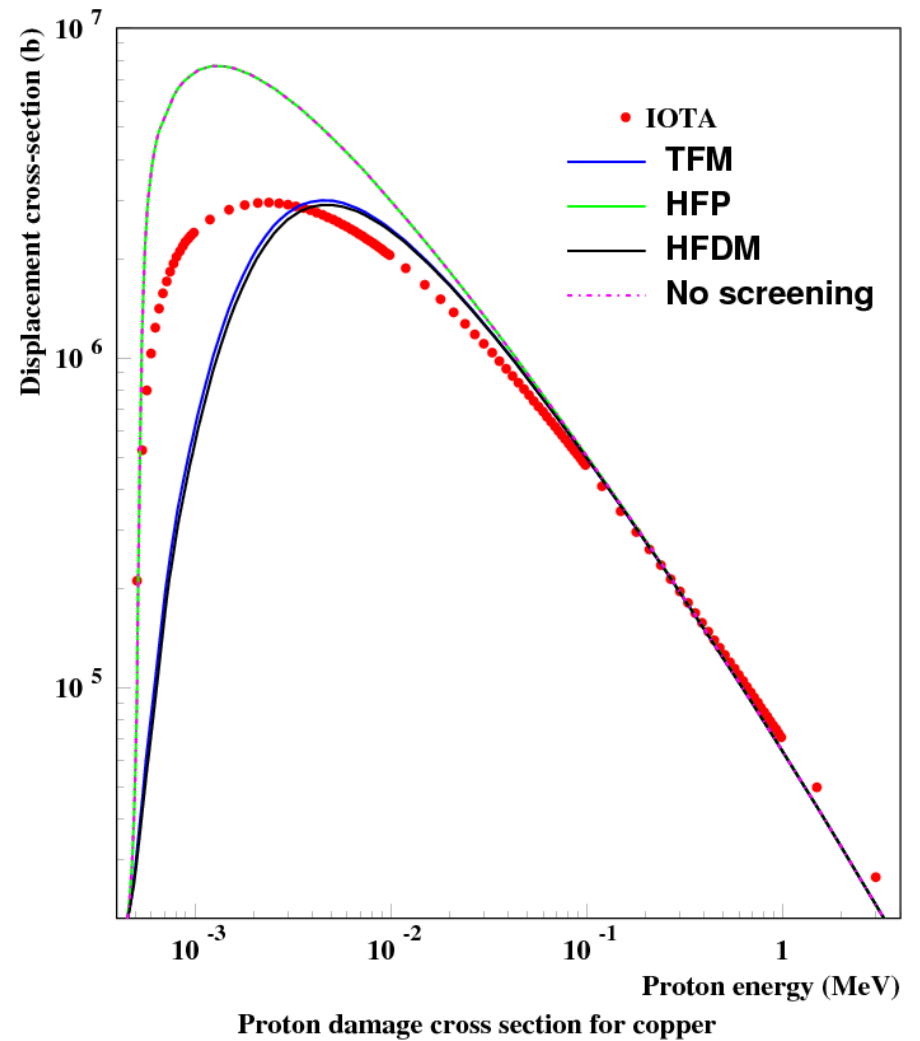
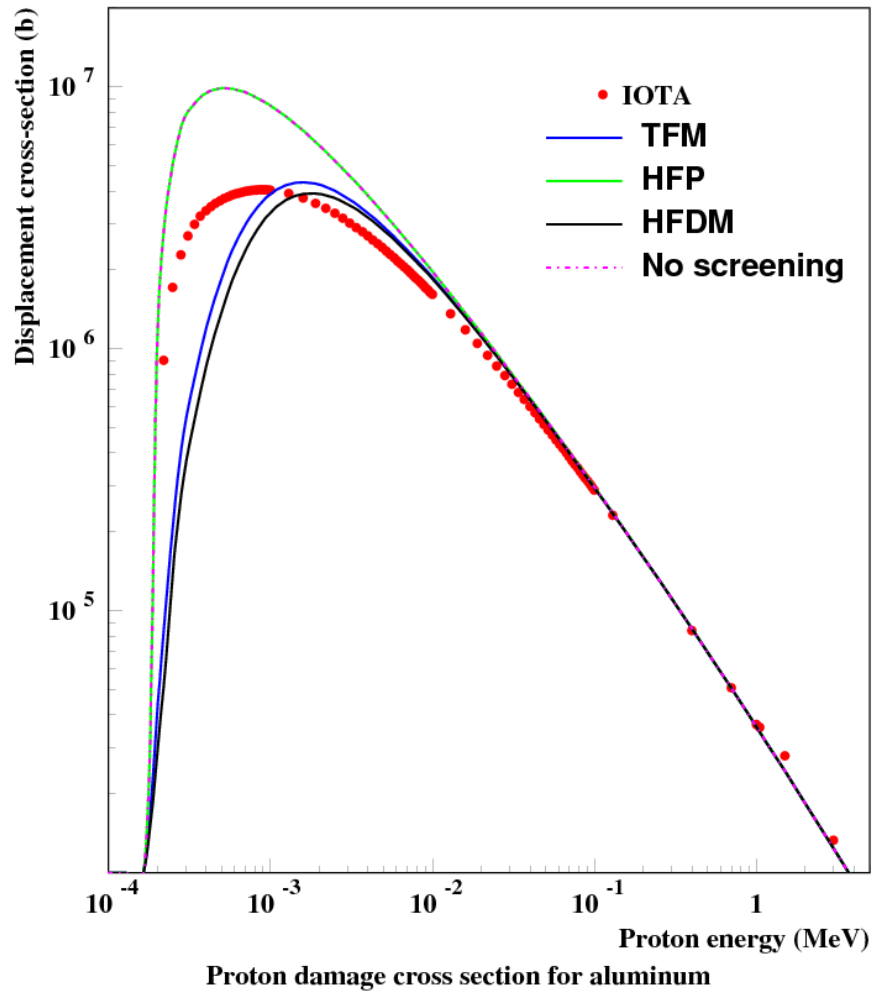


Proton NIEL for copper due the Coulomb scattering



Proton NIEL for lead due the Coulomb scattering

Comparison with other calculation - dpa



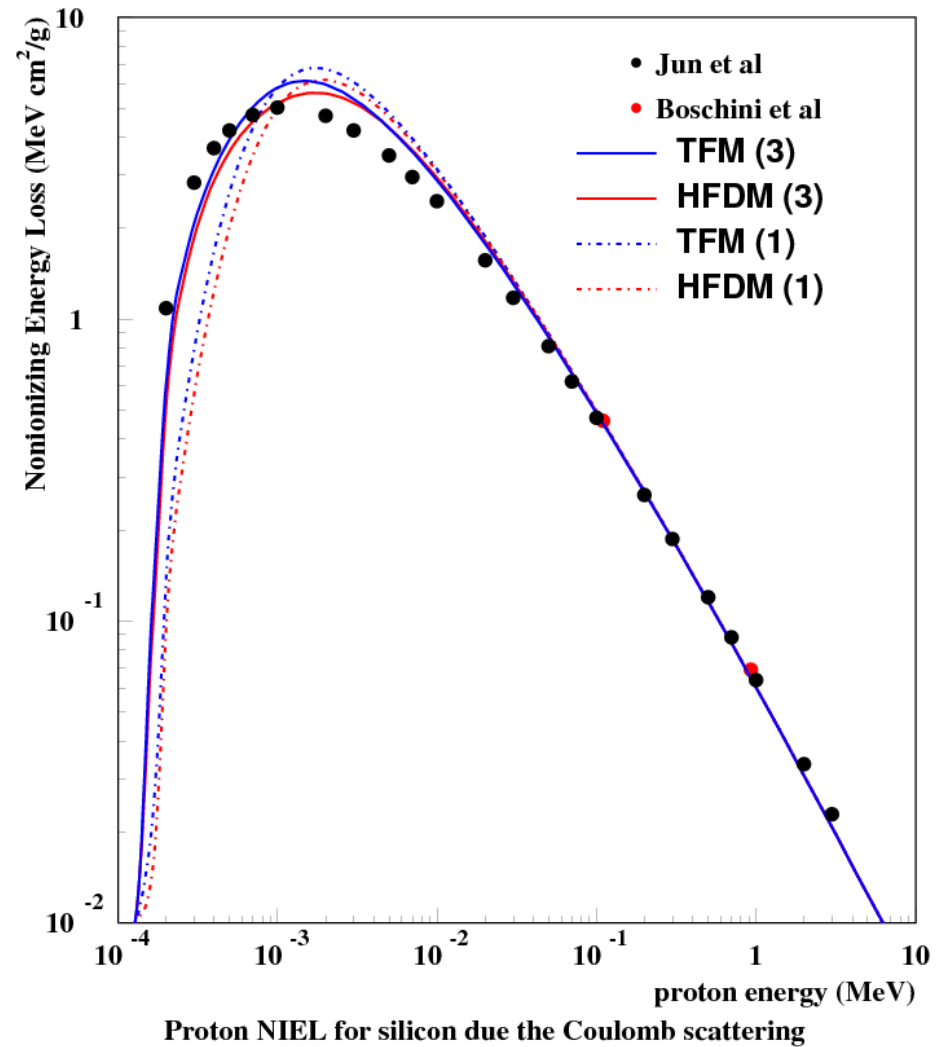
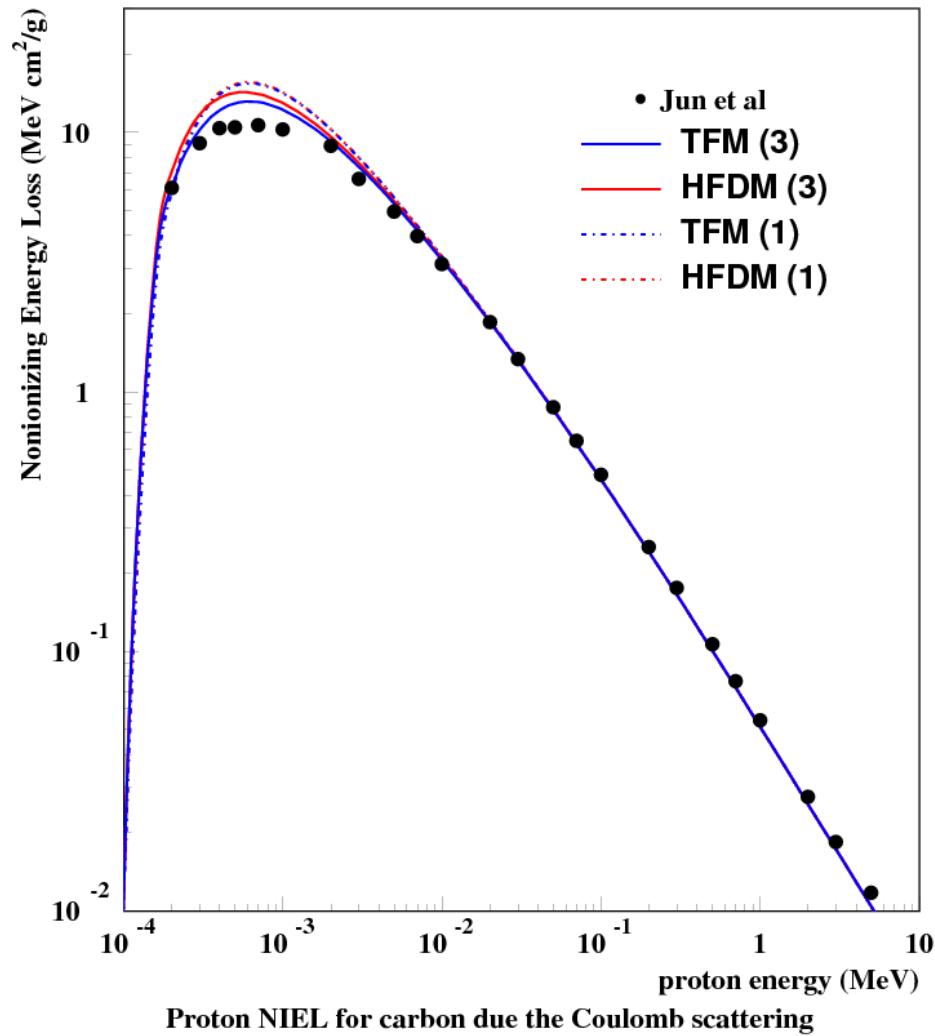
Full form factor against Moliere approximation

Moliere approximation - using one dipole term instead full form factor appears to be very useful to obtain analytical approximation of angular distribution due to multiple Coulomb scattering.

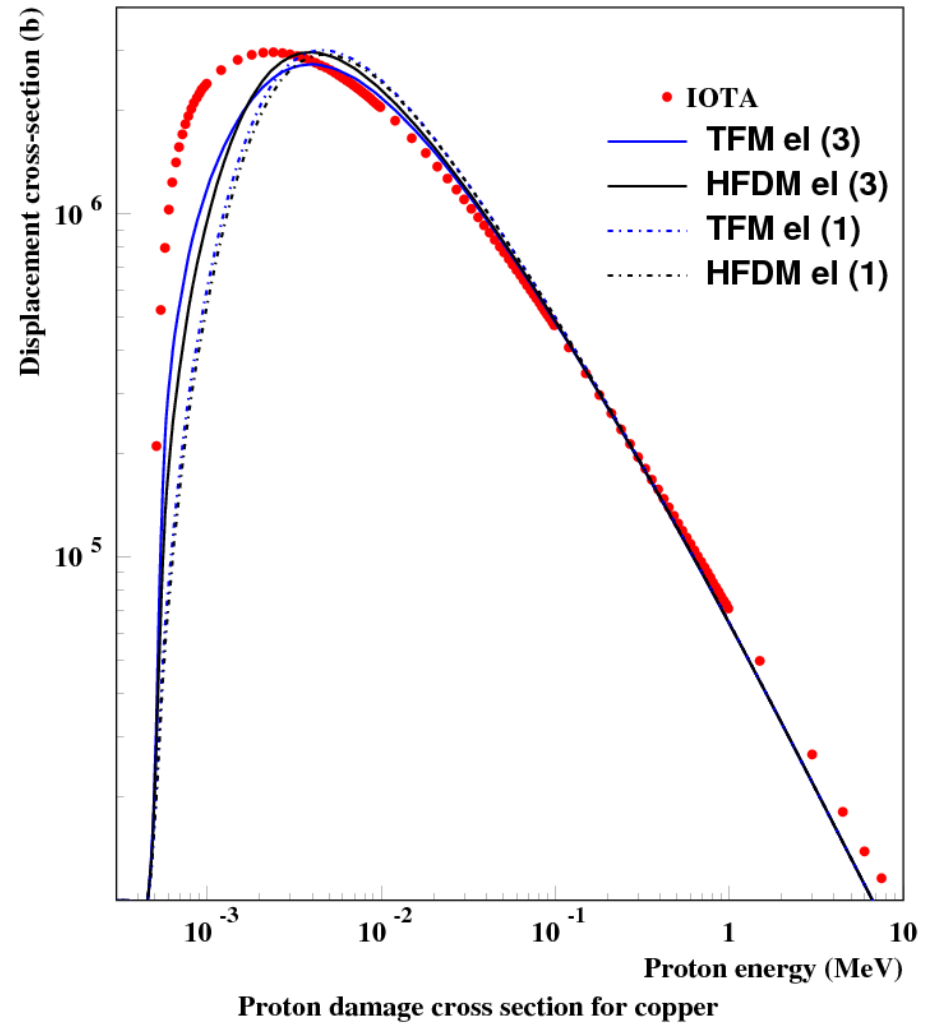
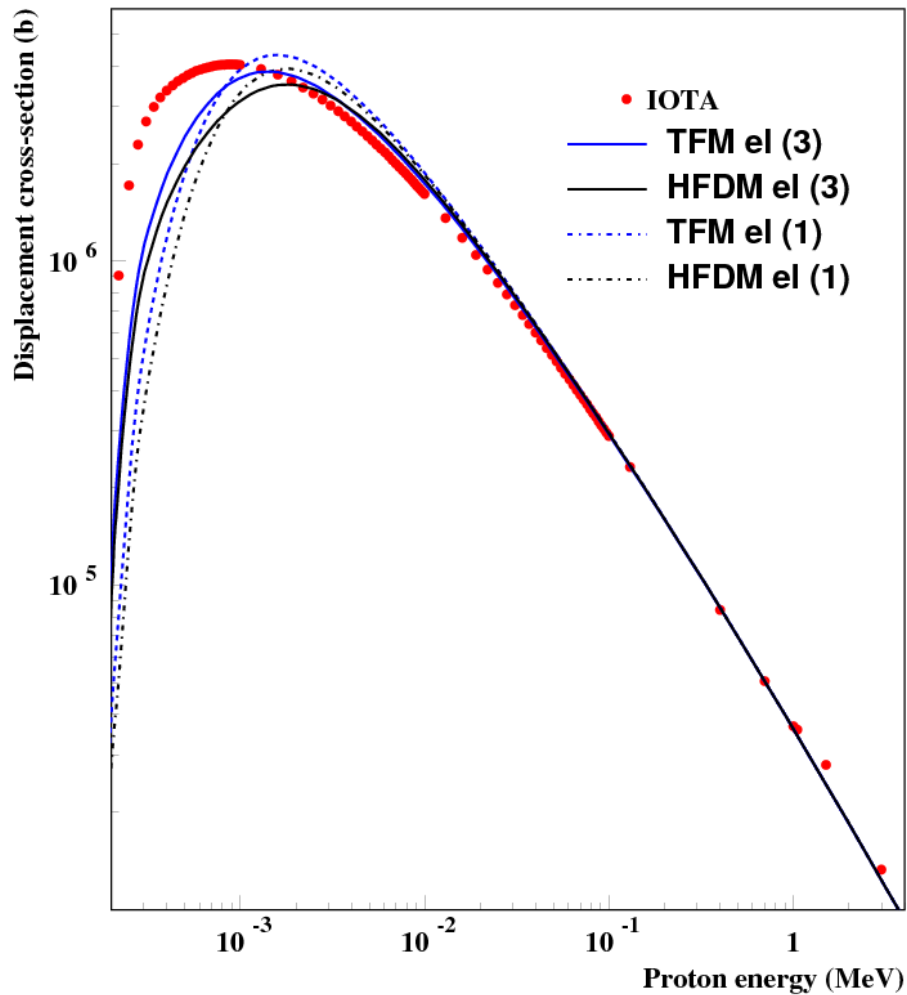
In calculation of radiation damage we do not radically simplify procedure by using Moliere's approximation, but can lose precision.

Let's compare NIEL and dpa obtained by integration Moliere's dipole approximation and more precise cross section including all 3 terms in form factor description.

Full form factor against Moliere approximation

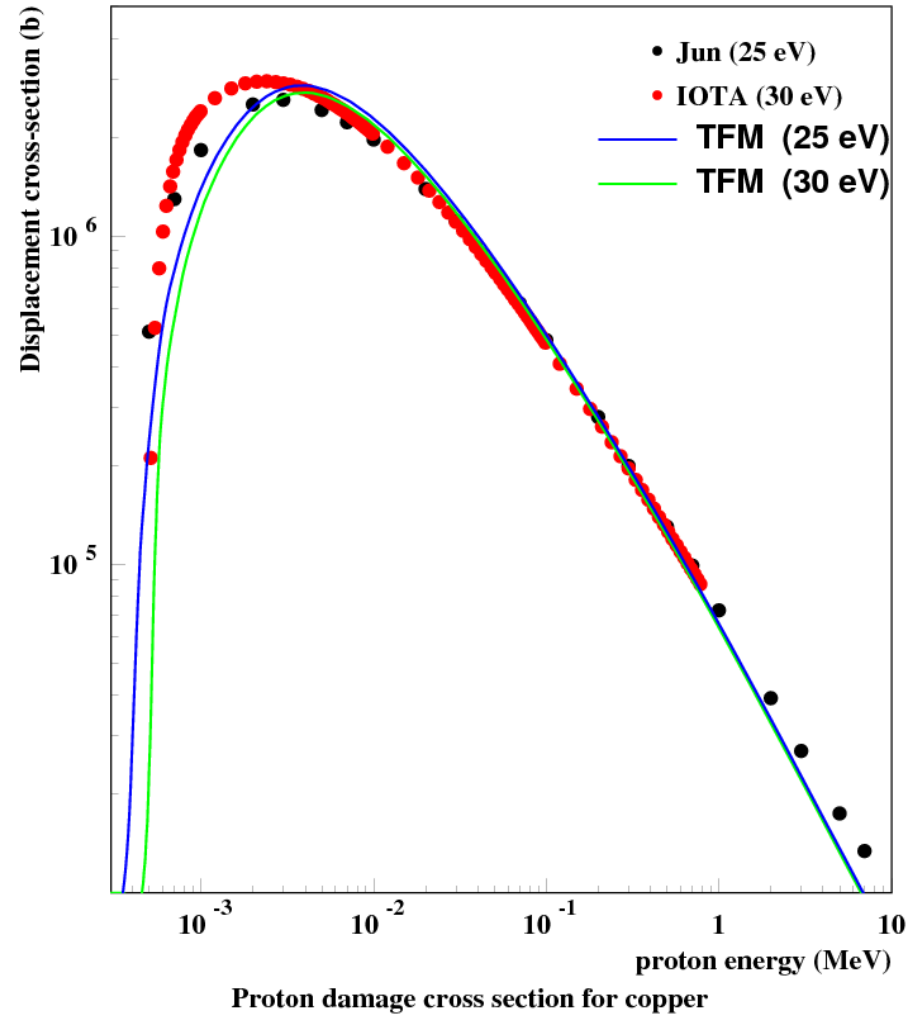
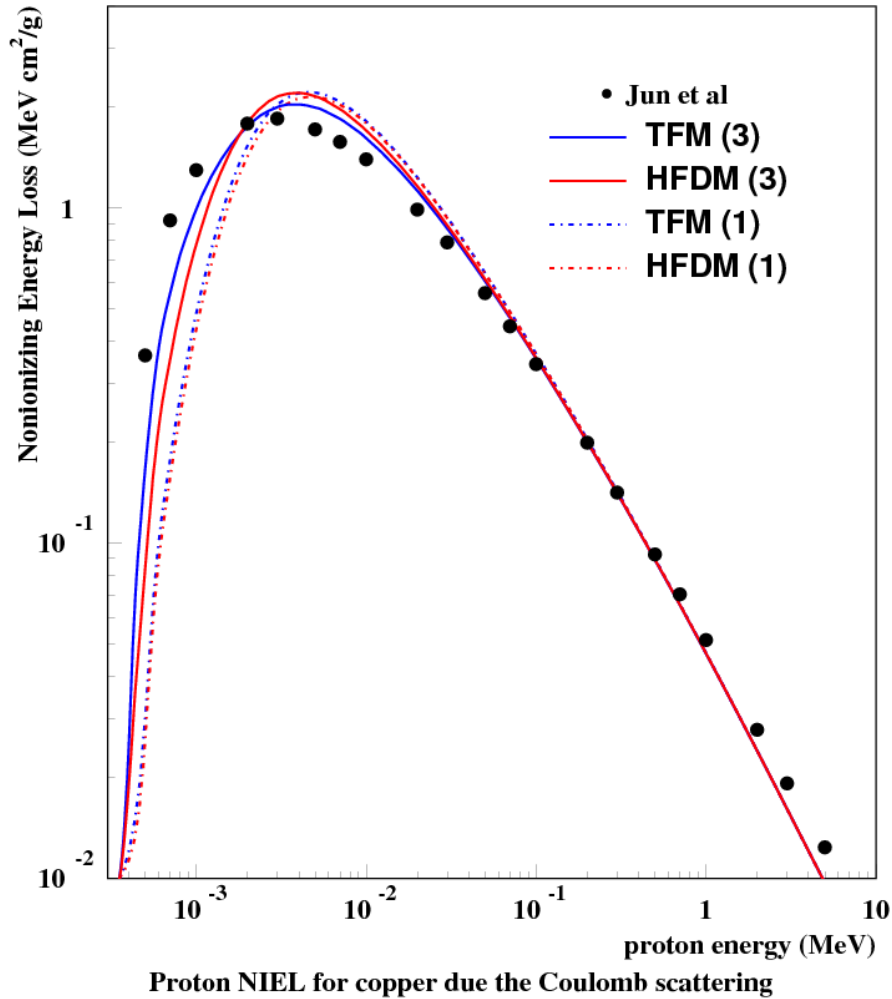


Full form factor against Moliere approximation



Full form factor against Moliere approximation

Jun(25eV) > IOTA(30eV)?
Different atomic screening?



Conclusions

Calculations of NIEL and dpa based on classical and quantum mechanic approaches are in reasonable agreement for protons with energy larger than few keV

Calculations of NIEL and dpa are not very sensitive to atomic screening model. Energy dependence of screening parameter looks like much more important

Calculation of NIEL and dpa using precise description of atomic form factor improve precision at very low proton energies

Including of nuclear form factor significantly decreases calculated NIEL and dpa, especially for heavy nucleus

Comparison of Moliere's differential cross section with results of recently developed code (Salvat 2013) at low energies will be interesting