III.D. SELF-SHIELDING AND MULTIPLE-SCATTERING CORRECTIONS TO CAPTURE OR FISSION YIELDS

The theoretical capture or fission cross section may be calculated directly from the equations in Section II using the Reich-Moore (or other) approximation to the multilevel R-matrix. However, in order to compare with experiment, corrections must be made for the finite (non-infinitesimal) size of the sample. Both "self-shielding" and "multiple-scattering" effects must be included in the calculation. (Note: for the rest of this section, "capture" will be taken to mean "capture or fission" to avoid arduous repetition; the corrections described here apply to both.)

Derivation of the appropriate expressions for self-shielding and multiple-scattering corrections, including details of the methods of calculation, is non-trivial and will not be presented here. Results of comparison tests with Monte Carlo calculations indicate good agreement between Monte Carlo results and results obtained via SAMMY, as reported in [NL02]. See Section X.M for a description of the Monte Carlo code used for such comparisons.

The capture yield $Y(E)$ can be written as the sum of four components, each of which is described separately below; that is,

$$Y(E) = Y_0(E) + Y_1(E) + Y_2(E) + Y_{ns}(E) \quad . \tag{III D.1}$$

Self-shielding

Self-shielding is the reduction in the observed capture cross section due to interactions of incident neutrons with other nuclei in front of the current position. The probability that capture will occur at depth z (within dz) can be written as

$$\frac{n}{D} e^{-n\sigma_t z/D} \sigma_c \, dz \quad , \tag{III D.2}$$

where n is the sample thickness in atoms/barn and D is the sample thickness in the same units as z. Subscripts t and c denote total and capture cross sections, respectively. Integrating over z (from 0 to D) gives the self-shielded capture yield

$$Y_0 = \left\{ 1 - e^{-n\sigma_t} \right\} \left(\frac{\sigma_c}{\sigma_t} \right) \quad . \tag{III D.3}$$

(See the end of this section for a discussion of the normalization options for capture yields.)

Single scattering

The scattering correction is the increase in the observed capture cross section due to capture of neutrons that have been scattered out of the original beam path. Calculation of the scattering effect is more complicated than the self-shielding because it involves the product of (1) the probability of reaching a position (x,y,z) inside the sample, (2) the probability of scattering from that position into solid angle Ω within $d\Omega$, (3) the probability of those scattered nuclei reaching position

q within *dq* along that direction, and (4) the probability of being captured at that location. This product is then integrated over the position *q*, over solid angle, and over the sample volume, giving the *single*-scattering result. If the *z* axis is defined by the beam line, this expression can be reduced to the form

$$Y_1(E) = \frac{1}{S}\int dx \int dy \frac{n}{D}\int dz \exp\left(-\frac{n}{D}\sigma_t z\right)\int d\Omega \frac{d\sigma}{d\Omega}\sigma'_c \frac{n}{D}\int dq \exp\left(-\frac{n}{D}\sigma'_t q\right) \quad , \text{(III D.4)}$$

in which primes indicate evaluation at the scattered energy, rather than at the incident energy of the neutron. The scattered energy is given by

$$E' = E\left[\frac{\cos\theta}{1+r} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2\theta}{(1+r)^2}}\right]^2 = E\varepsilon(\theta) \quad , \text{(III D.5)}$$

where *r* is the ratio of the mass of the target nuclide to the mass of the neutron. [See Section II.C.2 and especially Eq. (II C2 b.3) for a derivation of this equation.]

Explicit evaluation of the expression in Eq. (III D.4) requires detailed knowledge of the geometry of the sample and its positioning relative to the neutron beam, as shown in the sketch in Figure III D.1. In the case where the sample is a round disk, with a flat surface perpendicular to the beam, the expression can be reduced to

$$Y_1(E) = Y_{1\infty f} + Y_{1\infty b} + Y_{1cf} + Y_{1cb} \quad , \text{(III D.6)}$$

where the subscripts "*f* " and "*b*" refer to forward and backward scattering, respectively. The subscript "∞" indicates that this term assumes the sample extends to infinity in the dimensions perpendicular to the beam; subscript "*c*" indicates that this term is the correction for finite size. (NOTE: Corrections for a rectangular shape, rather than a round disk, will be available in future releases of the code.)

The "infinite" terms in Eq. (III D.6) are one-dimensional integrals,

$$Y_{1\infty f}(E) = \frac{1}{2}\int_0^1 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}}\left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} + \frac{e^{-n\sigma_{tot}} - e^{-n\sigma'_{tot}/\mu}}{\sigma_{tot} - \sigma'_{tot}/\mu}\right) \quad \text{(III D.7)}$$

and

$$Y_{1\infty b}(E) = \frac{1}{2}\int_{-1}^0 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}}\left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} - \frac{1-e^{-n(\sigma_{tot}-\sigma'_{tot}/\mu)}}{\sigma_{tot} - \sigma'_{tot}/\mu}\right) \quad , \text{(III D.8)}$$

in which $\mu = \cos(\theta)$. The "finite" corrections involve four-dimensional integrals of the form

$$Y_{1cf}(E) = \frac{1}{2}\int_0^1 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}} Q_f(\mu, \sigma_{tot}, \sigma'_{tot}) \qquad \text{(III D.9)}$$

and

$$Y_{1cb}(E) = \frac{1}{2}\int_{-1}^0 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}} Q_b(\mu, \sigma_{tot}, \sigma'_{tot}) \quad . \qquad \text{(III D.10)}$$

Here the three-dimensional integral Q_f is given by

$$Q_f(\mu, \sigma, \sigma') = \int dz\, e^{-n\sigma' D/z} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D} \right) \qquad \text{(III D.11)}$$

and Q_b by

$$Q_b(\mu, \sigma, \sigma') = \int dz\, e^{-n\sigma'(D-z)/z} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D} \right) \quad , \qquad \text{(III D.12)}$$

where L is the actual path length, within the sample, available for travel by the scattered neutron; note that L is geometry dependent. The integration over d^2S in this expression for Q is over the beam cross section; the integration over z is over the thickness of the sample. SAMMY evaluates Q on a separate grid and interpolates to produce the required values for Eqs. (III D.9) and (III D.10).

Values for Q are generated in advance (in segment SAMPAR) and stored in a file named SAMMY.SSM. This file may be renamed and reused for subsequent runs, as long as the geometry remains the same.

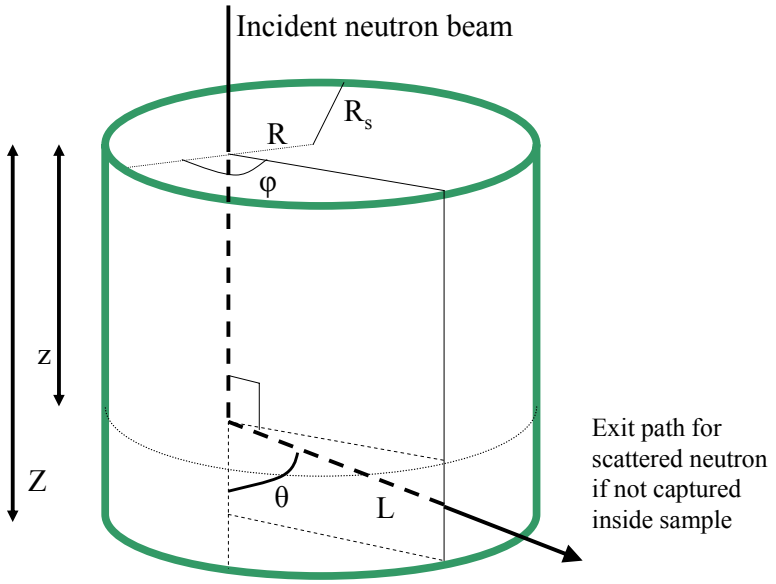

Figure III D.1. Geometry for the single-scattering correction to capture or fission yield, for a neutron incident on the flat surface of a cylindrical sample.

More than one scatter

Derivation of the effect of two or more scatters followed by capture is accomplished in a similar manner to the derivation of the single-scattering effect. The exact expression for *k* scatters involves $(3k+3)$ embedded integrations; it is therefore necessary to make severe approximations in order to derive an expression that can be calculated in a finite amount of time. The approximation currently employed by SAMMY is borrowed from Moxon [MM89], based on a derivation by Case et al. [KC53]; an independent derivation was developed in preparation for implementation into the SAMMY code. The approximation assumes that after two scatterings, neutrons are uniformly distributed both in direction of motion and in position within the sample. This approximation has the effect of decoupling 2*k* of the embedded integrals, so that they can be performed separately from the others. Quantization of this approximation is achieved by assuming that the escape probability for a neutron after *k* scatterings (i.e., at energy $E^{(k)}$) depends only on the energy; specifically, the escape probability is given by the formula

$$p_{escape}\left(E^{(k)}\right) = \frac{1}{n\sigma^{(k)}}\left[\frac{1}{2}-\int_1^\infty u^{-3}e^{-n\sigma^{(k)}u}du\right]\frac{1+2n\sigma_{tot}^{(k)}}{1+\dfrac{2n\sigma_{tot}^{(k)}}{1+Z/R}} \quad , \qquad \text{(III D.13)}$$

where *R* is the radius of the sample. With this approximation, one can recursively define a function *y* via

$$y_{j-1} = \int d\Omega_j \frac{d\sigma^{(j-1)}}{d\Omega_j}\left(\sigma_c^{(j)}+y_j\right)\left(1-p_{escape}\left(E^{(j)}\right)\right) \quad , \qquad \text{(III D.14)}$$

in which the superscript denotes the energy at which the cross section is to be calculated. The initial estimate for a neutron scattered *k* times is

$$y_{k-1} \approx 2\pi\int d\mu_k \frac{d\sigma^{(k-1)}}{d\Omega_k}\sigma_c^{(k)}\left(1-p_{escape}\left(E^{(k)}\right)\right) \quad . \qquad \text{(III D.15)}$$

This function *y* can then be used to estimate the capture yield for two or more scatterings,

$$Y_2(E) = \frac{1}{S}\int dx\int dy\frac{n}{E}\int dz\, e^{-\frac{n}{D}\sigma_{tot}z}\int d\Omega\frac{d\sigma}{d\Omega}y_l\frac{n}{D}\int dq\, e^{-\frac{n}{D}\sigma'_{tot}q} \quad . \qquad \text{(III D.16)}$$

In this form the multiple-scattering capture yield has the same mathematical properties as the single-scattering capture yield of Eq. (III D.4). Similar computational techniques can therefore be used to evaluate both quantities.

Alternative for more than one scatter

For very thick samples and/or very strong resonances, the crude approximation described above for double-plus scattering may be woefully inadequate. For those situations, tabulated values can be for Y_2. The tabulated values are generated with a series of three runs, first SAMMY with the command

```
PREPARE INPUT FOR MOnte carlo simulation,    or simply
MONTE CARLO  .
```

Next, the SAMSMC code is run to perform the Monte Carlo calculation. Then SAMGY2 reads the output from SAMSMC, smooths the Y2 curve, and creates a file named SAMY2.DAT that contains the tabulated Y2 values for use in the next SAMMY run. For that run, the command

```
Y2 VALUES ARE TABULAted
```

is inserted into the INPut file, and the name of the file must be included in the input stream.

Only the values of Y_2 are given in this manner; derivatives are still generated as though the original form were used. Caution must be exercised when using this option, especially when varying resonance parameters, since (1) the tabulated values of Y_2 do not change unless the entire process is repeated and (2) derivatives are inaccurate.

Simulation sim009 makes use of this option.

Neutron sensitivity

In capture experiments, not only gamma rays but also scattered neutrons reach the detector. The detector is not always able to distinguish between the two; hence, corrections must be made for the neutron sensitivity of the detector. Following Borella [AB05] with only notational changes, this correction term has the form

$$Y_{ns}(E) = A\left\{1 - e^{-\sigma_{tot}}\right\}\frac{\sigma_n}{\sigma_{tot}}\frac{\varepsilon_n}{\varepsilon_c} \quad , \qquad \text{(III D.17)}$$

in which ε_n represents the neutron sensitivity of the detector and ε_c the capture sensitivity. The ratio of these sensitivities as a function of energy was provided by Peter Schillebeeckx [PS06], and log-log interpolation gives the value at a particular energy. The multiplier A is an input parameter whose value is the binding energy of the target nuclide. Nevertheless, A may be flagged as a variable or as a PUP when the user wishes to include an estimate of the uncertainty on the neutron sensitivity. See line 12 of card set 11 of Table VI B.2 for input details for this feature.

Normalization and input options

Capture yield data may be normalized in a variety of ways; therefore, SAMMY allows the user to choose which normalization is to be taken. The normalization generally referred to as

capture "yield" is the one shown in the equations in this section; this choice has the property that values are in the range from 0 to 1. Another commonly used normalization requires dividing by thickness *n*; in this case, the value approaches the capture cross section in the limit of zero thickness. Finally, the data may be normalized as $\left(1-e^{-n\sigma_{tot}}\right)\sigma_{tot}$, that is, by multiplying the yield by the total cross section. To use these options, the appropriate phrase must be included in the alphanumeric section of the INPut file:

```
NORMALIZE AS CROSS Section rather than yield
NORMALIZE AS YIELD Rather than cross section
NORMALIZE AS (1-E)SIgma
```

No default is assumed for normalization; instead, SAMMY requires that one of the above options be specified by the user.

The default mode in SAMMY is to <u>not</u> include self-shielding and multiple-scattering corrections; therefore, to invoke these corrections, users will need to include one or more of the following phrases in their INPut file:

For self-shielding but no multiple-scattering correction:

```
USE SELF SHIELDING Only, no scattering, or
SELF SHIELD
```

For self-shielding, single-scattering (with edge-effects), and no double-scattering correction:

```
USE SINGLE SCATTERINg plus self shielding, or
SINGLE
```

For self-shielding, single-scattering (infinite slab approximation), and no double-scattering corrections:

```
SINGLE
INFINITE SLAB
```

For self-shielding, single-scattering (with edge-effects correction), and multiple-scattering corrections:

```
INCLUDE DOUBLE SCATTering plus single scattering, or
DOUBLE
```

For self-shielding, single-scattering (infinite-slab approximation), and multiple-scattering corrections:

```
DOUBLE
INFINITE SLAB
```

When finite-size corrections (for single scattering) are wanted, additional input is needed to express the geometric properties of the beam and of the sample. These include the dimensions of the sample, the cross-sectional dimensions of the beam if smaller than the sample, and integers that determine the accuracy to which the function *Q* will be calculated. Details are given in Table VI A.1, card set 11.

Examples using multiple-scattering corrections can be found in test cases tr039, tr052, tr064, tr099, and others.