



Simulation of Nucleon Elastic Scattering in the MARS14 Code System*

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Abstract – *Correct modeling of nucleon elastic scattering is of special importance in many applications at high energy accelerators, such as deep penetration, beam loss and collimation studies. In present paper, the work performed to update the MARS elastic scattering model at $E < 5$ GeV is described. Modern evaluated nuclear data as well as fitting formulae are used in the new model. For protons as projectiles, Coulomb scattering and Coulomb-nuclear interference are taken into account in addition to nuclear elastic scattering. Comparisons with experimental angular distributions and calculations by means of other codes are presented.*

I. INTRODUCTION

Correct description of nucleon elastic scattering distributions is of special importance in numerous applications at high energy accelerators. In many cases particles scattered at small angles determine radiation field at large distances from the source of radiation. At nucleon energies above 5 GeV a reasonable systematics exists¹ which reproduces smooth dependence of considered distributions on projectile energy and target nucleus mass. Below 20 MeV the most correct description of neutron transport in matter can be performed by means of the MCNP computer code.² Recently this region has been extended for a number of important nuclides up to 150 and 250 MeV for neutrons and protons as projectiles, respectively. It gave rise to development of the MCNPX radiation transport code as an advanced alternative to LAHET-MCNP coupling.³ In the energy region from 150 MeV up to 5 GeV a systematics is used usually which reproduces diffraction scattering more or less adequately.

The multi-purpose MARS14 code system was developed for simulation of radiation transport in matter in the energy region up to 100 TeV.¹ While the extremely high upper en-

ergy limit is pertinent to frontier physics research, the lower energy region (below 5 GeV) is very important from the practical standpoint. In present paper the work performed to update the elastic scattering model in this lower energy region is described.

II. CALCULATION MODEL

Neutron elastic scattering is pure nuclear scattering and described by means of tabulated distributions in existing evaluated nuclear data libraries. For protons as projectiles, in addition to nuclear elastic scattering, one takes into account Coulomb scattering as well as Coulomb-nuclear interference. As a rule, charged particle small- and large-angle collisions are simulated separately⁴: (i) dominant small-angle scattering, i.e. multiple Coulomb scattering, is described by means of analytical distributions taking into account nuclear finite size; (ii) large-angle scattering events are considered as discrete nuclear reactions. In modern evaluated nuclear data libraries proton elastic scattering distributions are often presented as tabulated “*nuclear + interference*” ones⁵ which makes it impossible to extract the pure *nuclear* component and implement the simplest approach. Therefore, Coulomb-nuclear interference is taken into account in our elastic scattering model whenever relevant data on interference component is available.

II.A. Evaluated nuclear data used in MARS code

At present the most comprehensive collection of evaluated nuclear data files for neutron energies up to 150 MeV (250 MeV for protons) is contained in the ENDF/B-VI library.³ At the same time, there are several evaluations for nucleon energies up to a few GeV,⁶ in particular, for nuclides ¹²C, ⁵⁶Fe, and ²⁰⁸Pb. Thus, for these three nuclides we use evaluated nuclear data from both the sources, with Coulomb-nuclear interference having been ignored in the latter evaluated data files

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for protons.⁶ For several nuclides, in addition to the ENDF/B-VI library, we use other evaluated data.⁷⁻⁹ All the data used in the MARS14 code system are listed in Tables I and II.

TABLE I. Evaluated nuclear data for incident neutrons used in MARS14

Nuclide	E_{max} (MeV)	Reference	Reference date
1. 1-H-1	150	3	1999
2. 6-C-12	5000	3, 6, 8	1999 1996, 2000
3. 7-N-14	150	3	1999
4. 8-O-nat	150	3	1999
5. 13-Al-27	150	3	1999
6. 14-Si-28	150	3	1999
7. 15-P-31	150	3	1999
8. 20-Ca-nat	150	3	1999
9. 26-Fe-56	1000	3, 6	1999, 1988
10. 28-Ni-58	150	3, 9	1997, 2000
11. 29-Cu-63	150	3	1997
12. 41-Nb-93	150	3	1997
13. 74-W-184	150	3	1999
14. 82-Pb-208	1000	3, 6	1999, 1990
15. 92-U-238	150	7	2000

II.B. Simulation procedure

Angular distribution of elastically scattered neutrons at low incident energies can be represented as a Legendre polynomial series:⁵

$$f(\mu, E) = 2\pi \frac{\sigma(\mu, E)}{\sigma_s(E)} = \sum_{l=0}^{l_{max}} \frac{2l+1}{2} a_l(E) P_l(\mu), \quad (1)$$

where μ is cosine of the scattering angle, E is the projectile energy in the laboratory system, $\sigma_s(E)$ is scattering cross sec-

TABLE II. Evaluated nuclear data for incident protons used in MARS14

Nuclide	E_{max} (MeV)	Reference	Reference date
1. 6-C-12	5000	3, 6, 8	1996 1996, 2000
2. 26-Fe-56	1000	3, 6	1996
3. 28-Ni-58	150	9	2000
4. 82-Pb-208	1000	3, 6	1996
5. 92-U-238	150	7	2000

tion, $\sigma(\mu, E)$ is differential scattering cross section (b/sr), and $a_l(E)$ is the l^{th} Legendre polynomial coefficient, with $a_0(E)$ being equal to 1. The above representation implies azimuthal symmetry and correct normalization for the probability density function, $f(\mu, E)$. Evaluated nuclear data libraries contain tabulated values of $a_l(E)$ and $\sigma_s(E)$. At high energies, adequate representation of strongly forward-peaked angular distributions would require a lot of coefficients $a_l(E)$. Their absolute values decrease fast with l which involves additional computational tricks to prevent loss of accuracy. Therefore, above 20 MeV (and sometimes below 20 MeV as well) tabulated values of the probability density function, $f(\mu, E)$, are used instead of such a polynomial expansion.

A proton differential scattering cross section (assuming that projectile and target are not identical) can be written as:⁵

$$\sigma(\mu, E) = \sigma_c(\mu, E) + \sum_{l=0}^{l_{max}} \frac{2l+1}{2} a_l(E) P_l(\mu) - \frac{2\eta}{1-\mu} \operatorname{Re} \left\{ \exp \left(i\eta \ln \frac{1-\mu}{2} \right) \sum_{l=0}^{l_{max}} \frac{2l+1}{2} b_l(E) P_l(\mu) \right\}, \quad (2)$$

where $\eta = Z_1 Z_2 \left[(2.48058 \times 10^4) m_1 / E(eV) \right]^{1/2}$, $\sigma_c(\mu, E)$ is the differential Coulomb scattering cross section, m_1 is the projectile mass (a.m.u.), a_l are real coefficients for expanding the pure nuclear scattering cross section, and b_l are complex coefficients for expanding the trace of the nuclear scattering amplitude matrix. The integrated cross section for the expression (2) is not defined and not required for the elastic scattering simulation procedure. From practical standpoint, a useful approach to represent the differential cross section (2) is to tabulate only “nuclear + interference” components:⁵

$$\sigma_{ni}(E) = \int_{\mu_{min}}^{\mu_{max}} [\sigma(\mu, E) - \sigma_c(\mu, E)] d\mu \quad (3)$$

and

$$p_{ni}(\mu, E) = \frac{\sigma(\mu, E) - \sigma_c(\mu, E)}{\sigma_{ni}(E)}, \mu_{min} \leq \mu \leq \mu_{max}, \quad (4)$$

$$= 0, \text{ otherwise}, \quad (5)$$

where $\mu_{min} = -1$, if target and projectile are not identical, otherwise μ_{min} equals to 0, and μ_{max} is as close to 1 as possible. When using the last representation, evaluated nuclear data libraries contain tabulated values $\sigma_{ni}(E)$ and $p_{ni}(\mu, E)$. For neutrons, in addition to the tabulated values $\sigma_s(E)$, $a_l(E)$, and/or $f(\mu, E)$, the tabulated total cross section $\sigma_t(E)$ is used as well. To extract from the ENDF/B files all the values required for nucleon elastic scattering simulation procedure, a set of processing routines has been developed for MARS14.

For both neutrons and protons as projectiles a non-analog procedure is used when sampling cosine of the center-of-mass scattering angle, μ . However, the particles are treated differently because of different description of their angular distributions in evaluated nuclear data files.

For neutrons, a biased probability density function (p.d.f.), $p(\mu, E)$, is introduced which reproduces forward-peaked behaviour of the distributions:

$$p(\mu, E) = \frac{1}{\sigma_\mu} \sqrt{\frac{2}{\pi}} \exp \left[\frac{-(1-\mu)^2}{2\sigma_\mu^2} \right], \quad (6)$$

where $\sigma_\mu(E)$ is a function of projectile energy and target nucleus mass. The value of $\sigma_\mu(E)$ is determined from the equality condition for $p(\mu, E)$ and $f(\mu, E)$ at $\mu = 1$, resulting in:

$$\sigma_\mu(E) = \left[\sqrt{\frac{\pi}{2}} \sum_{l=0}^{l_{max}} \left(l + \frac{1}{2} \right) a_l(E) \right]^{-1}. \quad (7)$$

Next step is to perform sampling of the μ values using the p.d.f. $p(\mu, E)$ with $\sigma_\mu(E)$ defined by expression (7). Let us consider numerical values of $\sigma_\mu(E)$ presented in Table III. One can see that the total numerical interval for $(1-\mu)$ values, namely $[0, 2]$, can contain from about two up to several hundred sub-intervals of width $\sigma_\mu(E)$. Taking this into account, the sampling the μ values is performed in the following manner:

- A total interval for the $(1-\mu)$ values is divided into sub-intervals $[0, \sigma_\mu]$, $[\sigma_\mu, 2\sigma_\mu]$, ..., $[k\sigma_\mu, 2]$, where k depends on $\sigma_\mu(E)$ for the target nucleus under consideration.
- A set of probabilities p_i , with $i = 1, \dots, k+1$, is assigned to this set of the sub-intervals. A probability to sample $(1-\mu)$ within $[0, \sigma_\mu]$ is supposed to be equal to 0.68, the probabilities for the subsequent sub-intervals ($[\sigma_\mu, 2\sigma_\mu]$ and so on) decreasing fast. For the last sub-interval, the probability is defined according to the expression $p_{k+1} = 1 - \sum_{i=1}^k p_i$.

- An importance function q_i , $\sum_{i=1}^{k+1} q_i = 1$, is brought into consideration to improve description of low-probability large-angle scattering events.
- A sub-interval $[(i-1)\sigma_\mu, i\sigma_\mu]$ (or $[k\sigma_\mu, 2]$) is sampled according to the probabilities q_i taking into account corresponding weight factors p_i/q_i .
- Sampling μ by means of the p.d.f. (6) within the sub-interval sampled at previous step.
- Having sampled the value $\tilde{\mu}$ at previous step, one takes into account the weight factor $f(\tilde{\mu}, E)/p(\tilde{\mu}, E)$.

TABLE III. Numerical values of $\sigma_\mu(E)$ from (7) for several target nuclei (for iron at higher energies tabulated values of $f(\mu, E)$ are used instead of expansion (1))

Nuclide	E(MeV)	
	14.5	150
1-H-1	1.65	0.70
6-C-12	0.13	0.031
26-Fe-56	0.061	-
92-U-238	0.024	0.0035

At higher energies, when tabulated values of $f(\mu, E)$ are used instead of the polynomial expansion (1), the sampling procedure looks more concise when comparing to the previous one:

- An importance function $q(\mu, E)$ is brought into consideration, with $\int q(\mu, E) d\mu$ being equal to 1.
- Sampling μ from the p.d.f. $q(\mu, E)$ is performed.
- A weight factor $f(\tilde{\mu}, E)/q(\tilde{\mu}, E)$ is taken into account, with the $\tilde{\mu}$ value sampled at the previous step.

For protons as projectiles, dominant small-angle scattering at $\mu \geq \mu_{max}$, i.e. multiple Coulomb scattering, is described by means of analytical distributions taking into account the nuclear finite size.¹⁰ Large-angle scattering events at $\mu < \mu_{max}$ are considered as discrete nuclear reactions and treated like neutron scatterings.

III. COMPARISON WITH EXPERIMENTAL DATA

All the experimental data used in comparisons presented below (see Figs. 1 through 4) were taken from the Experimental Nuclear Reaction Data File (EXFOR [CSISRS]).¹¹ The

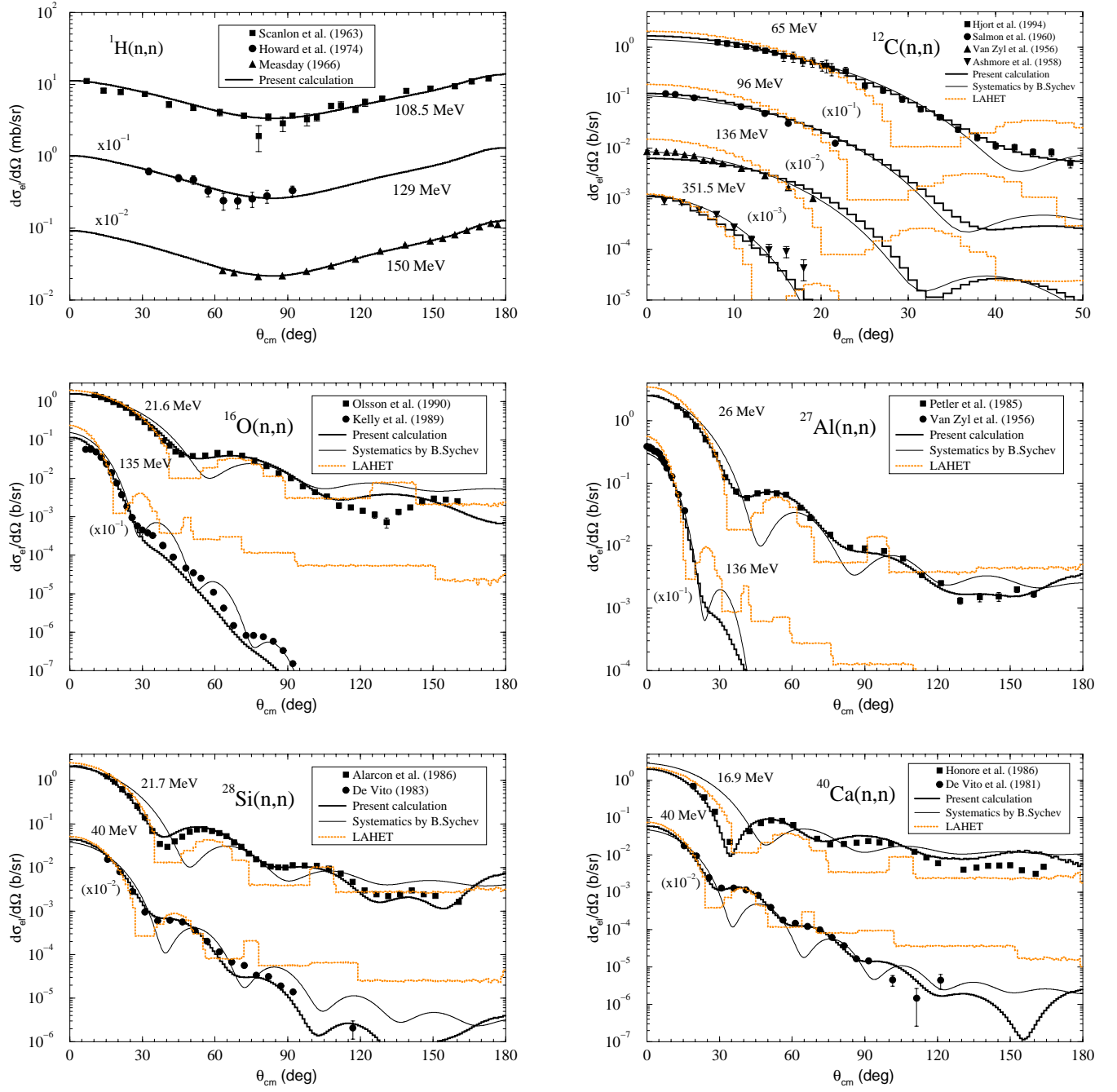


Fig. 1. Measured¹⁴ (symbols) and calculated (lines) neutron elastic scattering distributions on light nuclei. Present calculations were performed using the data from the ENDF/B-VI library³ except for the energy region above 150 MeV and distributions for carbon where other evaluations^{6,8} were used.

calculated nucleon angular distributions according to the LAHET 2.7 code¹² and systematics by B. S. Sychev¹³ are presented as well.

III.A. Neutrons

Comparisons between measured and calculated neutron elastic scattering distributions on several light, medium, and heavy nuclei are shown in Figs. 1 through 3. A good agreement is observed for all the nuclides. For heavy nuclei with discrete levels starting from a few tens of keV, one takes into

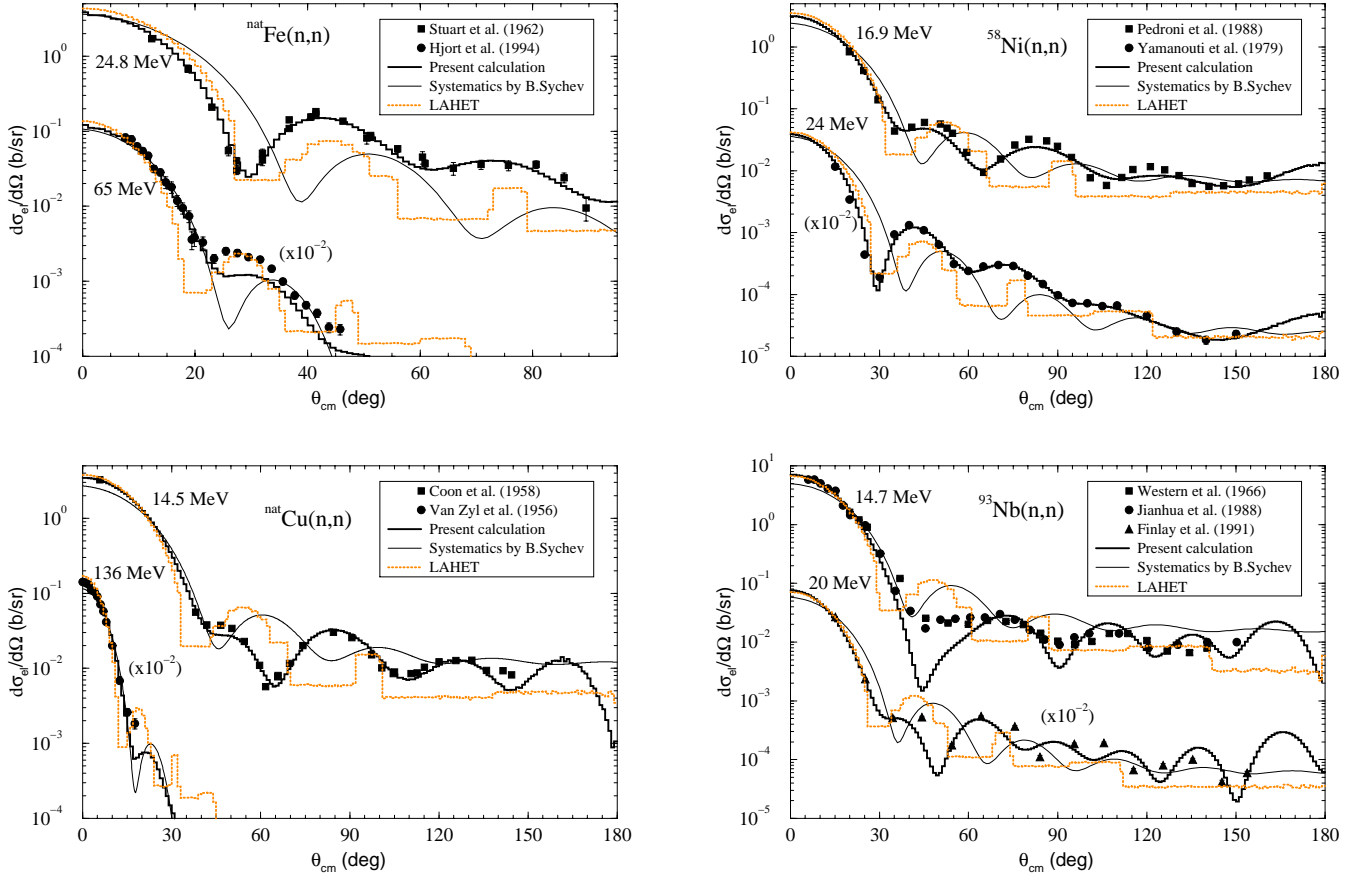


Fig. 2. Measured¹⁵ (symbols) and calculated (lines) neutron elastic scattering distributions on medium nuclei. Present calculations were performed using the data from the ENDF/B-VI library³ except for the distributions for ^{58}Ni in which case another evaluation⁹ was used. The distributions for ^{nat}Fe and ^{nat}Cu were calculated using the data for ^{56}Fe and ^{63}Cu , respectively.

account excitation of several low-lying levels when comparing to experiments with a low energy resolution (it was about 500 keV in the experiment by B. Ya. Guzhovskiy¹⁶). As for the other nuclides, not included presently in the MARS library (see Table I), several conclusions follow from the comparisons presented: (i) simulation with LAHET¹² is preferable below 150 MeV except for large-angle scattering on light nuclei, in which case the systematics by B. S. Sychev¹³ is preferable (at present we use the systematics for scattering angles above 20 degrees); (ii) above 150 MeV the systematics is preferable in the entire range of angles. Comparison with a recently developed version of LAHET¹⁸ would also be of interest.

III.B. Protons

While for neutrons most of available evaluated nuclear data cover the energy range below 150 MeV,³ for protons in accelerator applications such data is required mainly above that energy. Evaluations available at present for protons are less representative (with respect to target nuclei covered) than those

for neutrons. Comparisons between measured and calculated proton elastic scattering distributions for target nuclei of carbon, iron, and lead are presented in Fig. 4. Agreement is quite reasonable.

IV. APPLICATION TO ACCELERATOR SYSTEMS

Scattering on a stripping foil used in a beam injection system is considered as an example to demonstrate importance of correct description of elastic scattering. The foil strips two electrons off the incident H^- ions thus forming a circulating proton beam which, in turn, also traverses the foil. When considering different foil designs, heating and lifetime of the foil as well as beam loss due to scattering in it are important issues. We performed MARS modeling of proton transport through a carbon foil to estimate sensitivity of its predicted performance to nuclear data used. The following data sets were investigated: (i) nucleon cross sections according to systematics by V. S. Barashenkov *et al.*¹⁹ combined with elastic scattering

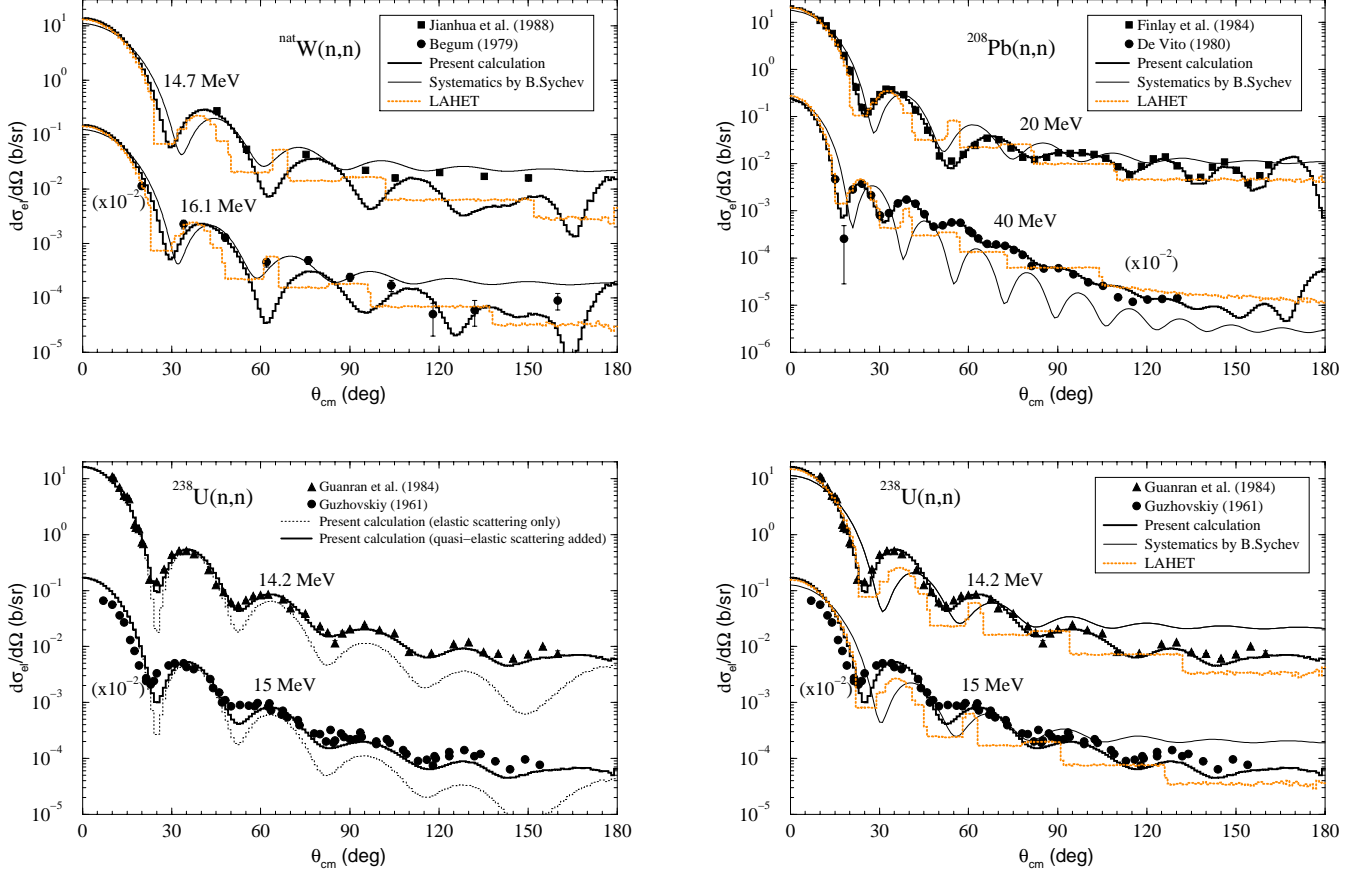


Fig. 3. Measured¹⁶ (symbols) and calculated (lines) neutron elastic scattering distributions on heavy nuclei. Present calculations were performed using the data from the ENDF/B-VI library³ except for the distributions for ²³⁸U in which case another evaluation⁷ was used. The distributions for ^{nat}W were calculated using the evaluated data for ¹⁸⁴W. In case of quasi-elastic scattering on ²³⁸U, excitation of the four lowest levels (45, 148, 307, and 517 keV) was taken into account.

procedure from the LAHET code¹² (data set 1); (ii) nucleon cross sections from the evaluated nuclear data files^{3,6} combined with the elastic scattering procedure described in this paper (data set 2). Results of the calculations are presented in Fig. 5 (multiple Coulomb scattering, which contributes for such a foil in the $0 - 2^\circ$ range mainly, is not shown in the Figure). The proton angular distributions reveal that contributions from elastic and inelastic scattering for the two data sets used behave differently. Namely, at small scattering angles, where elastic component dominates, evaluated nuclear data (data set 2) give rise to higher proton yield in accordance with the elastic cross sections used (78 and 146 mb according to the data sets 1 and 2, respectively) and distributions for a single scattering event (see Fig. 4). At larger angles, starting from approximately 15 degrees, the new algorithm predicts almost the same yields for both protons and neutrons as the data set 1 does. The results at large angles represent a small difference between the nonelastic cross sections used (216 and 228 mb according to the data sets 1 and 2, respectively). Thus, the

predicted angular distribution of a circulating beam formed by means of such a stripping foil depends significantly on the nuclear data used.

V. CONCLUDING REMARKS

The elastic scattering model for nucleons with energies in the range of 20-5000 MeV based on the evaluated nuclear data was developed and implemented in the MARS14 code system. Comparisons with experimental data reveal a good agreement for the wide range of target nuclei and projectile energies. Importance of the model is demonstrated in a typical example of a stripping foil used in a beam injection system.

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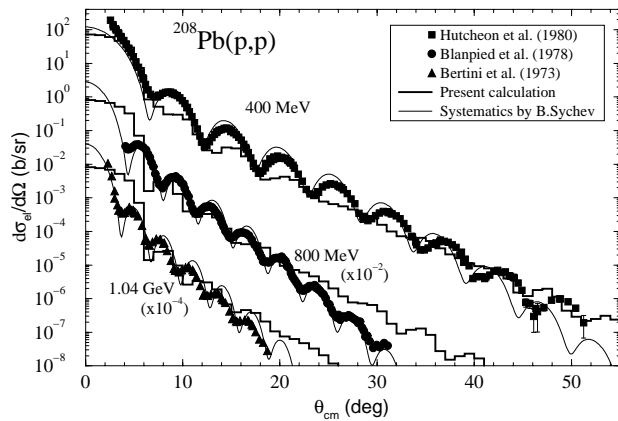
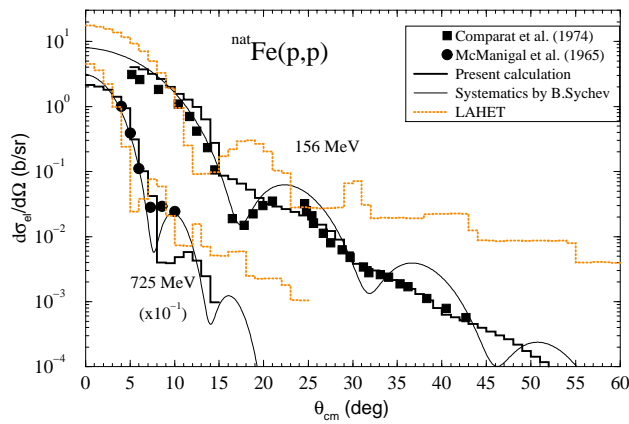
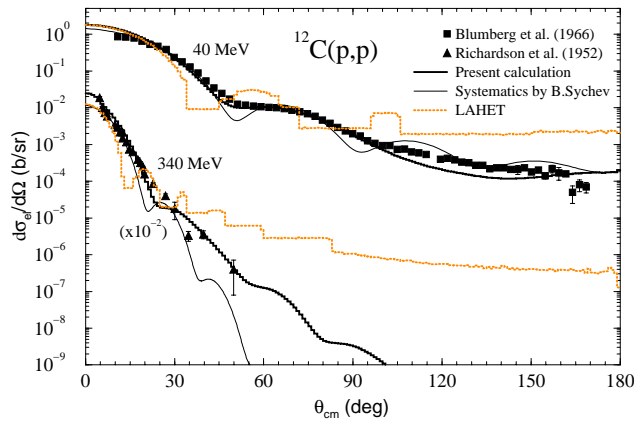


Fig. 4. Measured¹⁷ (symbols) and calculated (lines) proton elastic scattering distributions on different nuclei. Present calculations were performed using the evaluated data from the ENDF/HE-VI sublibrary⁶ above 250 MeV and other evaluations^{3,8} for iron and carbon, respectively, below this energy. For iron at 156 MeV experimental data for ⁵⁶Fe is used.

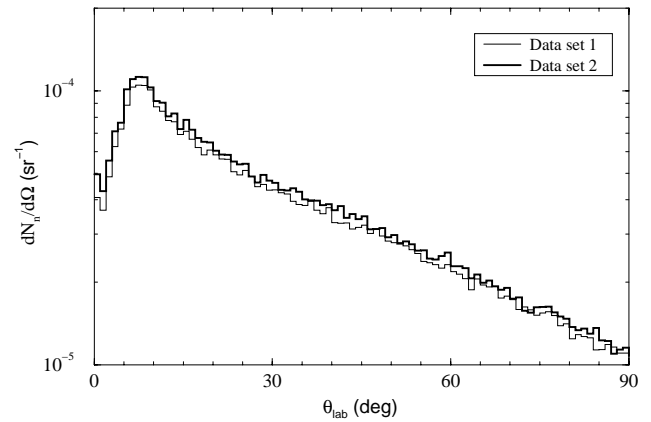
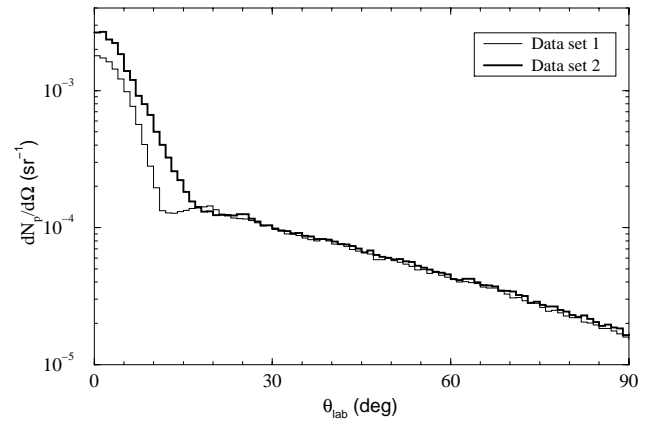


Fig. 5. Calculated with the MARS14 code angular distributions of protons (top) and neutrons (bottom) emitted from a carbon foil 100 μ m thick irradiated with a monodirectional 400 MeV proton beam. The nuclear data sets used are described above. A normalization is per one incident proton.

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