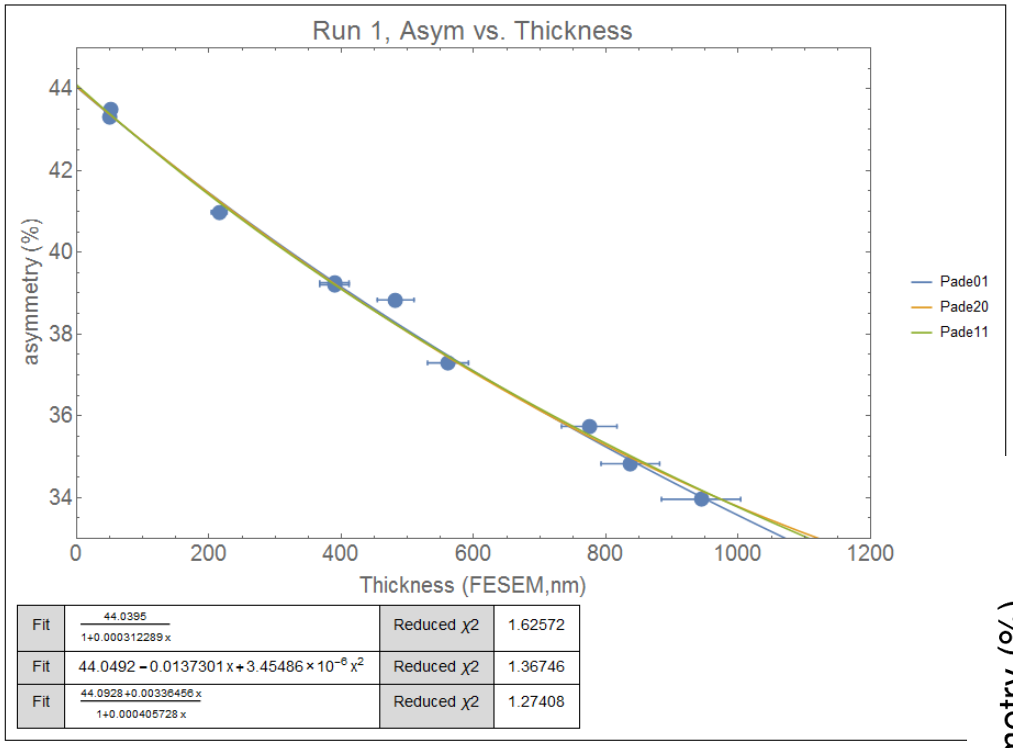
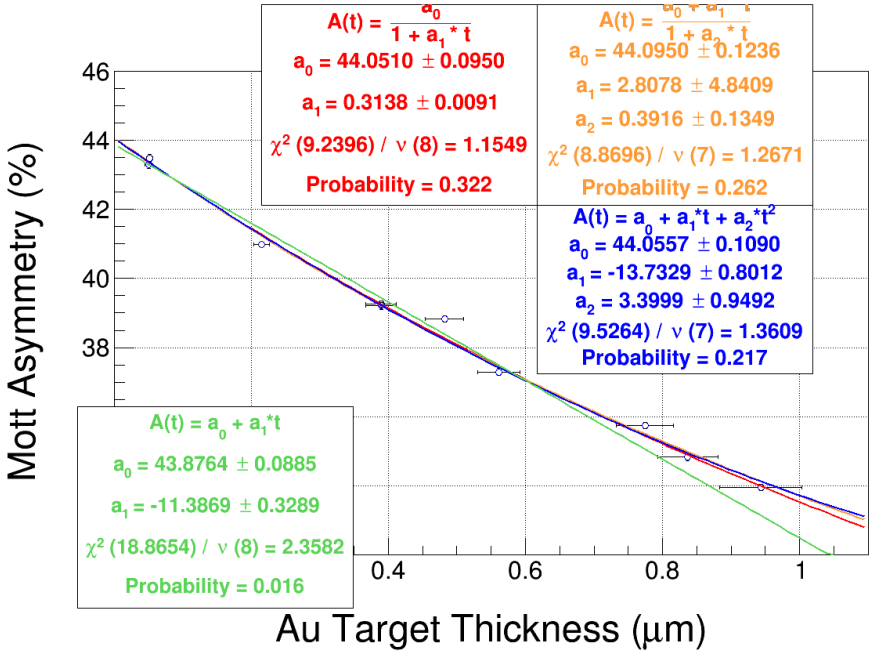
Mathematica fits vs. Root

17Jan 2017

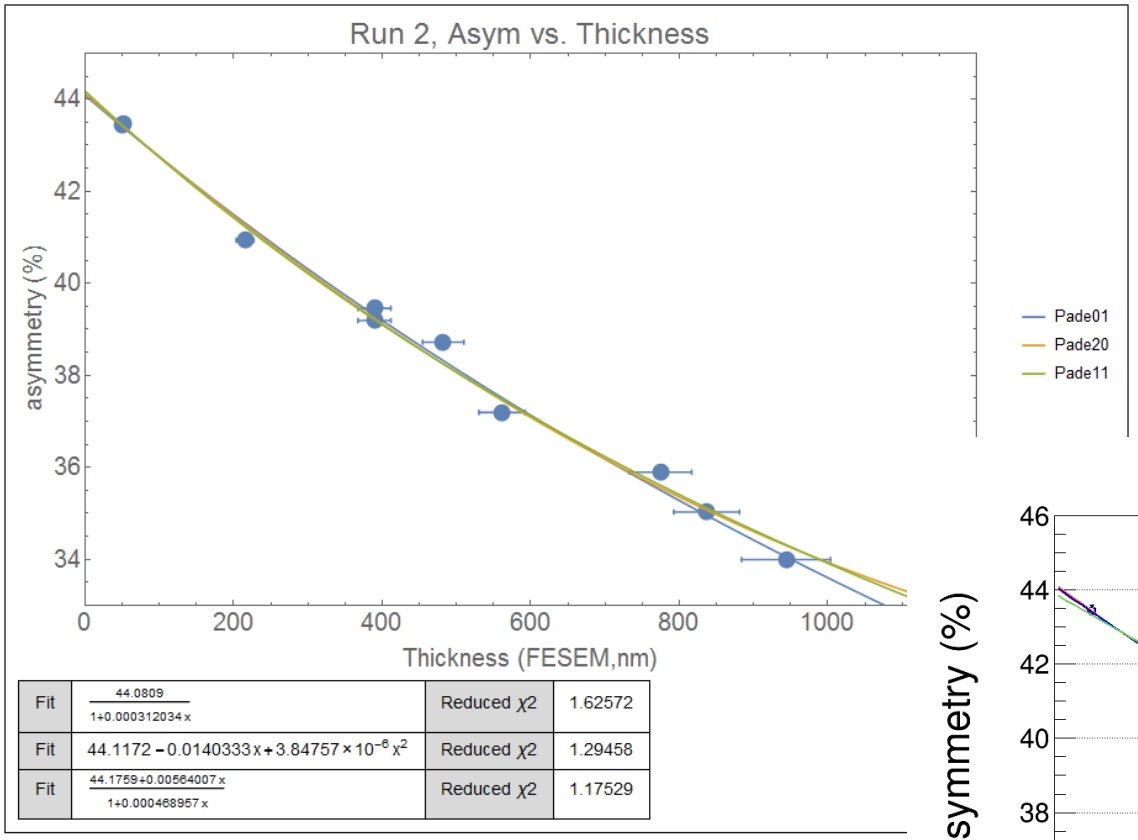
Asym vs. T, Run 1



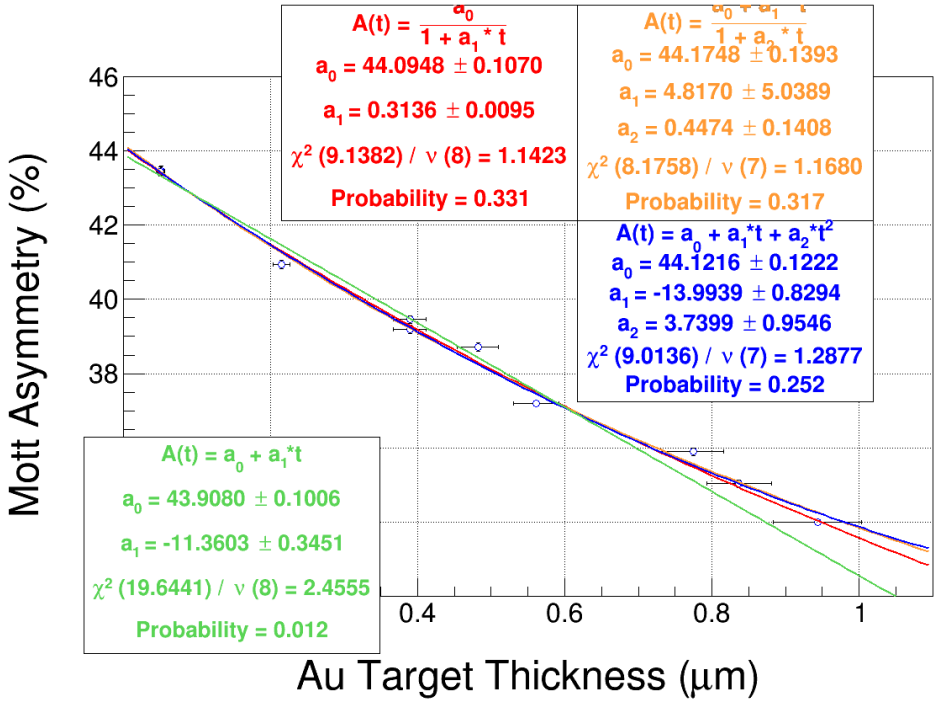
Fit	$\frac{44.0395}{1+0.000312289\,x}$	Reduced $\chi 2$	1.62572
Fit	$44.0492 - 0.0137301\,x + 3.45486\times10^{-6}\,x^2$	Reduced $\chi 2$	1.36746
Fit	$\frac{44.0928+0.00336456\,x}{1+0.000405728\,x}$	Reduced $\chi 2$	1.27408



Asym vs. T, Run 2



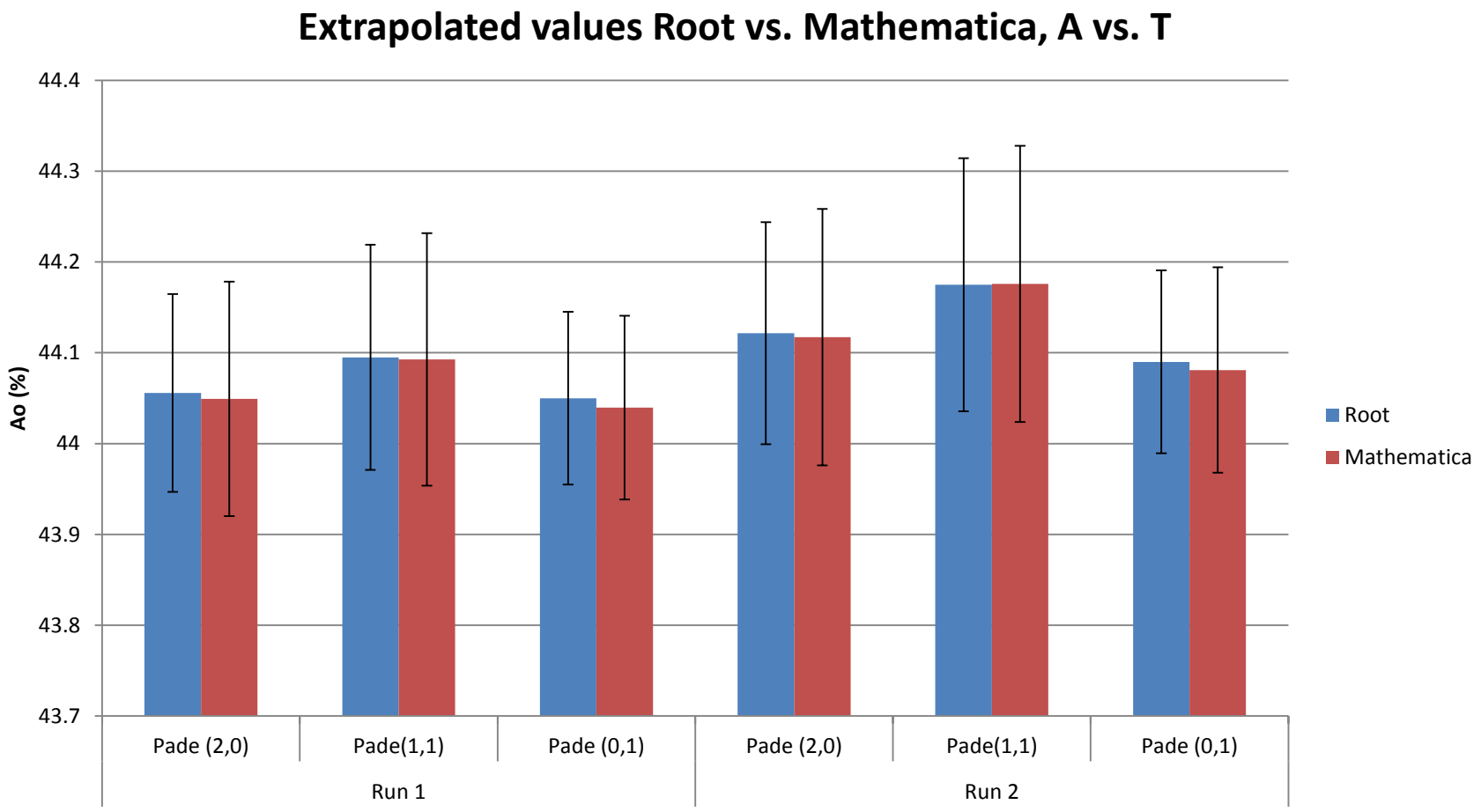
Fit	$\frac{44.0809}{1+0.000312034\,x}$	Reduced $\chi 2$	1.62572
Fit	$44.1172 - 0.0140333\,x + 3.84757\times10^{-6}\,x^2$	Reduced $\chi 2$	1.29458
Fit	$\frac{44.1759+0.00564007\,x}{1+0.000468957\,x}$	Reduced $\chi 2$	1.17529

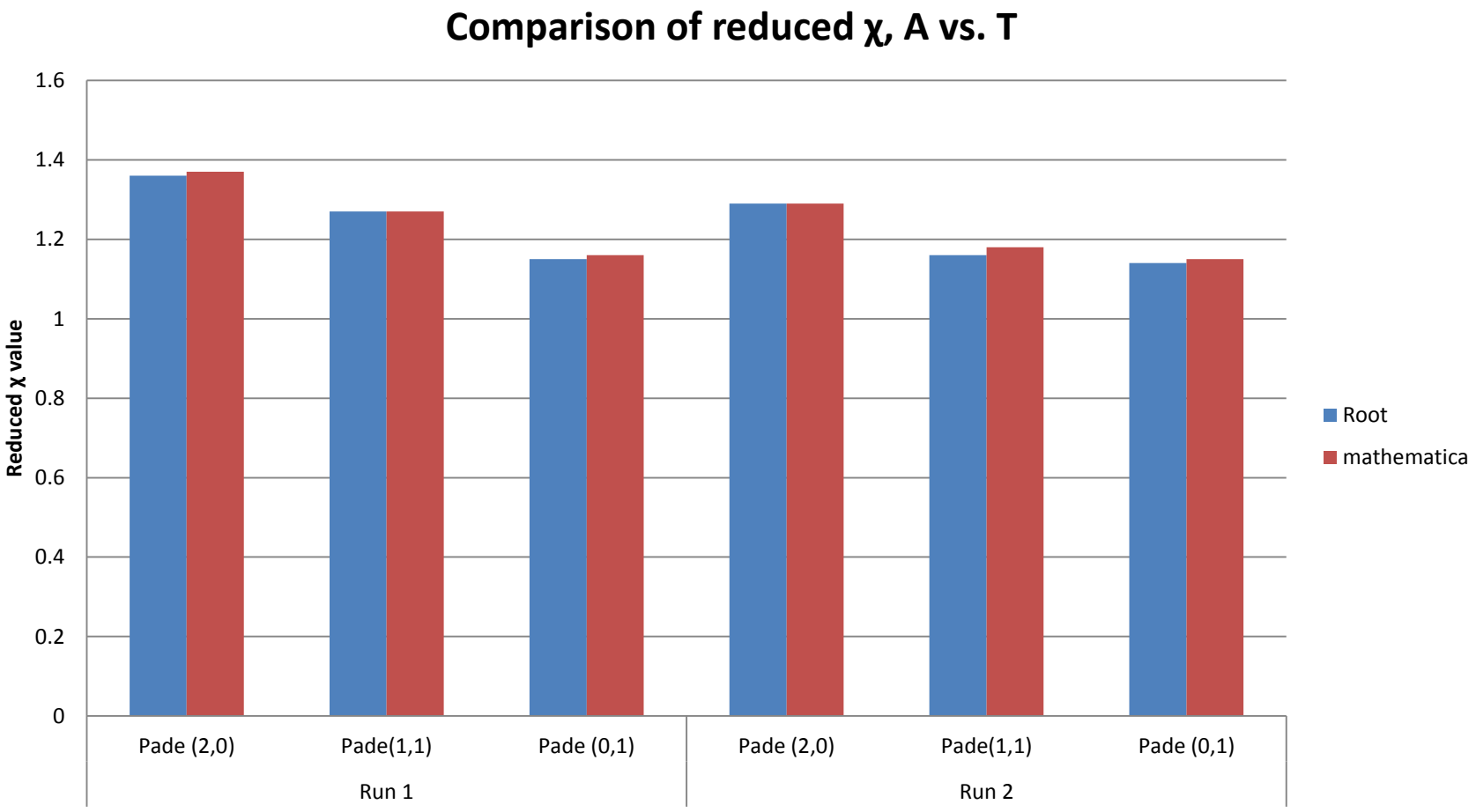


Root vs. Mathematica

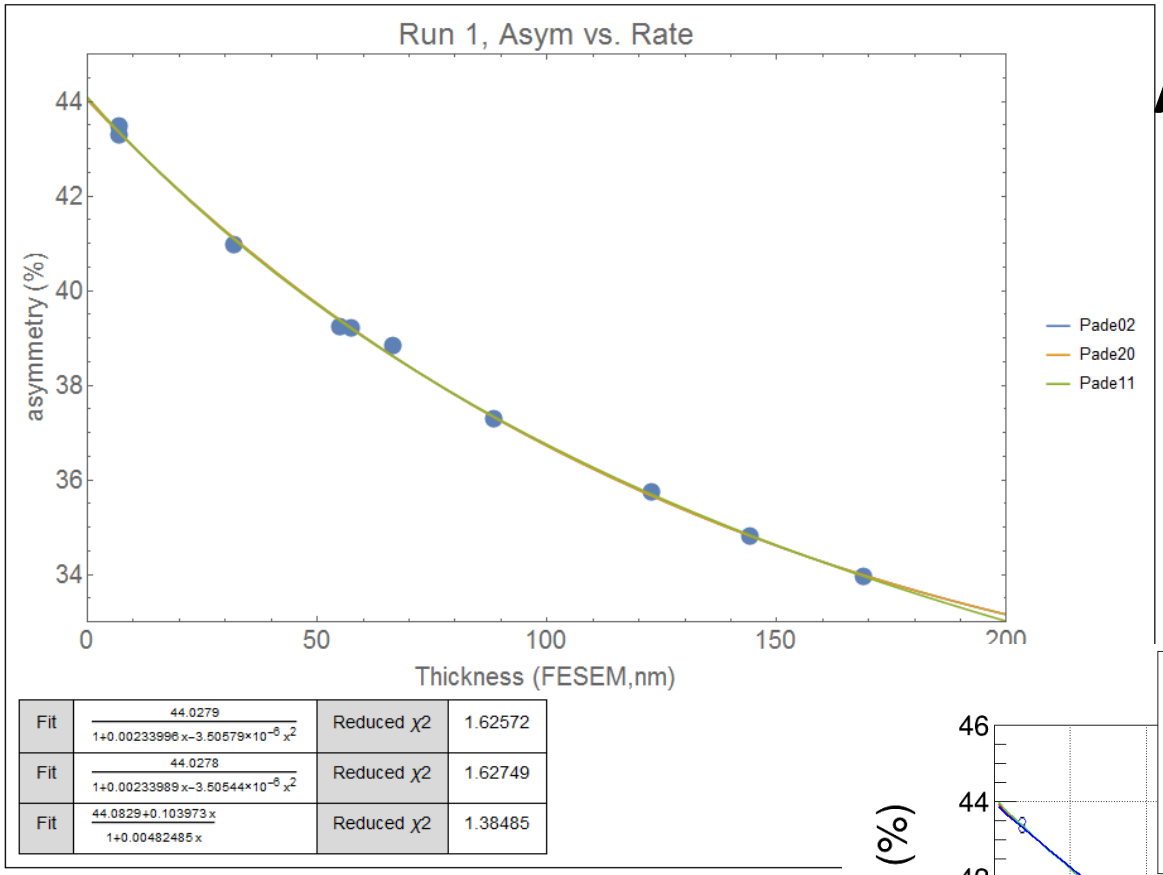
A vs. T	ao	Δao	a1	a2	b1	Chi sq	
Pade (2,0)	44.0557	.1090	-13.76	3.4		1.36	Root
Pade(1,1)	44.095	.124	2.8		0.39	1.27	Root
Pade (0,1)	44.05	0.095			0.31	1.15	Root
Pade (2,0)	44.1216	.1222	-13.99	3.74		1.29	Rt run2
Pade(1,1)	44.175	.1393	4.8		0.45	1.16	Rt run2
Pade (0,1)	44.09	0.1006	-11.36		0.3136	1.14	Rt run2

A vs. T	ao	Δao	a1	a2	b1	Chi sq	
Pade (2,0)	44.0492	0.129	-0.0137	3.45e-6		1.37	MM run 1
Pade(1,1)	44.0928	0.139	0.00336		0.0002747	1.27408	MM run 1
Pade (0,1)	44.0395	0.1012			0.0003122	1.16	MM run 1
Pade (2,0)	44.1172	0.1413	-0.014	3.85e-6		1.29	MM run 2
Pade(1,1)	44.1759	0.152	0.00564		0.000469	1.18	MM run 2
Pade (0,1)	44.0809	0.1131			0.000312	1.15	MM run 2

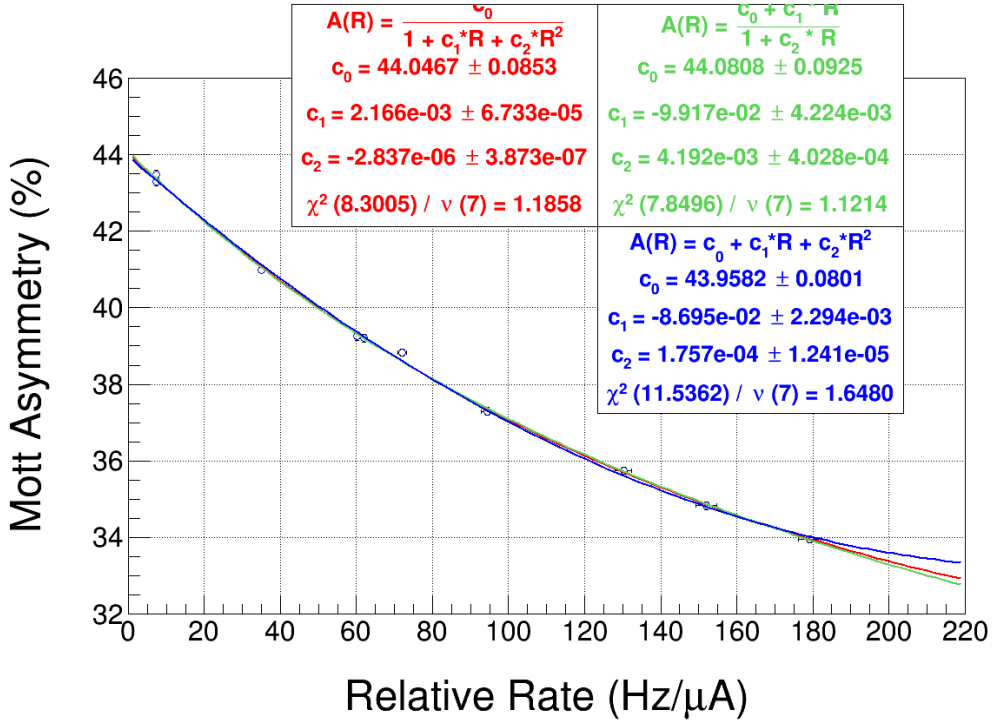

Extrapolated values Root vs. Mathematica, A vs. T
Ao (%)
44.4
44.3
44.2
44.1
44
43.9
43.8
43.7
Pade (2,0)
Pade(1,1)
Pade (0,1)
Pade (2,0)
Pade(1,1)
Pade (0,1)
Run 1
Run 2
Root
Mathematica


Comparison of reduced χ, A vs. T
Reduced χ value
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Pade (2,0)
Pade(1,1)
Pade (0,1)
Pade (2,0)
Pade(1,1)
Pade (0,1)
Run 1
Run 2
Root
mathematica

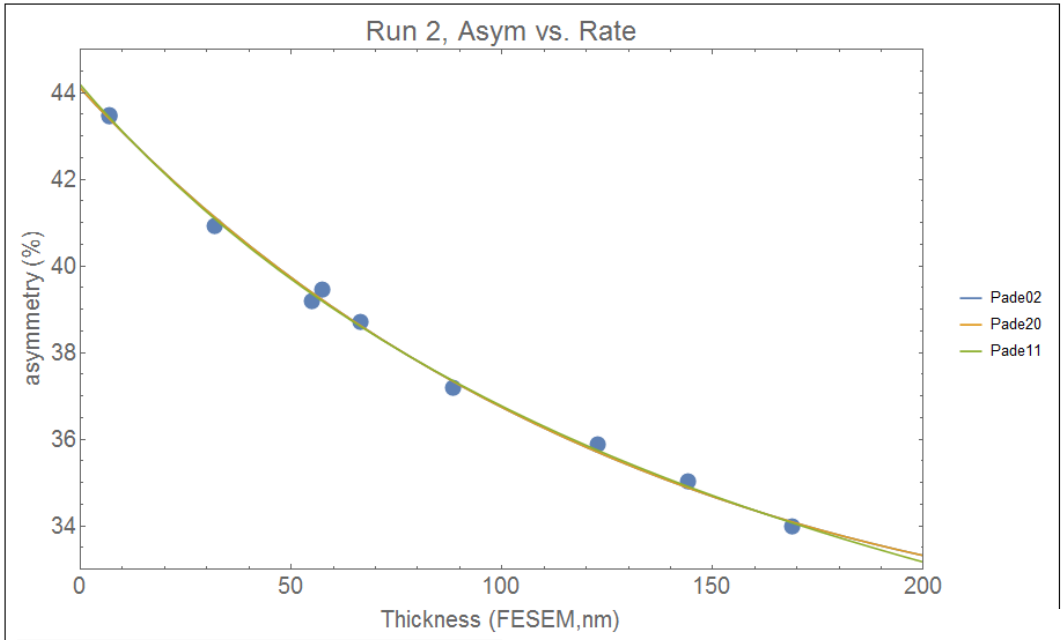
Asym vs. Rate run 1



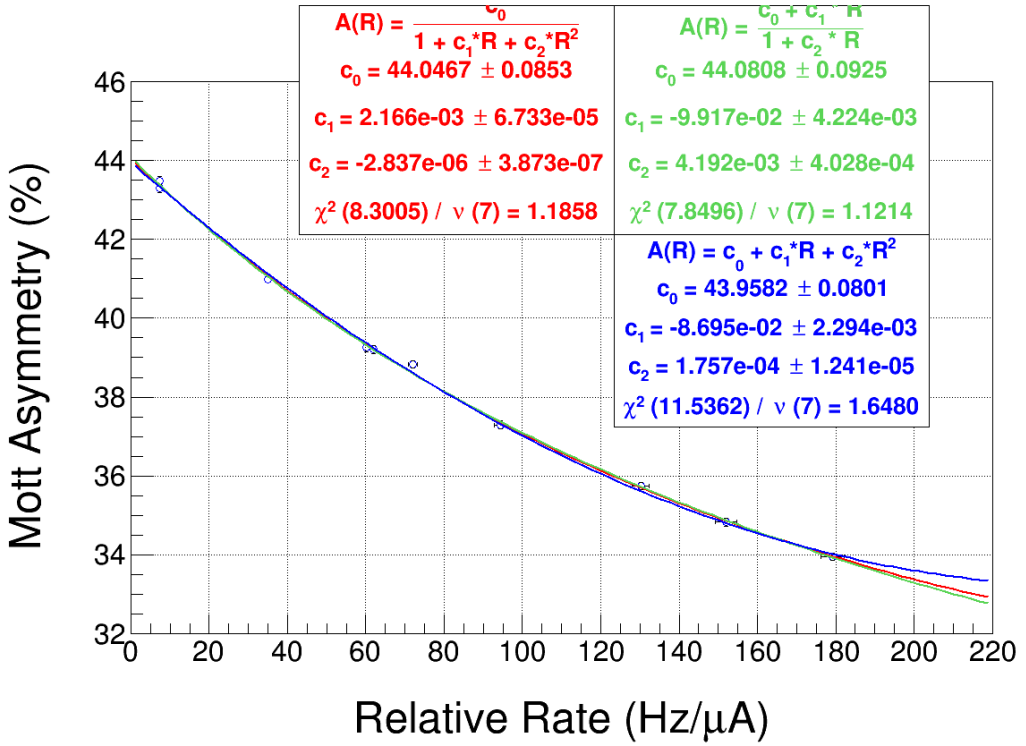
Fit	$\frac{44.0279}{1+0.00233996\,x-3.50579\times10^{-6}\,x^2}$	Reduced $\chi2$	1.62572
Fit	$\frac{44.0278}{1+0.00233989\,x-3.50544\times10^{-6}\,x^2}$	Reduced $\chi2$	1.62749
Fit	$\frac{44.0829+0.103973\,x}{1+0.00482485\,x}$	Reduced $\chi2$	1.38485



Asym. vs rate run 2



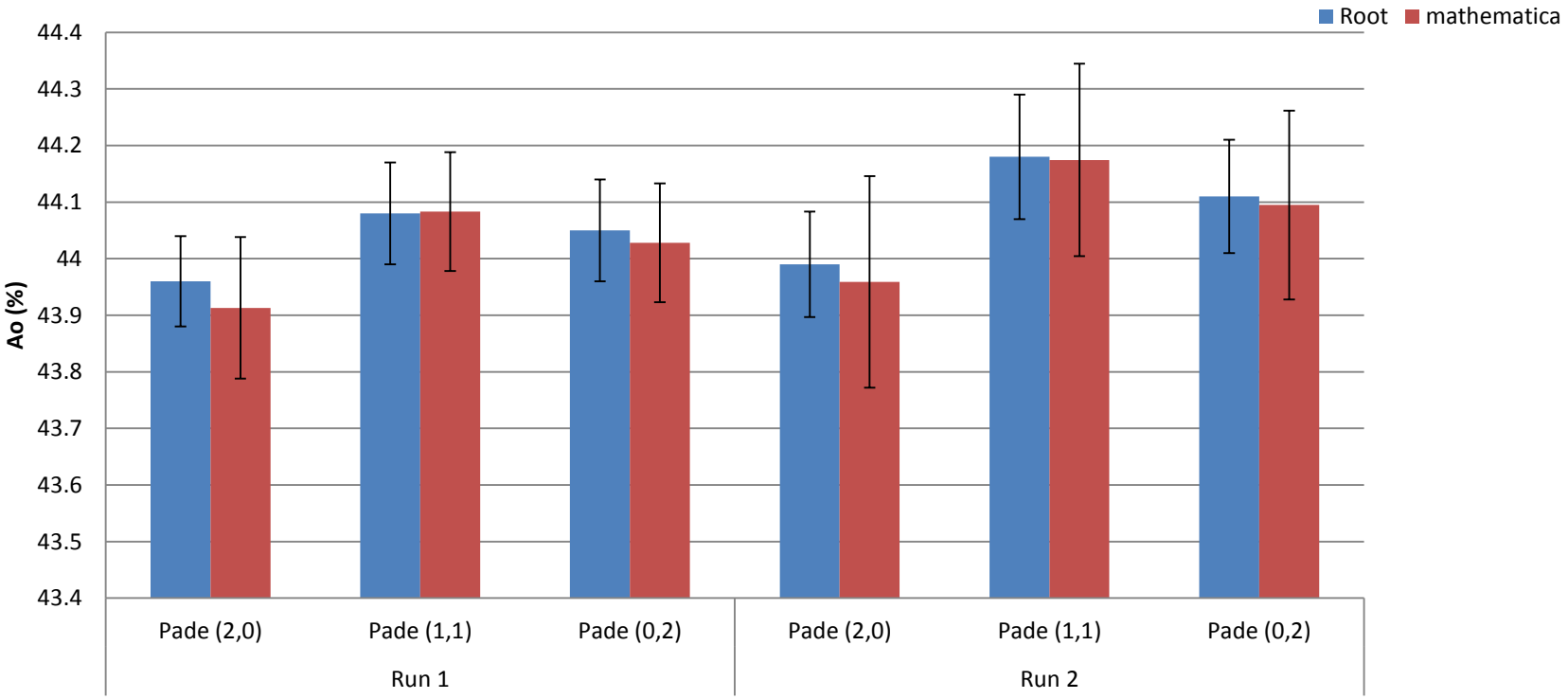
Fit	$\frac{44.0948}{1+0.00238883\,x-3.86058\times10^{-6}\,x^2}$	Reduced $\chi2$	2.95104
Fit	$\frac{44.0947}{1+0.00238879\,x-3.86036\times10^{-6}\,x^2}$	Reduced $\chi2$	2.95485
Fit	$\frac{44.1744+0.120627\,x}{1+0.00529568\,x}$	Reduced $\chi2$	2.54385

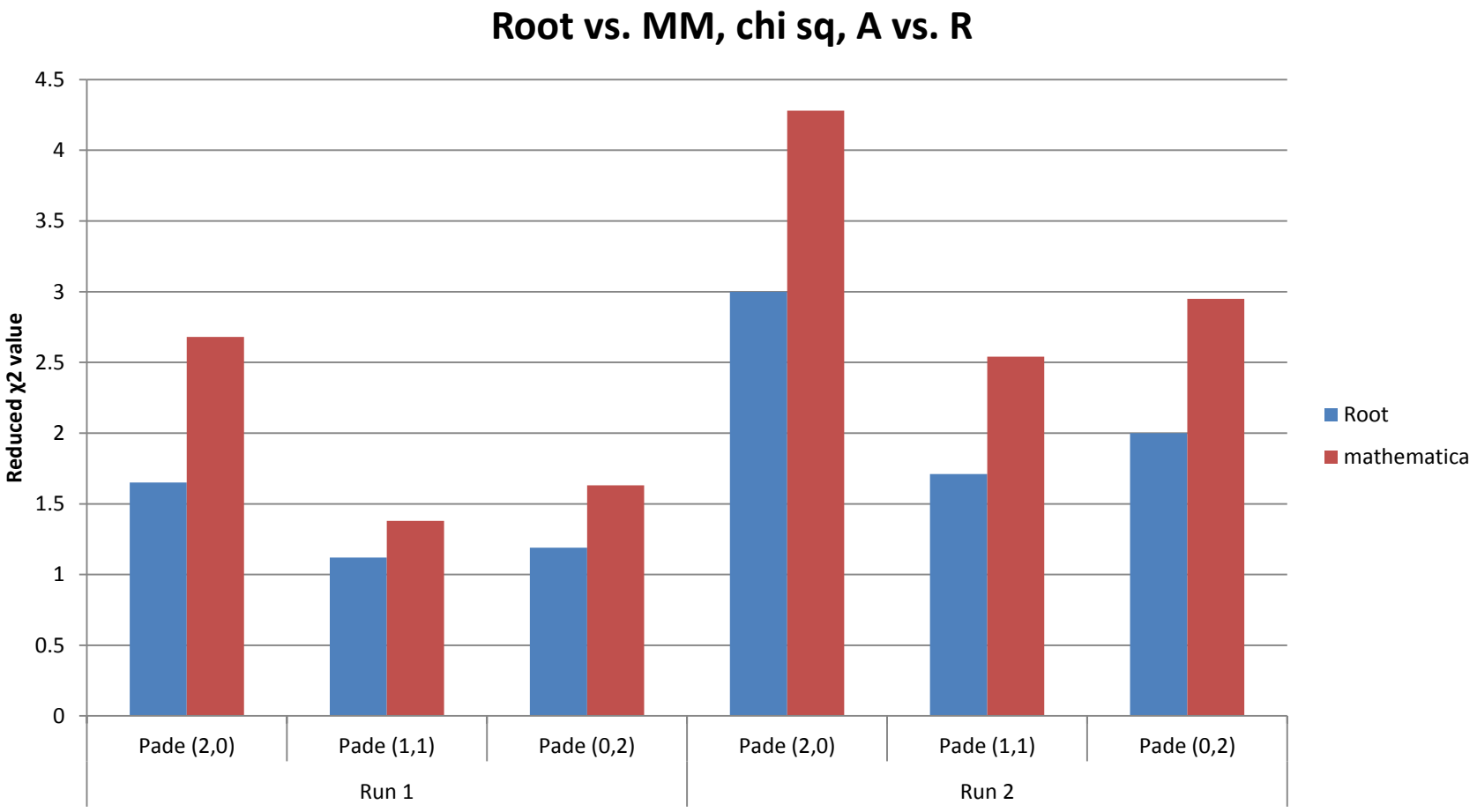


A vs. R	Ao	dAo	Chi squared	Run
Pade (2,0)	43.96	0.08	1.65	Root, 1
Pade (1,1)	44.08	0.09	1.12	Root, 1
Pade (0,2)	44.05	0.09	1.19	Root, 1
Pade (2,0)	43.99	0.093	3.00	Root, 2
Pade (1,1)	44.18	0.11	1.71	Root, 2
Pade (0,2)	44.11	0.100	2.00	Root, 2

A vs. R	Ao	dAo	Chi squared	Run
Pade (2,0)	43.913	0.125	2.68	MM, 1
Pade (1,1)	44.0829	0.105	1.38	MM, 1
Pade (0,2)	44.0279	0.105	1.63	MM, 1
Pade (2,0)	43.959	0.187	4.28	MM, 2
Pade (1,1)	44.1744	0.170	2.54	MM, 2
Pade (0,2)	44.0948	0.167	2.95	MM, 2

Root vs. MM, A vs. R




Root vs. MM, chi sq, A vs. R
Reduced χ2 value
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
Pade (2,0)
Pade (1,1)
Pade (0,2)
Pade (2,0)
Pade (1,1)
Pade (0,2)
Run 1
Run 2
Root
mathematica

Summary

- Extrapolated Ao in agreement with two methods (mathematica and root analysis of same data set)
- Some differences in the Chi squared values may come from slightly different methods for calculation, x-error bar handling
- Pick one, pick thickness units, proceed.

Math in mathematica

- Get y(x+dx), y(x-dx) for fitting function, add this dy due to x error bar in quadrature
- Use weighting function: w=(1/dy)^2 at each pt
- Use the mathematica “NonlinearModelFit” function – least squares, using weighted data points, standard error on Ao term
- Define χ2 (sum over all data pts)

  SUM{[(data pt – fit(xi))/Δyi]^2}
- Reduced χ2 :

  χ2 /(# data points - fit parameters)