Rate Calculations from `MottG4` Simulation

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2015-07-01

1 Calculating Rates and the Acceptance Function

The calculation of rates from simulation is of primary importance. The rate is the simplest quantity with which to compare simulations to data. The rate calculation from a given simulation is a prediction of the number of events that will hit our detector per unit current per unit time, using the assumptions in our simulation. All rates quoted in this note will have units of Hz/μA. The differential rate in our detector from one point in phase space $\vec{v}$ is:

$$d\mathcal{R}(\vec{v}) = \mathcal{L}(\vec{v})\sigma(\vec{v})\epsilon(\vec{v})dv, \tag{1}$$

where $\mathcal{L}(\vec{v})$ is the luminosity, $\sigma(\vec{v})$ is the cross-section of the physics of interest and $\epsilon(\vec{v})$ is the acceptance function of our detectors (essentially the chance that an event near $\vec{v}$ will be detcted). The total rate our detector sees is simply the integral of Eq. (1):

$$\mathcal{R} = \int_V d\mathcal{R}(\vec{v}). \tag{2}$$

While $\mathcal{L}(\vec{v})$ and $\sigma(\vec{v})$ are often known quantities, $\epsilon(\vec{v})$ is a value obtained solely by simulation. Figure ?? shows a plot of the acceptance function with respect to the different variables of single scattering. As is demonstrated in the figure, the acceptance function's behavior is well characterized solely by it's dependence upon scattering angle, χ and azimuthal angle ψ. Thus:

$$\epsilon(\vec{v}) = \epsilon(\chi, \psi). \tag{3}$$

2 Single Scattering Calculation

For a single scattering event, our phase space vector becomes $\vec{v} = (x, y, z, E, \chi, \psi)$ and the volume element is $dv = dxdydzdEd\chi d\psi$. The total rate in a detector is then:

$$\mathcal{R} = \int_V \mathcal{L}(\vec{v})\sigma(\vec{v})\epsilon(\vec{v})\sin\chi dv. \tag{4}$$

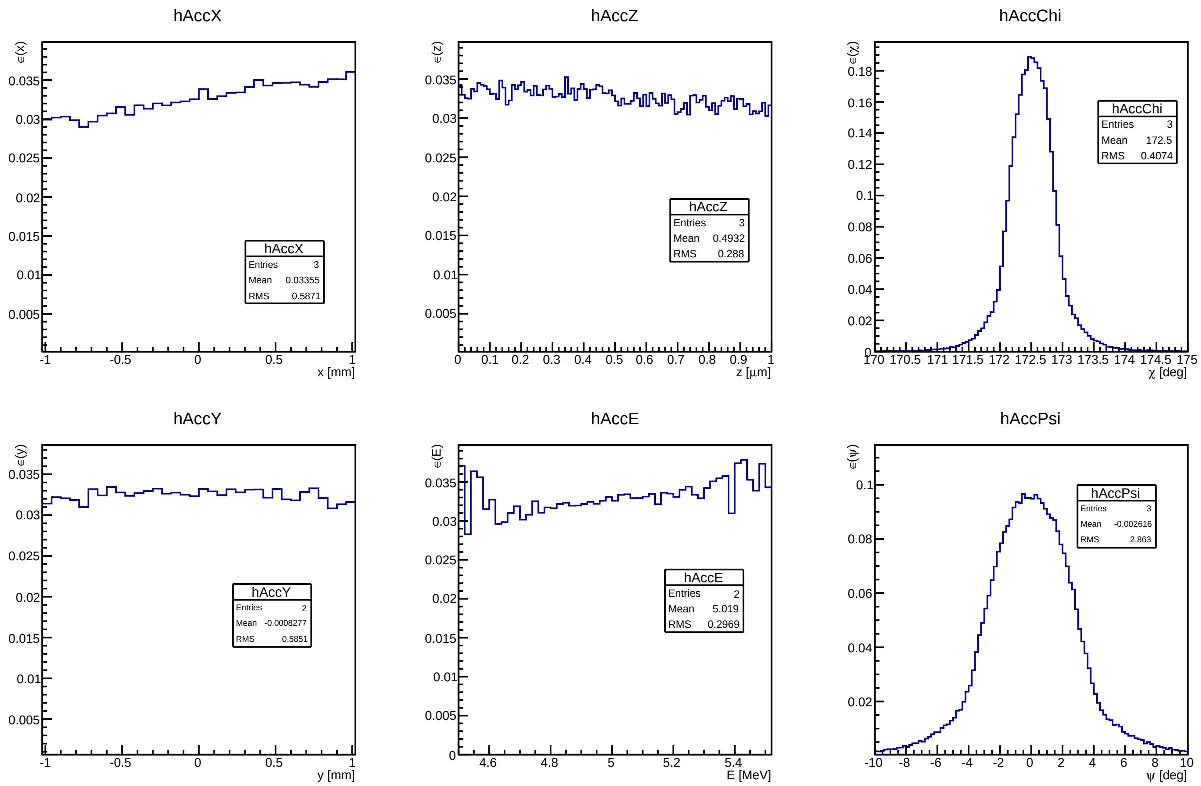

Figure 1: Simulated Acceptance Functions for each of the six degrees of freedom in single scattering. Results are from the Left detector for 10 million events thrown. Only $\epsilon(\chi)$ and $\epsilon(\psi)$ show large dependence.

The integrals over x, y are trivial. Additionally, the dependence of $\sigma(\vec{v})$ upon z and E are small enough to ignore in our case. This yields:

$$\mathcal{R} = \frac{N_A \rho}{A} N_B d \int_{\psi_{min}}^{\psi_{max}} \int_{\chi_{min}}^{\chi_{max}} \sigma(\chi, \psi) \epsilon(\chi, \psi) \sin \chi d\chi d\psi, \tag{5}$$

Where N_A is Avogadro's number, ρ is the density of the target foil, A is the atomic weight of the foil material, N_B is the number of electrons per second in 1 μA, and d is the target thickness. From this point there are two methods that I've attempted to approximate this integral numerically.

2.1 Method 1: Reimann Sum

We divide the 2D integral into $N_\chi \times N_\psi$ bins in χ and ψ of size $\Delta\chi\Delta\psi$. Then Eq. (5) can be estimated using

$$\mathcal{R} \approx \frac{N_A \rho}{A} N_B d \sum_{i=1}^{N_\chi} \sum_{j=1}^{N_\psi} \sigma_{ij} \epsilon_{ij} \sin \chi_i \Delta\chi\Delta\psi, \tag{6}$$

Where σ_{ij} is the average cross-section for all events thrown in the ij'th bin and ϵ_{ij} is the acceptance function for the bin. The uncertainty, $\delta\mathcal{R}$, from this method is given by

$$\delta\mathcal{R}^2 = \left(\frac{N_A\rho}{A}N_B d\Delta\chi\Delta\psi\right)^2 \sum_{i=1}^{N_\chi}\sum_{j=1}^{N_\psi}\left(\epsilon_{ij}^2\delta\sigma_{ij}^2 + \sigma_{ij}^2\delta\epsilon_{ij}^2\right)\sin^2\chi_i. \tag{7}$$

Figure 2 shows the binned cross-section and acceptance function for a run. This method gives good results which are in decent agreement with data as seen in Table 1.

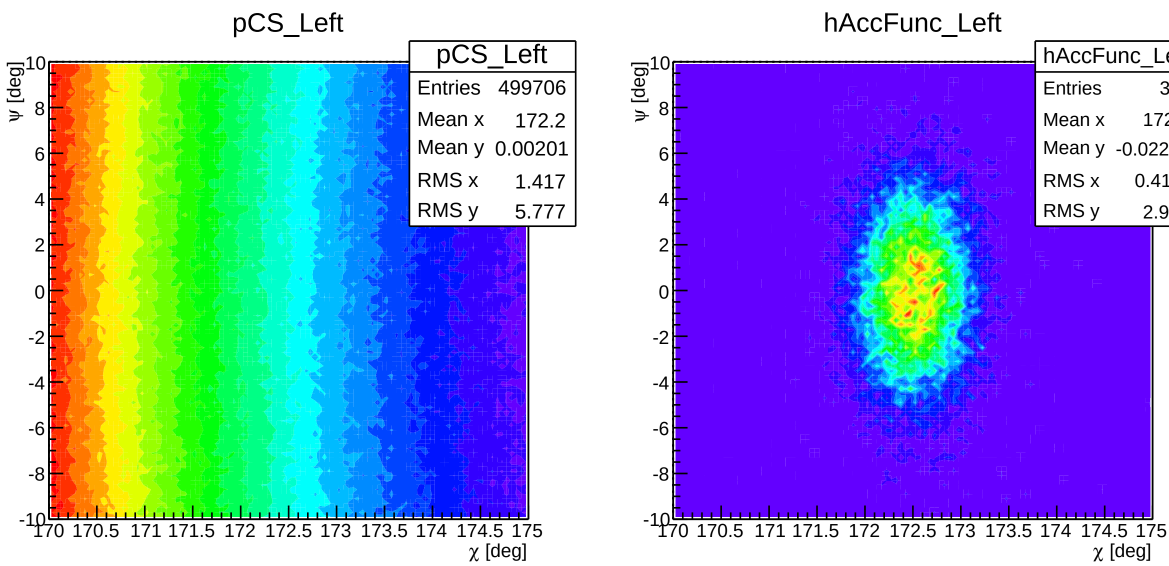

Figure 2: On the left: Simulated average cross-section as a function of scattering angle, χ, and azimuthal angle, ψ, for the left detector. On the right: Simulated acceptance function, $\epsilon(\chi,\psi)$. Results from a simulation of one million events and a 52 nm gold foil.

d (nm)	$\mathcal{R}_{\text{sim}}$	$\mathcal{R}_{\text{fit}}$	$\mathcal{R}_{\text{data}}$
52	10.25 ± 0.67	9.75 ± 0.50	9.93 ± 0.09
215	42.49 ± 1.46	40.32 ± 2.05	46.50 ± 0.48
389	77.15 ± 2.08	72.95 ± 3.70	82.58 ± 1.04
487	95.75 ± 2.40	91.33 ± 4.62	97.74 ± 1.00
561	109.89 ± 2.62	105.21 ± 5.34	128.66 ± 1.32
775	153.20 ± 3.28	145.34 ± 7.38	178.30 ± 1.86
837	163.88 ± 3.45	156.97 ± 7.97	209.30 ± 2.15
944	186.50 ± 3.77	177.04 ± 8.99	246.00 ± 2.53

Table 1: Comparison of simulated rates to data. $\mathcal{R}_{\text{sim}}$ are the simulated rates for single scattering calculated using the Reimann sum method on one million events at each target thickness. $\mathcal{R}_{\text{fit}}$ is the linear portion of the quadratic fit to data, $\mathcal{R}_{\text{data}}$. Data and fit taken from: `https://wiki.jlab.org/ciswiki/images/e/ef/Rates.pdf` . All rates are given in units of Hz/μA.

2.2 Method 2: Monte Carlo Integration

In this method we try to numerically estimate the integral in Eq. (4) with a Monte Carlo method. Examining Eq. (4) without simplifying, we see

$$\mathcal{R} = \frac{N_A \rho}{A} \frac{N_B}{(2\pi)^{3/2}\sigma_x \sigma_y \sigma_E} \int_V \exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(E-\mu_E)^2}{2\sigma_E^2}\right) \sigma(E,z,\chi,\psi)\epsilon(\chi,\psi)\sin\chi dv. \tag{8}$$

We define

$$g(\vec{v}) = \frac{1}{(2\pi)^{3/2}\sigma_x \sigma_y \sigma_E} \exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(E-\mu_E)^2}{2\sigma_E^2}\right) \sigma(E,z,\chi,\psi)\epsilon(\chi,\psi)\sin\chi. \tag{9}$$

The `GEANT4` code throws single scattering events by sampling the space V according to the probability distribution function,

$$f(\vec{v}) = C \exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(E-\mu_E)^2}{2\sigma_E^2}\right) \sin\chi, \tag{10}$$

with normalization condition,

$$\frac{1}{C} = \int_V \exp\left(-\frac{x^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2} - \frac{(E-\mu_E)^2}{2\sigma_E^2}\right) \sin\chi dv \tag{11}$$

$$= (2\pi)^{3/2}\sigma_x \sigma_y \sigma_E d \frac{\pi}{9}\left[\cos\frac{\pi}{36} - \cos\frac{\pi}{18}\right]. \tag{12}$$

Looking back at Eq. (8), we can write it in terms of $f(\vec{v})$ and $g(\vec{v})$ as

$$\mathcal{R} = \frac{N_A \rho}{A} N_B \int_V \frac{g(\vec{v})}{f(\vec{v})} f(\vec{v}) dv. \tag{13}$$

At this point we can estimate the integral using Monte Carlo integration

$$\mathcal{R} \approx \frac{N_A \rho}{A} N_B \sum_{i=1}^{n} \frac{g(\vec{v}_i)}{f(\vec{v}_i)} \tag{14}$$

$$= \frac{\pi}{9}\left[\cos\frac{\pi}{36} - \cos\frac{\pi}{18}\right] \frac{N_A \rho}{A} N_B d \sum_{i=1}^{n} \sigma(E_i, z_i, \chi_i, \psi_i)\epsilon(\chi_i, \psi_i). \tag{15}$$

where n is the number of events thrown. Using this method we see some issues as highlighted in Table 4. In particular, the rates are similar at small foils and then diverge as d increases. Additionally, the uncertainty provided by the Monte Carlo method is much too small, particularly in light of Table 3, which shows the dependence upon n.

3 Double Scattering Rates

We look again at the differential form of the scattering rate. In this case we consider the rate by pieces. The rate from the initial scattering at position (x, y, z) and energy (prior to entering the

	Method 1		Method 2	
d (nm)	$\mathcal{R}_L$	$\mathcal{R}_R$	$\mathcal{R}_L$	$\mathcal{R}_R$
52	4.9925 ± 0.278161	15.328 ± 0.857051	4.70594	14.3801
215	20.6304 ± 1.15056	64.3406 ± 3.5734	18.5732	58.4646
389	37.5026 ± 2.08311	116.799 ± 6.47384	33.9492	105.638
487	46.318 ± 2.59238	145.19 ± 8.07558	41.5134	130.262
561	53.9568 ± 3.00251	165.831 ± 9.26319	48.2993	147.777
775	74.3995 ± 4.14572	232.009 ± 12.8863	66.7659	205.792
837	80.1061 ± 4.47106	247.645 ± 13.8336	71.5765	222.249
944	90.757 ± 5.04853	282.25 ± 15.6653	80.4706	253.798

Table 2: Simulated single scattering results for one million simulated events using both Methods. It is apparent that the two methods diverge at higher target thickness.

	Method 1		Method 2	
# Events (M)	$\mathcal{R}_L$	$\mathcal{R}_R$	$\mathcal{R}_L$	$\mathcal{R}_R$
1	95.755	297.138	85.6182	267.592
1	95.3268	297.042	87.8213	276.02
3	95.9154	296.887	89.9372	279.687
4	95.6782	297.705	90.9824	283.096
5	95.6821	298.066	91.6055	286.014
6	95.655	298.174	92.0939	288.068
7	95.7495	298.209	92.6041	289.371
8	95.7276	298.514	92.8742	290.194
9	95.7947	298.681	93.103	290.973
10	95.9183	298.902	93.3508	291.551

Table 3: A comparison of results from each method for a target 1000 nm thick all results are in Hz/μA. It should be noted that the uncertainty for Method 1 is constant as well (it's dominated by the averaging over target positions, energies etc.) with values of $\delta\mathcal{R}_L = 5.34$ Hz/μA and $\delta\mathcal{R}_R = 16.58$ Hz/μA. Thus the two methods are consistent with around 5 million events.

target), E towards the second scattering position along direction (θ, ϕ) is given by:

$$d\mathcal{R}_1(\vec{v}) = \mathcal{L}(\vec{v})\sigma_1(\vec{v})dv \tag{16}$$

$$= \frac{N_A\rho}{A}\frac{N_B}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_E}\exp\left[\frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{E^2}{2\sigma_E^2}\right]\sigma_1(z, E, \theta, \phi)\sin\theta dxdydzdEd\theta d\phi \tag{17}$$

The rate that our detector sees then from the second scattering is then:

$$d\mathcal{R}(\vec{v}) = \frac{N_A\rho}{A}d\mathcal{R}_1(\vec{v})\sigma_2(z, E, \xi, \theta, \phi, \chi, \psi)\epsilon(\chi, \psi)\sin\chi d\xi d\chi d\psi. \tag{18}$$

We define

$$g(\vec{v}) = \exp\left[\frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{E^2}{2\sigma_E^2}\right]\sigma_1(\vec{v})\sigma_2(\vec{v})\epsilon(\chi, \psi)\sin\theta\sin\chi \tag{19}$$

	Method 1		Method 2	
d (nm)	$\mathcal{R}_L$	$\mathcal{R}_R$	$\mathcal{R}_L$	$\mathcal{R}_R$
52	5.02 ± 0.28	15.44 ± 0.86	5.05	15.57
215	20.67 ± 1.15	63.96 ± 3.56	20.20	62.52
389	37.10 ± 2.07	115.52 ± 6.43	35.84	112.35
487	46.51 ± 2.60	144.83 ± 8.063	44.82	139.50
561	53.81 ± 3.00	167.01 ± 9.29	51.70	160.60
775	74.49 ± 4.15	231.14 ± 12.86	70.98	221.97
837	80.22 ± 4.47	249.79 ± 13.89	76.92	239.72
944	91.07 ± 5.06	282.06 ± 15.68	87.01	270.56

Table 4: Simulated single scattering results for five million simulated events using both Methods. Now both methods are in better agreement. All rates are in Hz/μA.

and note that our `GEANT4` simulation samples the double scattering phase space, V, according to the probability density function

$$f(\vec{v}) = C \exp\left[\frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{E^2}{2\sigma_E^2}\right] \sin\theta \sin\chi. \tag{20}$$

With the normalization condition:

$$1 = \int_V g(\vec{v}) dv \tag{21}$$

$$\frac{1}{C} = I \times \int_{-\infty}^{\infty} e^{-x^2/2\sigma_x^2} dx \int_{-\infty}^{\infty} e^{-y^2/2\sigma_y^2} dy \int_{-\infty}^{\infty} e^{-E^2/2\sigma_E^2} dE \int_0^{2\pi} d\phi \int_{\psi_{min}}^{\psi_{max}} d\psi \int_{\chi_{min}}^{\chi_{max}} \sin\chi d\chi \tag{22}$$

Where

$$I = \int_0^d \int_0^\pi \left[\int_0^{\xi_{max}(\theta,z)} d\xi\right] \sin\theta d\theta dz \tag{23}$$

The variable ξ refers to distance from the first scattering point and $\xi_{max}(\theta, z)$ is the maximum distance the second scattering can be generated given the initial scattering position and angle. Since the simulation also has the caveat that all electrons generated must not have lost more than 500 keV in the target (these would not be counted in our physical asymmetry in any case), we put a distance limit, $D = 157\,\mu$m, for those particles travelling at $\theta \approx \pi/2$. Thus we define:

$$\xi_{max}(\theta, z) = \begin{cases} \frac{d-z}{\cos\theta}\left[1 - H\left(\frac{d-z}{\cos\theta} - D\right)\right] + DH\left(\frac{d-z}{\cos\theta} - D\right) & \text{if } \theta \leq \pi/2 \\ \frac{-z}{\cos\theta}\left[1 - H\left(\frac{-z}{\cos\theta} - D\right)\right] + DH\left(\frac{-z}{\cos\theta} - D\right) & \text{if } \theta > \pi/2, \end{cases} \tag{24}$$

where $H(x)$ is the Heaviside step function. Plugging this in we have

$$I = \int_0^d \int_0^\pi \xi_{max}(\theta, z) \sin\theta d\theta dz. \tag{25}$$

Examining the integral over θ we see

$$\int_0^{\pi} \xi_{max}(\theta, z) \sin\theta d\theta = (d - z) \int_0^{\alpha_1} \tan\theta d\theta + D \int_{\alpha_1}^{\alpha_2} \sin\theta d\theta + (-z) \int_{\alpha_2}^{\pi} \tan\theta d\theta, \tag{26}$$

where $\cos\alpha_1 = (d - z)/D$ with $0 \leq \alpha_1 < \pi/2$ and $\cos\alpha_2 = -z/D$ with $\pi/2 \leq \alpha_2 < \pi$. We then see:

$$(d - z) \int_0^{\alpha_1} \tan\theta d\theta = -(d - z) \log(\frac{d - z}{D}), \tag{27}$$

$$D \int_{\alpha_1}^{\alpha_2} \sin\theta d\theta = d, \tag{28}$$

$$-z \int_{\alpha_2}^{\pi} \tan\theta d\theta = z \log(\frac{z}{D}), \tag{29}$$

$$\therefore \int_0^{\pi} \xi_{max}(\theta, z) \sin\theta d\theta = d \left[1 - \log(\frac{d - z}{D})\right] + z \left[\log(\frac{d - z}{D}) + \log(\frac{z}{D})\right]. \tag{30}$$

Therefore we see

$$I = \int_0^{d} \left(d \left[1 - \log(\frac{d - z}{D})\right] + z \left[\log(\frac{d - z}{D}) + \log(\frac{z}{D})\right]\right) dz \tag{31}$$

$$= d^2 \tag{32}$$

regardless of our initial choice of D (so long as it is a physically possible value). Returning to the normalization condition on $f(\vec{v})$, we see:

$$\frac{1}{C} = \left(d^2\right) \left(\sqrt{2\pi}\sigma_x\right) \left(\sqrt{2\pi}\sigma_y\right) \left(\sqrt{2\pi}\sigma_E\right) (2\pi) \left(\frac{\pi}{9}\right) \left(\cos\frac{\pi}{36} - \cos\frac{\pi}{18}\right). \tag{33}$$

Given the definitions above, we can calculate the rate from double scattering

$$\mathcal{R} = \left(\frac{N_A \rho}{A}\right)^2 \frac{N_B}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_E} \int_V \frac{f(\vec{v})}{g(\vec{v})} g(\vec{v}) dv \tag{34}$$

Using the Reimann sum method is not available to us due to the high dimension of the integral and the difficulty of the integration limits. So we instead try to integrate numerically with a Monte Carlo estimator:

$$\mathcal{R} = \frac{1}{n} \left(\frac{N_A \rho}{A}\right)^2 \frac{N_B}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_E} \sum_i^n \frac{f(\vec{v}_i)}{g(\vec{v}_i)} \tag{35}$$

$$= \frac{1}{C} \frac{1}{n} \left(\frac{N_A \rho}{A}\right)^2 \frac{N_B}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_E} \sum_i^n \sigma_1(\vec{v}_i)\sigma_2(\vec{v}_i)\epsilon(\chi_i, \psi_i) \tag{36}$$

$$= \frac{2\pi^2}{9} \left(\cos\frac{\pi}{36} - \cos\frac{\pi}{18}\right) N_B \left(\frac{N_A \rho d}{A}\right)^2 \frac{1}{n} \sum_i^n \sigma_1(\vec{v}_i)\sigma_2(\vec{v}_i)\epsilon(\chi_i, \psi_i) \tag{37}$$

Results of this method are shown in Table 5. Combined results of single and double scattering rates can be seen in Table 6 and Fig. 3.

d [nm]	$\mathcal{R}_{\text{fit}}$	$\delta\mathcal{R}_{\text{fit}}$	$\mathcal{R}_{\text{sim}}$	$\delta\mathcal{R}_{\text{sim}}$
52	0.188	0.047	0.160	0.019
215	3.213	0.795	2.573	0.365
389	10.517	2.603	8.650	1.320
487	16.483	4.079	13.957	2.266
561	21.873	5.413	19.158	3.227
775	41.743	10.331	29.984	4.853
837	48.690	12.050	47.164	10.156
944	61.934	15.328	64.584	10.977

Table 5: Results of simulations of 100,000,000 events from the double scattering generator compared with the quadratic fit to data from `https://wiki.jlab.org/ciswiki/images/e/ef/Rates.pdf` . All rates are given in units of Hz/μA.

d [nm]	$\mathcal{R}_{\text{data}}$	$\delta\mathcal{R}_{\text{data}}$	$\mathcal{R}_{\text{sim}}$	$\delta\mathcal{R}_{\text{sim}}$
52	9.93	0.09	10.42	0.23
215	46.50	0.48	45.06	1.01
389	82.58	1.04	85.41	2.15
487	97.74	1.00	110.39	3.11
561	128.66	1.32	129.56	4.05
775	178.30	1.86	182.92	5.92
837	209.30	2.15	213.02	10.79
944	246.00	2.53	252.15	11.73

Table 6: Results of summed simulations for both single and double scattering compared with data from `https://wiki.jlab.org/ciswiki/images/e/ef/Rates.pdf`. All rates are given in units of Hz/μA.

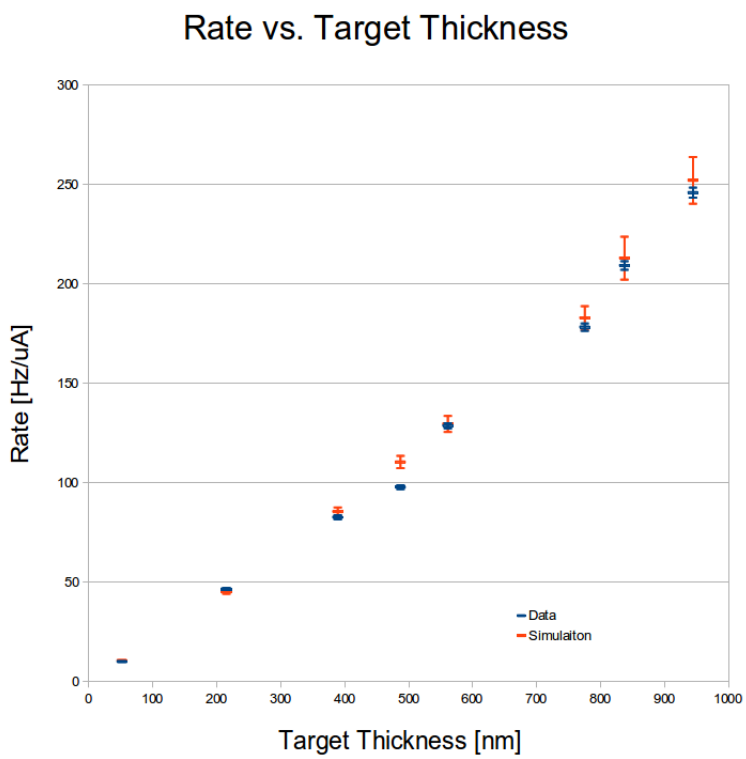

Figure 3: Combined rates from single and double-scattering simulations (red) compared to results from data (blue). Data from `https://wiki.jlab.org/ciswiki/images/e/ef/Rates.pdf`.

4 Combined Asymmetry

With the rates in both left and right detectors for single and double scattering, we can calculate the Mott asymmetry as:

$$A = \frac{\mathcal{R}_L^1 + \mathcal{R}_L^2 - \mathcal{R}_R^1 - \mathcal{R}_R^2}{\mathcal{R}_L^1 + \mathcal{R}_L^2 + \mathcal{R}_R^1 + \mathcal{R}_R^2}, \tag{38}$$

where the subscript refers to the left or right detector and the superscript refers to single or double scattering. The results of these calculations can be seen in Fig. 4 and Table

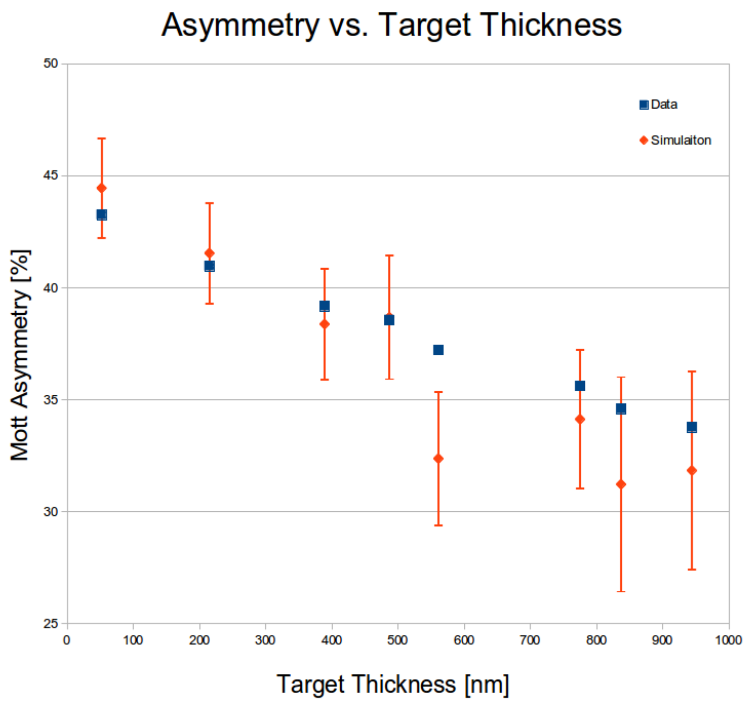

Figure 4: Simulated asymmetries (red) compared with data (blue).

d	A_{sim}	δA_{sim}	A_{data}	δA_{data}
52	44.45	2.23	43.26	0.11
215	41.54	2.24	40.97	0.07
389	38.38	2.48	39.18	0.08
487	38.68	2.77	38.56	0.08
561	32.37	2.98	37.21	0.08
775	34.13	3.11	35.61	0.08
837	31.22	4.79	34.59	0.08
944	31.84	4.41	33.77	0.08

Table 7: Asymmetry as a function of target thickness for simulation and data.