SHIELD – a Monte Carlo Hadron Transport Code

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Abstract

SHIELD is a universal code for Monte Carlo simulation of hadron cascades in complex macroscopic targets. One can calculate a nucleon, pion, kaon, antinucleon, and muon transfer in energy range up to 100 GeV.

To obtain an exclusive description of hadron-nucleus interactions, the SHIELD code includes well-known hA-generators: the Dubna version of intranuclear cascade model as well as the independent quark-gluon string model generator at the higher particle energies; nuclear deexcitation code permits to take into account the Fermi break up, multifragmentation, and evaporation/fission processes.

During a hadron tree generation in target the sources of "evaporated" neutrons and electromagnetic particles are being formed. Subsequent neutron transport is simulated with the original neutron code LOENT based on 26-group neutron constant system BNAB. The interface between SHIELD and EGS4 codes is realized to simulate electromagnetic showers.

Each hadron cascade tree is stored without any loss of physical information during its simulation, allowing to divide completely a modeling and registration parts of the code. The SHIELD code's open architecture presumes its modification and improvement depending on specific problems. The results of the spallation process investigation in heavy targets are presented as example of the code application.

1 Introduction

As is generally known, there are two main approaches to Monte Carlo simulation of hadron cascades in complex macroscopic targets – inclusive and exclusive ones, according to the method of description of hadron-nucleus (hA) interaction.

In inclusive approach a single-particle distributions of secondary particles are used for description of the hA-interaction. Evidently the essential convolution of an information occurs because a many-particle distribution of secondary particles is being integrated over all secondaries variables excluding a single particle. This way permits to calculate the fields of secondary particles of each type and functionals of them. This is enough for many applications, in the first place for the most of radiation physic problems on high- and superhigh energy accelerators. The advantage of inclusive approach is a moderate requirements to computer power and slow increase of CPU time expense with the primary energy. On the other hand, due to mentioned above convolution, this approach doesn't permit to study any correlations in hadron cascade as well as any fluctuations of separate cascades. On the same reason the energy-momentum conservation law is obeyed on the average only, over a whole ensemble of hadron cascades, while having been violated in each separate hadron cascade as well as in each hA-interaction in target. The latter excludes, in particular, the straightforward modeling of a nuclear deexcitation and nuclei-product yields. Further discussion of the inclusive approach, including well-known inclusive codes MARS, CASIM, KASPRO one can find, for example, in survey [1].

On the contrary, the exclusive approach is based on a many-particle distribution of secondaries for description of the hA-interaction. It implies the calculation of all individual characteristics of each hA-interaction, i.e. of energy and direction of each secondary particle as well as the individual variables of the residual nucleus (A, Z, kinetic and excitation energy), the conservation laws are being obeyed in each interaction. In practice an exclusive hadron-nucleus Monte Carlo generator is included into the hadron transport code to simulate in detail the hA-interaction (usually this is an intranuclear cascade model coupled with some nuclear deexcitation model). Therefore the exclusive approach allows to get not only the differential hadron fluences, as inclusive one, but also the yields of residual nuclei in the target, distributions of neutron and electromagnetic sources as well as some correlation characteristics, e.g. effective mass spectra of given hadron group. There is a specific area of applications of this approach (resolution of hadron calorimeters and some other tasks of experimental installation modeling, simulation of spallation targets) where the inclusive method is not applicable. However the payment for some advantages of the exclusive approach is large expense of CPU time as compared to inclusive one with increase in energy.

There is, besides, the "quasiexclusive" approach describing hA-interaction by means of a model representations, experimental data, and semiempirical single-particle distributions, the approximate conservation laws execution is being obeyed using some special shifts. It is possible to treat as "quasiexclusive" the high energy oriented codes GHEISHA [2] (up to 0.5 TeV) and FLUKA [3] (up to 20 TeV) included in popular GEANT package.

At present the most of exclusive investigations at intermediate hadron energies are carried out using the HETC code [4], which has become a standard de-facto for such calculations. Really several modifications of this code, including early version NMTC [5], are being used in different Laboratories.The most of the HETC code versions are based on Bertini intranuclear cascade model [6], the evaporation/fission competition at deexcitation stage is taken into account as a rule. All versions permit to simulate the pion-nucleon cascades in the target at energy up to 3 GeV (exactly up to 30 GeV, having extrapolated the results of the hA-interaction above 3 GeV). A single exclusion is the high-energy version HETC88 [7], which uses above

5 GeV the modified "quasiexclusive" hA-generator from the FLUKA code. The modifications include improvements in energy-momentum conservation in separate hA-interaction. So the HETC88 code is applicable up to 20 TeV. However only pion-nucleon cascades are considered in a whole energy range similar to initial HETC version. Other mesons and baryons beard by FLUKA hA-generator are converted into pions and nucleons. It excludes from consideration the kaon and antinucleon transport in the target, representing an independent interest, in particular in "kaon factory" energy range (10÷50 GeV).

Thus, at present time, the exclusive simulation of the hadron cascades in a medium at intermediate energies is closed in fact on the HETC code. Meanwhile the presence of other independent original codes would be useful for progress in this research field, in particular from the viewpoint of an intracontrol intended to guarantee a scientific community's trust in obtained computational results. The SHIELD code is such independent original code.

An initial version of the SHIELD code [8,9] was elaborated in 1968-70. Being quite independent it turned out to be ideologically similar to the HETC code and had approximately the same power. Dubna version of cascade-evaporation model [10], having been included into SHIELD as hA-generator, provided the exclusive simulation of pion-nucleon cascades in a medium at energy region up to 3-5 GeV. In further the SHIELD code was successfully applied to a set of specific researches. Since 1989 a full revision and rewriting of the SHIELD code was made taking into account a current experience and an increased problem field. Today the SHIELD code is a universal, completely exclusive hadron transport code for energy region up to 100 GeV. The name "SHIELD" is not quite good for universal code but this workname is strong pasted during the code lifetime.

Below the necessarily short write-up of the SHIELD code is given. The results of the modeling of spallation process in fissile and nonfissile targets are presented as example of the code application to the intensive pulsed neutron source problematics. At present the SHIELD code is being also used for modeling of radiation damages of materials under proton beam, calculation of muon background behind massive hadron absorber, absorber optimization, etc.

2 The SHIELD code write-up

2.1 The areas of application and main features

The SHIELD code allows calculations to be made for macroscopic targets involving a number of geometric bodies bounded by surfaces of the second degree. The chemical composition of a material inside of any geometric zone can be essentially arbitrary: a pure matter of natural or a given isotopic composition; an alloy or other mixture; a chemical compound with a given formula (including hydrogen-bearing ones).The original geometric modulus GEMCA of the SHIELD code is completely compatible with the CG-modulus of the MORSE code [11] on input data. Its advantages as compared with CG-modulus are higher speed and more simple inclusion into a transport code procedure. Of course, the CG-modulus can be immediately used in the SHIELD code.

The SHIELD code enables to simulate the transfer of nucleons, pions, kaons, antinucleons, and muons in energy range up to 100 GeV. This bound can be enlarged if required because the used hA-generator is applicable for higher energies (see sect. 2.2). In fact this bound is defined by real field of problems and by available computer power.

To simulate the hadron interaction pass length and to sample the interaction type (elastic or inelastic) the total and inelastic hadron-nucleus cross sections are required. These values are calculated on a basis of compilation [12] and preceding preprints. The tabulated representation of the cross sections is used in the SHIELD code with specially adopted and detailed enough energy mesh (up to 50 points) for each hadron type and for 20 support nuclei in the region from hydrogen to uranium. Binary search in the tables together with a linear interpolation on the energy provides an acceptable calculation speed and accuracy for support nuclei. The interpolation as $A^{2/3}$ is used for other nuclei.

If the inelastic hA-interaction is realized in the pass endpoint, the hA-generator runs. Otherwise elastic scattering is simulated. The hadron scattering angle is sampled from diffractionlike distribution while a recoil nucleus momentum is calculated with the two-particles kinematic.

The algorithm of the interaction pass length simulation in the SHIELD code is based on the relation pass–energy–optical depth for charged particles and on dependence of the total macroscopic cross section on the energy for neutral ones. Having known these relations one can calculate the accumulated optical depth OPTDEP(R) when the distance R is covered along a hadron trajectory, and energy E(R) for charged particles. As a result the interaction pass length RANGE sampling procedure is reduced to numerical solving of the equation OPTDEP(RANGE)=$-\ln(\xi)$, where ξ is the uniformly [0,1] distributed random variable. The algorithm is well adopted to the complex targets where the hadron trajectory crosses several different materials. The cases of the hadron flying out from the target and absorption in target due to ionization loss are realized automatically. The relations pass-energy-optical depth and energy-macro cross section are calculated by the SHIELD code during the preliminary stage, before the Monte Carlo simulation has began, and are represented in tabulated form with detailed enough energy mesh for each hadron type and for all media constituting the target. Binary search in the tables together with linear interpolation is thereafter used to calculate the needed values.

The modified algorithm of the charged particle pass sampling is also realized in the SHIELD code to take into account the ionization loss fluctuations.

The SHIELD code permits to simulate the main modes of pion and kaon decays. The decay kinematic is simulated over phase space in any case. However, only the following decays are liable to direct simulation: $\pi^0 \rightarrow 2\gamma$ (immediately in π^0 birthpoint), $K_S^0 \rightarrow 2\pi$ (the interaction-decay competition is realized), and π^+ and K^+ decays at rest. (The stopped π^- and K^- mesons are absorbed by nucleus and give rise a nuclear reaction). At the same time the decays of the $\pi^\pm$, $K^\pm$, and K_L^0 mesons in a fly are not liable to direct simulation due to very large decay length as compared to the interaction pass length and, in typical cases, to ionization pass length and target dimensions. Therefore the forced decay of these particles in a fly is realized in the SHIELD code. The statistical weight of the decay products is proportional to the decay probability on the interaction (or ionization loss, or target flying out) pass. The weighted transport of the decay products is then simulated. The forced decay is initiated in a special tasks only (e.g. muon background calculation).

During hadron cascade simulation the sources of the "evaporated" neutrons ($E<10.5$ MeV) are formed as well as the sources of gamma-quants, electrons/positrons, and neutrinos (as a meson decay products). All these particles are individually stored in corresponding source arrays and are transported on completion of the hadron cascade simulation (excluding neutrinos).

The electromagnetic showers are simulated by means of the EGS4 code [13]. Special interface between the SHIELD and EGS4 codes allows the latter to use the same geometric modulus as well as the sources created by the former. The descriptions of the target chemical composition are agreed also.

The neutron transfer is simulated with the help of original neutron transport code LOENT on the basis of the 26-group neutron constants BNAB [14]. The elastic and inelastic neutron scattering, (n,2n) reaction, neutron capture and neutron induced fission are taken into account. The elastic scattering is treated according to linear-anisotropic approximation. Any other neutron transport code can be connected with SHIELD instead of the LOENT code, in particular the MORSE code. The compatibility of the geometric module of the SHIELD and MORSE codes is provided foreseeing this potentiality.

Both direct and weighted simulation of the hadron cascades are foreseen in the SHIELD code. The availability of the weighted mode enables to apply standard techniques for rare events simulation, as in the case of forced meson decays, and reserves also the possibility of inclusion of weighted inclusive hA-generators into the SHIELD code.

It is pertinent to note here that the SHIELD code was designed bearing in mind the ease of the code modification and development. In particular, the inclusion of a new particles in hadron cascade was foreseen as well as the replacement of hA-generator (or inclusion of an alternative ones), enlargement of inner storage with the hadron energy, etc. The code's open architecture has proven itself in actual practice.

The main original features of the SHIELD code, in our opinion, are the following: (1) complete memorizing of the hadron cascade tree during its generation; (2) using of created in Russia advanced exclusive hA-generator which is not used in other transport codes (see sect. 2.2).

Memorizing of the hadron tree is being performed in special arrays: all individual characteristics of the secondary particles over all generations are stored as well as all events of particle decay, flying out of the target or absorption due to ionization loss; all acts of elastic or inelastic hA-interaction including individual variables of each residual nucleus (nuclei) are stored also. The tree is stored having been coupled with the geometric configuration of the target, i.e. for each particle the inlet and outlet coordinates and energies are being stored in each crossed geometric zone, etc. Simultaneously the neutron and $e^{\pm}\gamma$-sources are being stored as mentioned above. As a result, on completion of the hadron tree generation it finds itself stored without any loss of physical information. Such organization of simulation allows to separate completely a modeling and registration parts of the code, to store trees into magnetic media if required, and facilitates the tree visualization and consideration in time.

It is impossible to describe here the tree memorizing algorithm even briefly. Let us notice only that in practice it turns out very reliable and fast enough. The requirements on memory size are moderate: memorizing of a single tree at primary energy range of $1\div3$ GeV requires up to 24 Kb. At 100 GeV and for large complex targets up to 800 Kb is needed. As trees are stored dynamically, at tree processing operations appears the actual tree arrays length but not the maximal one. A simple procedure of the tree arrays enlargement is foreseen if required.

2.2 Simulation of inelastic hadron-nucleus interaction

The capabilities and quality of a hadron transport code depends substantially on a hA-generator used. The exclusive hadron-nucleus generator of the SHIELD code involves presently the following nuclear models: Dubna version of the intranuclear cascades model CASCAD detailed in monograph [10] and survey [15]; hadron-nucleus and nucleus-nucleus generator QGSM based on an independent quark-gluon string model [16]; extended nuclear deexcitation model DEEX [17] considering the Fermi break up, multifragmentation and evaporation/fission processes.

Simultaneous presence of two models (CASCAD and QGSM) for description of a fast nuclear reaction stage is caused by the following. The CASCAD model uses continuous nuclear density approximation which provides an adequate description of nuclear reaction for medium and heavy nuclei at the energies of incident hadrons (nucleons or pions) up to $3\div5$ GeV. However this approximation is not quite correct for light nuclei. Besides, the changes in nuclear density during interaction process are not taken into account in the CASCAD model with a consequent distortion of results with increase in energy [15]. On the contrary, in the QGSM model the location of intranuclear nucleons is described with individual coordinates according to nuclear density distribution. This allows to take automatically into account the changes in nuclear density and consider all nuclei including the lightest ones. The QGSM model is applicable in energy range up to 0.5 TeV due to an independent quark-gluon string model is used for description of the hadron-nucleon intranuclear interactions. On the same reason, apart from pions and nucleons, the kaons, antinucleons and some other mesons and barions are included in interaction process. At the same time the QGSM generator requires much more CPU time in comparison with CASCAD one, especially in the case of heavy nuclei.

Therefore the CASCAD generator is used in the SHIELD code for incident pions and nucleons with energies below 1 GeV and for nuclei heavier then oxygen. In all other cases the QGSM generator is used. Special comparison has demonstrated that these two generators are very well butted on the boundary.

After a fast stage of hA-interaction is completed the simulation of a deexcitation stage begins according to the DEEX model. For light excited residual nuclei with A $\leq$ 16 the classic Fermi break up mechanism starts. It results in two or more light nonexcited fragments and nucleons with known momentum. For heavier residue the multifragmentation or equilibrated decay (evaporation) processes are possible. As multifragmentation mechanism is significant at high excitations only [18] it starts if excitation energy exceeds 2 MeV/nucleon. (Let us note that simulation of multifragmentation requires much more CPU time as compared with evaporation). As a result either several excited nuclear fragments can be formed or, if the multifragmentation process was not realized, the equilibrated decay occurs. The latter is true for excitations lower then 2 MeV/nucleon. Evaporation of neutrons, protons, deuterons, tritons, ^3He-nuclei, and alphas is taken into account. The evaporation-fission competition [19] for heavy nuclei can results in two fission fragments with known individual parameters (A,Z, kinetic and excitation energy). Excited multifragmentation and fission fragments deexcite, in turn, according to the above scheme. As a result the individual characteristics of all particles and nuclear fragments formed on deexcitation stage are defined. The physical models realized in the DEEX code are detailed in [18,19]. The above numerical parameters are found from computational experience and comparison with experimental data.

2.3 Registration

Once a hadron tree generation and storage have been completed the tree processing begins to build up the distributions and functionals of interest.

As the tree is stored without any loss of physical information one can, knowing the structure of the tree arrays, write a tree processing subroutine to extract any desirable results. At the same time the SHIELD code contains a special subroutine for registration of some general characteristics, such as:

- energy spectra of hadrons which escaped a target
- energy spectra of all particle sources over a whole target
- distribution of energy deposition in a target on the geometric zones for different processes separately (ionization loss, $e^{\pm}\gamma$-showers etc.)
- similar distribution of elastic and inelastic interactions

- (A,Z)-distribution of residual nuclei over a whole target

In addition some results of a neutron transport calculation are registered by the LOENT code:

- energy spectrum of neutrons which escaped a target
- distribution of neutron-induced reactions of each type on the geometric zones

These results display general picture of hadron transport process, in particular the total energy balance. In some calculations this output turns out quite enough and no additional tree processing subroutine is required. It is true for example presented below.

The SHIELD code is written on FORTRAN 77. Source code size is about 50000 lines, load module volume - up to 5 Mb. Presently the SHIELD code runs on VAX-11/780 (under VMS), IBM PC AT-386/387 (MS-DOS) and SUN SPARCclassic (SunOS). To achieve sufficient statistical accuracy at incident energy about 1 GeV in the typical tasks from one to a few hours of CPU time are required (on VAX-11/780). At 100 GeV of energy and for large targets the required CPU time rises by a factor of 10^2.

3 Interaction of 0.3÷70 GeV proton beam with tungsten and uranium targets

To demonstrate the operation of the SHIELD code, in this section the results of simulation of intermediate energy proton beam interaction with fissible and nonfissible massive targets are presented.

These results are interested in the context of existing conceptions of intensive pulsed neutron sources based on the high-intensity proton accelerators. The most commonly encountered and realized by this time scheme is based on a "meson factory" (beam energy about 1 GeV at an average current of 1 mA). At the same time there is an alternative conception [20] with the using of "kaon factory" (beam energy 10÷50 GeV at respectively lower current). The advantages of this scheme are associated with lower energotension in a target and, what is more important, lower particle fluence at the target inlet ("the first wall problem"). The neutron yield from the target increases strongly with the energy while the beam energy fraction pumped into electromagnetic showers due to π^0 decay rises progressively. The results given below enable to discuss quantitatively the optimal target-beam parameters of a neutron source.

The target at the computations was a cylinder 20 cm in diameter and 60 cm in length consisting of metallic natural tungsten or uranium−238. The pencil proton beam was directed along the axis of the cylinder, proton energies were of 0.3, 0.6, 0.8, 1, 1.5, 3, 10, 30, and 70 GeV. Cylinder was broken down in depth along the beam direction into 20 geometric zones (10 zones of 1 cm plus 10 zones of 5 cm).

Fig.1−6 show calculated data for tungsten target, Fig.7−12 demonstrate analogous results for uranium one while Fig.13 gives some comparison of them.

First we consider some values integrated over a whole target versus beam energy.

In Fig.1a,7a show fractions of the beam energy expended for forming of a source of neutrons with kinetic energies less then 10.5 MeV (this fraction includes kinetic and binding energies) and for energy deposition in the target as well as energy leakage from the target during hadron cascade development as a percentage of beam energy.

A structure of energy deposition of the hadron and electromagnetic(EM) cascades in the target is presented in Fig.1b,7b. Taking the total release energy as 100% it is pictured what a fraction was realized due to ionization loss of charged particles, electromagnetic showers and as kinetic energy of residual nuclei. The residual excitation energy once nuclear deexcitation completed is presented also. As can be seen, the latest fraction going into electromagnetic deposition is small all over the beam energy area.

Fig.2a,8a give total number of the source neutrons, the neutron yield all over a target surface, number of inelastic interactions ("stars") in the target, and number of stars involving fast fission.

The neutron yield across lateral area and both end-walls of the target separately is presented in Fig.2b,8b.

Fig.3,9 illustrate the charge distribution of nuclei-products formed during hadron cascade development for beam energies of 1,10, and 30 GeV.

Further some spatial distributions (in target depth) are considered. Calculated histogramms were smoothed out for ease of visual perception.

Fig.4,10 display the profiles of full energy deposition for some beam energies under consideration. The net all over the target energy deposition is indicated near each curve.

Notice that the correct account of energy transfer by electron-photon showers becomes essential for forming of the proper energy deposition profile (including maximum location) as beam energy increases. While at low beam energy it is acceptable to consider that the electromagnetic energy is releazed locally at the π^0 decay point, this is wrong for higher energies, as Fig.5,11 illustrate.

Fig. 6,12 exhibit the spatial distribution of the neutron source and star density which, can be seen to be propotional to each other.

It is pertinent to compare some parameters for fissible and nonfissible targets. Fig. 13a shows total energy deposition in W and U targets including contribution from source neutrons transport calculation by means of the LOENT code which presented separately as a whole. The contributions of residual nuclei (fission fragments) kinetic energy in the hadron cascade to the energy release are shown also. As can be seen, in the uranium target the contribution of fission (both fast and neutron-induced one) prevails all over beam energy area while in tungsten one the energy deposition is determined by ionisation loss and electromaghnetic showers.

Fig. 13b demonstrates the specific number of source neutrons and specific neutron yield (E < 10.5 MeV) for both targets.

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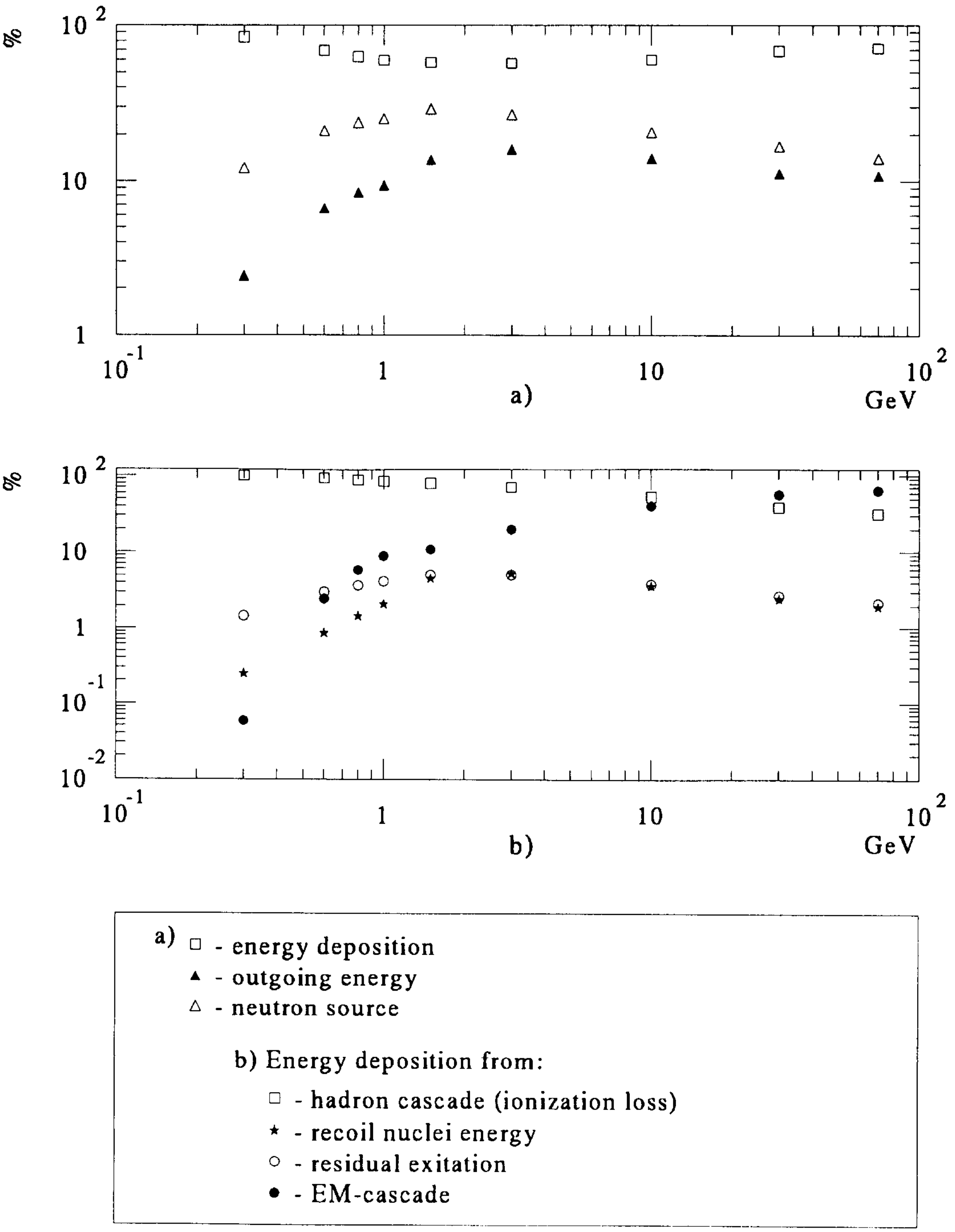

Figure 1: W target: a) Fraction of proton beam energy (in percents) have been spent on neutron source forming, target warming and removed from target (by hadron and electromagnetic cascades); b) Structure of heat release in dependence of primary proton energy (100 % – energy deposition from hadron and EM cascades).

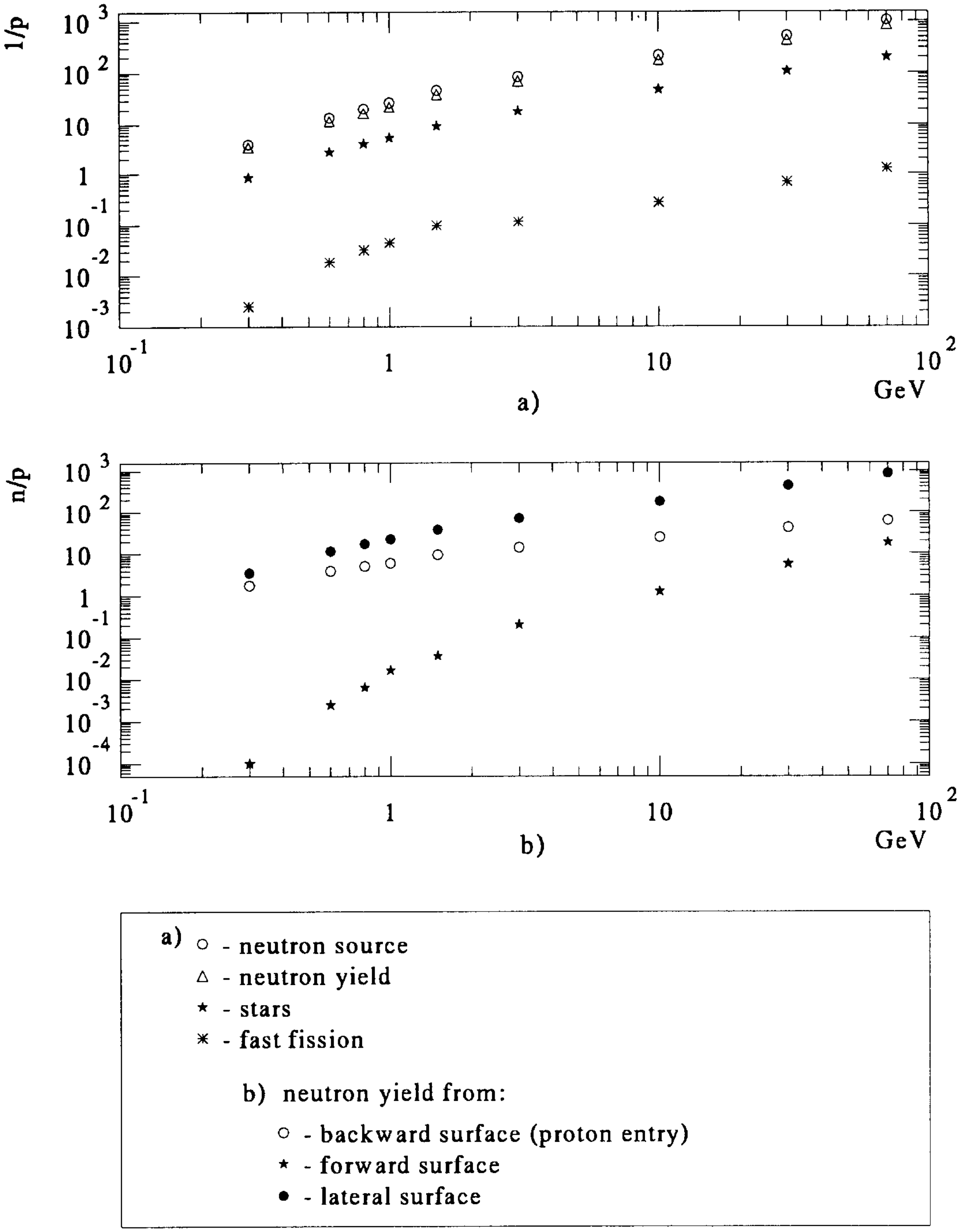

Figure 2: **W target: a) Neutron source, neutron yield ($E_n < 10.5$ MeV) and number of stars in target. ; b) Neutrons yield for different sides of target.**

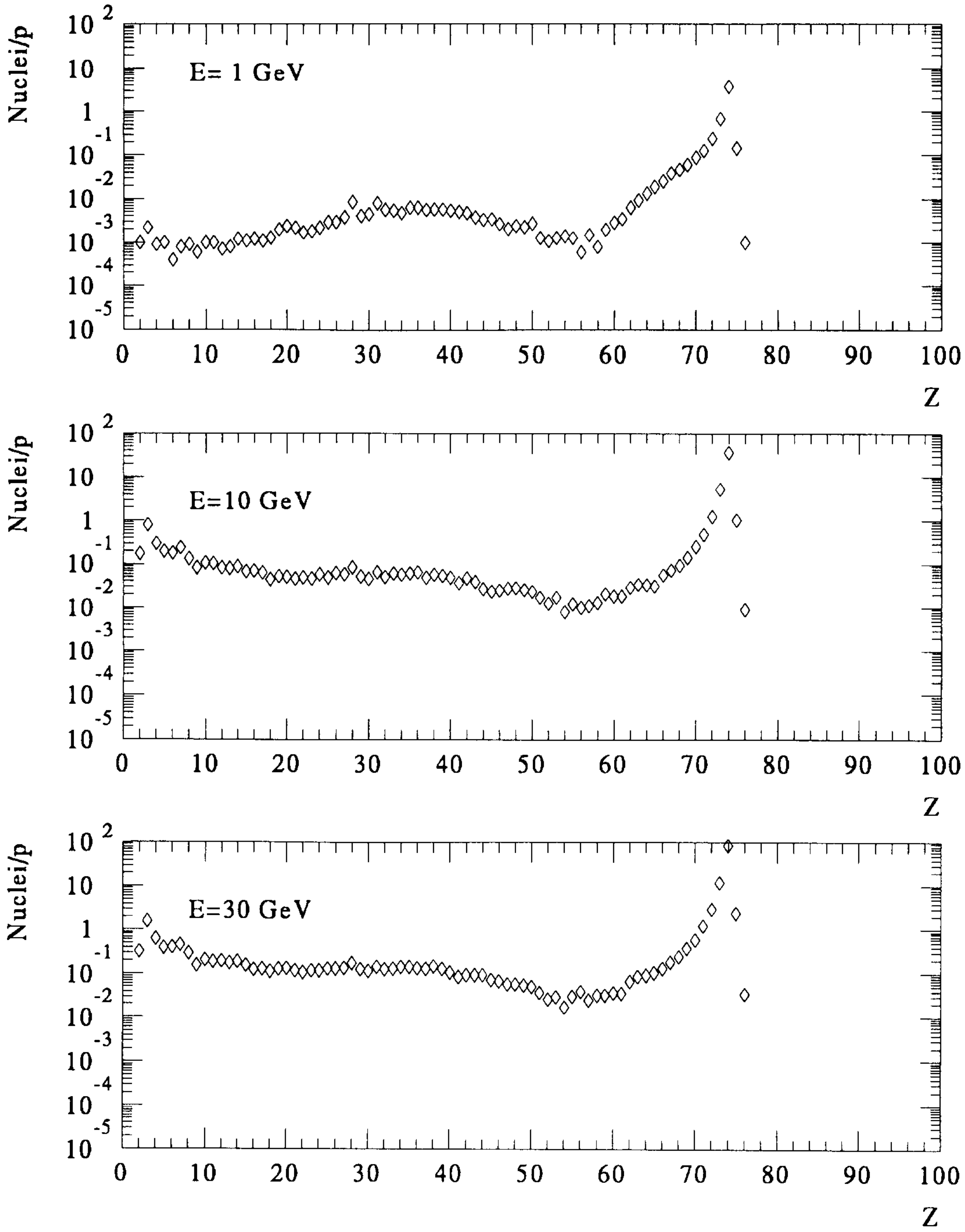

Figure 3: W target: Spallation products yield charge distribution for different beam energies.

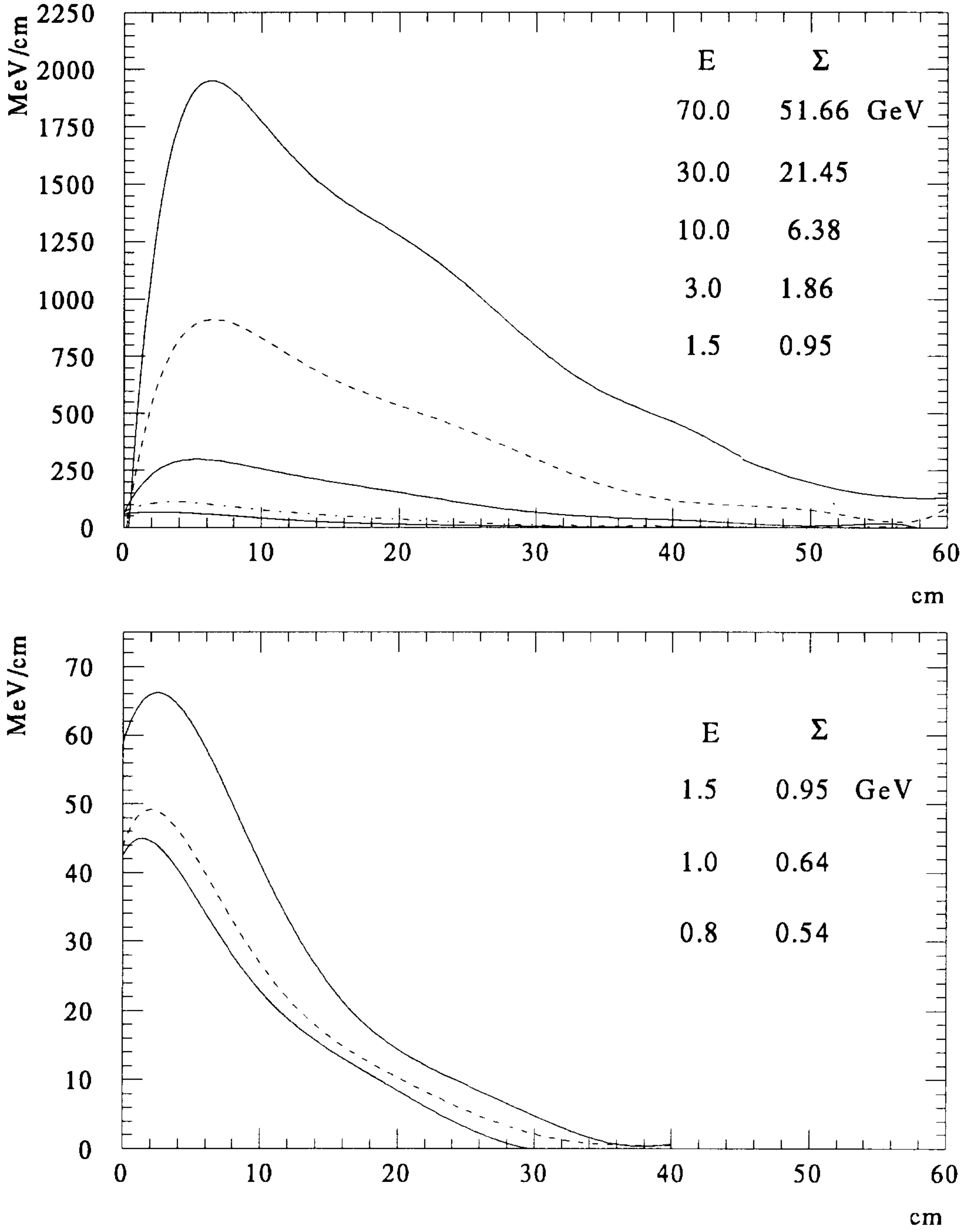

Figure 4: W target: Profile of full energy deposition at target depth (E - energy of primary proton, Σ - energy deposition for whole target).

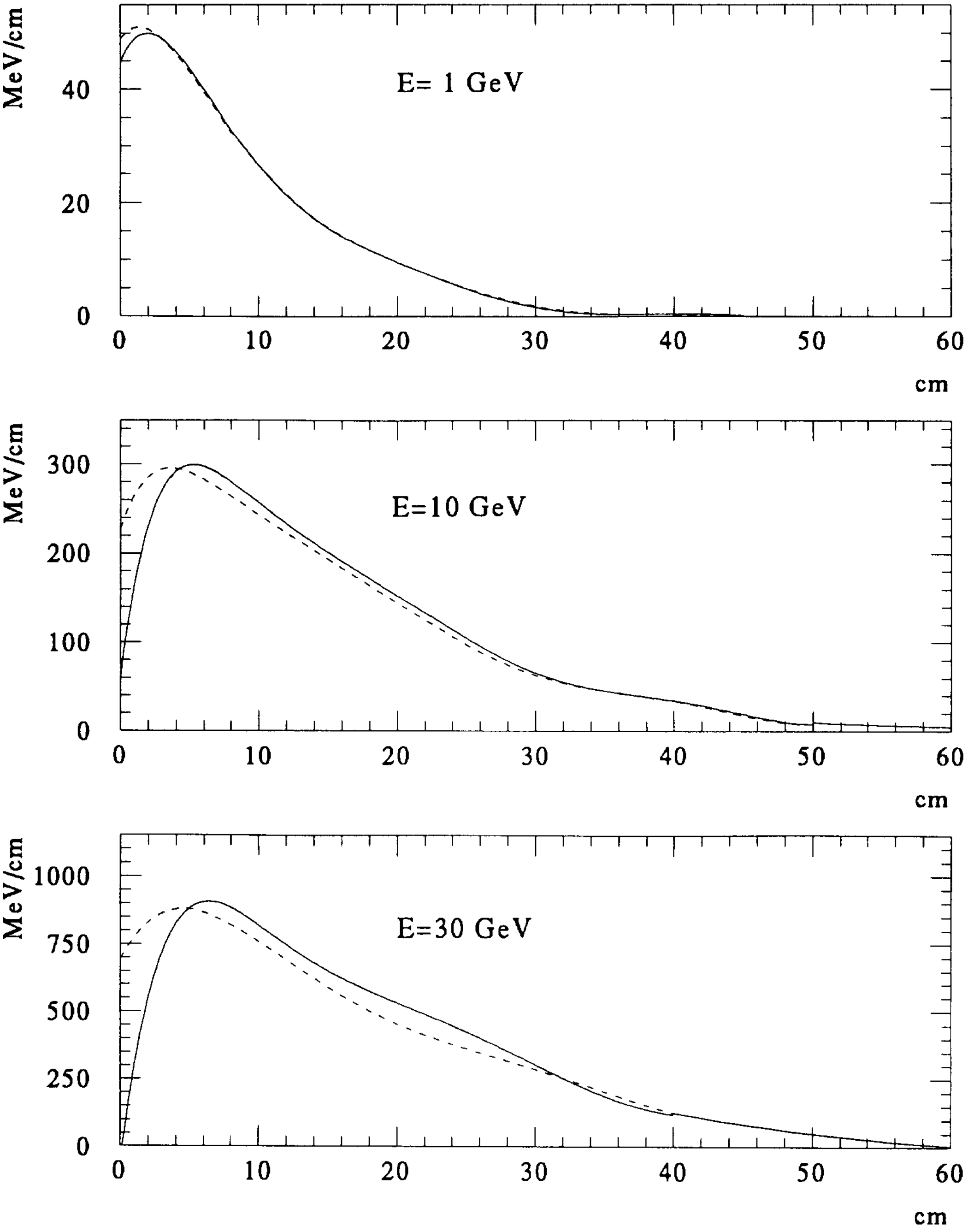

Figure 5: **W target: Profile of full energy deposition at target depth: solid line – calculation with consideration of EM-cascade (EGS4), dashed line – calculation in approximation of local energy release at point of π^0 decay.**

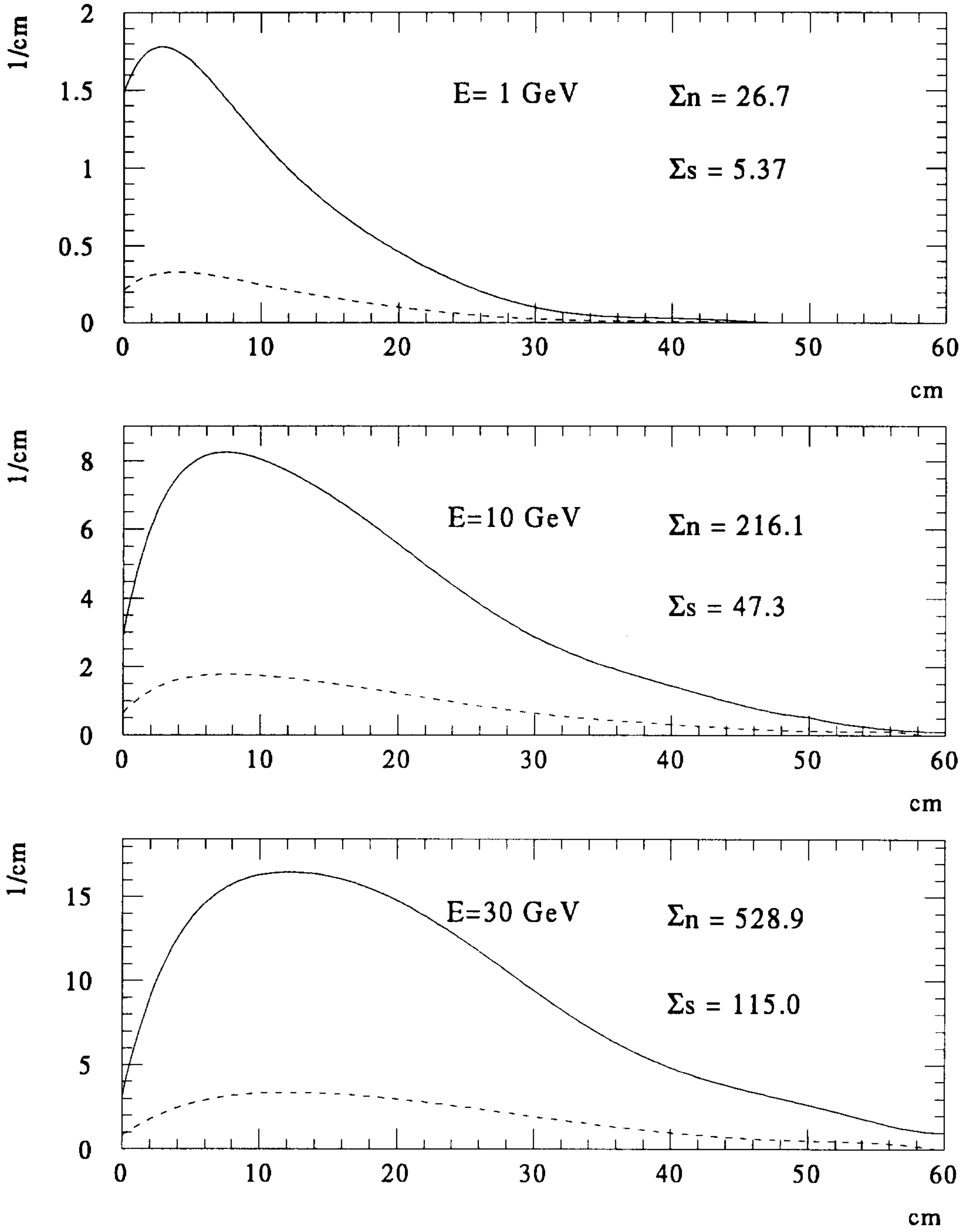

Figure 6: W target: Profiles of neutron source and star density at target depth (E - energy of primary proton, Σ - value for whole target; solid line – neutron source, dashed line – stars).

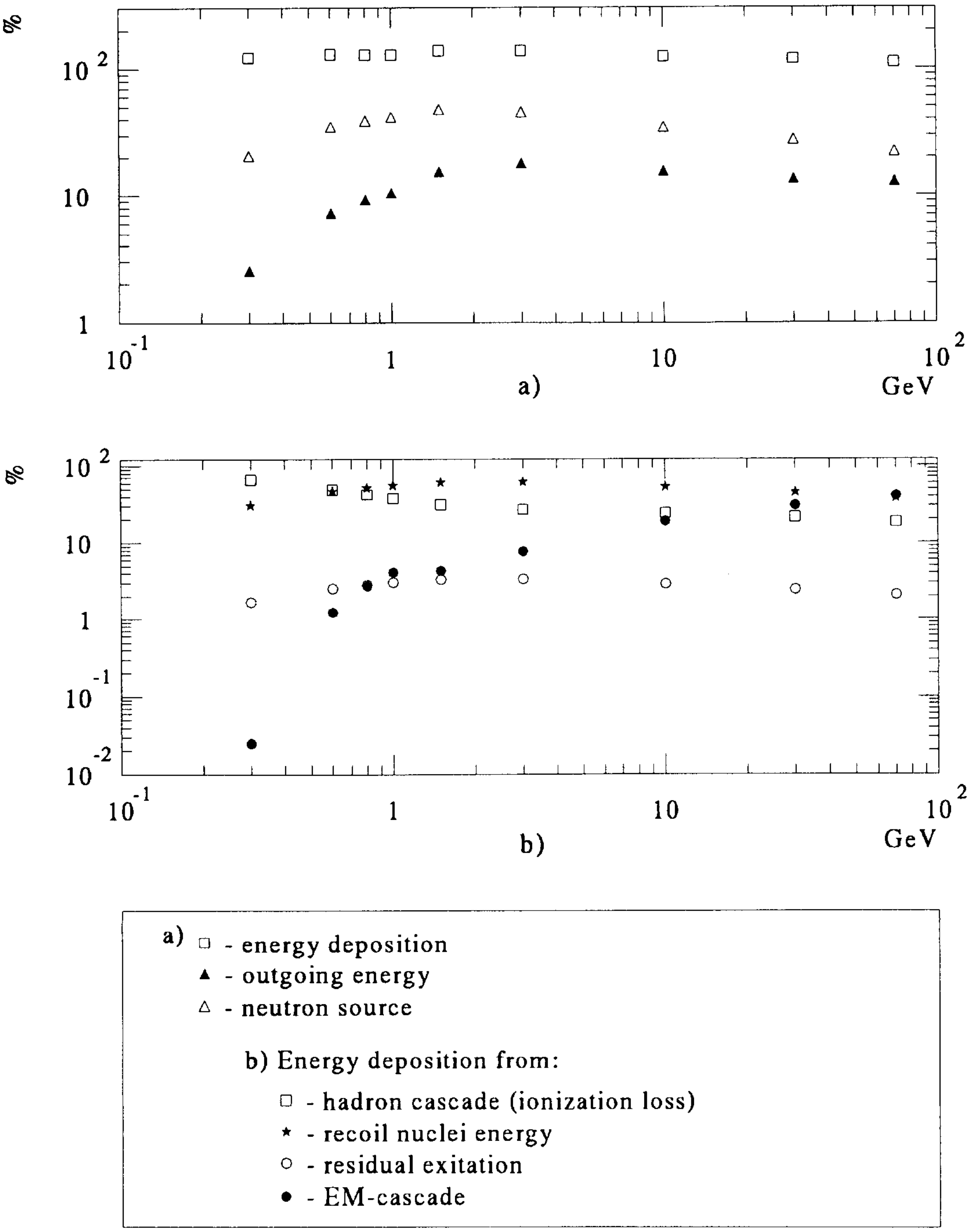

Figure 7: The same as Fig.1 for U target. (Energy deposition exceeds beam energy due to fast fission)

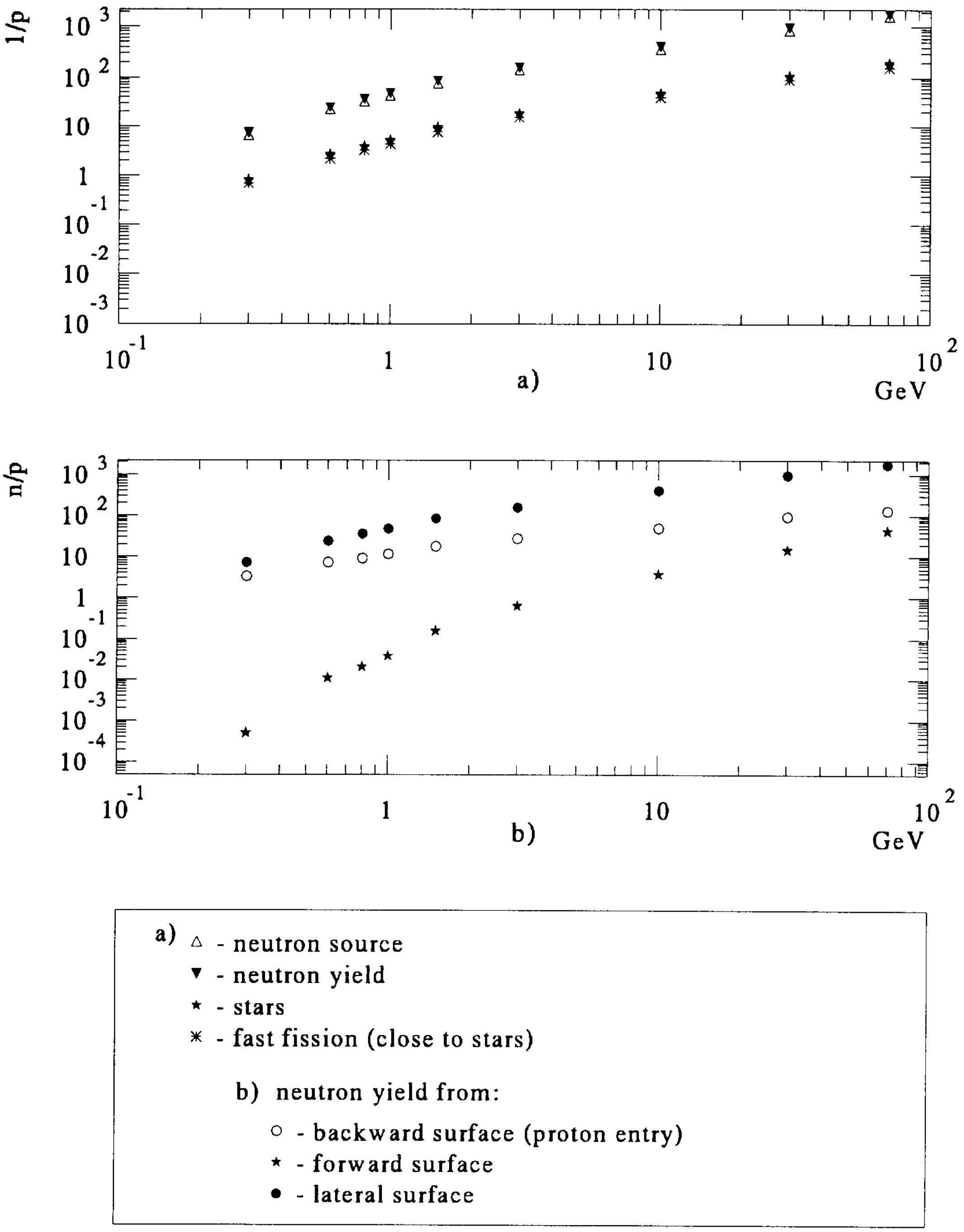

Figure 8: The same as Fig.2 for U target.

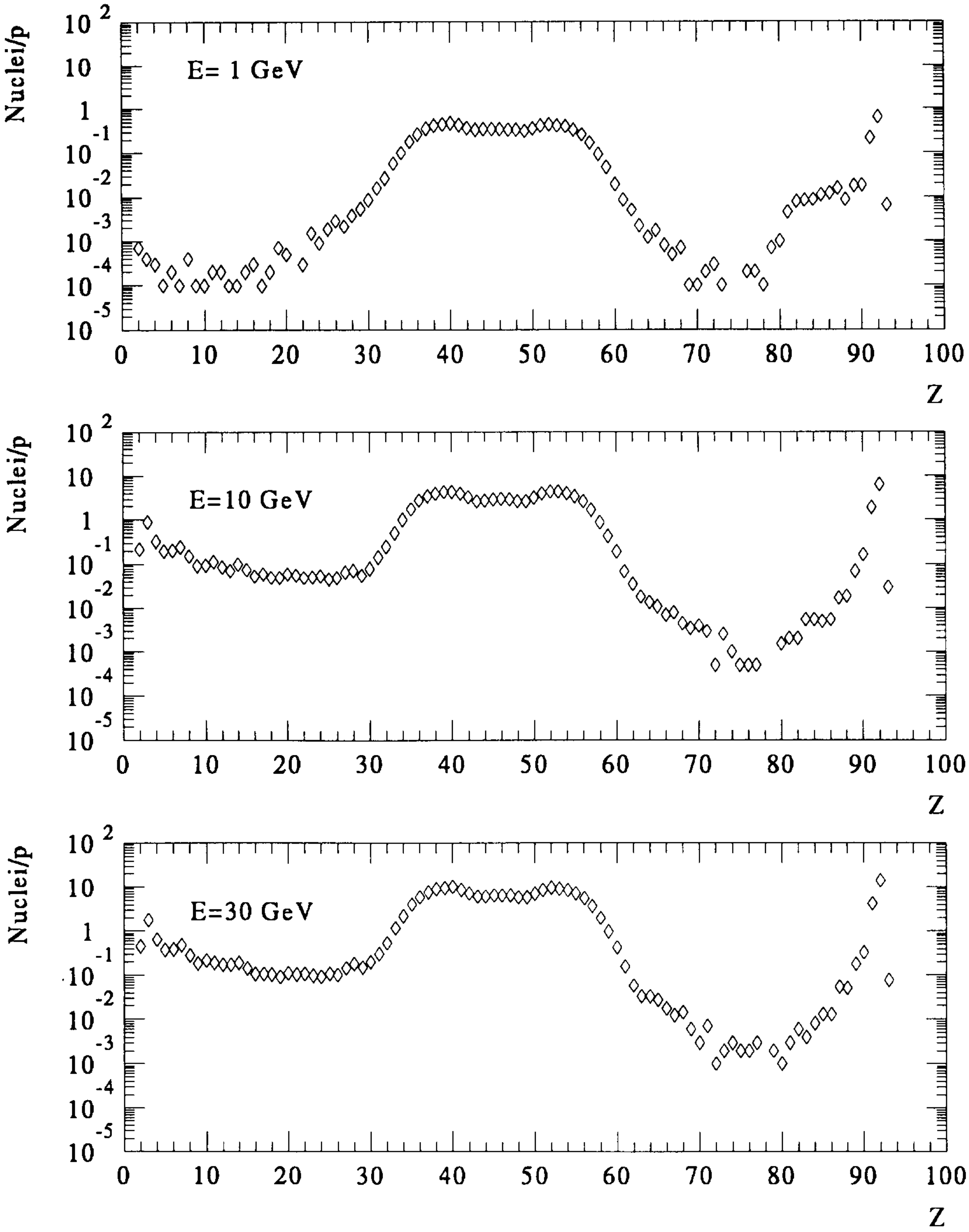

Figure 9: The same as Fig.3 for U target.

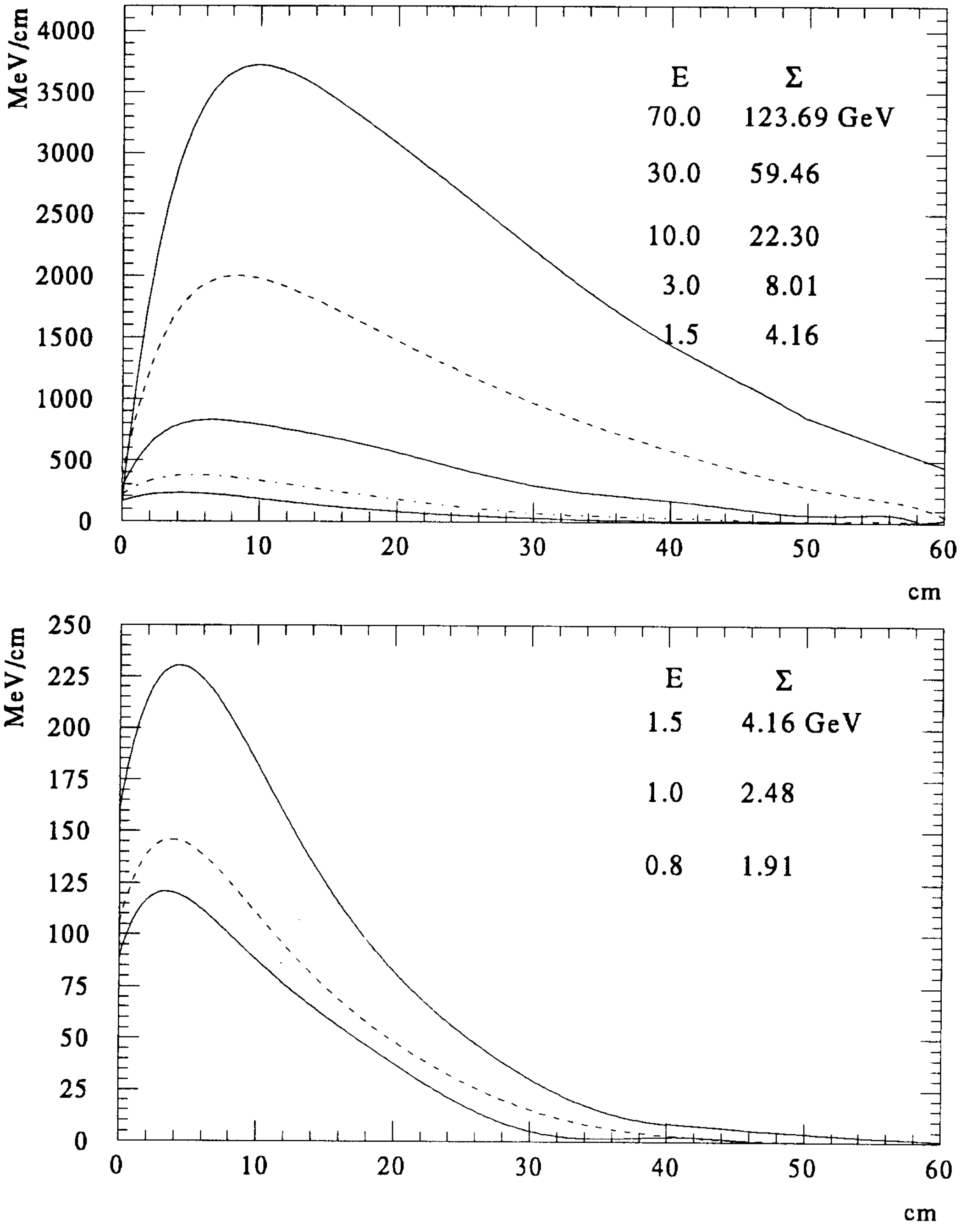

Figure 10: The same as Fig.4 for U target.

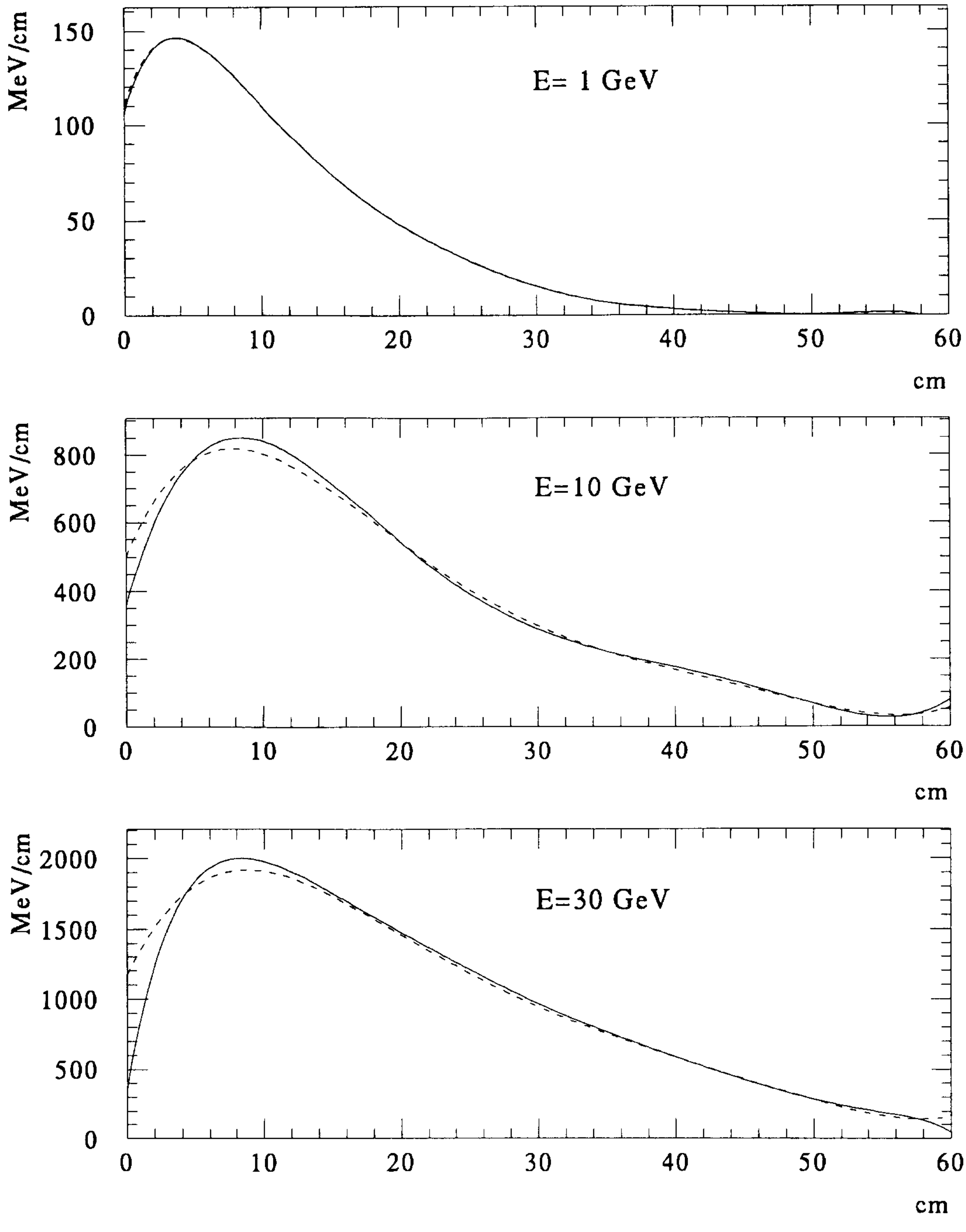

Figure 11: The same as Fig.5 for U target.

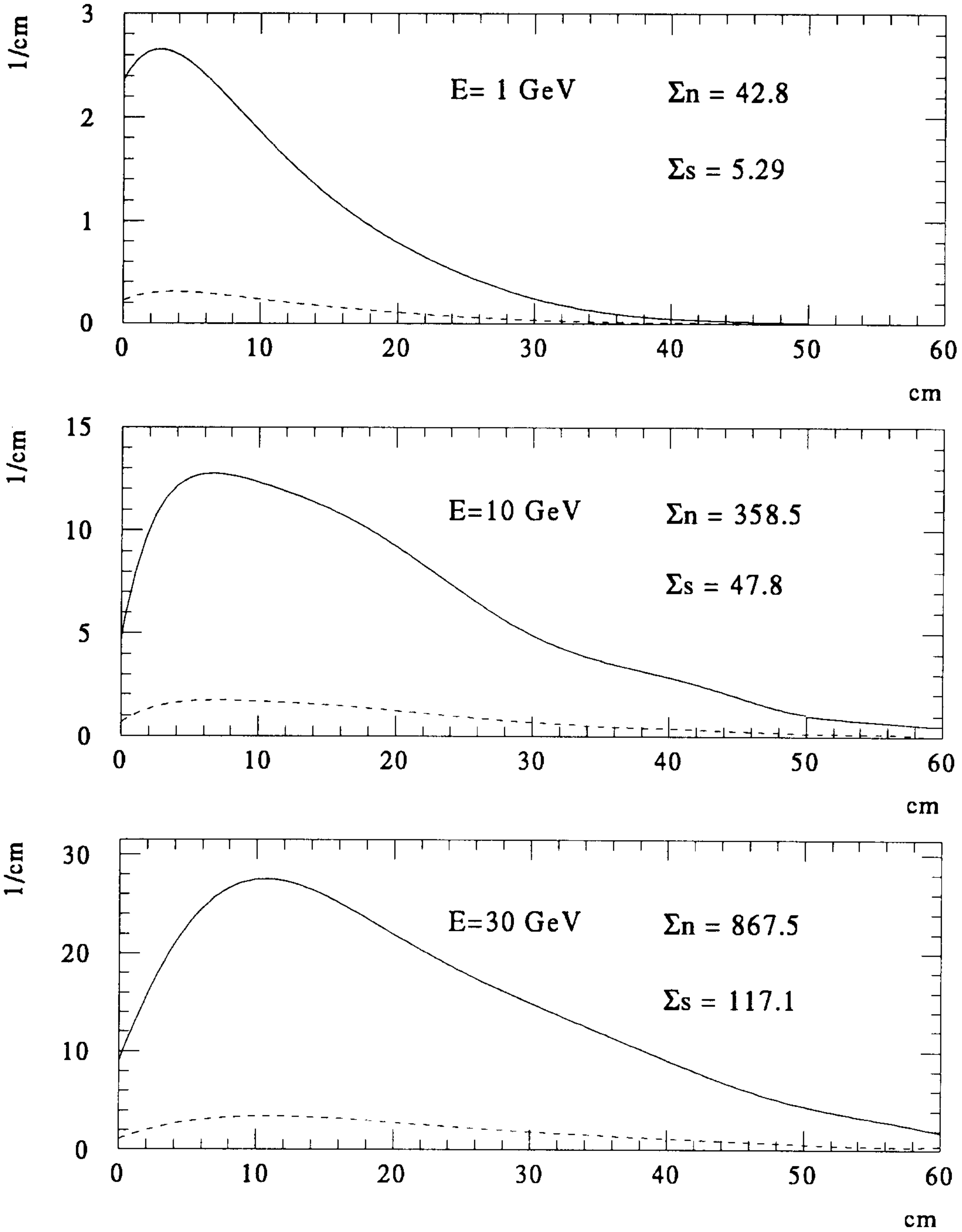

Figure 12: The same as Fig.6 for U target.

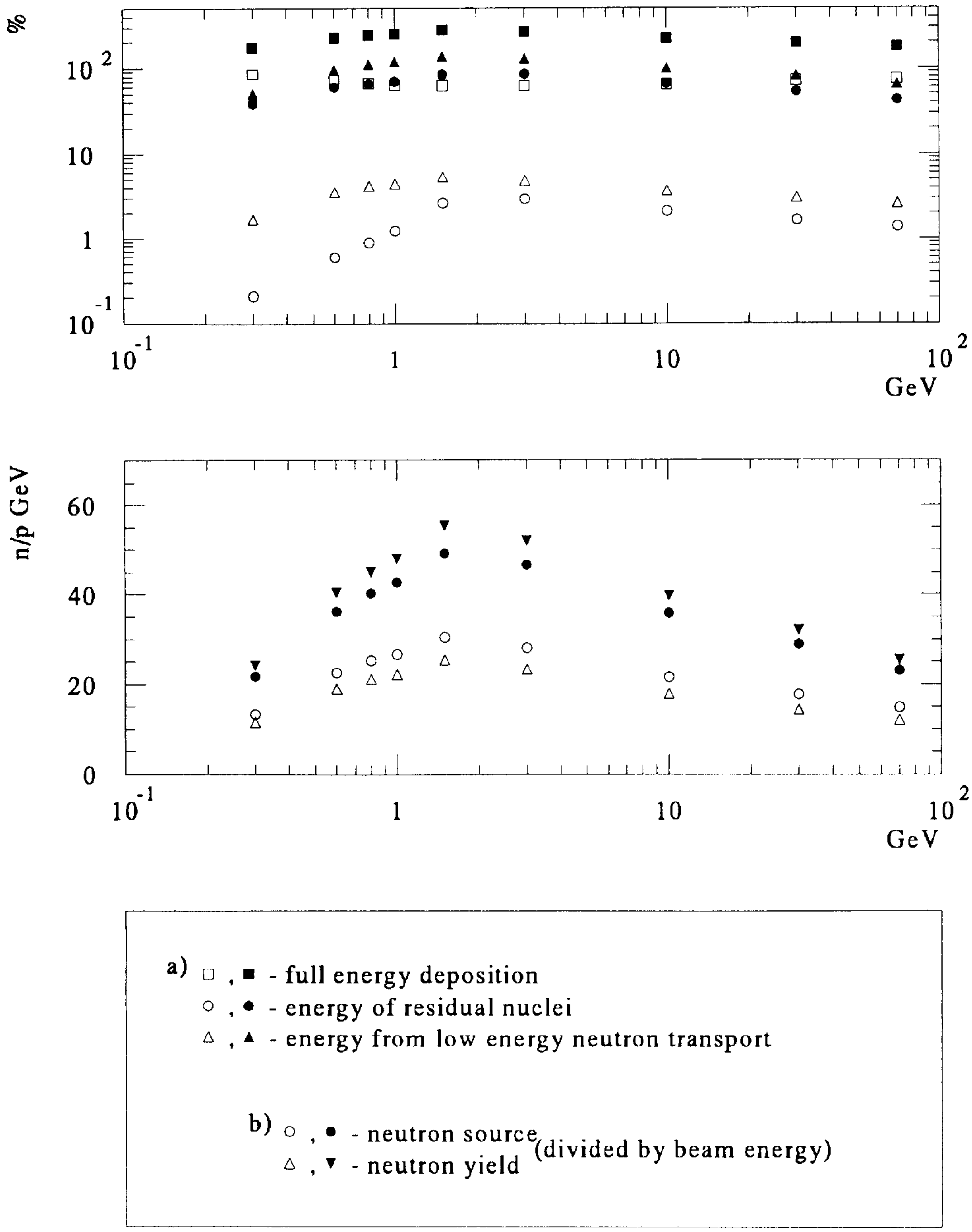

Figure 13: **Energy deposition (a) and specific neutron source an yield (b) for both targets (W – light symbols, U – dark symbols).**