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GEANT4 SIMULATION OF ENERGY LOSSES OF IONS

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Abstract

The algorithm for the simulation of energy losses of heavy ions is described. The details of its implementation in Geant4 are discussed. The comparison of the simulation results with the experimental data is presented.

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1 Introduction

GEANT4[1] is a toolkit for Monte Carlo particle transport simulation for a wide range of applications, based on the Object Oriented technology. The GEANT4 model of electromagnetic interaction of protons with matter at low energies was discussed in detail in our previous publication [2]. Concerning fast ions with higher Z, q model for the simulation of energy losses of such ions is implemented in Geant4 [3]. In this report we describe a model devloped for the extension of GEANT4 electromagnetic interactions of ions down to lower kinetic energies. This extension is necessary for the precise simulation of the stopping of low energy ions in matter, required by various types of analysis. For example, in space applications, the increasing use of sensitive components has lead to a higher susceptibility to heavy ion-induced failures and operational interruptions. The growing prolonged presence of man in space, especially in the context of the new International Space Station, will mean an increased astronaut health hazard. In this context heavy ions are thought to be particularly harmful from cellular and DNA damage point of view. On the other hand, in the medical field heavy ions are used for irradiation treatment, and in this application very accurate knowledge is required of the ion range and stopping power at low energies. A wide range of other important uses for low-energy ion transport simulation is also foreseen.

2 Physics Models

The energy loss of fast ions moving through the matter is mainly due to the process of ionisation of target atoms (electronic stopping power). The mean value of the energy loss is given by the Bethe-Bloch formula [2,4]. This energy loss is a function of the ion velocity; for $\beta > 0.05$ the Bethe-Bloch formula provides an accuracy better than 1 %. According to this formula the energy loss of any fast ion can be expressed via the energy loss of an another ion using the scaling relation. Therefore the energy loss of the ion S_{ei} is proportional to the energy loss of a proton with the same velocity

$$S_{ei}(T) = Z_i^2 \cdot S_{ep}(T_p), \tag{1}$$

where T is the kinetic energy of the ion, Z_i is the charge of the ion, S_{ep} is the stopping power of a proton with the same velocity, which corresponds to the so-called “reduced” kinetic energy T_p

$$T_p = T\frac{M_p}{M_i}, \tag{2}$$

where M_p is the proton mass and M_i is the ion mass. At lower energies the energy loss exhibits the behaviour of the Bragg’s peak, but no precise theory is available. So, an

accurate simulation of energy losses at low energies ($T_p < 2\ MeV$) can only be based on experimental data. The data on the ionisation of protons and α particles in all available target atoms were reviewed and parameterised by J.F. Ziegler in 1977 [5,6]. Old and more recent data were analysed in the ICRU report in 1993, and previous Ziegler's parameterisation coefficients were consequently upgraded [7].

A later review of the energy losses of low energy heavy ions was also performed by J.F. Ziegler [9,10]. It was shown that the scaling relation (1) must be substituted by

$$S_{ei}(T) = Z_{eff}^2 \cdot S_{ep}(T_p), \tag{3}$$

where Z_{eff} is effective charge of the ion. This effective charge approach takes into account the fact that a slow ion picks up electrons from the medium and its energy loss decreases.

For very slow ions with reduced energy $T_p < 1\ keV$ no precise data are available, but the free electron gas model [8] can be used, which predicts the electronic stopping power to be proportional to the ion velocity. At the same time, for very slow ions the energy transfer to the nuclei of the medium (nuclear stopping power) is not negligible [9,7] and must be taken into account.

3 Energy Loss of α Particles

The accuracy of the data for the ionisation losses of α particles in all elements [6,7] is comparable to the accuracy of the data for proton energy losses [5,7]. This provides the possibility of an accurate simulation of the α particle energy losses based on the experimental data and of a detailed check of the effective charge approach (3). In the GEANT4 energy loss model for α particles the Bethe-Bloch formula is used for kinetic energy $T > T_2$, where T_2 is the arbitrary parameter, currently set to $8\ MeV$. For lower energies the parameterisation is performed using three different models, which will be described below.

In the energy range of the Bragg's peak of ionisation losses, $1\ keV < T < 10\ MeV$, the Ziegler parameterisation [6,7] is used:

$$\begin{aligned} S_e &= \frac{S_{low} S_{high}}{S_{low} + S_{high}}, \\ S_{low} &= A_1 T^{A_2}, \\ S_{high} &= \frac{A_3}{T} \ln\left(1 + \frac{A_4}{T} + A_5 T\right), \end{aligned} \tag{4}$$

where S_e is the electronic stopping power in $[eV/10^{15} atoms/cm^2]$, T is the kinetic energy of α particles in MeV, A_i are five fitting parameters found individually for each atom for atomic numbers from 1 to 92.

For higher energies $T > 10\ MeV$ (this model is used only in case if $T_2 > 10\ MeV$) J.F. Ziegler suggested another parameterisation

$$S_e = exp\left(A_6 + A_7 E + A_8 E^2 + A_9 E^3\right),\ E = ln(1/T). \tag{5}$$

To ensure a continuous dE/dx function from the energy range of the Bethe-Bloch formula to the energy range of the parameterisation, the factor

$$F = \left(1 + B\frac{T_2}{T}\right) \tag{6}$$

is multiplied by the value of S_e as predicted by the Bethe-Bloch formula for $T > T_2$. The parameter B is determined for each element of the material in order to ensure the continuity at $T_p = T_2$. The value of B for different atoms is usually less than 0.01.

For kinetic energies of α particles $T < 1\ keV$ the model of free electron gas [8] is used

$$S_e = A\sqrt{T}, \tag{7}$$

The parameter A is defined for each atom by requiring the stopping power to be continuous at $T = 1\ keV$.

Since the ICRU report provides both the table of the fitting parameters and the one of the stopping powers, it is possible to perform a cross check of the computation algorithm (Fig.1). The two available parameterisations (ICRU's [7] and Ziegler's [6]) are the same for most of the elements and are different only for a few elements. It is also seen from the figure that even for the kinetic energy of α particles 1 MeV the ionisation strongly depends on the target atom shell structure. This dependence disappears with increasing energy and becomes more pronounced with decreasing energy (fig.2).

4 Effective Charge of Ions

According to the relation (3) the process of the energy losses of ions can be described in the framework of ion effective charge. The ion effective charge is usually expressed via the ion charge Z_i and the fractional effective charge of ion γ_i

$$Z_{eff} = \gamma_i Z_i. \tag{8}$$

For fast ions the effective charge of the ion is equal to the ion charge Z_i. Lower energy ions pick up electrons of medium, thus leading to lower average ion charge.

For helium ions ionisation losses are parameterised for all elements with a good accuracy, as it was described in the previous chapter. The results of Ziegler analysis [6] confirm the effective charge approach (3) and a universal parameterisation of effective charge is obtained [9]

$$(\gamma_{He})^2 = \left(1 - \exp\left[-\sum_{j=0}^{5} C_j Q^j\right]\right)\left(1 + \frac{7 + 0.05 Z_t}{1000}\exp(-(7.6 - Q)^2)\right)^2, \quad (9)$$

$$Q = \max(0, \ln T_p), \quad (10)$$

where the coefficients C_j are the same for all elements, the helium ion kinetic energy is in keV/amu, and Z_t is the charge of the target nucleus. In the framework of this model the α particle effective charge is a function mainly of its kinetic energy and the dependence on Z_t is negligible (Fig.3).

Parameterisations for both protons and for α particles are implemented in GEANT4. Using the helium effective charge formula (10) it is possible to derive the proton stopping power from the α particle stopping power (Fig.4). The comparison demonstrates a very high precision of this approach for the reduced energy range $T_p > 100\ keV$. It is seen also that some disagreement in the calculation of the energy loss of protons exists at lower energies. To study this difference as a function of the kinetic energy, the electronic stopping powers of α particles were derived from parameterisations of both α particle and proton energy loss. The results are shown for carbon (Fig.5), aluminum (Fig.6), iron (Fig.7), and copper (Fig.8). It is seen that for very slow α particles ($T < 10\ keV$) the accuracy of the effective charge formula (10) strongly depends on the absorbers. For aluminum and copper the accuracy is relatively high, while for carbon and iron it is not. For α particle energies $T > 1\ MeV$ (reduced energy $T_p > 250\ keV$) the effective charge approach is precise.

5 Energy Loss of Heavy Ions

The effective charge approach is the framework that describes the energy loss of various ions. As it was demonstrated for helium ions (Fig.3), for fast ions ($T > 10 Z_i M_i MeV \cdot amu$) the effective charge of the ion is equal to the ion charge Z_i. Lower energy ions pick up electrons of the medium and the average ion charge can be expressed as $Z_{av} = qZ_i$, where q is the fractional average charge of the ion. In general, the value of q does not coincide with the value of γ_i and Z_{av} does not coincide with Z_{eff}, because the electrons of a moving heavy ion have a spatial distribution which modifies the ion stopping power from the one of a point-like charge.

Following Ref.[10] we use the expression derived from Brandt-Kitagava theory [11]

$$\gamma_i = \left(q + \frac{1-q}{2} \left(\frac{v_0}{v_F} \right)^2 \ln\left(1+\Lambda^2\right) \right) \left(1 + \frac{(0.18 + 0.0015 Z_t) \exp(-(7.6-Q)^2)}{Z_i^2} \right), \tag{11}$$

where v_0 is the Bohr velocity with the corresponding kinetic energy $T_p = 25\ keV/amu$, v_F is the Fermi velocity of the electrons in the target medium, Λ is the term taking into account the screening effect. In the Ref.[11] it is estimated as:

$$\Lambda = 10 \frac{v_F}{v_0} \frac{(1-q)^{2/3}}{Z_i^{1/3}(6+q)}. \tag{12}$$

The Fermi velocity of the medium is of the same order as the Bohr velocity. Its exact value depends on the detailed electronic structure of the medium. Experimental data on Fermi velocity exist for many elements [9] and these data are included in the GEANT4 implementation.

The expression for the fractional average charge of the ion is the following:

$$q = [1 - \exp(0.803 y^{0.3} - 1.3167 y^{0.6} - 0.38157 y - 0.008983 y^2)], \tag{13}$$

where y is a parameter that depends on the ion velocity v_i

$$y = \frac{v_i}{v_0 Z^{2/3}} \left(1 + \frac{v_F^2}{5 v_i^2} \right). \tag{14}$$

Note that the parameterisation described in this chapter is only valid, if the reduced kinetic energy of the ion is higher than the lower limit of the energy

$$T_p > \max\left(3.25\ keV, \frac{25\ keV}{Z_t^{2/3}} \right). \tag{15}$$

If the ion energy is lower, then the free electron gas model (7) is used to calculate the stopping power. An example of GEANT4 simulation of electronic stopping powers for carbon and argon ions in aluminum and the comparison with experimental data [12] is shown in Fig.9

6 Energy loss of Ions in Compounds

To obtain the energy losses of ions in a mixture or compound, the absorber can be thought of as made up of thin layers of pure elements with weights proportional to the electron density of the element in the absorber (Bragg's rule)

$$S_e = \sum_j S_{ej}, \tag{16}$$

where the sum is taken over all elements of the absorber. This rule is very accurate for relativistic particles, when the interaction of electrons with a nucleus is negligible; but at low energies the accuracy of Bragg's rule is limited [10]. The GEANT4 model of electronic stopping power of any ion in any absorber is based on the implementation of chemical effects described in details in Ref.[2].

For stopping powers of protons and α particles the coefficients for the parameterisation formula (4) in 11 compounds [2] are provided in the ICRU report. ICRU has also published the alternative parameterisation of D. Powers for α particle stopping power in 30 elements and compounds (table 2):

$$S_e = \left[1 - \exp(-c_2 T^{c_6 - 2})\right] \cdot \left[\left(\frac{c_1 \ln T}{T} + \frac{c_3}{T}\right) \exp(-c_5 T^{-c_7}) + \frac{c_4}{T}\right], \qquad (17)$$

which is also implemented in GEANT4. The GEANT4 method of simulation is the following:

- if experimental data on the stopping power for a compound as a function of the ion kinetic energy are available, then the direct parameterisation of the data for this material is performed;
- if the data on the stopping power of the ion in the compound are available for only one incident energy ($T_p = 125\ keV$), then the computation is performed based on Bragg's rule and effective charge approach; the result is multiplied by the chemical factor of the compound.
- if there are no data for the ion, the computation is performed using effective charge approach and Bragg's rule for protons or α particles.

Note that the effective charge approach requires two parameters of the compound: Fermi velocity v_F and average target element number Z_t. In the current implementation these parameters are obtained as average values

$$v_F = \frac{\sum_j N_j V_{Fj}}{\sum_j N_j},\ Z_t = \frac{\sum_j N_j Z_j}{\sum_j N_j}, \qquad (18)$$

where the sum in taken over all elements of the compound, N_j is the electron density of the j-th element, Z_j is its number, and V_{Fj} is its Fermi velocity. In future upgrades of the code it is foreseen to provide the capability to define the values v_F and/or Z_t for the specific compound from experimental data or from a theoretical model.

The type of parameterisation (table 1) can be selected by the Geant4 user.

The comparison of the energy dependence of α particle electronic stopping powers obtained from different parameterisations is shown for water (fig.10). Note, that the D. Powers parameterisation coincides with the J.F. Ziegler parameterisation.

7 Nuclear Stopping Powers

Low energy ions transfer their energy not only to electrons of a medium but also to the atom's nuclei of the medium due to the elastic Coulomb collisions. This contribution to the energy loss is called "nuclear stopping power". The theory of nuclear stopping power is based on Screen Coulomb Potential approach. It was shown by J.F. Ziegler [6,9] and confirmed in ICRU report [7] that it is possible to describe the nuclear stopping power using a universal parameterisation for reduced ion energy ϵ:

$$\epsilon = \frac{32.536 T M_t}{Z_i Z_t (M_i + M_t)\sqrt{Z_i^{0.23} + Z_t^{0.23}}}. \tag{19}$$

The universal reduced nuclear stopping power s_n is determined by J. Moliere in the framework of Thomas-Fermi potential [13]. The corresponding tabulation is included in ICRU report [7] and implemented in GEANT4. To transform the value of nuclear stopping power from reduced units to $[eV/10^{15} atoms/cm^2]$ the following formula is used:

$$S_n = s_n \frac{8.462 Z_i Z_t M_i}{(M_i + M_t)\sqrt{Z_i^{0.23} + Z_t^{0.23}}}. \tag{20}$$

The effect of nuclear stopping power in very small at high energies, but it is of the same order of magnitude as electronic stopping power for very slow ions (fig.11).

8 GEANT4 Implementation of Energy Losses of Slow Hadrons

For the implementation of energy losses of slow ions in GEANT4 a new class **G4ionLowEnergyIonisation** has been designed. This class inherits from the class **G4hLowEnergyIonisation**, described in detail in our previous work [2], which inherits from the based class **G4hEnergyLoss**. The user has the choice to include one of these classes in his **G4PhysicsList** for the simulation of energy losses of either hadron or ion. The main difference between these two classes is that only in the **G4ionLowEnergyIonisation** class the effective charge approach is implemented.

The list of available parameterisations (table 1) is common to these classes and for each hadron/ion the user can choose the model by the void member function **SetStoppingPowerTableName("TheTableName")**. The user also has the possibility to switch on the calculation of nuclear stopping powers using the void member function **SetNuclearStoppingOn()** or to switch it off by the void member function **SetNuclearStoppingOff()**.

Table 1: The list of different parameterisations available in GEANT4.

Name	Particle	Source
UrbanModel	proton	GEANT4 beta version [3]
Ziegler1977H	proton	J.F. Ziegler parameterisation [5]
Ziegler1977He	He^4	J.F. Ziegler parameterisation [6]
ICRU_R49p	proton	ICRU parameterisation [7]
ICRU_R49He	He^4	ICRU parameterisation [7]
ICRU_R49PowersHe	He^4	J. Powers ICRU parameterisation [7]

Table 2: The list of chemical formulas of compounds for which **ICRU_R49p** provides D. Powers parameterisations.

Number	Chemical formula	Number	Chemical formula
1.	H_2	16.	CaF_2
2.	Be	17.	CO_2
3.	C	18.	Cellulose-Nitrat
4.	Graphite	19.	C_2H_4
5.	N_2	20.	LiF
6.	O_2	21.	CH_4
7.	Al	22.	Nylon
8.	Si	23.	Polycarbonate
9.	Ar	24.	(CH_2)_N-Polyethylene
10.	Cu	25.	PMMA
11.	Ge	26.	(C_8H_8)_N
12.	W	27.	SiO_2
13.	Au	28.	CsI
14.	Pb	29.	H_2O
15.	C_2H_2	30.	H_2O-Gas

9 Conclusion

The first version of a precise parameterisation methods for the stopping powers of slow ions has been implemented in GEANT4. Both ICRU's and J.F. Ziegler's evaluated data are available. The design of the method provides wide possibilities to continuously improve the accuracy of simulations, by using new or additional experimental data.

References

[1] GEANT4: LCB Status Report/RD44, CERN/LHCC-98-44, 1988.

[2] V.N. Ivanchenko et al., GEANT4 Simulation of Energy Losses of Slow Hadrons, CERN-99-121, INFN/AE-99/20, (September 1999).

[3] http://wwwinfo.cern.ch/asd/geant4/G4UsersDocuments/UserGuid es/ PhysicsReferenceManual/html/index.html/

[4] C.Caso et al. (Particle Data Group) Europ. Phys. Jour. **C 3** 1 (1998).

[5] H.H. Andersen and J.F. Ziegler, The Stopping and Ranges of Ions in Matter. Vol.3, Pergamon Press, 1977.

[6] J.F. Ziegler, The Stopping and Ranges of Ions in Matter. Vol.4, Pergamon Press, 1977.

[7] ICRU (A. Allisy et al), Stopping Powers and Ranges for Protons and α Particles, ICRU Report 49, 1993.

[8] J. Linhard and A. Winther, Mat. Fys. Medd. Dan. Vid. Selsk. **34**, No 10 (1963).

[9] J.F. Ziegler, J.P. Biersack, U. Littmark, The Stopping and Ranges of Ions in Solids. Vol.1, Pergamon Press, 1985.

[10] J.F. Ziegler and J.M. Manoyan, Nucl. Instr. and Meth. **B35**, 215 (1988).

[11] W. Brandt and M. Kitagawa, Phys. Rev. **B25**, 5631 (1982).

[12] H. Paul,http://www.uni-linz.ac.at/fak/TNF/atomphys/STOPPING/welcome.htm

[13] G. Moliere, Theorie der Streuung schneller geladener Teilchen I; Einzelstreuungam abbgeschirmten Coulomb-Feld, Z. f. Naturforsch, **A2**, 133 (1947).

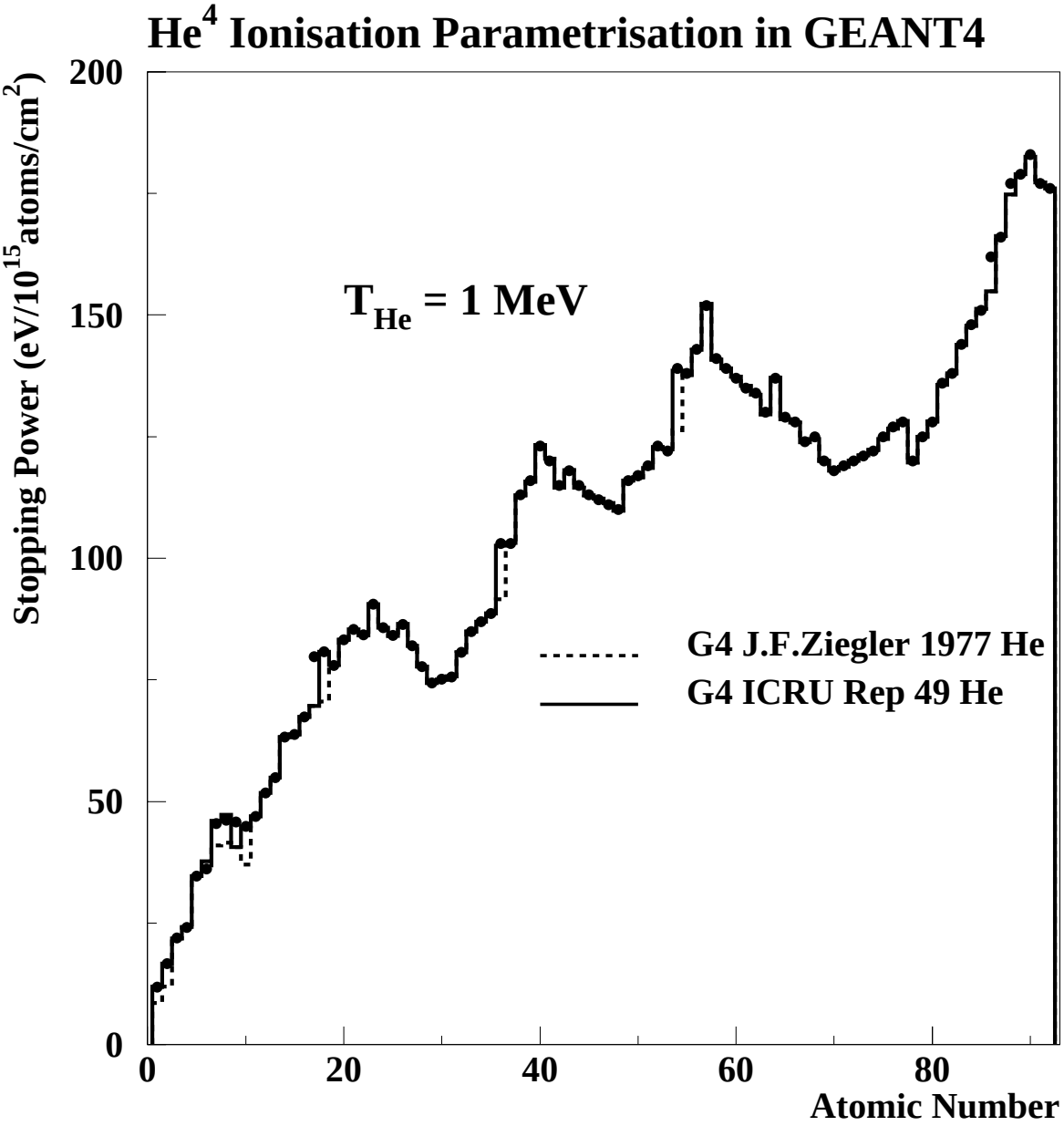

Figure 1: Cross check of the implementation of the α particles stopping power parameterisation for all elements with $Z < 93$. Solid line - ICRU's parameterisation, dashed line - J.F. Ziegler parameterisation, points - the data from ICRU report 49.

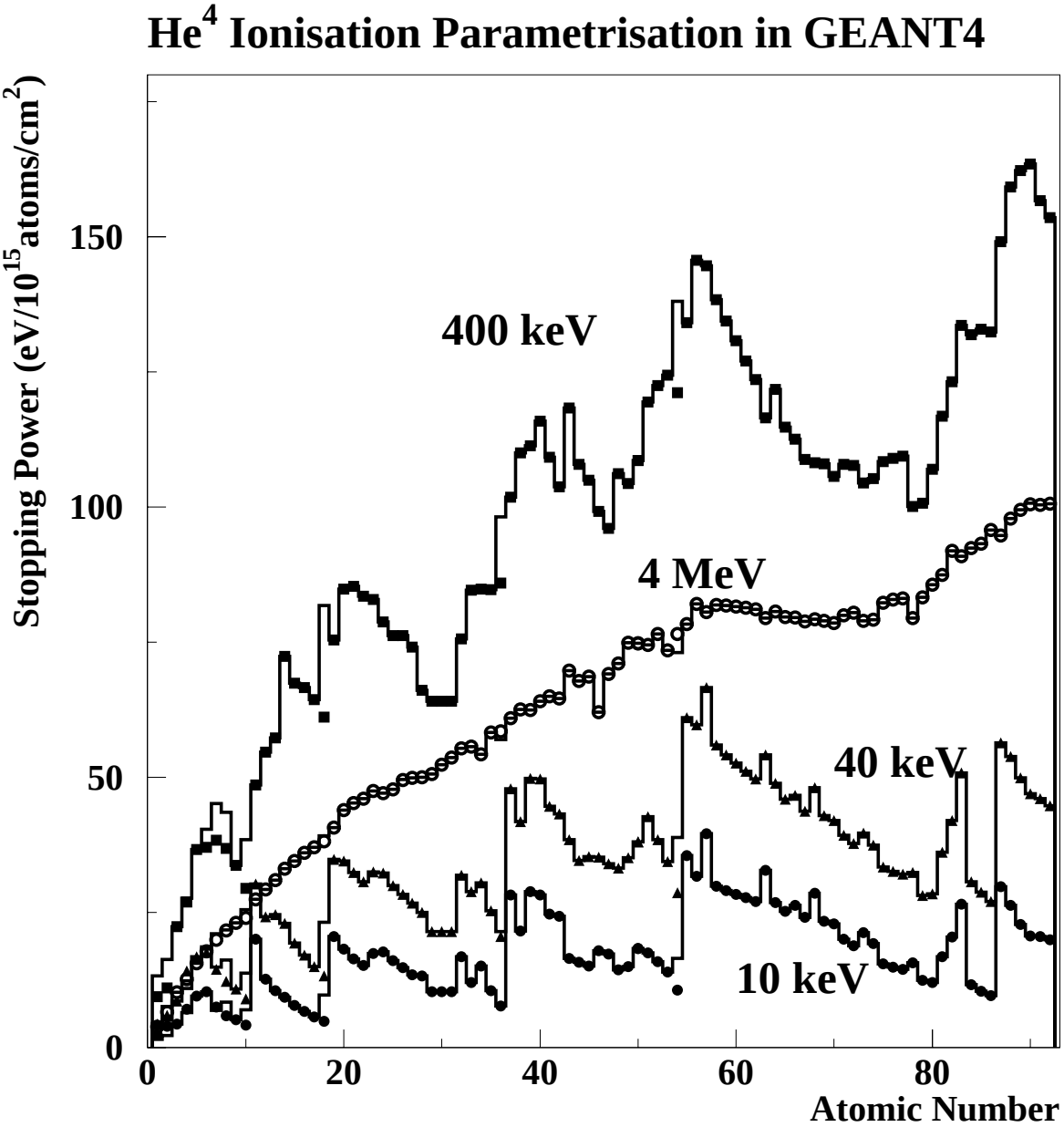

Figure 2: Stopping power in all atoms with $Z < 93$ for various α particle energies. Histograms - J.F. Ziegler's parameterisation, points - ICRU's parameterisation.

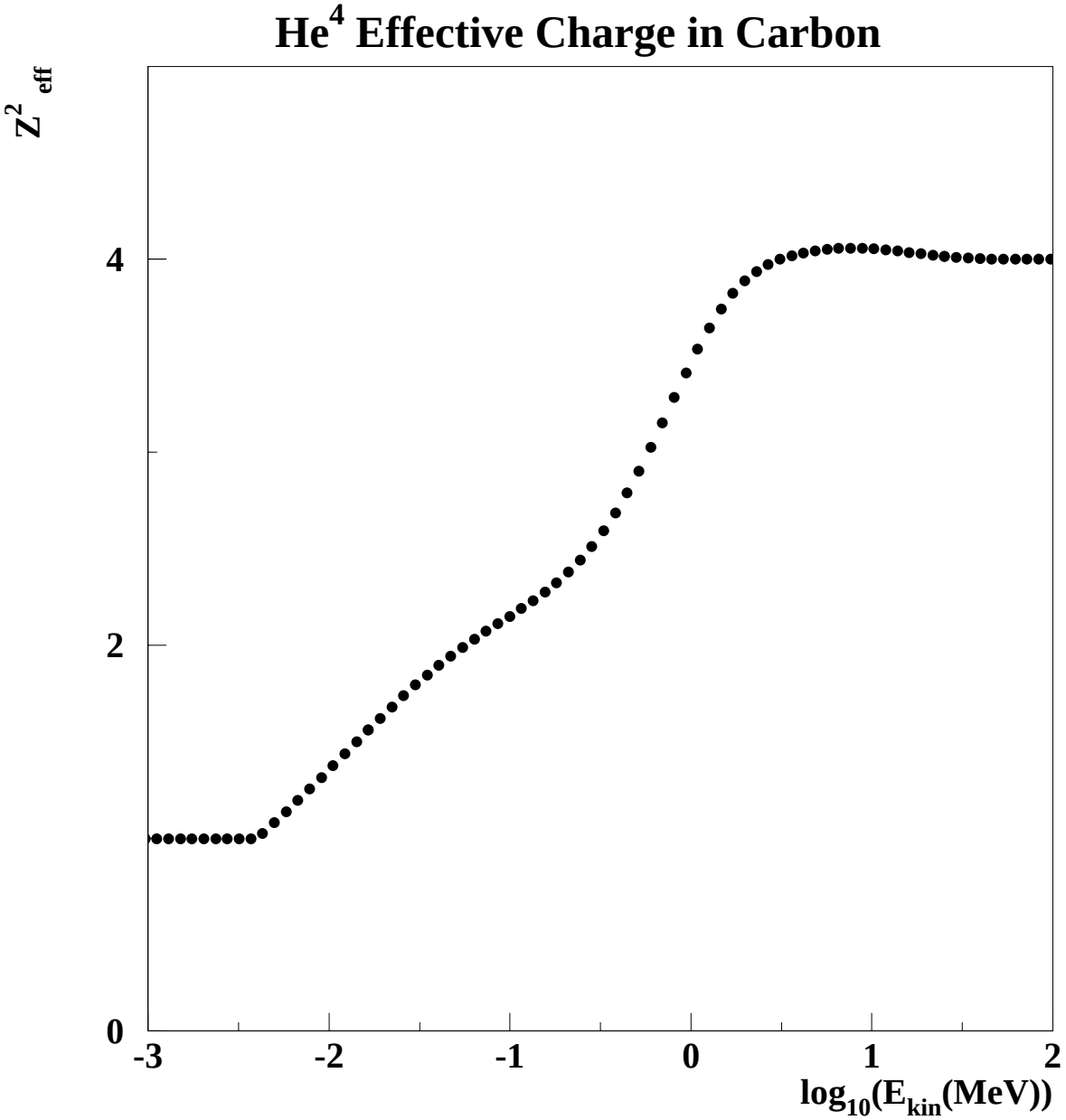

Figure 3: α particle effective charge square parameterisation.

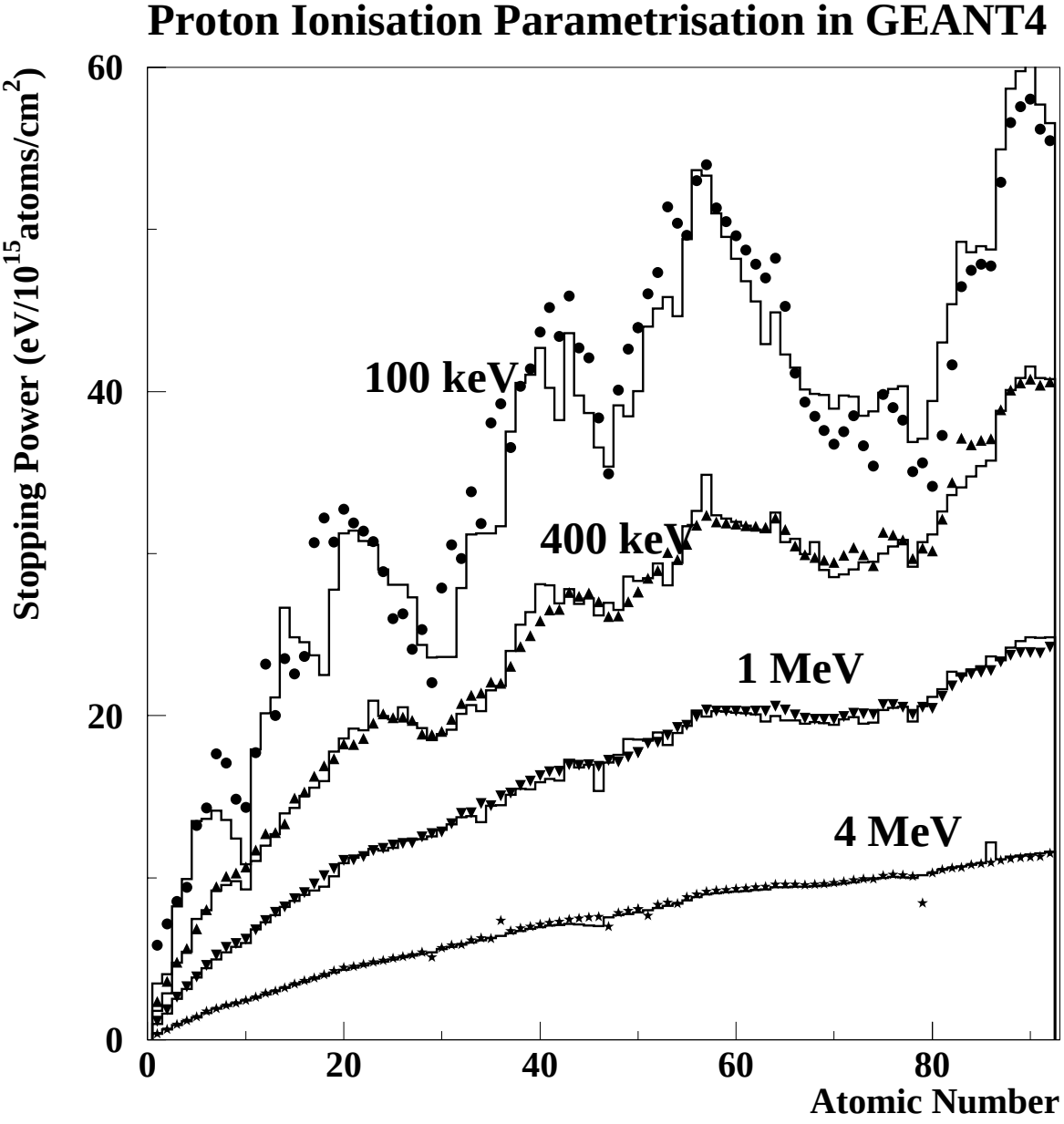

Figure 4: Protons stopping power parameterisation for all elements with $Z < 93$. Points - derived from the ICRU's parameterisation for α particles, histograms - ICRU's parameterisation for protons.

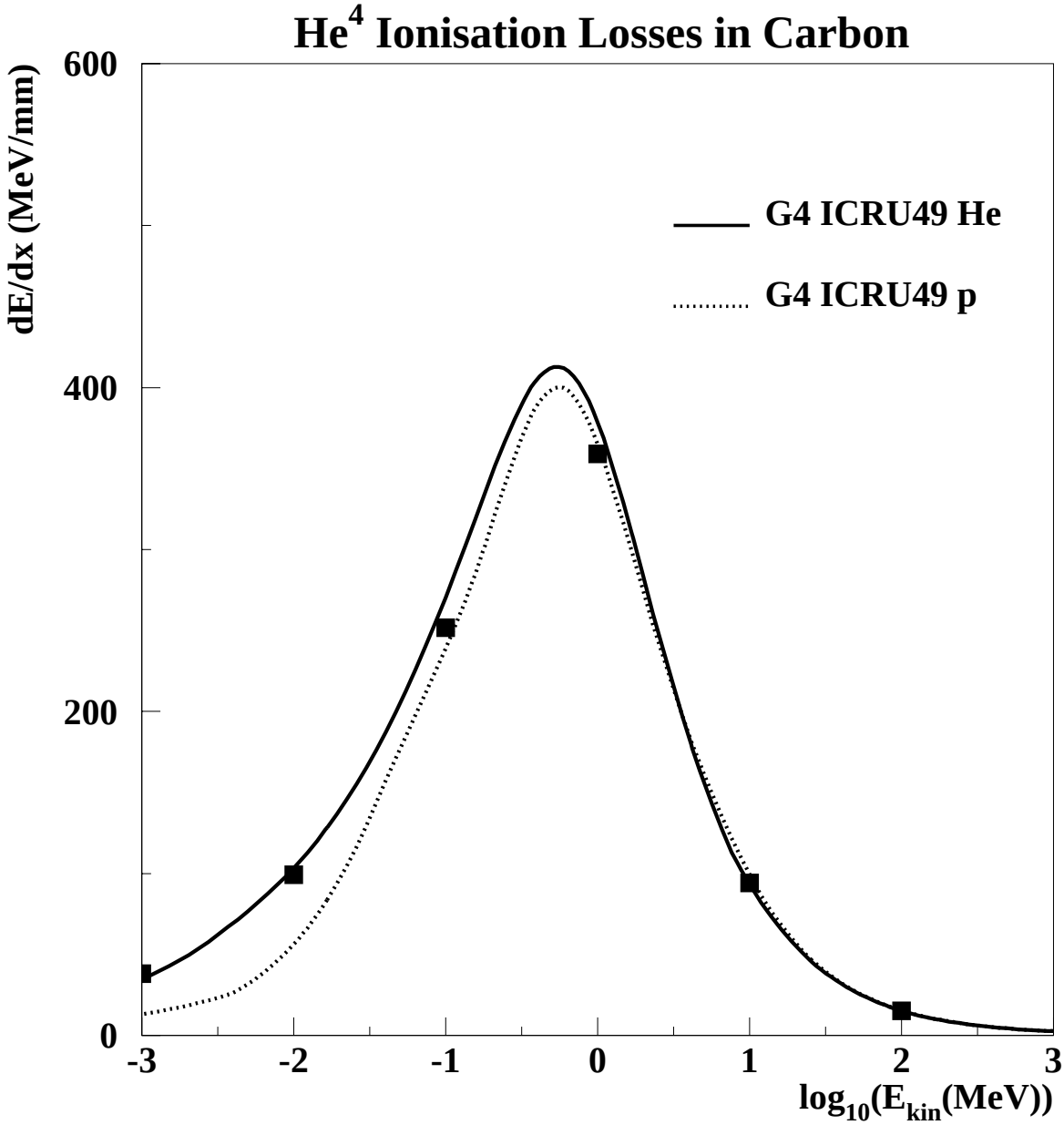

Figure 5: α particles stopping power in carbon. Points - data from ICRU report, solid line - the ICRU's parameterisation for α particles, dashed line - derived from ICRU's parameterisation for protons.

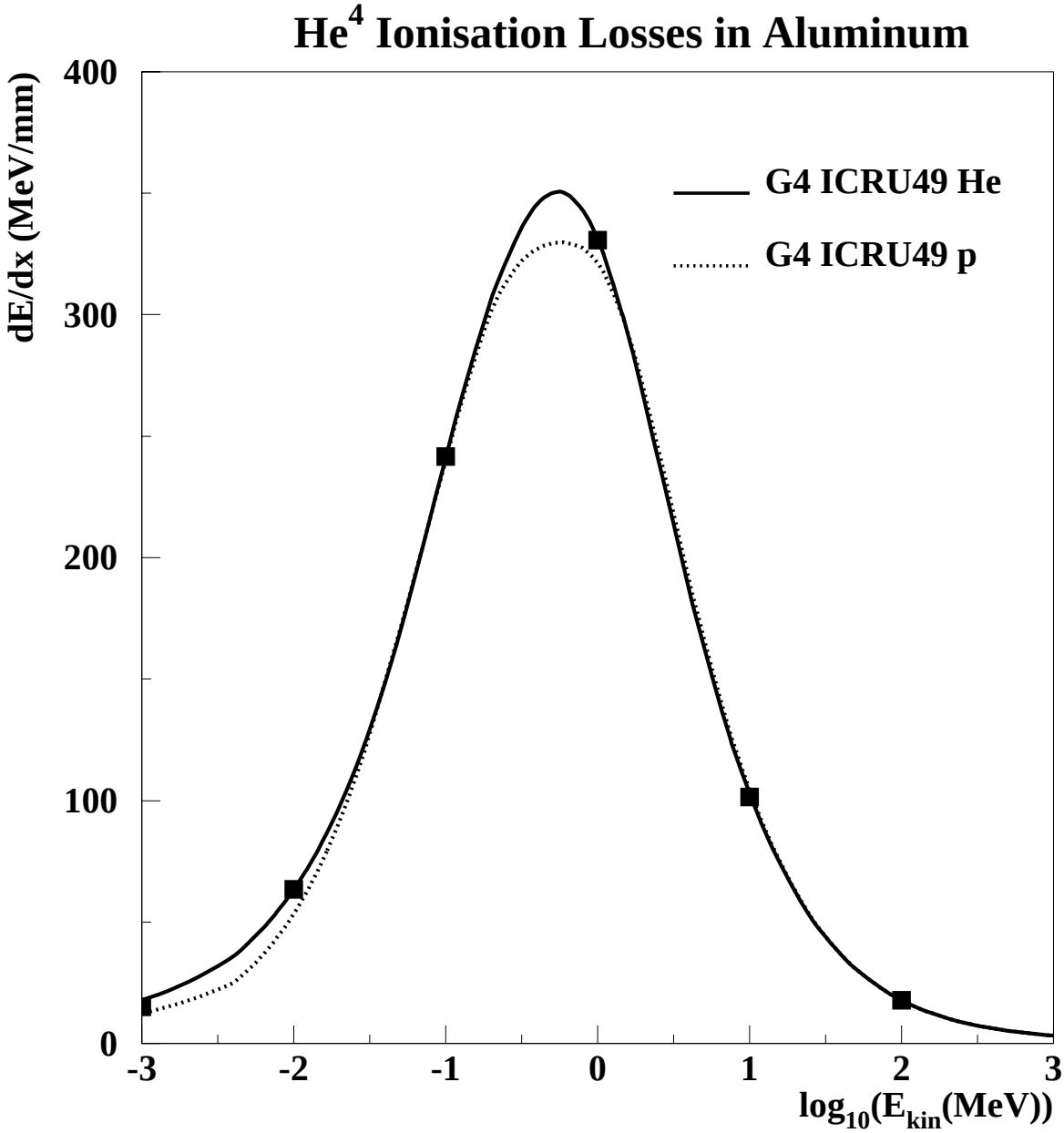

Figure 6: α particles stopping power in aluminum. Points - data from ICRU report, solid line - the ICRU's parameterisation for α particles, dashed line - derived from ICRU's parameterisation for protons.

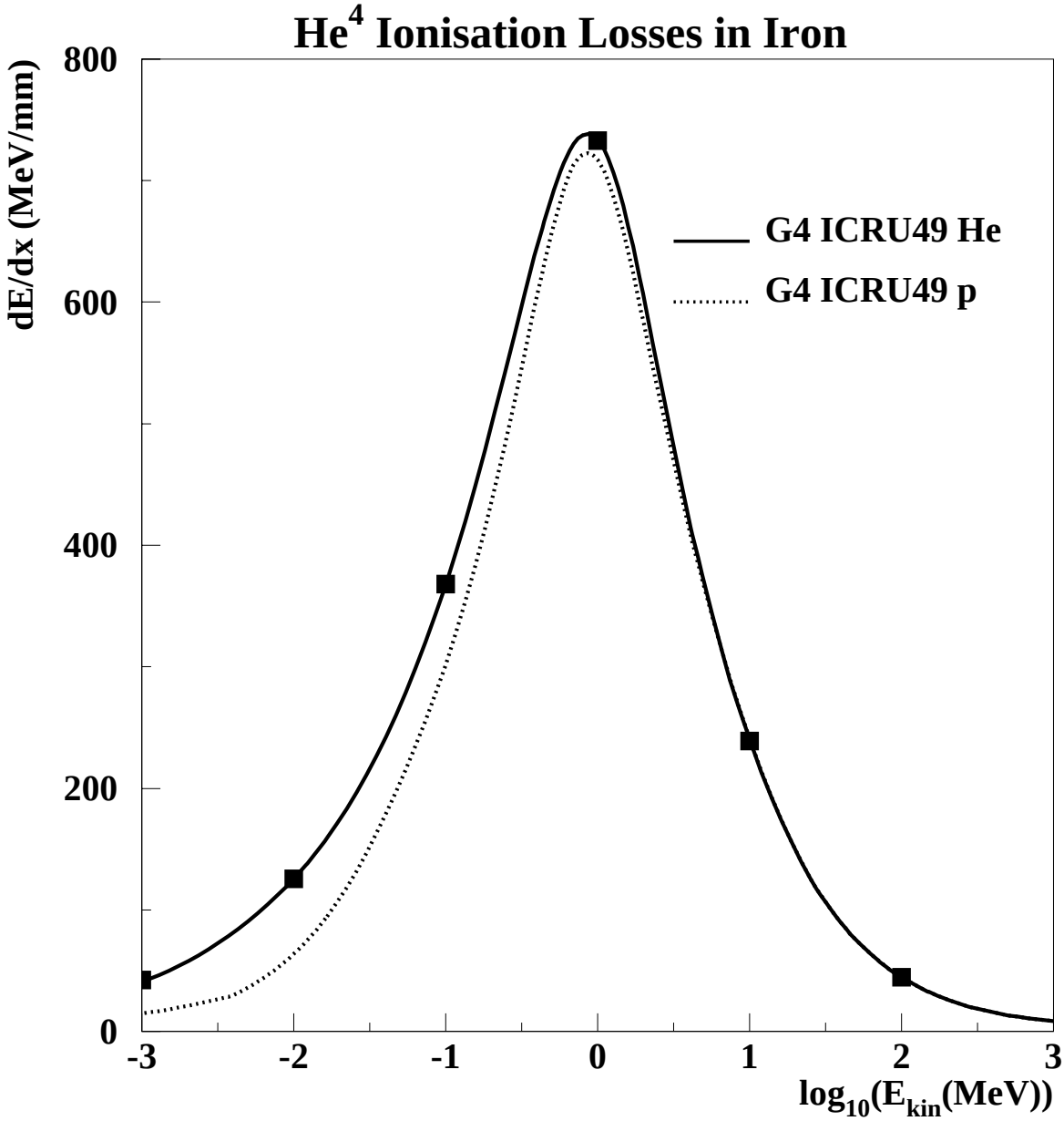

Figure 7: α particles stopping power in iron. Points - data from ICRU report, solid line - the ICRU's parameterisation for α particles, dashed line - derived from ICRU's parameterisation for protons.

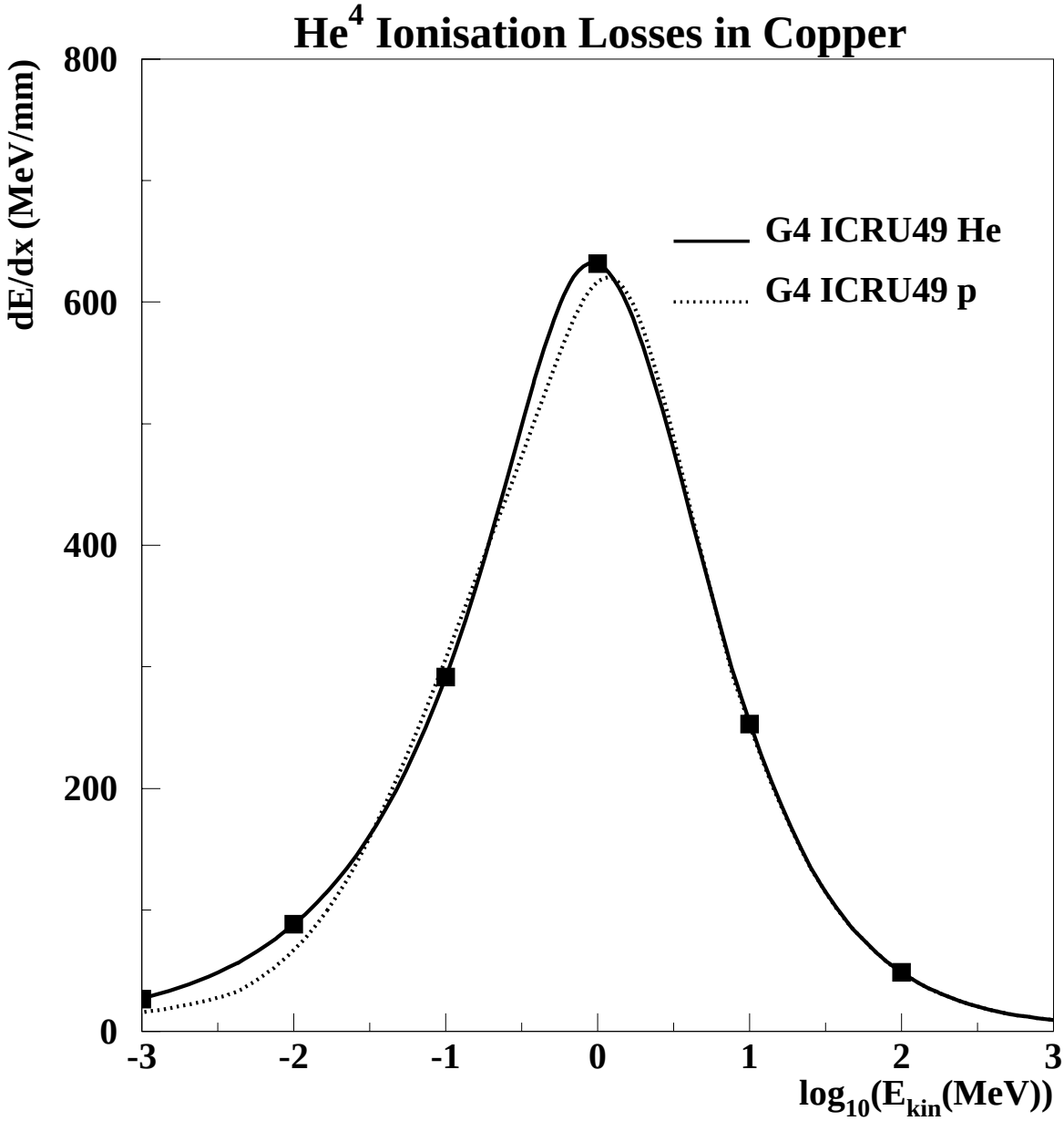

Figure 8: α particles stopping power in copper. Points - data from ICRU report, solid line - the ICRU's parameterisation for α particles, dashed line - derived from ICRU's parameterisation for protons.

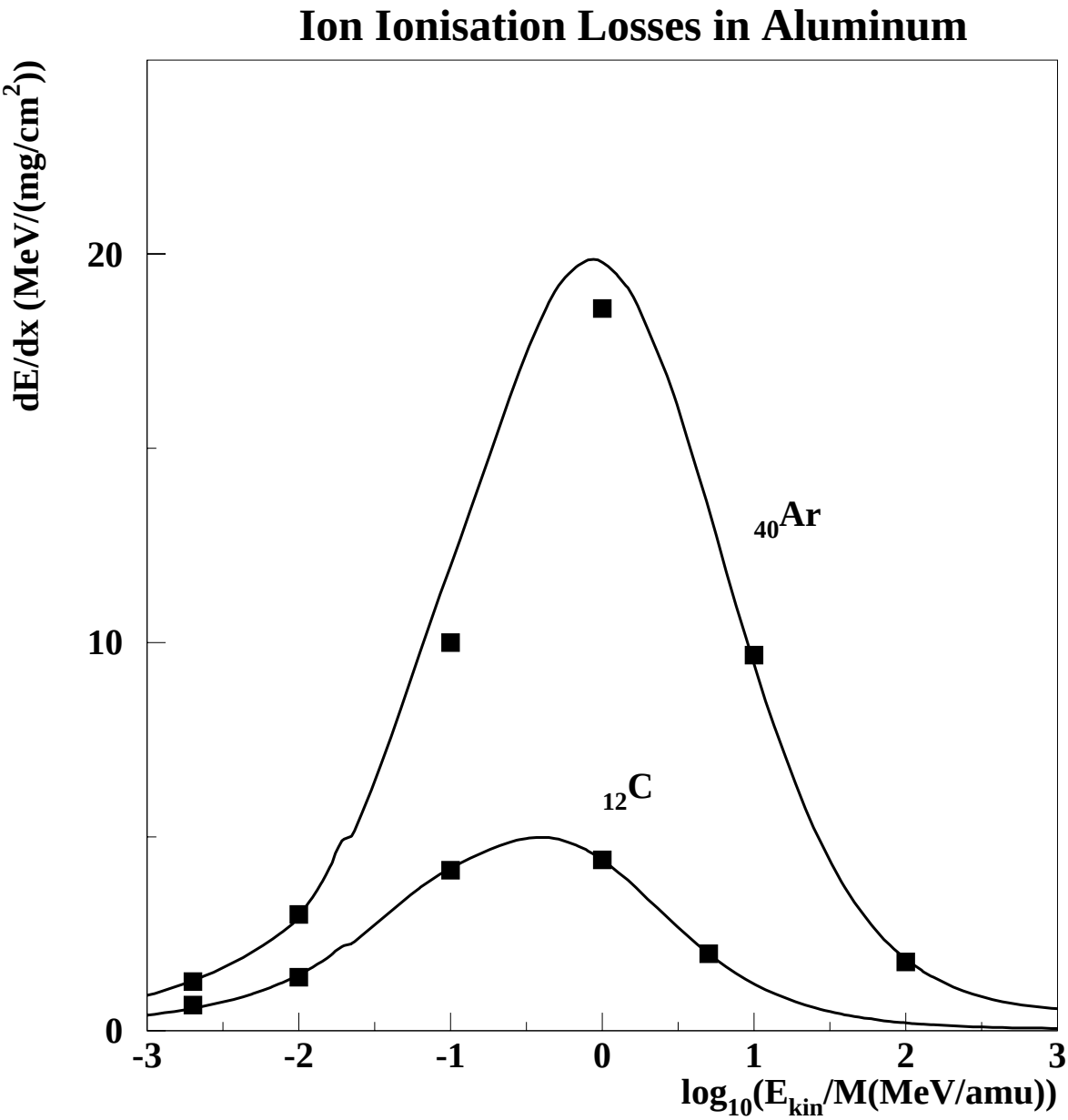

Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.

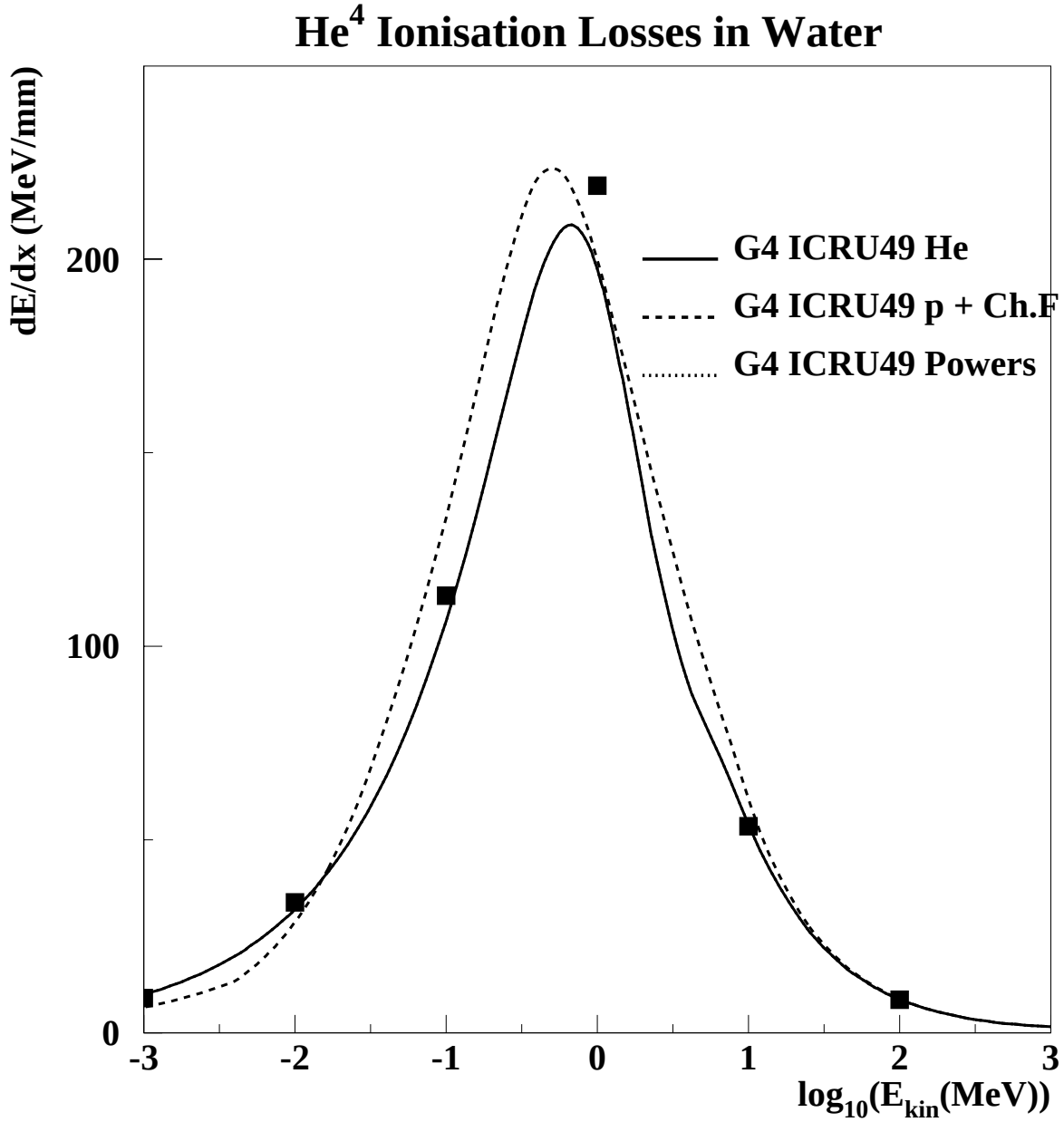

Figure 10: α particles stopping power in water. Points - data from ICRU report, solid line - the two ICRU's parameterisation for α particles (dotted line is not seen), dashed line - derived from ICRU's parameterisation for protons taking into account the "chemical factor".

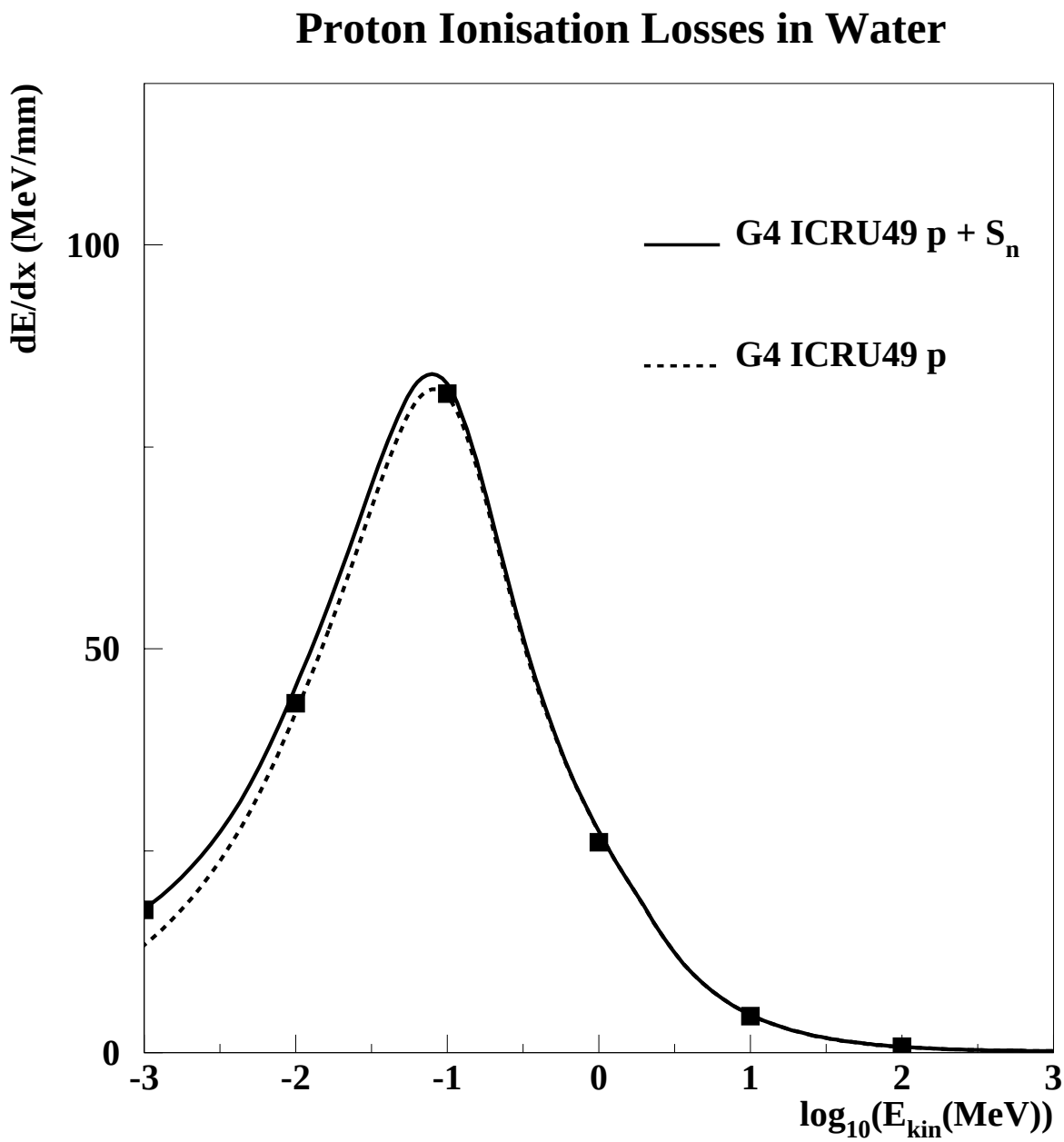

Figure 11: Protons stopping power in water. Points - data from ICRU report, solid line - the ICRU's parameterisation for protons with nuclear stopping power, dashed line - without nuclear stopping power.