Neutrons Update

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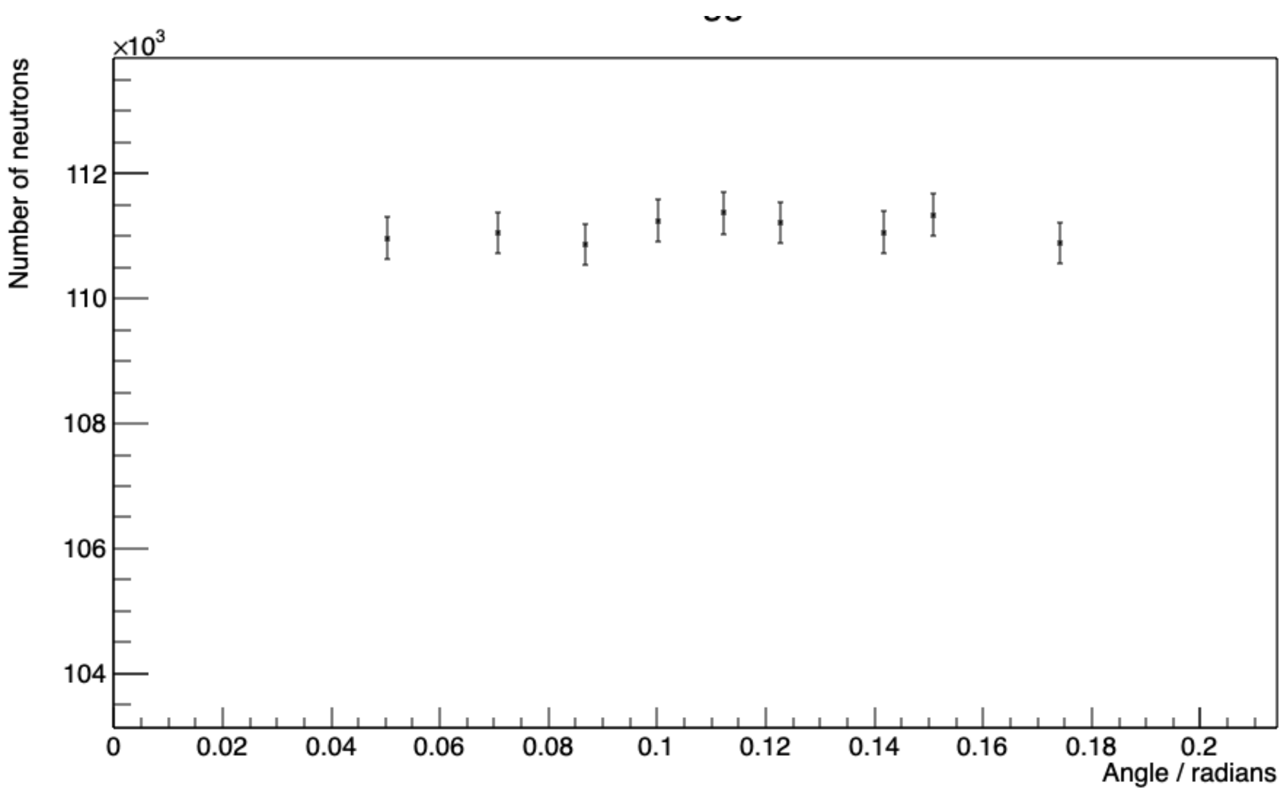
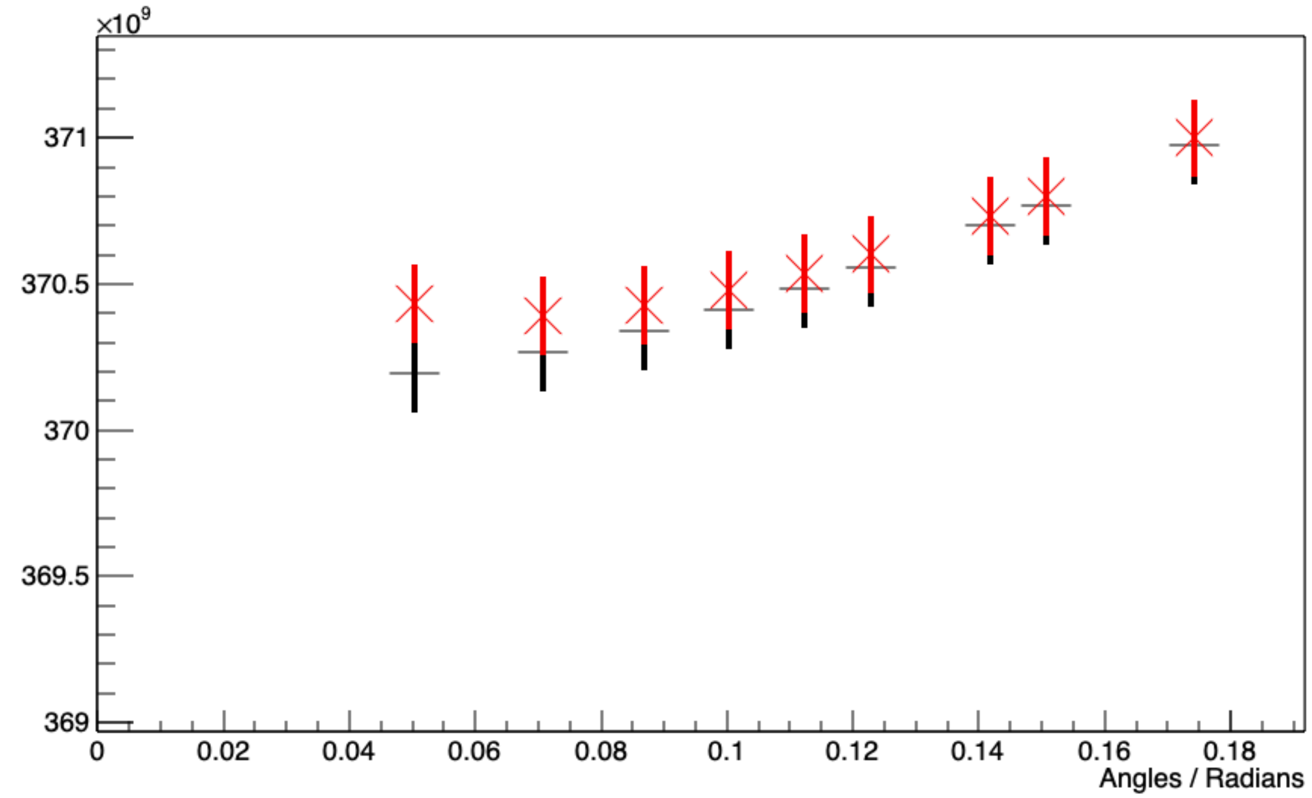
Monte Carlo Details

- Set (arbitrary) cutoff for Miller indices ($h,k,l < 3$ right now)
- Get all index combinations h,k,l such that no degeneracies in θ_{hkl}.
    - E.g. cubic lattice $\theta_{hkl} = \arcsin(\lambda/2\alpha\,(h^2 + k^2 + l^2))$ so only count 100 and ignore 010, 001. (000) is not a valid plane.
    - Reason for this: Miller families is what counts. Families = equivalence class of planes related by symmetries of unit cell. E.g. {100} = (100), (010), (001) (-100) (0 -1 0) (0 0 -1) are all faces of a unit cube.
- Simulate n particles and randomly pick a Miller plane for each. Populate histogram with angles. Should be uniformly distributed if done right with large enough n. Errors are $\sqrt{N}$.
- For nonzero bins in angle histogram, get centre of bin θ and evaluate $I = |F_{hkl}|^2$ at that angle θ. Multiply by number of particles in that bin to get intensity I.

Example: N = 1e6 particles



Angle Distribution



Intensity (red = with new force)

Y axis: Intensity $I = \sigma N$ (fm^{-2})

Errors: $\delta I = \sigma^* \delta N = \sigma\sqrt{N}$

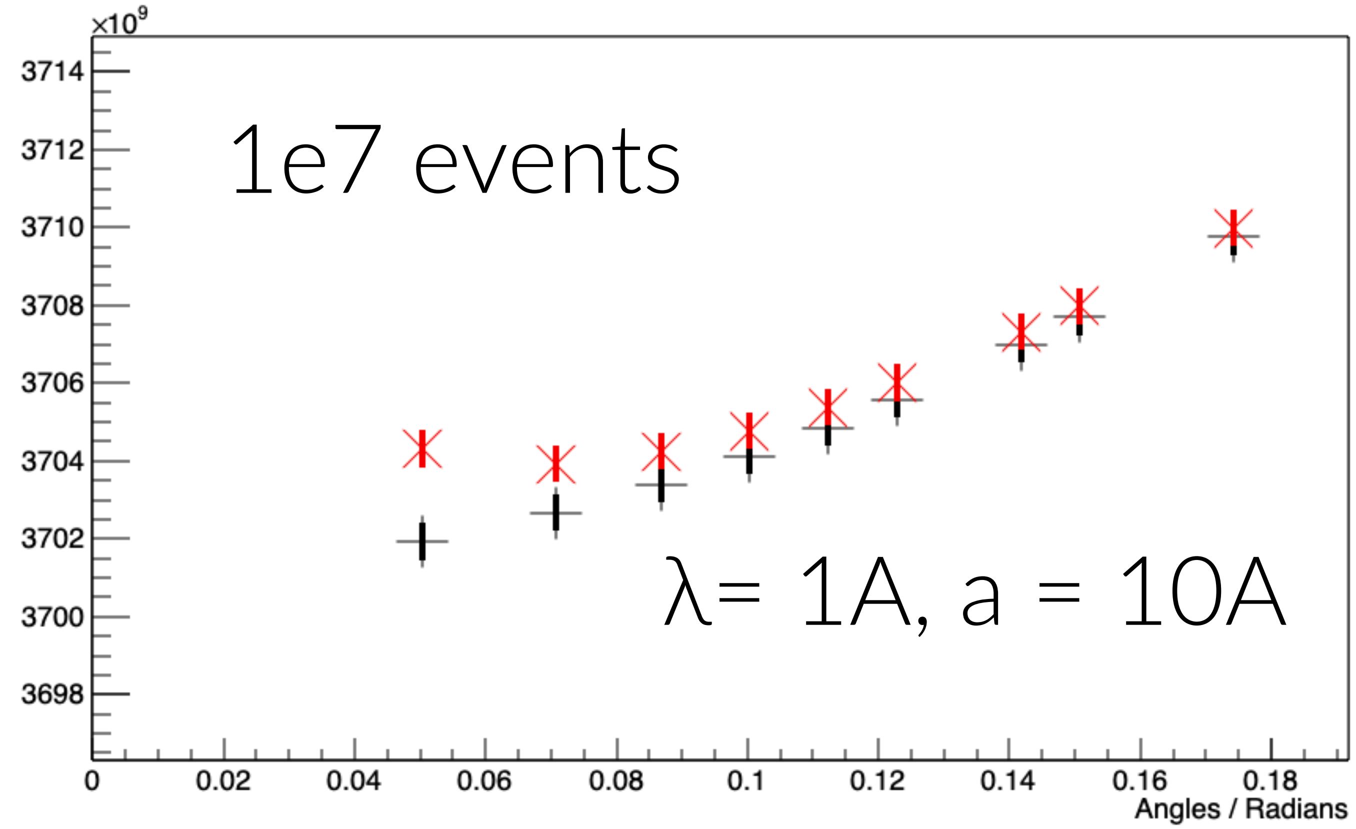
Can get > 1σ separation between signals at N = 1e7 events.

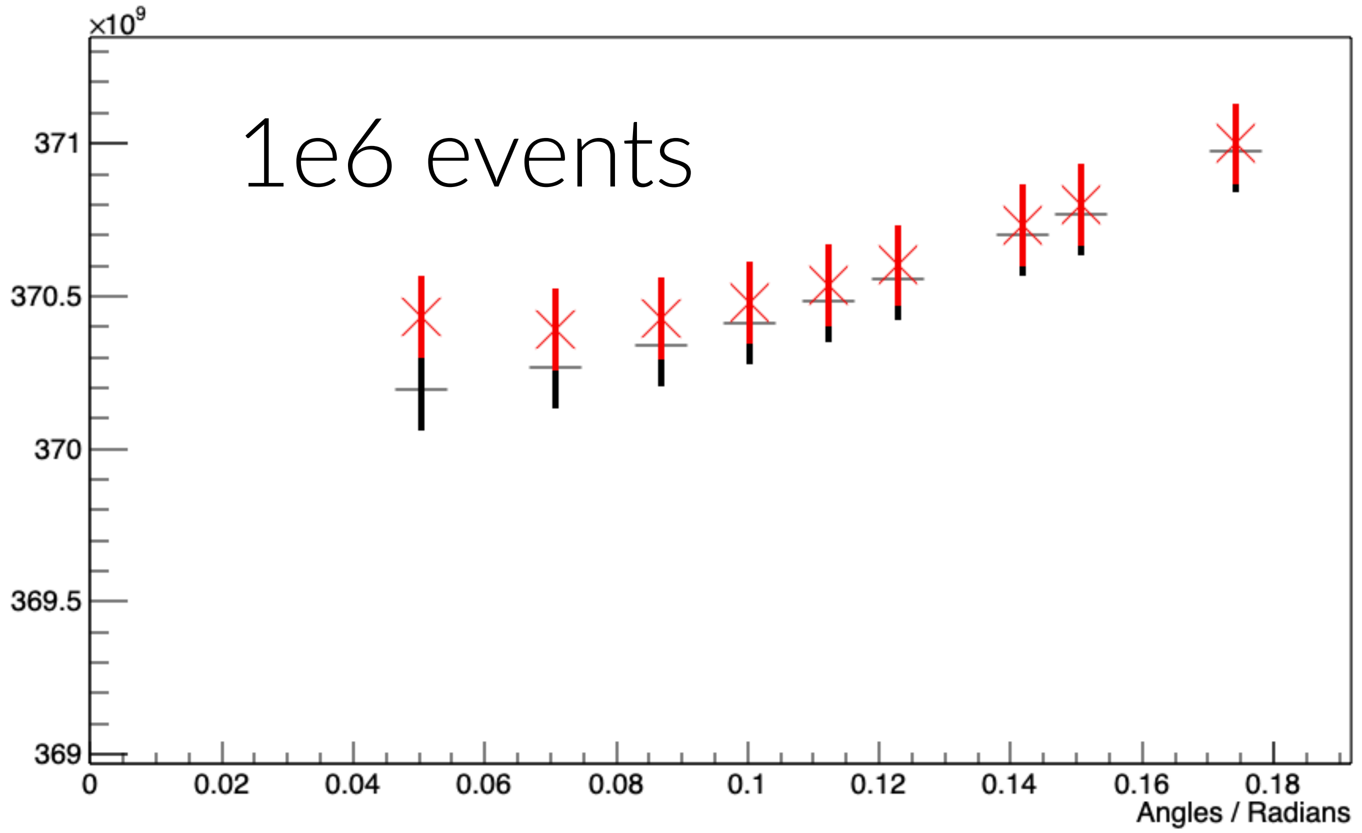
From table of neutron fluxes:

$\Phi \sim 1e6\ cm^{-2}$

$A = 25 \times 50\ mm^2$

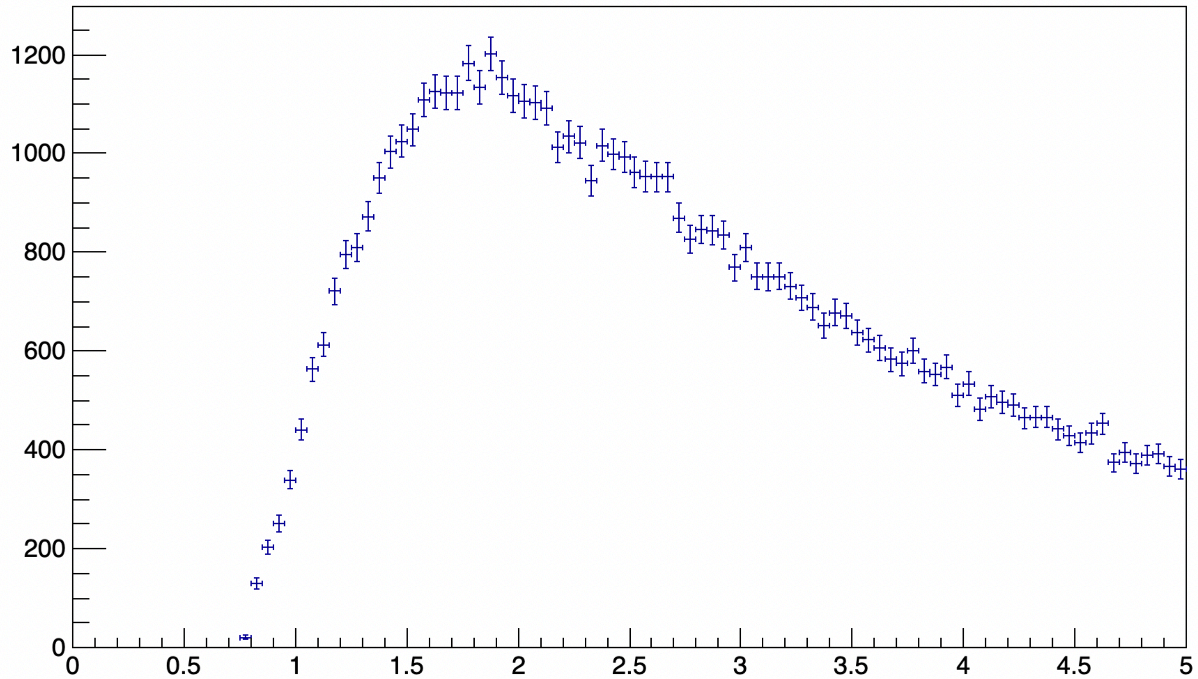
$N = \Phi A \sim 1e7$



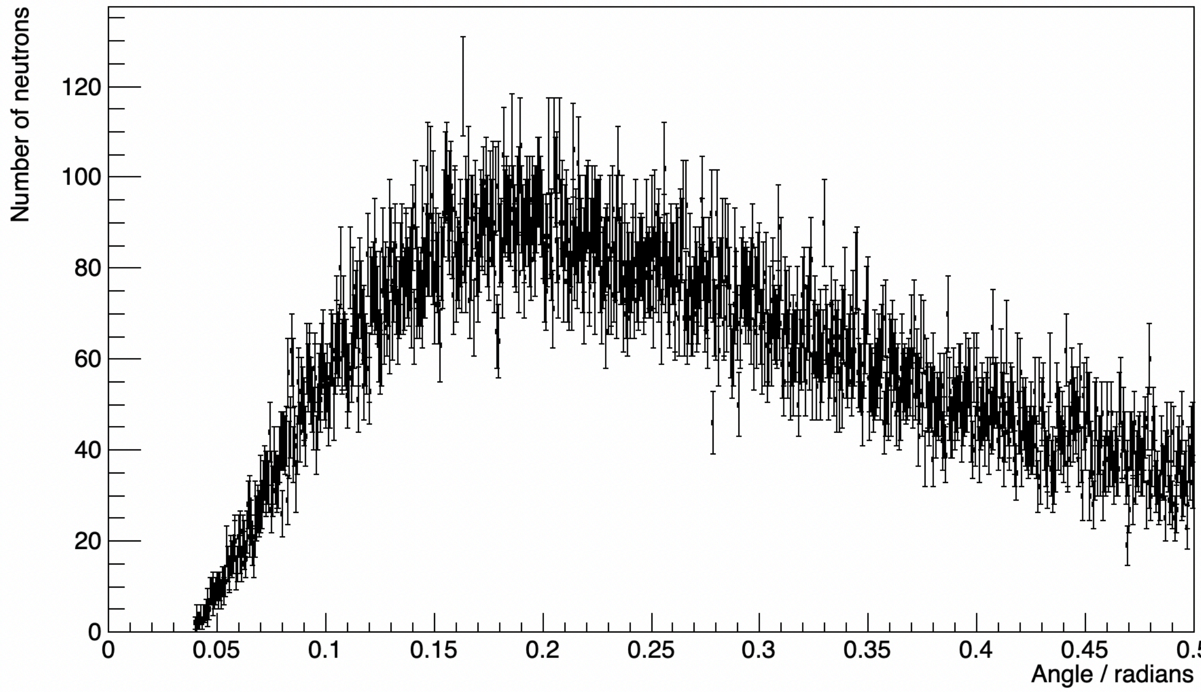


- Now add wavelength distribution.
- Neutron velocity distributed according to 1D M-B distribution.
- $E = 1/2\ mv^2$ & $\lambda = h/\sqrt{(2mE)} \rightarrow \lambda \sim 1/v$
- After getting wavelength, do the same steps as above to get final intensity plot.

T = 290K (peak λ ≈ 1.8 A), a = 10 A

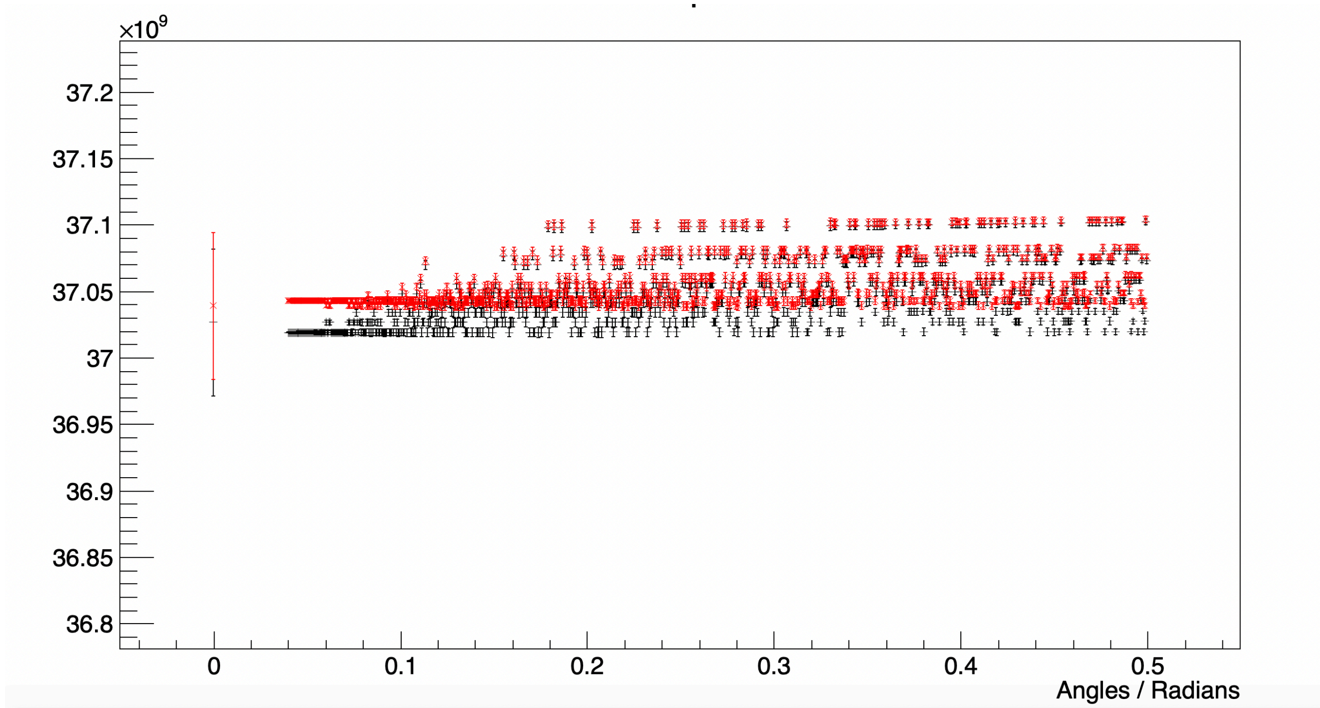


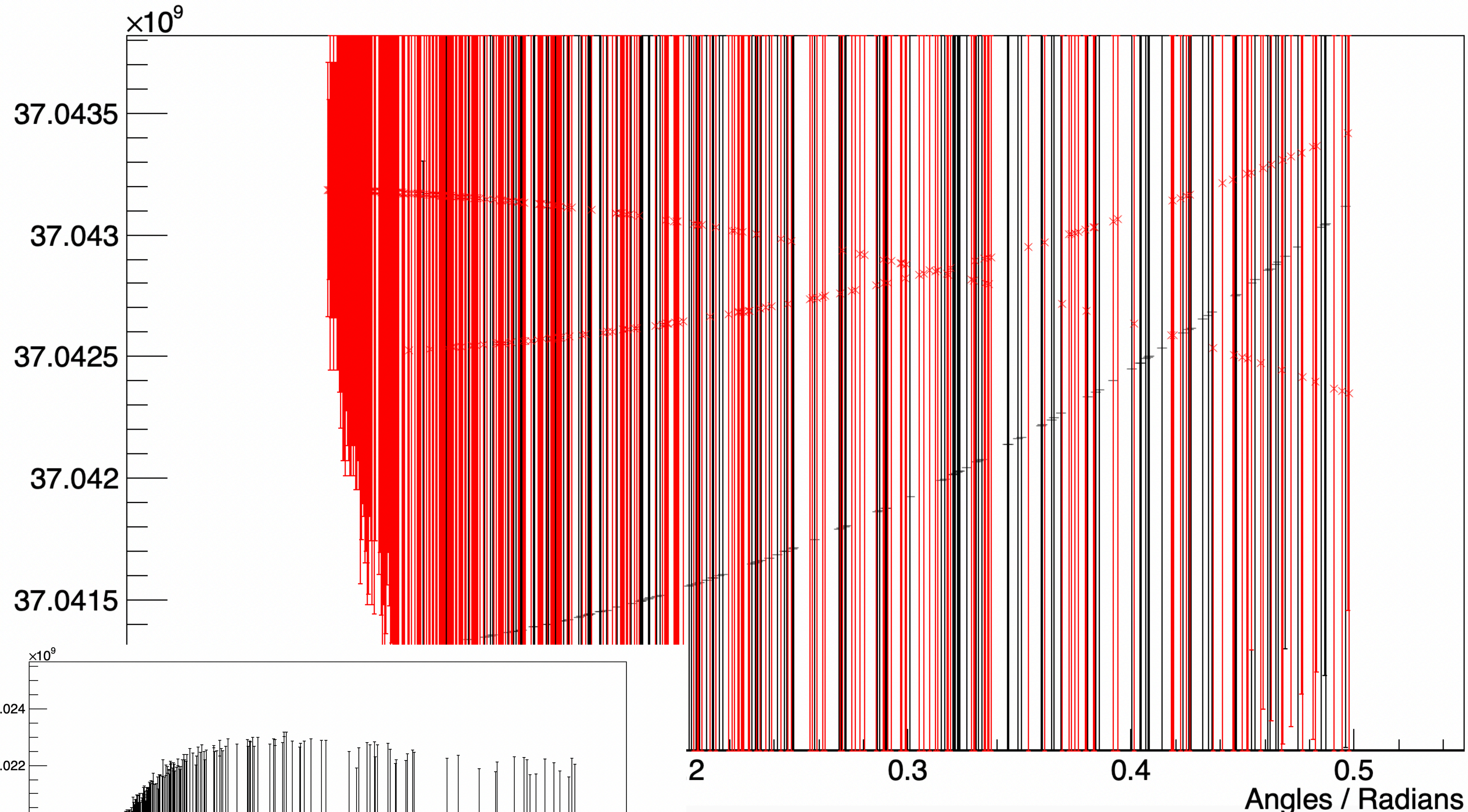
Wavelength Distribution (A)

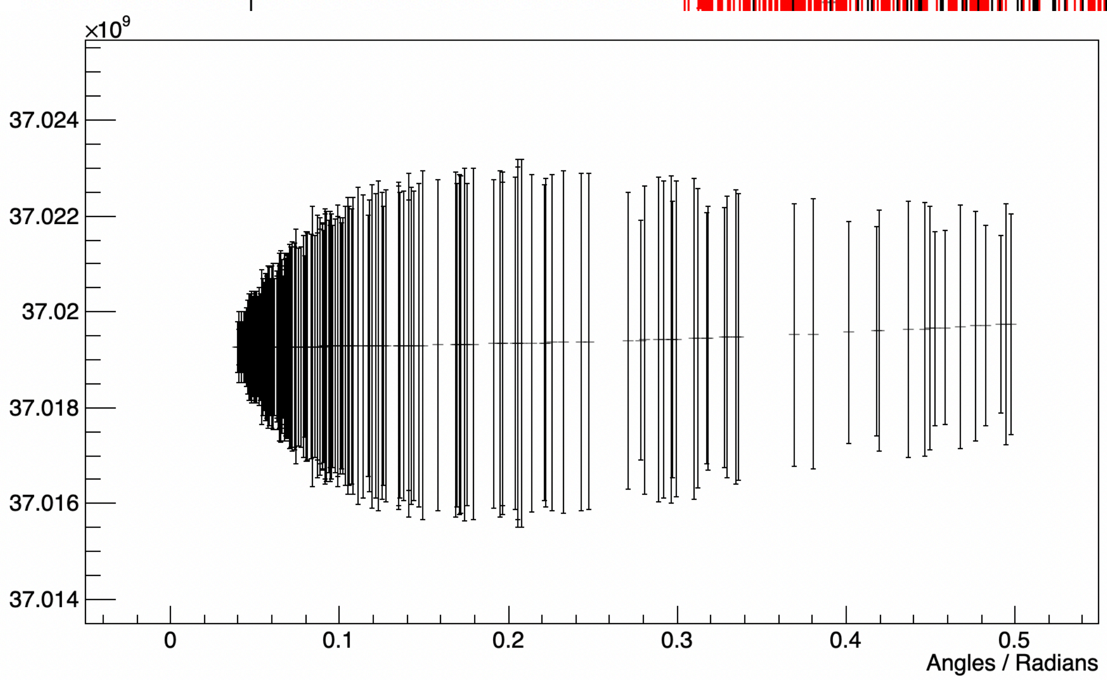


Lattice Angular Distribution

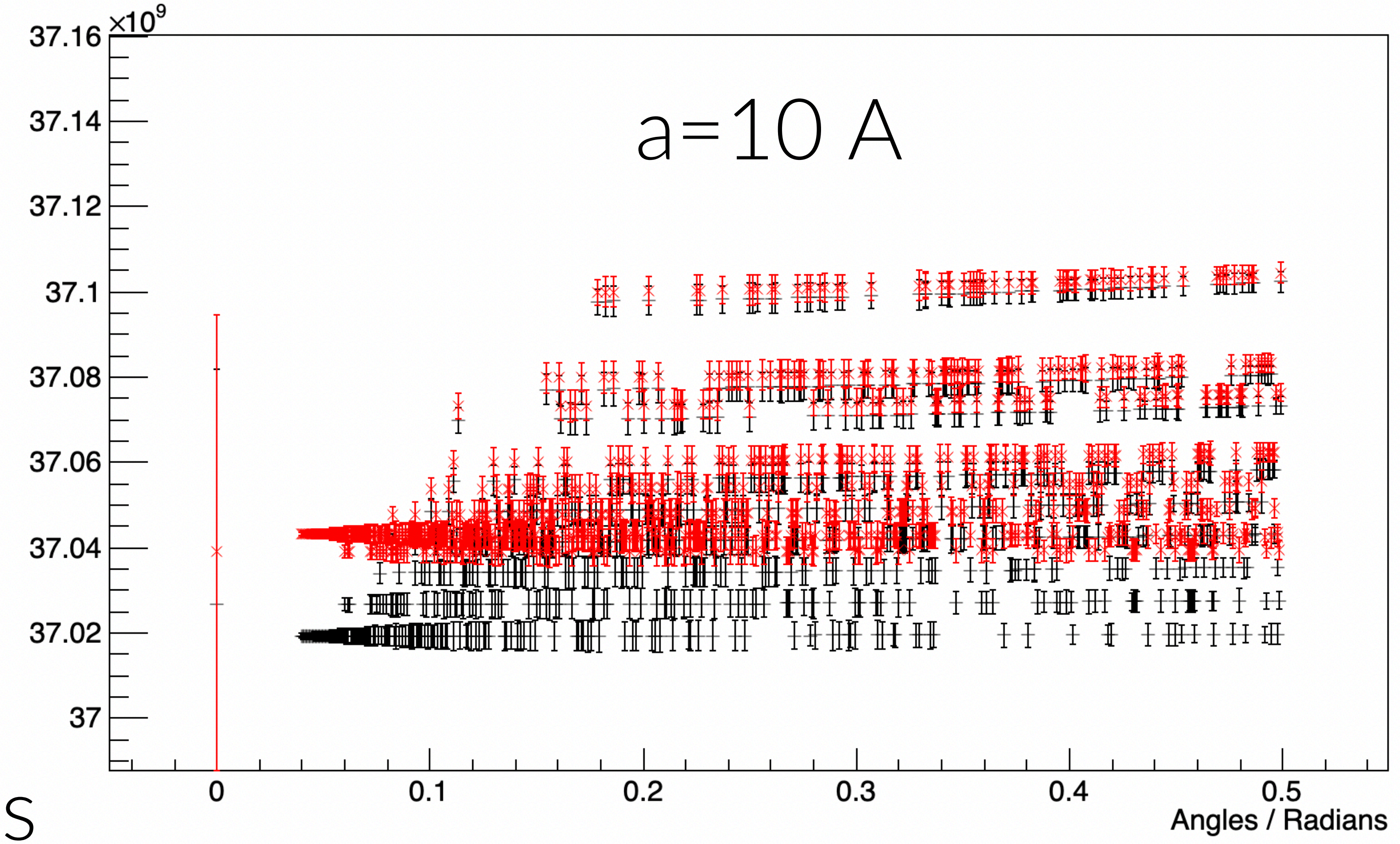
Intensity (looks like a mess)



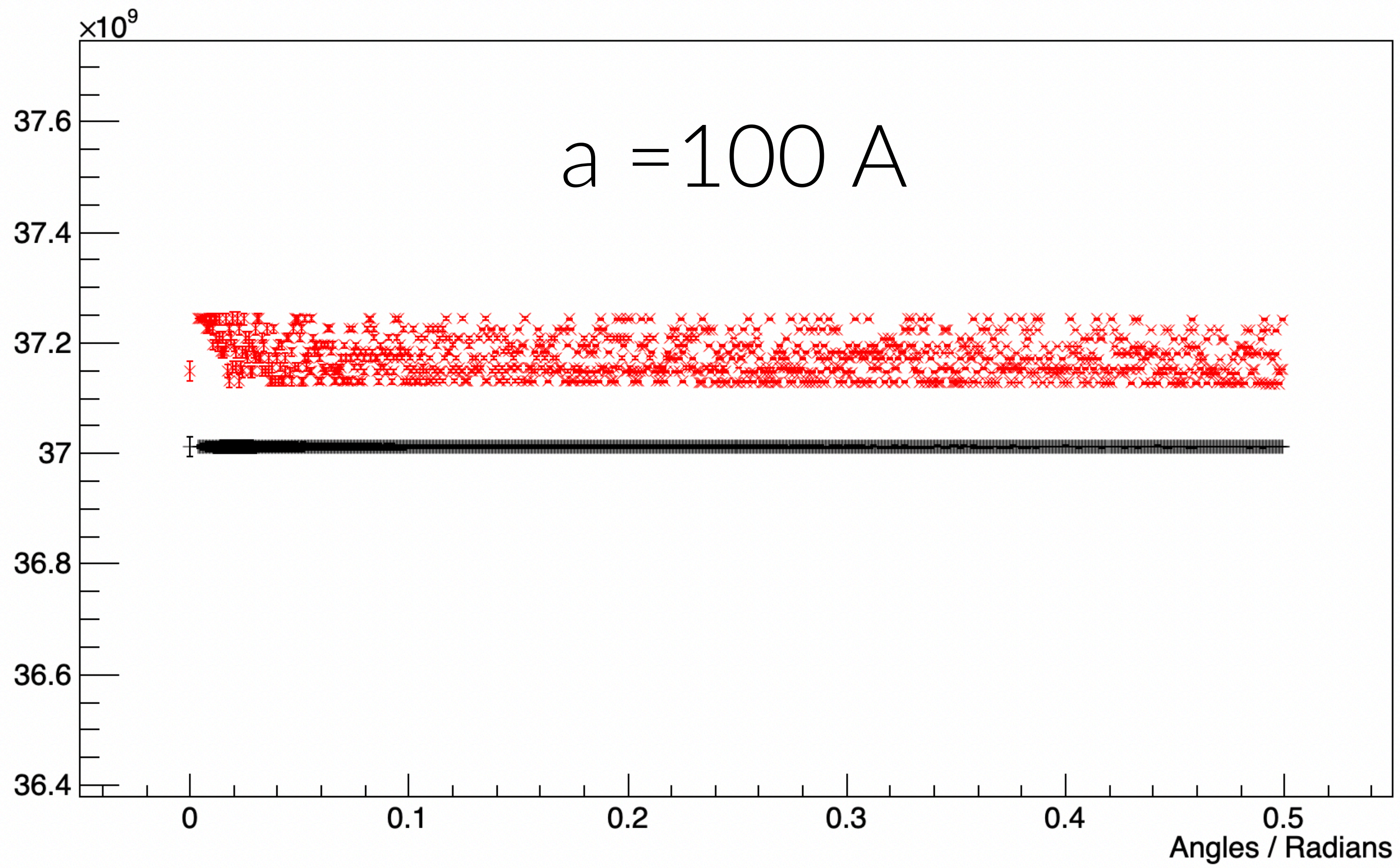




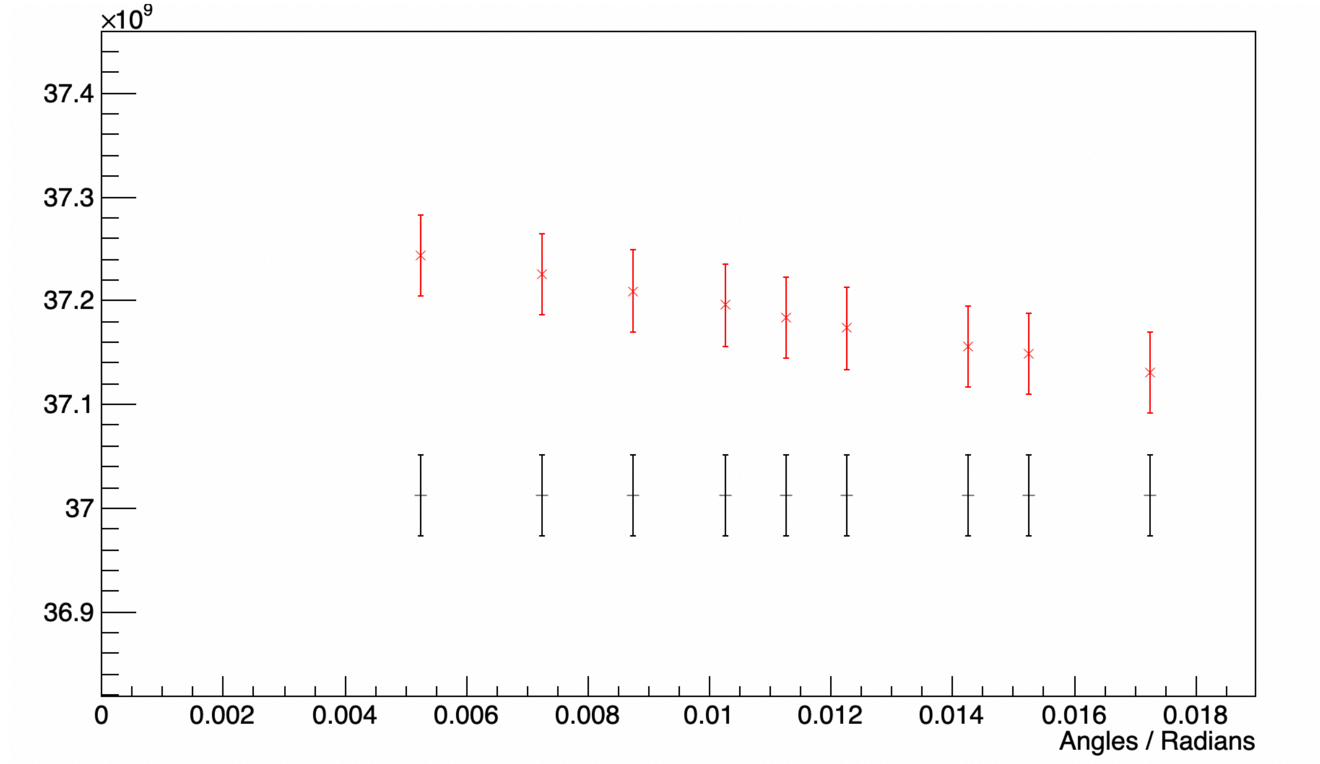
Zoom in on mess


×10^9
37.16
37.14
37.12
37.1
37.08
37.06
37.04
37.02
37
a=10 A
0
0.1
0.2
0.3
0.4
0.5
Angles / Radians

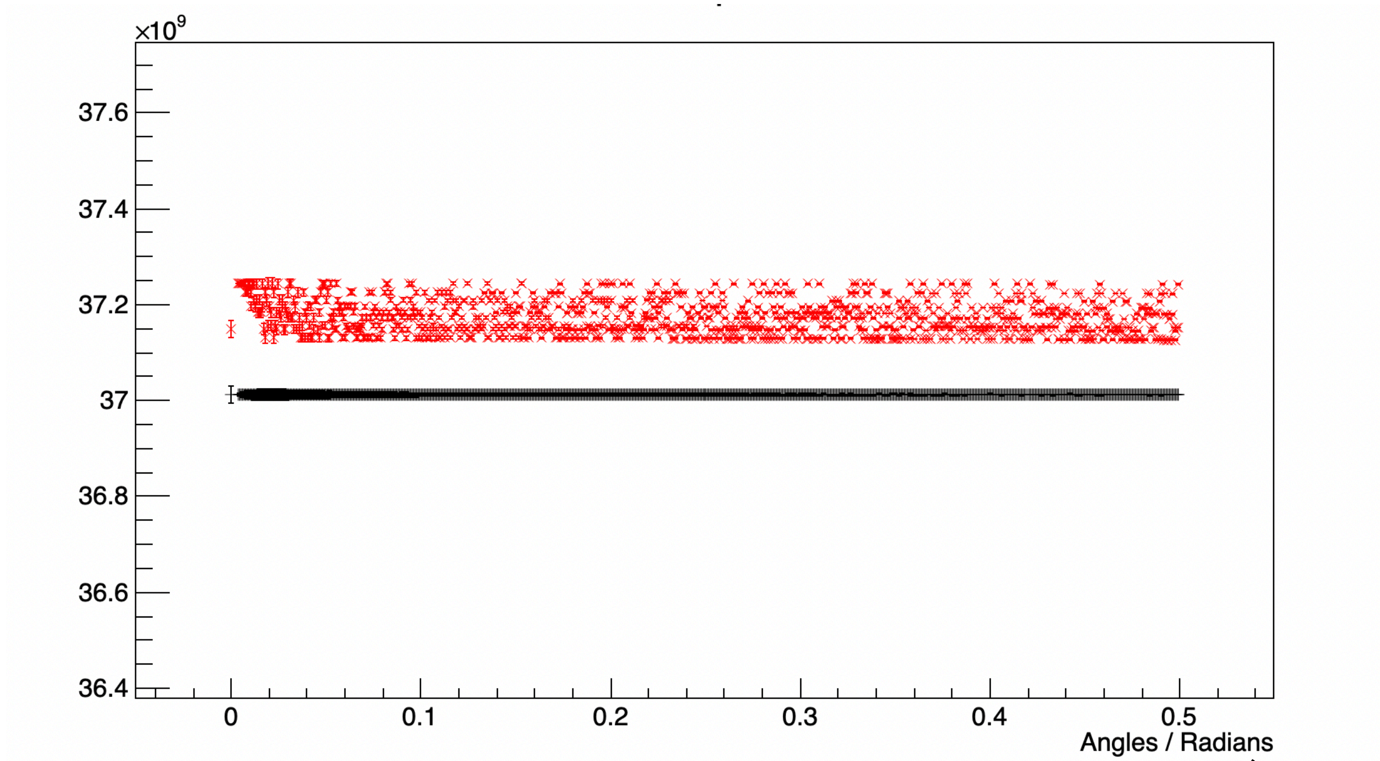
1e5 events


×10^9
37.6
37.4
37.2
37
36.8
36.6
36.4
a =100 A
0
0.1
0.2
0.3
0.4
0.5
Angles / Radians

λ = 1.0 A, a = 100 A



T = 290K (λ = 1.8 A),
a = 100 A



Cleaner separation over larger angle range in second case (both N = 1e5). Doesn't smear out if a is large enough relative to wavelength (lower λ/a is good)