The Mott asymmetry extrapolated to zero foil thickness depends on the functional form of the fit of the data. In parallel with simulations to determine if the effects of single and double scattering could be modelled sufficiently to explain the Mott scattering data, a statistical investigation of fitting functions was undertaken. Many extrapolation formulae have been used previously to approximate the data and extrapolate to the zero foil thickness for comparison with theoretical calculations. However, there had not previously been clear consensus regarding the functional form that this fit of asymmetry vs. thickness should follow. While a χ2 value can be calculated for the goodness of data to a function, it relies on the fact that the function is truly the parent distribution for the data, so both differences between the data and the function as well as between the function tested and the true parent distribution of the data are included in the χ2 value. This leads to the conclusion that merely finding a function with a good χ2 value is not sufficient to determine that that functional form is the best form for extrapolating to find Ao.

To determine the uncertainty in the asymmetry extrapolated to zero thickness from the foil thickness measurements, we studied the dependence of the value of the zero thickness intercept while varying the extrapolation function between both historically used functions and using Pade approximates. Pade approximates are a class of rational fractions which are typically well behaved and converge more rapidly than Taylor series approximations to a set of data for extrapolation. The Pade approximant take the form



for m≥0 and n≥1. To determine the Pade approximant order (Pade (m,n)) required for the zero thickness extrapolation, the statistical F-test was used. The F-test gives guidance for the validity of adding an nth term to a function is defined as: (bevington, 1st ed, p 203)

$$F\_{χ}=\frac{χ\_{\left(n-1\right)}-χ\_{\left(n\right)} }{χ\_{\left(n\right)}/(N-n-1)}$$

where N is the number of data points, n+1 is the number of parameters in the fit, and X(n) is defined as

$$χ^{2}=\sum\_{}^{}\frac{\left(y\_{i}-f(x\_{i})\right)^{2}}{\left(σ\_{i}\right)^{2}}$$

where yi are the data points, f(xi) the function at that same point, σi the uncertainty in the data, and the function is summed over all data points.

A note on the fitting: fitting was done for these studies both using the root program (details) and Mathematica, where the fitting was performed by defining the function and using the “NonlinearModelFit” routine with the weight option set with each point weighted by wi= 1/σi2. Although the uncertainties in thickness are much larger than the uncertainties in the measured asymmetry at each thickness, the data were plotted with asymmetry vs. thickness to make both the extrapolation to zero thickness and the determination of the uncertainty in the measurement more straightforward for this test. For each data point, the uncertainty in thickness (x) was transformed, using the linear fit to the data for slope and intercept, to an equivalent uncertainty in asymmetry based on thickness. The actual y asymmetry uncertainty and the asymmetry uncertainty due to the thickness uncertainty were added in quadrature. This is the default procedure as well for common fitting programs such as root when the program is asked to fit functions with both x and y uncertainties.

The Pade orders tested were the following:

Pade (1,0): A= a0+a1T

Pade (2,0): A= a0+ a1T+a2T2

Pade (3,0): A= a0+ a1T+ a2T2+ a3T3

Pade (0,1): A=1/(1+b1T)

Pade (0,2): A=1/(1+b1T+b2T2)

Pade (1,1): (a0+a1T)/(1+b1T)

Pade(1,2): A= a0+a1T /(1+b1T+b2T2)

Pade (2,1): A= (a0+ a1T+a2T2) /(1+b1T)

Since these Pade approximant orders are nested functions, the F-testing procedure described above can be used to determine if adding the next term in the series can be rejected to a given confidence level. Higher order Pade functions were also investigated, but as shown below, eliminated due to the statistical F-test results.

The functions that have been historically used (ref Dunning and Gay review 1992) for fitting Mott foil thickness extrapolations are listed here. Many of them are of the form of the Pade approximants listed above, and are noted as such.

A=a+bT (Pade (1,0))

A=a/(1+bT) (Pade (0,1))

1/A=a+bT (equivalent to Pade (0,1))

1/√A=a+bT (equivalent to Pade (0,2))

ln(A)=a+bT (raise both sides to e, becomes a subset of exponential fit)

A=a+becT (only historical fit not captured in Pade approximants)

## Summary of fits

The results of the Pade approximant study of the fitting function for the Run 1 data, with the cuts of ‑0.5σ to +2σ, with the dilution subtraction as described in \_\_\_ are summarized in Table xx.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)****Run 1** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.85 | 0.145 | 2.24 | 9 | n/a |  |  |
| (2,0) | 44.12 | .121 | 0.96 | 8 | 12.95 |  |  |
| (3,0) | ~~44.35~~ | 0.142 | 0.63 | 7 | 5.23 | Reject: Ftest 95% conf. |  |
| (0,1) | 44.086 | 0.0974 | .980 | 8 | 12.6 |  |  |
| (0,2) | ~~44.17~~ | 0.124 | 0.99 | 7 | 0.94 | Reject: Ftest |  |
| (1,1) | 44.17 | 0.128 | 1.14 | 7 | 11.7 |  |  |
| (1,2) | ~~44.28~~ | 0.601 | 1.19 | 6 | 0.733 | Reject: Ftest |  |
| (2,1) | 43.78 | 0.210 | 2.97 | 6 | -2.41 (constrained) | Reject: Ftest |  |
| A=a+be^(cT) | 44.0635 | 8.58 | 1.43 | 9 | 4.89 vs. linear |  |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Rcode****Run1 larger** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.833 | .123 |  |  |  |  |  |
| (2,0) | 44.01 | .115 |  |  |  |  |  |
| (3,0) |  |  |  |  |  | Reject: Ftest 95% conf. |  |
| (0,1) | 43.98 | 0.114 |  |  |  |  |  |
| (0,2) |  |  |  |  |  | Reject: Ftest |  |
| (1,1) |  |  |  |  |  |  |  |
| (1,2) |  |  |  |  |  | Reject: Ftest |  |
| (2,1) |  |  |  |  |  | Reject: Ftest |  |
| A=a+be^(cT) |  |  |  |  |  |  |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)****Run 1 without 2%** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.8208 | .127 | 2.99 | 9 | n/a |  |  |
| (2,0) | 44.0407 | .1187 | 1.06 | 8 | 8.9 |  |  |
| (3,0) | ~~44.2315~~ | 0.151 | 0.8419 | 7 | 3.1 |  |  |
| (0,1) | 44.055 | 0.092 | 1.003 | 8 | 9.9 |  |  |
| (0,2) | ~~44.0753~~ | 0.124 | 1.137 | 7 | 0.06 |  |  |
| (1,1) | 44.0768 | 0.125 | 1.33 | 7 | 7.53 |  |  |
| (1,2) | ~~44.0827~~ | .224 | 1.58 | 6 | 0.022 |  |  |
| (2,1) | ~~45.2861~~ | 6.17 | 1.14 | 6 | 2.44 |  |  |
| A=a+be^(cT) | 44.0647 | 8.52 | 1.54 | 9 | 5.83 |  |  |

As shown in Table xx, many of the higher order Pade fits are rejected to a 95% confidence level by the F-test, leaving the Pade (1,0), Pade(2,0), Pade (0,1) and Pade(1,1) as viable fitting functions for the extrapolation to the asymmetry value at zero foil thickness. The values of the reduced χ2 in the table suggest that the error in the data may be overestimated.

**For the collaboration to discuss: Taking into consideration that we have included a 2% thickness error for foil nonuniformity and a 5% error for sibling nonuniformity, these maybe should be combined to be the overall nonuniformity? These additionally dominate the uncertainties.**

Reframe these to be thickness vs. asym to check difference in uncertainties

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)****Run 1** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.85 | 0.145 | 2.24 | 9 | n/a |  |  |
| T=a+bA | 43.99 | 0.0039 | 3.39 | 9 | n/a |  |  |
| (2,0) | 44.12 | .121 | 0.96 | 8 | 12.95 |  |  |
| T=a+bSqrt(A) | ~~44.0205~~ | 0.017 | 2.80 | 9 | 1.86 |  |  |
| (0,1) | 44.086 | 0.0974 | .980 | 8 | 12.6 |  |  |
| T=a+b/A | ~~44.1208~~ | 0.0458 | 1.93 | 8 | 7.80 |  |  |
| (1,1) | 44.17 | 0.128 | 1.14 | 7 | 11.7 |  |  |
| T=(a+bA)/(1+dA) | ~~44.17~~ | 0.0013 | 2.06 | 7 | 7.7 |  |  |
|  |  |  |  |  |  |  |  |
| A=a+be^(cT) | 44.15 | 0.057 | 1.43 | 9 | 17.06 (vs linear) |  |  |

Run 2 data: Table ?? (thickness error bars converted to dy using quadratic)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)** **Run 2** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.87 | .140 | 2.27 | 9 | n/a |  | .01 |
| (2,0) | 44.13 | .117 | .972 | 8 | 13.0 (vs Pade 1,0) |  | .45 |
| (3,0) | ~~44.37~~ | .135 | .605 | 7 | 5.9 (vs Pade 2,0) | Reject: Ftest | .75 |
| (0,1) | 44.09 | .0970 | 1.04 | 8 | 11.7 (vs Pade 1,0) |  | .4 |
| (0,2) | ~~44.18~~ | 0.119 | 0.98 | 7 | 1.44 (vs Pade 0,1) | Reject: Ftest | .4 |
| (1,1) | 44.20 | 0.124 | 1.12 | 7 | 12.2 (vs Pade 1,0) |  | .3 |
| (1,2) | ~~44.34~~ | 0.62 | 1.11 | 6 | 1.1 (vs Pade 1,1) | Reject: Ftest | .35 |
| (2,1) | 44.00 | 0.22 | 1.78 | 6 | -1.21 (vs Pade 1,1) | Reject: Ftest | .10 |
| A=a+be^(cT) | 44.1533 | 5.43 | 1.43 | 9 | 4.39 (vs. lin) |  | .15 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)** **Run 2****Without 2% uncertainty** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | 43.8335 | 0.149 | 3.65 | 9 | n/a |  |  |
| (2,0) | 44.1134 | .125 | 1.05 | 8 | 12.723 |  |  |
| (3,0) | ~~44.3496~~ | .146 | .697 | 7 | 5.13 | Reject f? |  |
| (0,1) | 44.0803 | 0.101 | 1.07 | 8 | 12.41 |  |  |
| (0,2) | ~~44.1622~~ | .129 | 1.08 | 7 | 0.9 | Reject f |  |
| (1,1) | 44.17 | .132 | 1.25 | 7 | 11.5 |  |  |
| (1,2) | ~~44.68~~ | 3.74 | 1.19 | 6 | 1.34 | Reject F |  |
| (2,1) | ~~43.1059~~ | 0.50 | 15.51 | 6 | -4.45 | Reject chi |  |
| A=a+be^(cT) | 44.1497 | 5.479 | 1.56 | 9 | 5.51 |  |  |

The other fits that have been historically used but are not equivalent to Pade approximants are the exponential and natural log functions, which are appended to the tables in the last row.

The distribution of values of Ao vs. the non-excluded fitting functions is shown in Figure \_\_ below. There is a clear clustering of the values around 44.06, with the Pade(1,0), or linear fit the farthest outlier. A Gaussian representation of the mean and standard deviation of the full data set is shown by the blue curve, and the distribution for the mean and std dev of the data with the Pade(1,0) removed from the data set is shown by the green curve.

The Pade(1,0), or linear fit, to the data appears to be a poor fit by eye. However, the fit cannot be excluded based on an F test since it has no lower order function to compare to, nor can it be rejected outright based on the χ2 value. To investigate the dependence of the linear fit to the data on the number of target foils in the data set, successive target foils were removed from the fit starting with the thickest. Indeed, the Pade(1,0) fit increases with each foil removed toward a value more consistent with the other values, but when removing successive target foils from the data set, the other functions approximating the data also have deviations when, in particular, the foilset is reduced to the thinnest 5 and 6 data points

 (Add images of Daniels successive fits here if we are keeping this section)

These need to be redone with corrected values

Summarizing the viable fits for both run 1 and run 2

The viable Pade approximants for the fitting of asymmetry vs. rate are the orders Pade(1,1), Pade(0,1) and Pade(2,0), with Pade(1,0) a potentially non-excluded fitting function but one that yields an outlier in the intercept value. The other functions that have traditionally been investigated for the fitting function are the ln(A)=a+bT (or A=ae^bT) and the exponential A=a+be^cT.  **Looking at this, I am kicking out the ln since it is a subset of the exponential and therefore less precise. It is also giving a poorer fit.**

The non-excluded rational fraction fitting functions and the exponential fit of the data agree well, giving a value of Ao of

The alternative to using the measured foil thickness to extrapolate to zero thickness is to rather use asymmetry vs rate for the extrapolation to the asymmetry at zero rate. These have been investigated using the pade approximant formalism, and are summarized here for first run 1 then run 2.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)** **Run 1****A vs. Rate** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | ~~42.76~~ | .343 | 44 | 9 | n/a | Reject: χ2 |  |
| (2,0) | 43.95 | .100 | 1.59 | 8 | 241 |  |  |
| (3,0) | ~~44.05~~ | .110 | 1.30 | 7 | 2.84 | Reject: Ftest |  |
| (0,1) | ~~43.36~~ | .236 | 18.0 | 8 | 14.07 | Reject: χ2 |  |
| (0,2) | 44.07 | .090 | 1.25 | 7 | 108 |  |  |
| (0,3) | 43.96 | 0.105 | 2.02 | 6 | -1.64 | Reject Ftest |  |
| (1,1) | 44.12 | 0.100 | 1.56 | 7 | 248 |  |  |
| (1,2) | ~~44.28~~ | 0.270 | 3.16 | 6 | -2.03 | Reject Ftest |  |
| (2,1) | ~~44.04~~ | 0.118 | 1.80 | 6 | 0.21 | Reject Ftest |  |
| A=a+be^(cT) | 44.06 | 0.0355 | 1.78 | 9 | 216 |  |  |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Pade(n,m)** **Run 2****A vs. Rate** | **intercept** | **dA** | **red. χ2** | **dof** | **Ftest** | **Accept/Reject** | **χ2 liklihood table** |
| (1,0) | ~~42.71~~ | .381 | 46.9 | 9 | n/a | Reject: χ2 |  |
| (2,0) | 43.96 | .205 | 5.74 | 8 | 65.5 |  |  |
| (3,0) | ~~44.20~~ | .217 | 4.36 | 7 | 3.53 | Reject: Ftest |  |
| (0,1) | ~~43.29~~ | .288 | 23.53 | 8 | 9.95 | Reject: χ2 |  |
| (0,2) | 44.11 | .193 | 5.02 | 7 | 30.5 |  |  |
| (0,3) | ~~43.97~~ | .217 | 7.53 | 6 | 0 | Reject: Ftest |  |
| (1,1) | 44.19 | .201 | 5.35 | 7 | 72.9 |  |  |
| (1,2) | ~~44.31~~ | .320 | 6.26 | 6 | 0.13 | Reject Ftest |  |
| (2,1) | ~~44.26~~ | .291 | 6.26 | 6 | 0.13 | Reject Ftest |  |
| A=a+be^(cT) | 44.12 | 0.074 | 6.94 | 9 | 61.9 |  |  |