Summary: Thickness measurements and extrapolation function for Ao

16 February 2016

FESEM measurement summary

- FESEM measurements of sibling foils for all but one of the 50 nm foils
- Statistical uncertainties
  - Variation between nominally identical images
  - Variation in repeated analysis of the same image
- Systematic uncertainties
  - FESEM resolution 1.2 nm
  - ± 4 pixel uncertainty in ends of line
  - Tilt uncertainty (up to 0.4% error)
  - Working distance error (1%)
  - 5% batch uniformity – Lebow spec
  - 2% foil uniformity – Lebow spec

Are these redundant?

Uncertainty calculation summary

		Au_5385_B	Au_3057_C	Au_5134_B	Au_7028_B	Au_5275_C	Au_5613_D	Au_7029_B	Au_6809_B
	nominal thickness (nm)	*1000*	*870*	*750*	*625*	*500*	*355*	*225*	*50*
	mean thickness (all data, nm)	**943.7**	**836.8**	**774.6**	**561.2**	**482.0**	**389.4**	**215.2**	**52.0**
Stat.	Stdev, nom. identical data (nm)	29.0	7.1	9.1	8.0	9.7	4.5	1.9	2.3
	stdev image reanalysis (nm)	22.5	7.7	9.4	7.5	4.0	2.7	1.8	2.1
Syst.	Image analysis: ± 4 Pixel	20.0	8.0	10.0	8.0	8.0	8.0	2.6	2.6
	Resolution (1.2 nm inherent)	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2
	Tilt (0.4%)	4.6	4.2	3.9	2.8	2.5	1.9	1.1	0.3
	Focus (1%)	9.4	8.4	7.7	5.6	4.8	3.9	2.2	0.5
	Different spots (Lebow: 2%)	18.9	16.7	15.5	11.2	9.6	7.8	4.3	1.0
	Sibling difference (Lebow:5%)	47.2	41.8	38.7	28.1	24.1	19.5	10.8	2.6
Totals									
	stat uncertainty (nm)	36.7	10.5	13.1	11.0	10.5	5.2	2.6	3.1
	syst uncertainty (nm)	55.6	46.7	43.8	31.9	27.7	22.9	12.2	4.1
	total uncertainty (nm)	**66.6**	**47.9**	**45.7**	**33.7**	**29.6**	**23.5**	**12.5**	**5.1**

Are these redun-dant?

Fitting function

- No consensus on the ideal function for fitting data and extrapolating to zero foil thickness asymmetry value (Dunning and Gay 1992)
- Pade approximants (rational fractions) are excellent for extrapolating
- Consider Pade approximant approach to investigate extrapolation to zero thickness, determine uncertainty due to model dependence of Ao value

Pade approximates

In mathematics a **Padé approximant** is the "best" approximation of a function by a rational function of given order.

Given a function *f* and two integers *m* ≥ 0 and *n* ≥ 1, the *Padé approximant* of order [m/n] is the rational function

$$y = \frac{a_n x^n + a_{n-1} x^{n-1} + \ldots + a_2 x^2 + a_1 x + a_0}{b_m x^m + b_{m-1} x^{m-1} + \ldots + b_2 x^2 + b_1 x + b_0},$$

Taylor series expansions are one example of Pade' (Pade (1,0), Pade (2,0), Pade(3,0), but do not converge as quickly

The typical fitting function $A = \frac{Ao}{1+\gamma T}$ is also Pade' (0,1)

Pade approximants and traditional fitting functions

The Pade orders tested were the following: (higher orders were examined and not needed)

- Pade (1,0): $A= a_0+a_1T$
- Pade (2,0): $A= a_0+ a_1T+a_2T^2$
- Pade (3,0): $A= a_0+ a_1T+ a_2T^2+ a_3T^3$
- Pade (0,1): $A=1/(1+b_1T)$
- Pade (0,2): $A=1/(1+b_1T+b_2T^2)$
- Pade (1,1): $(a_0+a_1T)/(1+b_1T)$
- Pade(1,2): $A= a_0+a_1T /(1+b_1T+b_2T^2)$
- Pade (2,1): $A= (a_0+ a_1T+a_2T^2) /(1+b_1T)$

Functions traditionally used for extrapolation (ref Dunning and Gay review 1992)

note – many are actually covered in the Pade formulation above

- $A=a+bT$ (Pade (1,0))
- $A=a/(1+bT)$ (Pade (0,1))
- $1/A=a+bT$ (equivalent to Pade (0,1))
- $1/\sqrt{A}=a+bT$ (equivalent to Pade (0,2))
- $\ln(A)=a+bT$
- $A=a+be^{cT}$

Not covered by Pade unless you consider the Taylor expansion of ln or exp functions

F testing

- The goodness of a fit is typically found by looking at reduced χ^2 or reduced R^2, which show how far the fit is from the data
- It is possible to overfit functions looking only at these “goodness of fit” tests
- An “F-test” can be used to see, to a given degree of confidence, if adding the next order term in an expansion is justified. If the F-test fails, there is a n% chance that the term isn’t needed

$$F = \frac{S_{j-1} - S_j}{S_j}(N - j - 1)$$

is distributed as a Fisher–Snedecor $F(1, N - j - 1)$ variable if the j^{th} degree is not justified.

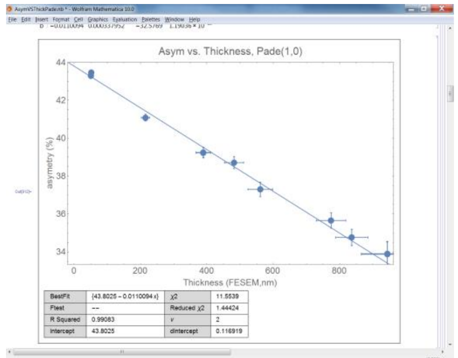
From the tabulated value of the F distribution one can then give the prescription in Table 10.2.

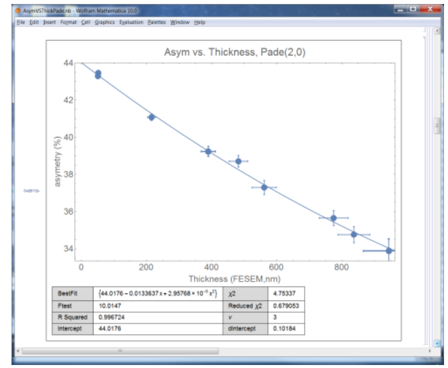
Table 10.2. Maximum degree needed in polynomial approximation.

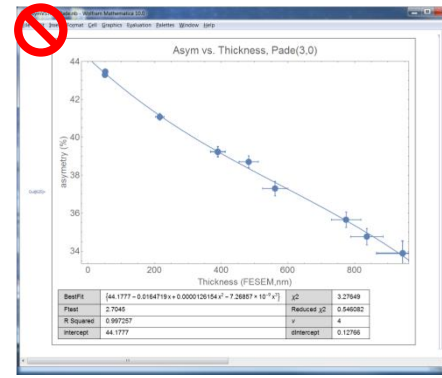
$N - j - 1$	2	3	4	6	8	12	20	60	120
Reject j^{th} order to 95% confidence level if F is smaller than	18.5	10.1	7.7	6	5.3	4.7	4.3	4	3.9

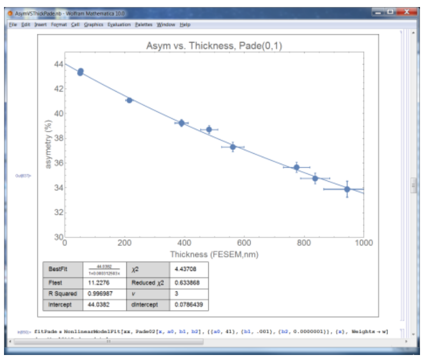
Frederick James,
Statistical methods in
experimental physics 2nd ed.

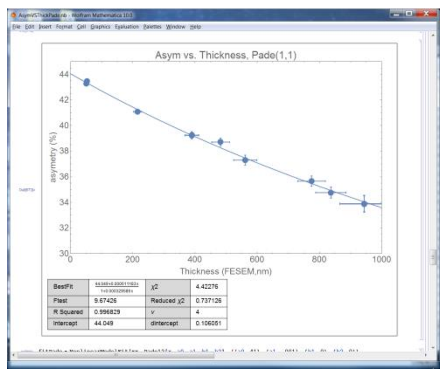
Asymmetry vs. Thickness

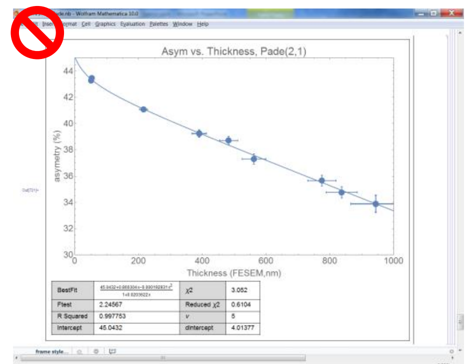


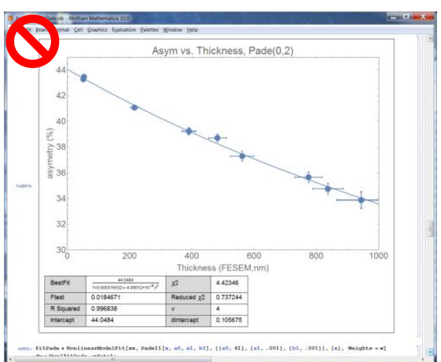


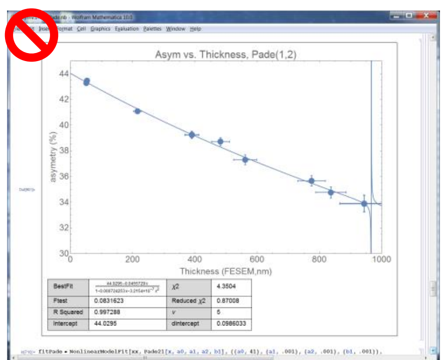












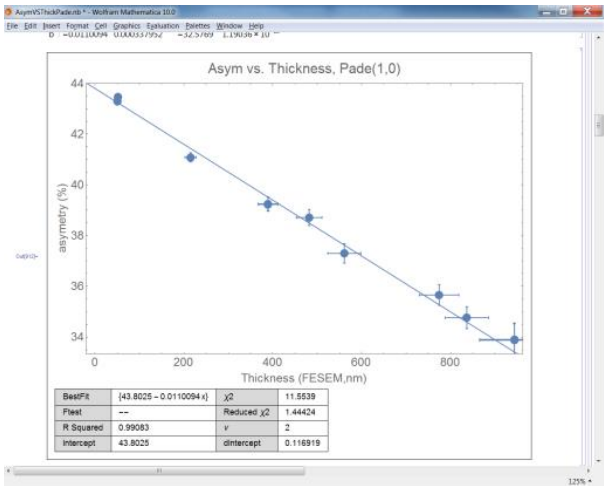
Y error bars have been manipulated to have the x uncertainty included since mathematical typically only fits with y uncertainty. Pade (0,1) (typical fit) used to transform error bars

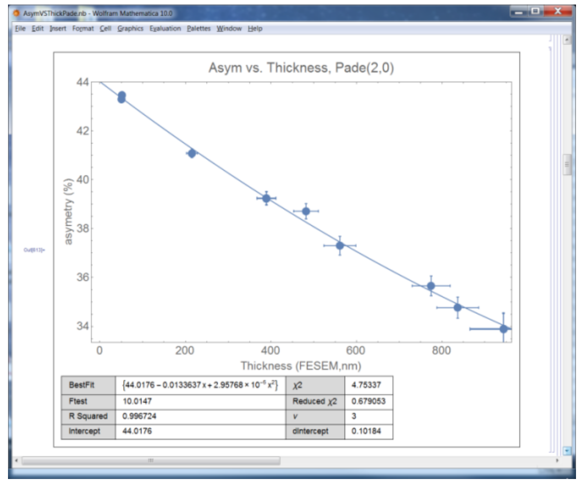
Pade(n,m) orders: Asy vs. Thick

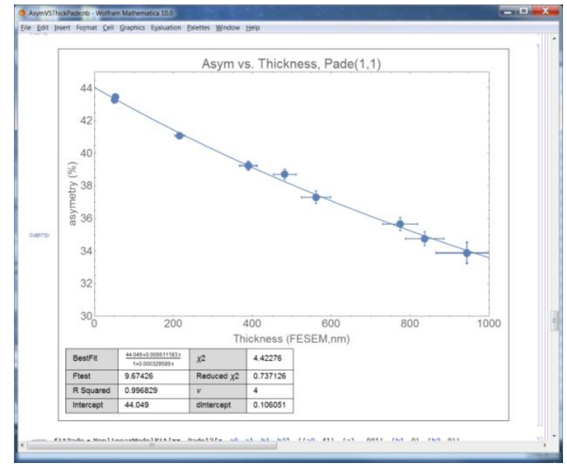
Pade(n,m)	intercept	dA	R^2	red. χ^2	Ftest
(1,0)	43.8025	0.1169	0.991	1.44	-- worst red. χ^2
(2,0)	44.0176	0.1018	0.997	0.679	10.01
(3,0)	~~44.1777~~	0.128	0.997	0.546	2.70 (rej F test)
(0,1)	44.0382	0.0786	0.997	0.634	11.23
(0,2)	~~44.0484~~	0.1057	0.997	0.737	0.0185 (rej ftest)
(1,1)	44.049	0.1061	0.997	0.737	9.67
(1,2)	~~44.0295~~	0.0986	0.997	0.870	0.083 (rej. Ftest)
(2,1)	~~44.043~~	4.014	0.998	0.6104	2.24 (rej. Ftest)

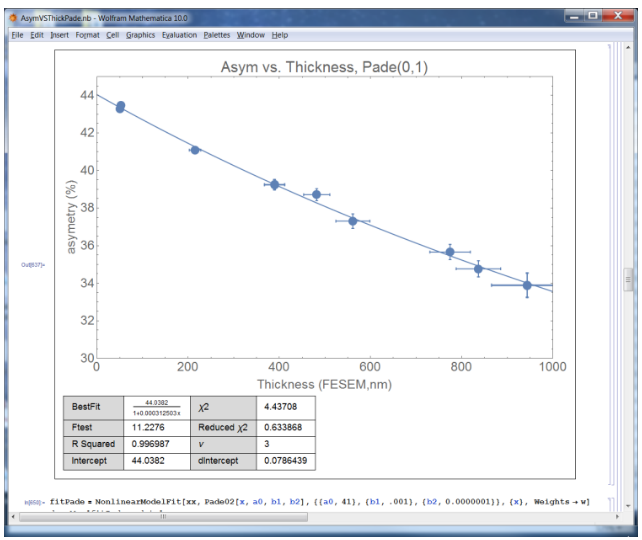
Run 1 data, -0.5σ to +2.0σ, may still require error bar adjustment

Potential fits: not statistically rejected









Pade(n,m)	Asym(%)	dA	red. X^2(dof)	
(1,0)	43.8025	0.1169	1.44 (9)	Linear -
(2,0)	44.0176	0.1018	.679 (8)	
(0,1)	**44.0382**	**0.0786**	**.634 (8)**	**Normal fit**
(1,1)	44.049	0.1061	.737 (7)	
averaged	**44.0352**	***~0.1***		***Additional uncertainty due to model***

Zero thickness extrapolation largely independent of fit function used, assuming statistically reasonable fits

Run 1 fits: Asy vs. Thick

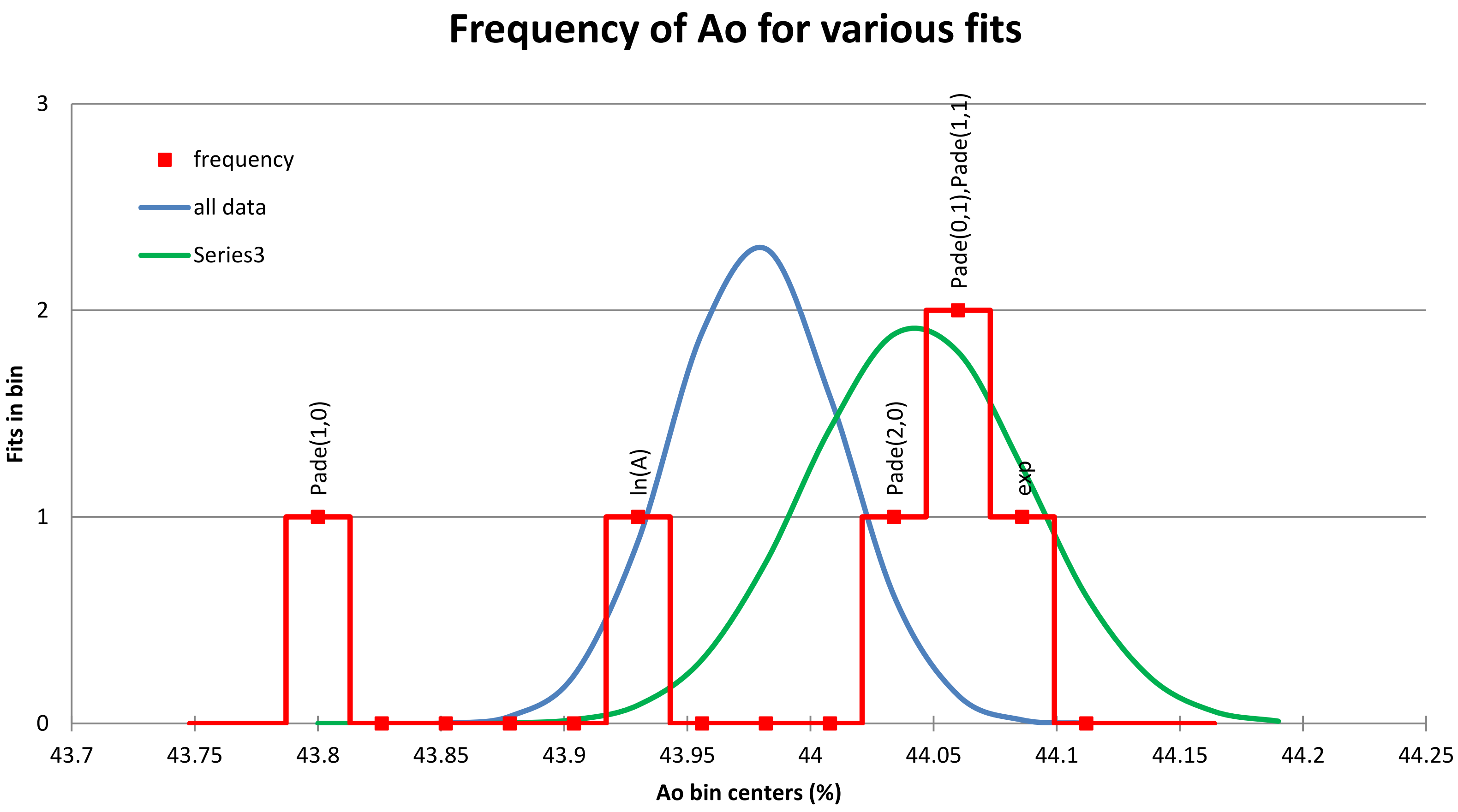
Pade(n,m) or fn	intercept	dA	R^2	red. χ^2	d.o.f.	Ftest
(1,0)	43.8025	0.1169	0.991	1.28	9	--
(2,0)	44.0176	0.1018	0.997	0.594	8	11.45
(0,1)	44.0382	0.0786	0.997	.554	8	11.23
(1,1)	44.049	0.1061	0.997	0.737	7	9.67
ln(A)=a+bT	43.9917	*0.058**	0.994	0.865	9	n/a
A=a+be^(cT)	44.0837	*0.087**	0.996	0.669	8	n/a

Run 2 fits: Asy vs. Thick

Pade(n,m) or fn	intercept	dA	R^2	red. χ^2	d.o.f.	Ftest
(1,0)	43.8437	0.1475	.984	2.28	9	--
(2,0)	44.1131	0.125	.993	1.01	8	12.21
(0,1)	44.0759	0.102	.994	1.04	8	11.61
(1,1)	44.1735	0.132	.993	1.19	7	9.67
ln(A)=a+bT	44.0562	*0.0726**	.984	1.77	9	n/a (not nested)
A=a+be^(cT)	44.22	*0.049**	0.991	1.16	8	n/a

Uncertainties for ln and exp functions need to be examined

All viable Pade approximants + ln, exp Run 1



Conclusions

- Unless we can rule out the other functions, we should be adding an uncertainty to our extrapolate Ao due to model uncertainty
- The uncertainty due to model dependence is small, ~0.25%
- Some refinement still needed for which are the viable fits to include in this uncertainty
- Is there a legitimate way to eliminate the Pade(1,0)=linear fit that looks bad, is outlier?

Still to do

- Verify and propogate best estimate at thickness uncertainty through these fits and Daniel’s root fits
- χ< 1: have we overestimated out uncertainty in thickness? How can/should we adjust?
- Do we get significant improvements in uncertainty with Asym vs. rate rather than Asym vs. thickness?