Fitting the 10 K, HF $CoFe_2O_4$ (Glassy, XTAL) Nanoparticles With SasView

Loading the 6 Column Data – Q, Intensity, ΔIntensity, Mean_Q, ΔQ, Shadow

Open SasView

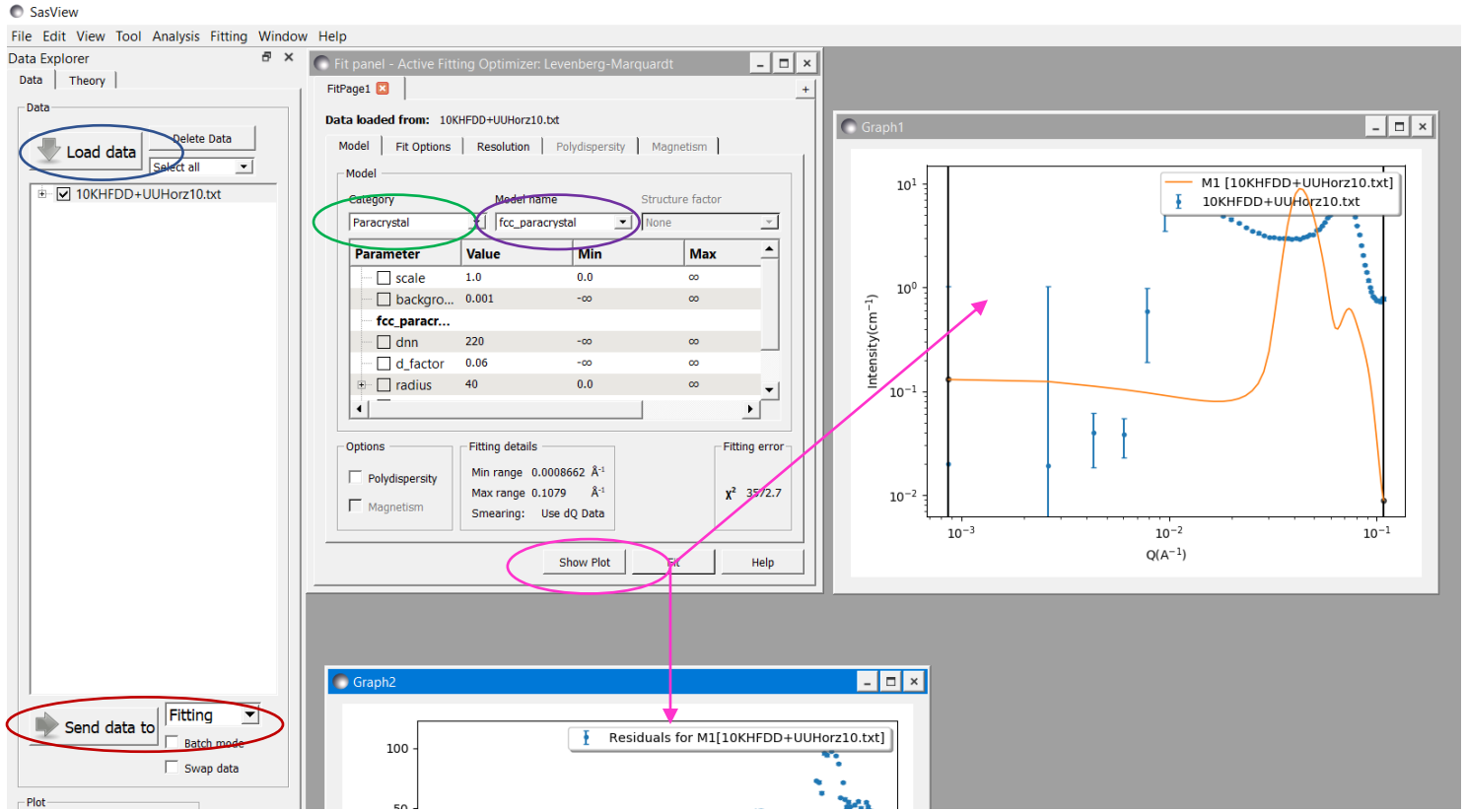
Load Data -> Choose Files -> 10KHFDD+UUHorz10.txt (in GlassyCoFe2O4_NG7SANSData_AllConditionsProcessed) → Open

Send Data To → Fitting (you could also create a new plot at this point, but you don't need to)

In FitPage1 Tab, Model -> Category -> Paracrystal

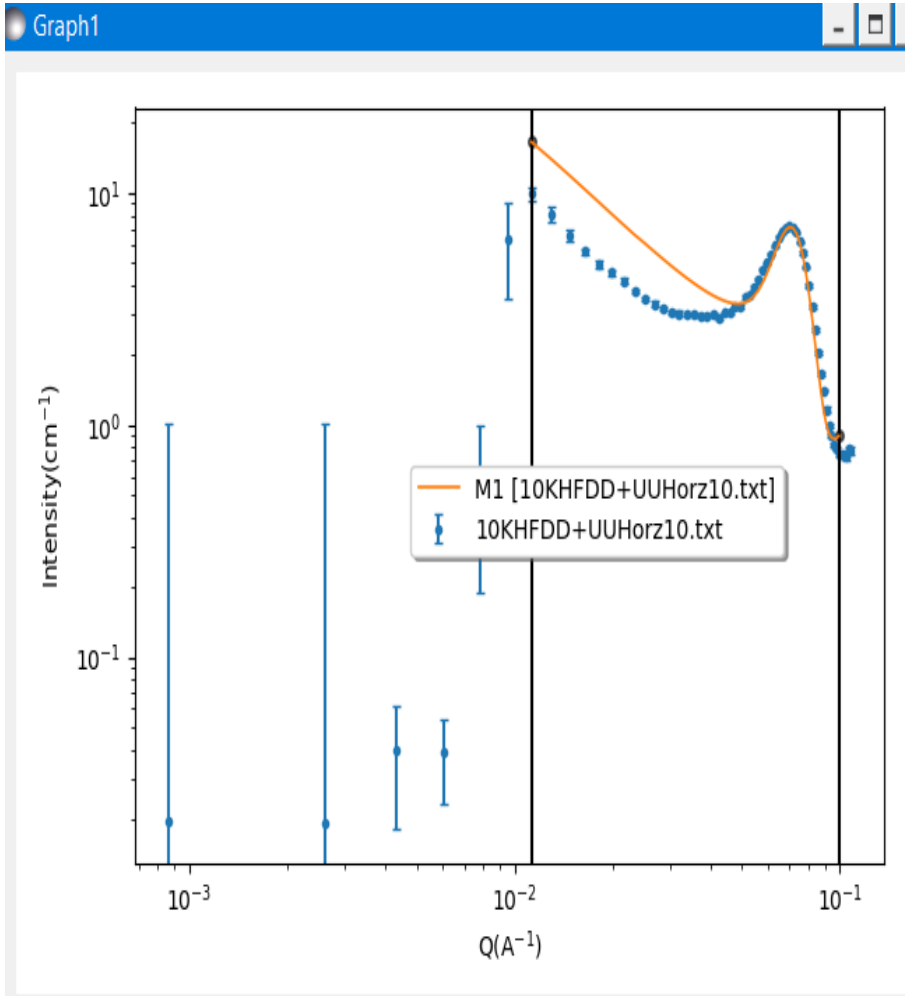
Model Name → FFC Paracrystal

Show Plot. Two plots will pop you; you may want to drag the residuals away to the bottom for now.



Fitting the 10 K, HF Nuclear Scattering (to set scale factor, etc.)

Scale is set by volume fraction and sample thickness (which we do not know)
Background is this case is dominated by incoherent scattering from hydrogen
Dnn is the spacing between nanoparticles
D_factor is the distortion of the FCC lattice (larger widens Bragg peak)
Radius of the nanoparticles is ≈46 Å (from TEM, modified by M_perp to be shown)
SLD of CoFe2O4 = 6.07
SLD of "solvent" = 0 (air)
Help at bottom describes the model in more detail



Before fitting the idea is to change the parameters within physically reasonable limits to get a near fit to the data (fitting before getting close often leads the model astray)

A decent hand fit can be obtained using:
Scale = 0.35
BKGD = 0.8
Dnn = 130
D_factor = 0.12

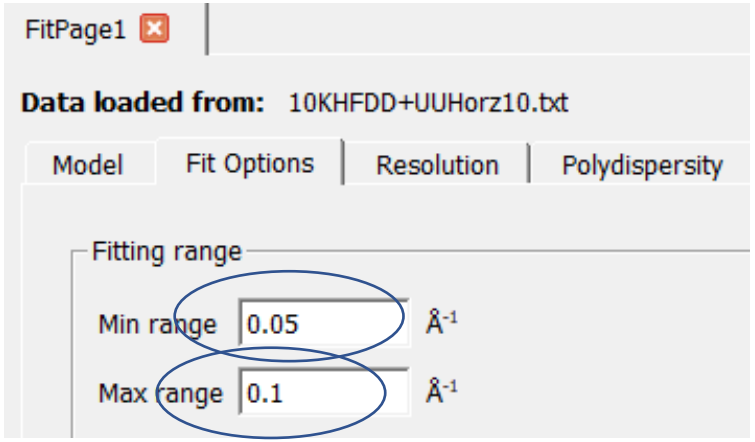
The overshoot at low-Q likely means D_factor is artificially large to cover some of the FCC stacking faults (a different form of disorder)

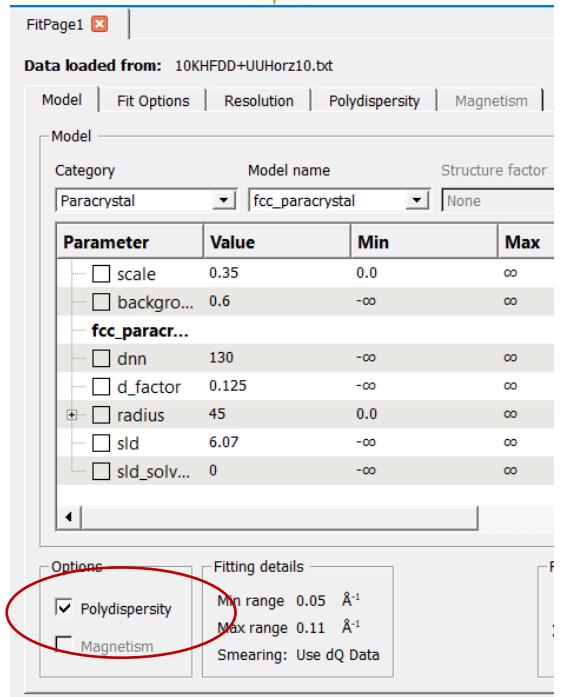
Fitting the 10 K, HF Nuclear Scattering, Continued

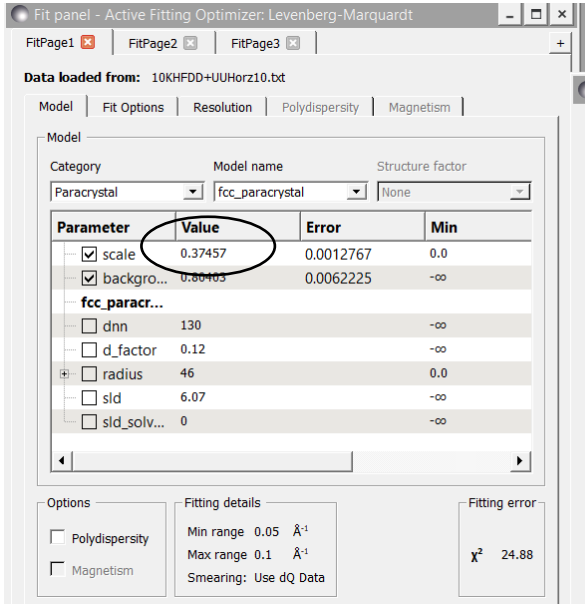
Let's restrict the Q-range being examined. Fit Options -> Min range = 0.05 and Max range = 0.10.

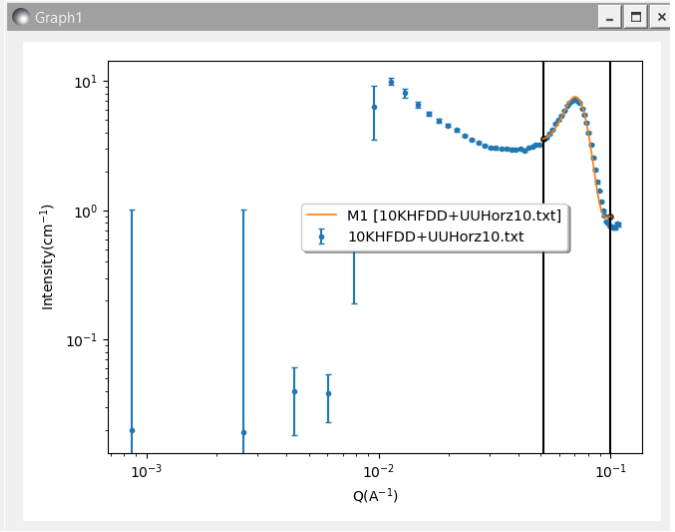
One could check Polydispersity box at bottom of Model. It slows model and isn't needed, so we will NOT use it today.

Go back to Model. Check Scale and BKGD only and then Fit. The fit returns something like scale of 0.37457. This should remain constant for all other cuts.



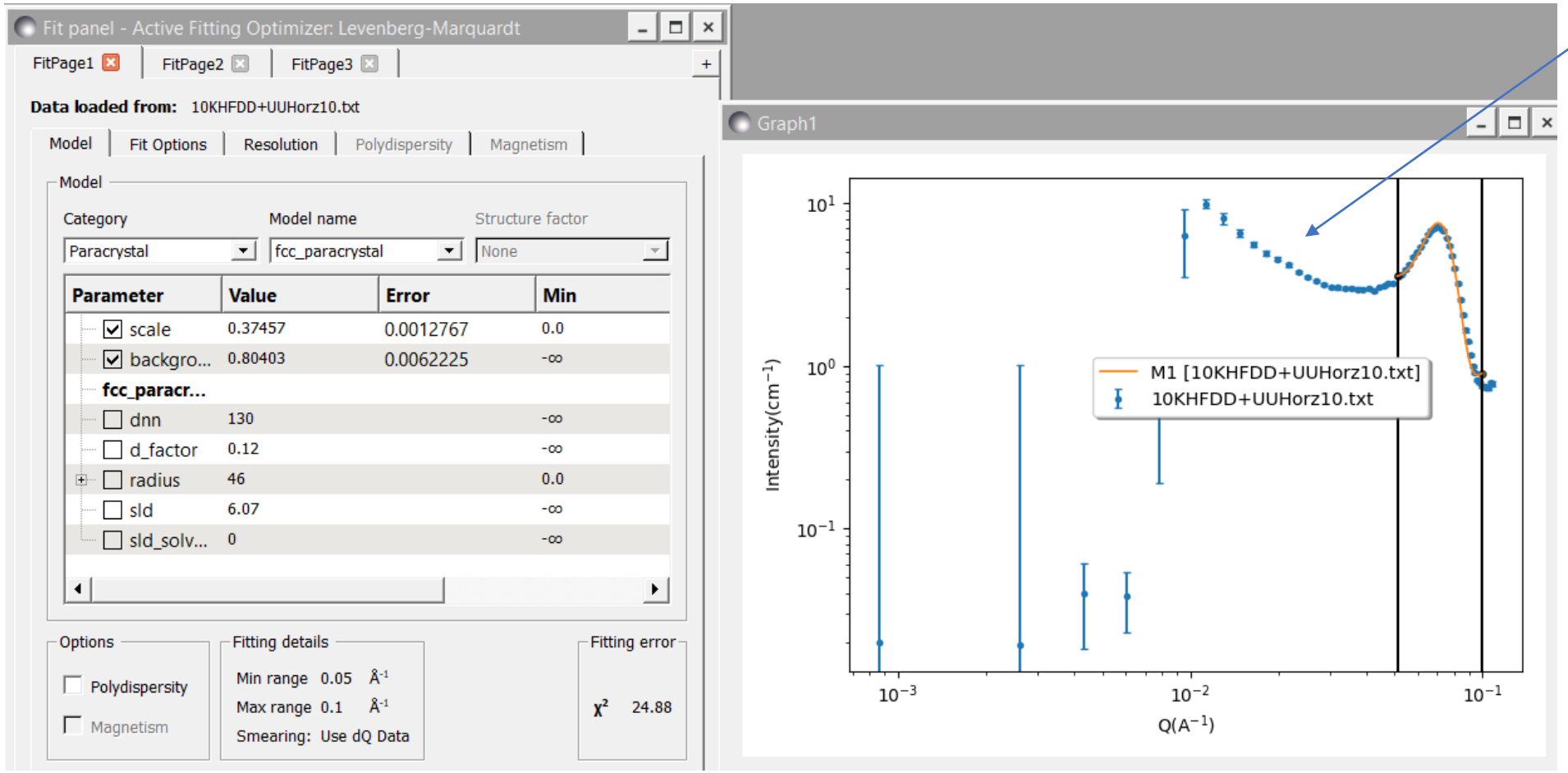






Note the model may try to include lower-Q in fit (this is OK, too).

10 K, HF Nuclear Scattering Fit:



FCC model overshoots at lower Q (true in PRB., too); It works somewhat better for M_Parl_H

Scale = 0.375

Modeling M_Parl_H (from $[DD_{Ver}t - UU_{Vert}]^2 / 8N^2$)

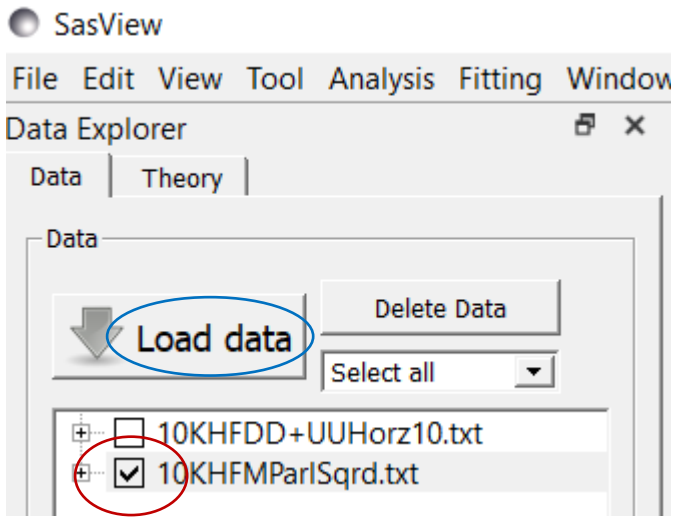
Load Data -> Choose Files -> 10KHFMParlSqrd.txt (in GlassyCoFe2O4_NG7SANSData_AllConditionsProcessed). Open.

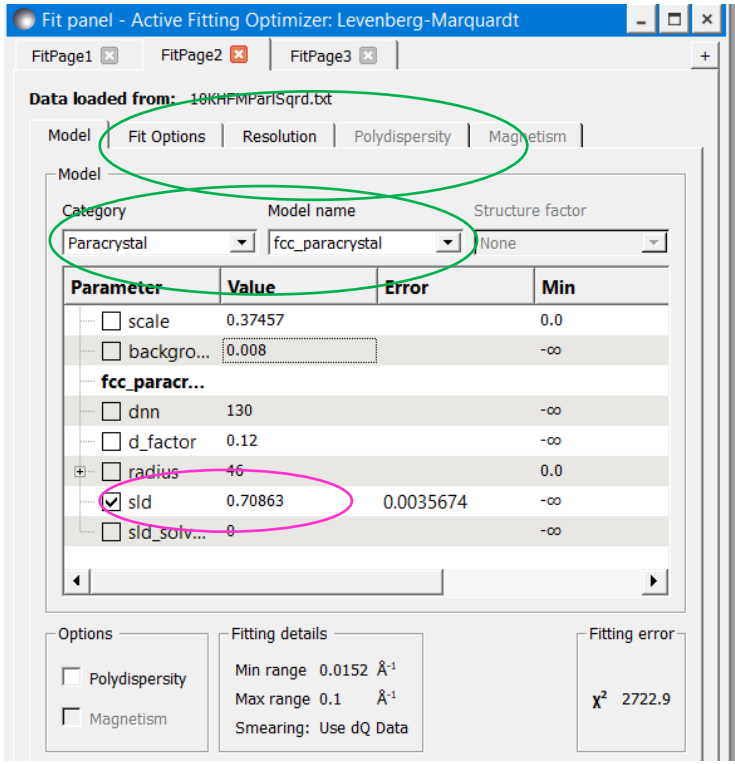
Check 10KHFMParlSqrd.txt only and then Send Data To → Fitting. This creates a fit page 2.

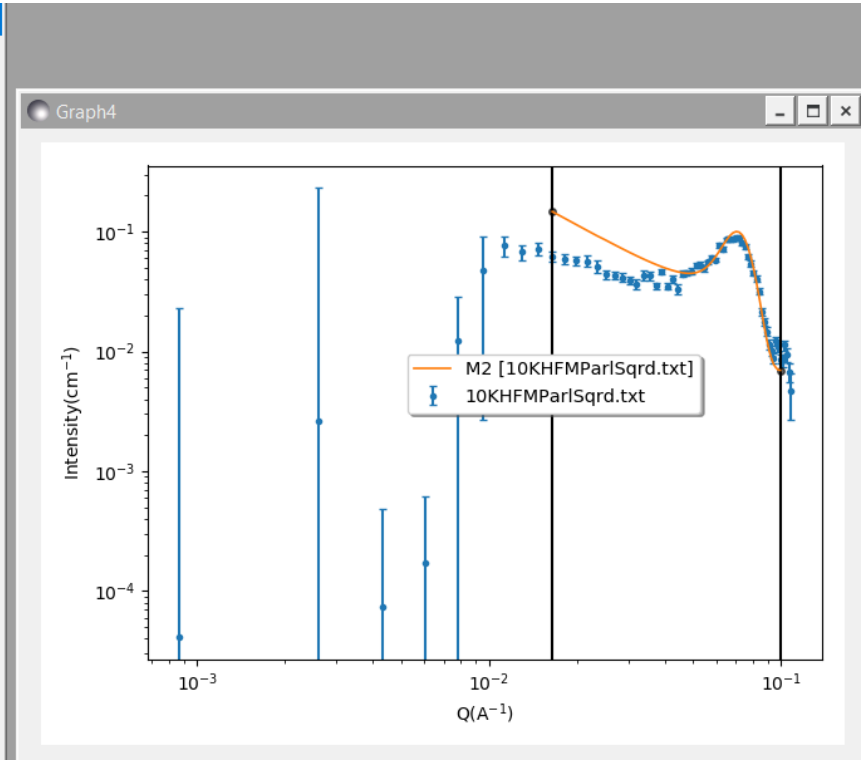
Set the parameters and Q-range to match that of the structural scattering.

Background should be close to zero due to difference taken (DD – UU). SLD 6.07 -> 1.42 (for max magnetism)

Now let the fit decide SLD only or can adjust by hand to save time -> 0.71 of possible 1.42!







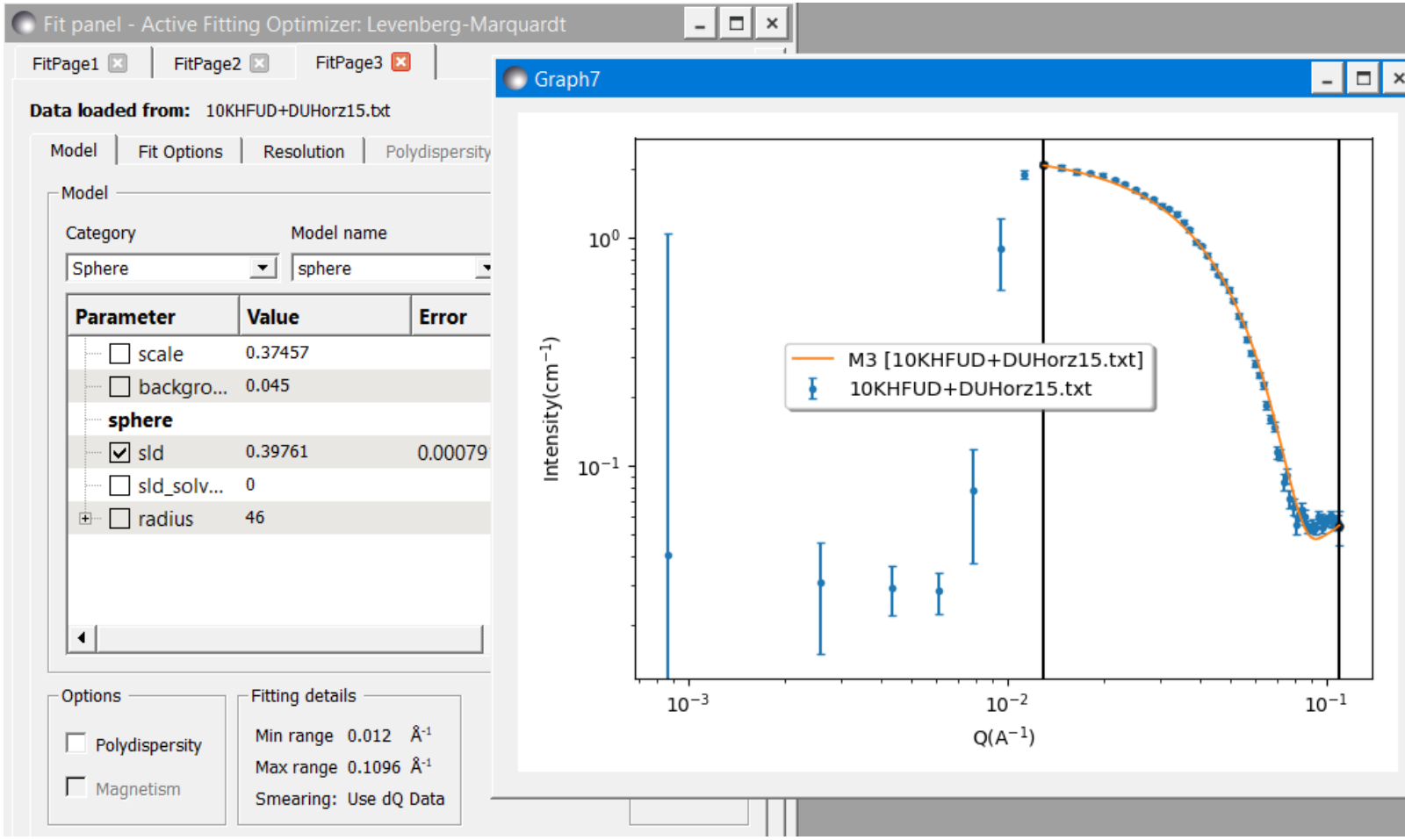
Modeling M_Perp_H

Load Data -> Choose Files -> 10KHFUD+DUHorz15.txt (in GlassyCoFe2O4_NG7SANSData_AllConditionsProcessed). Open.

Check 10KHFUD+DUHorz15.txt only and then Send Data To → Fitting. This creates a fit page 3.

Choose Category = Sphere, Model Name = Sphere. Scale = 0.422. Radius = 45. SLD (max) = 1.42. Set Q min = 0.012.

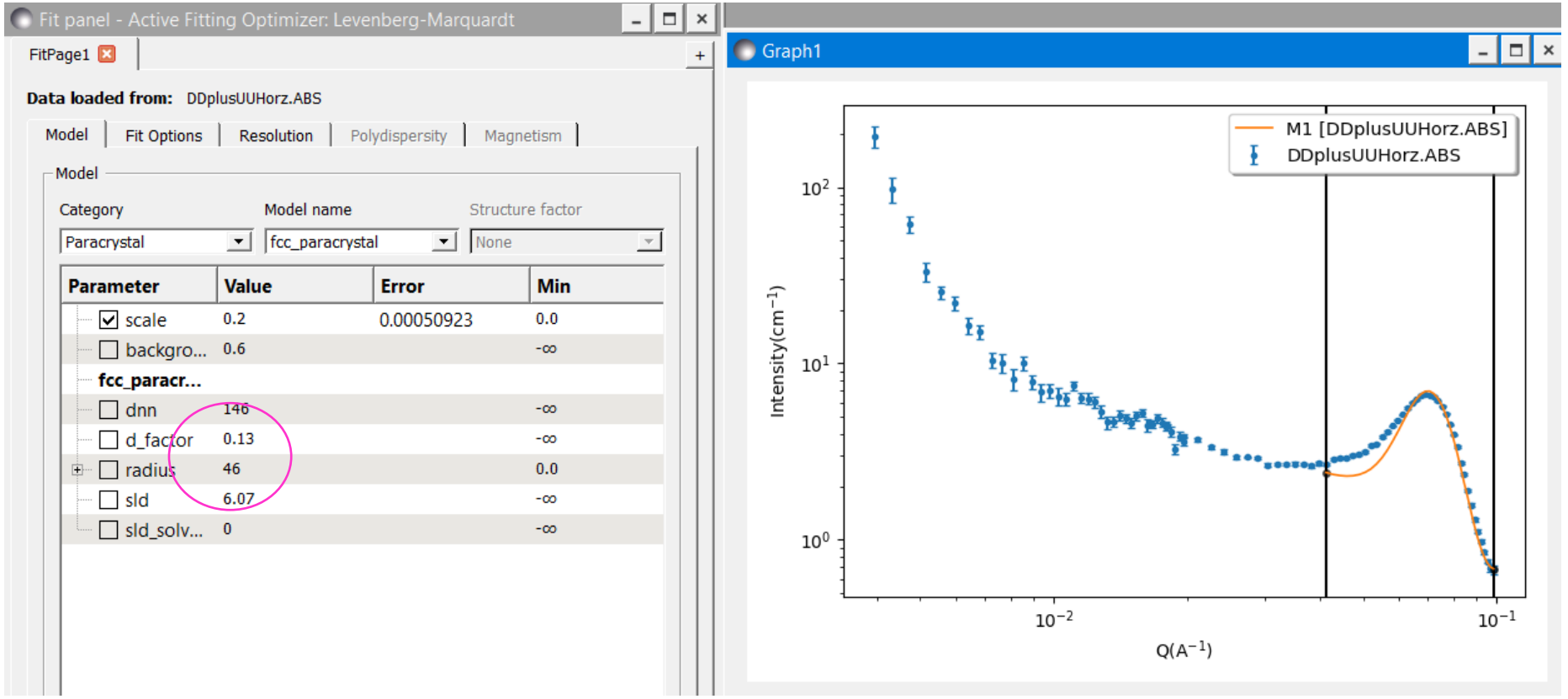
Now let the fit decide SLD only or can adjust by hand to save time -> 0.40 of possible 1.42!



(0.40 + 0.71)/1.42 = 78%

And what the other sample (the data set you reduced last session)?

N^2 from DDplusUUHorz.ABS (GlassyCoFe2O410KHF_Ng7SANSData)



M_{Parl}^2 from MParlSqrd10KHF.txt (GlassyCoFe2O410KHF_Ng7SANSData)

Fit panel - Active Fitting Optimizer: Levenberg-Marquardt

FitPage1 | FitPage2 | +

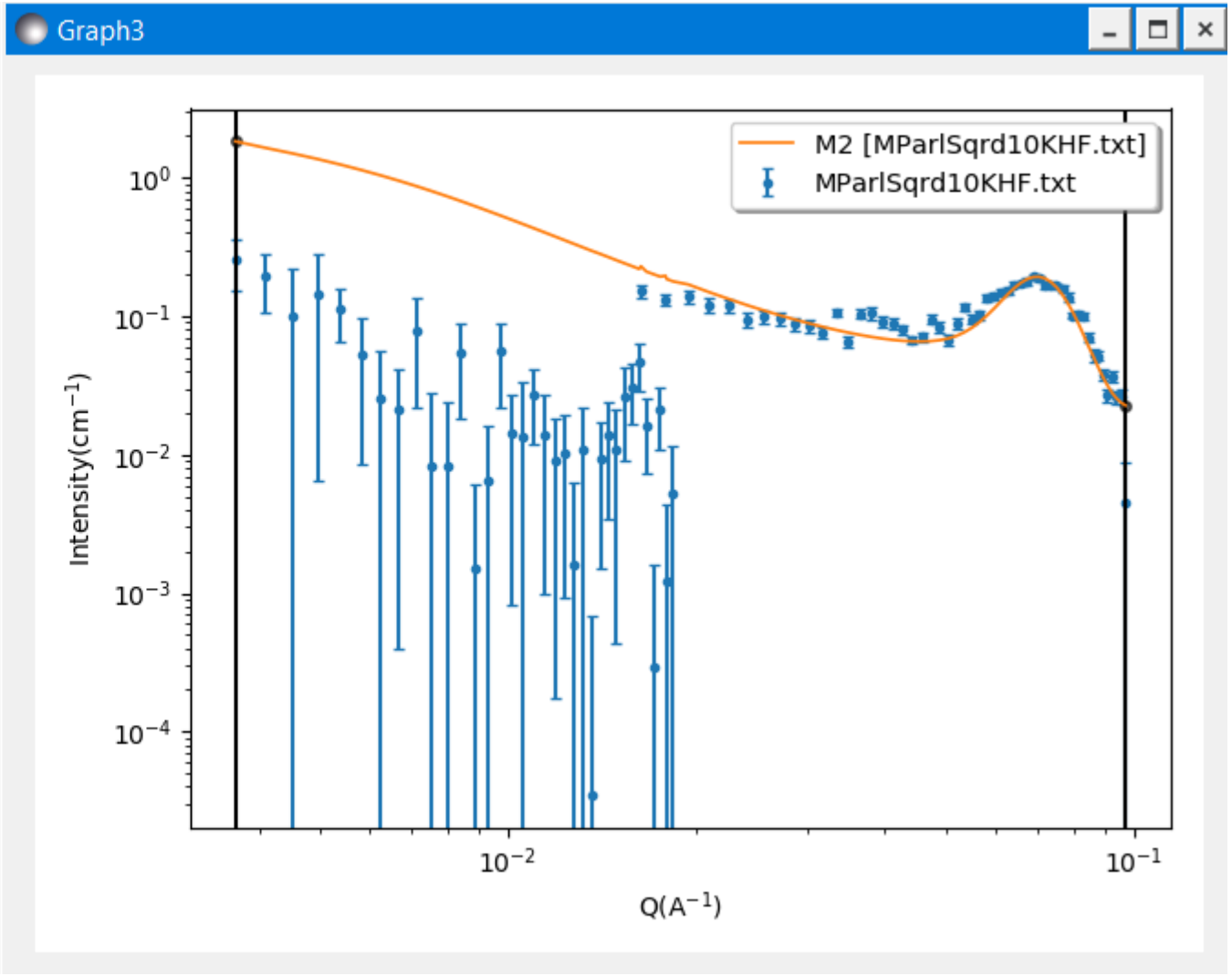
Data loaded from: MParlSqrd10KHF.txt

Model | Fit Options | Resolution | Polydispersity | Magnetism

Model

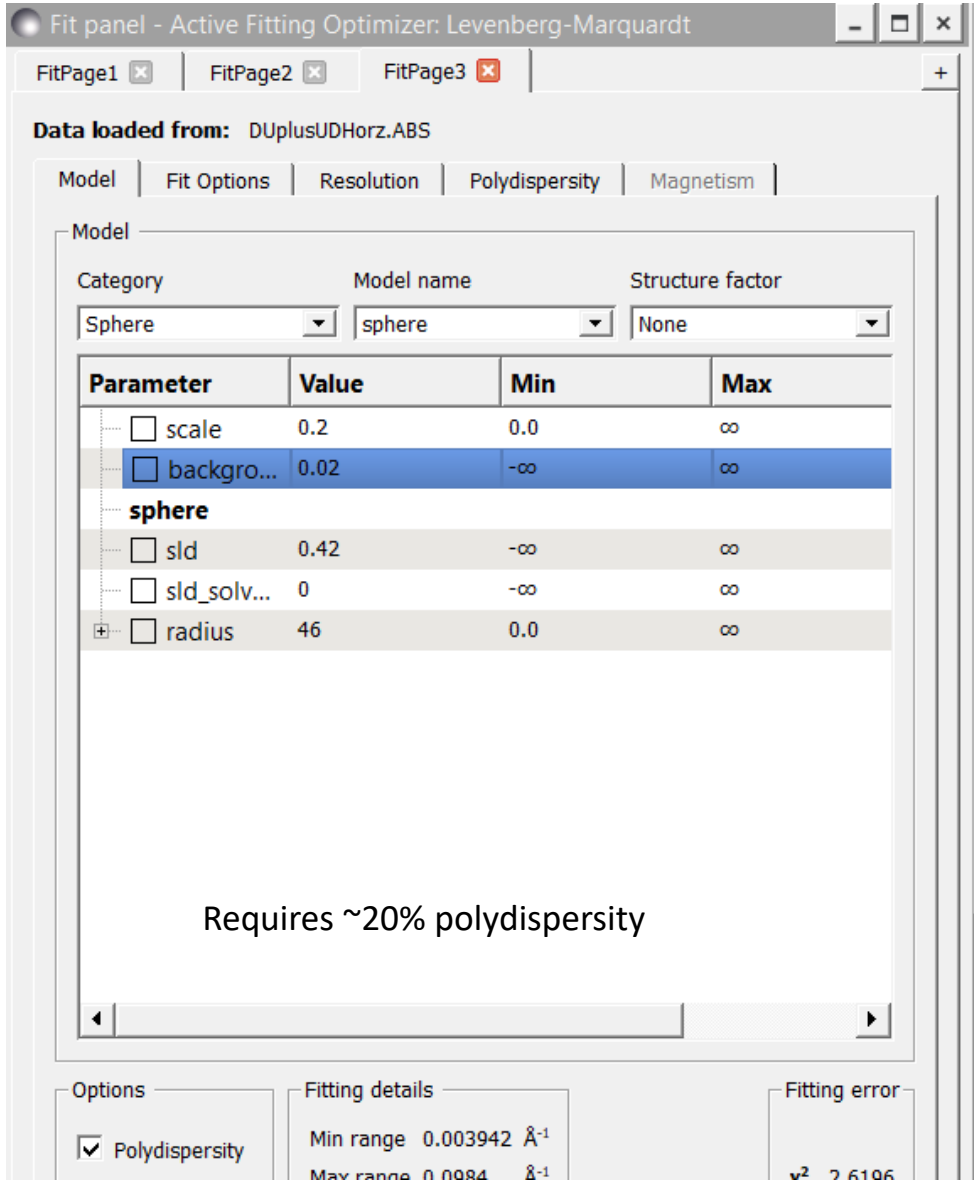
Category: Paracrystal | Model name: fcc_paracrystal | Structure factor: None

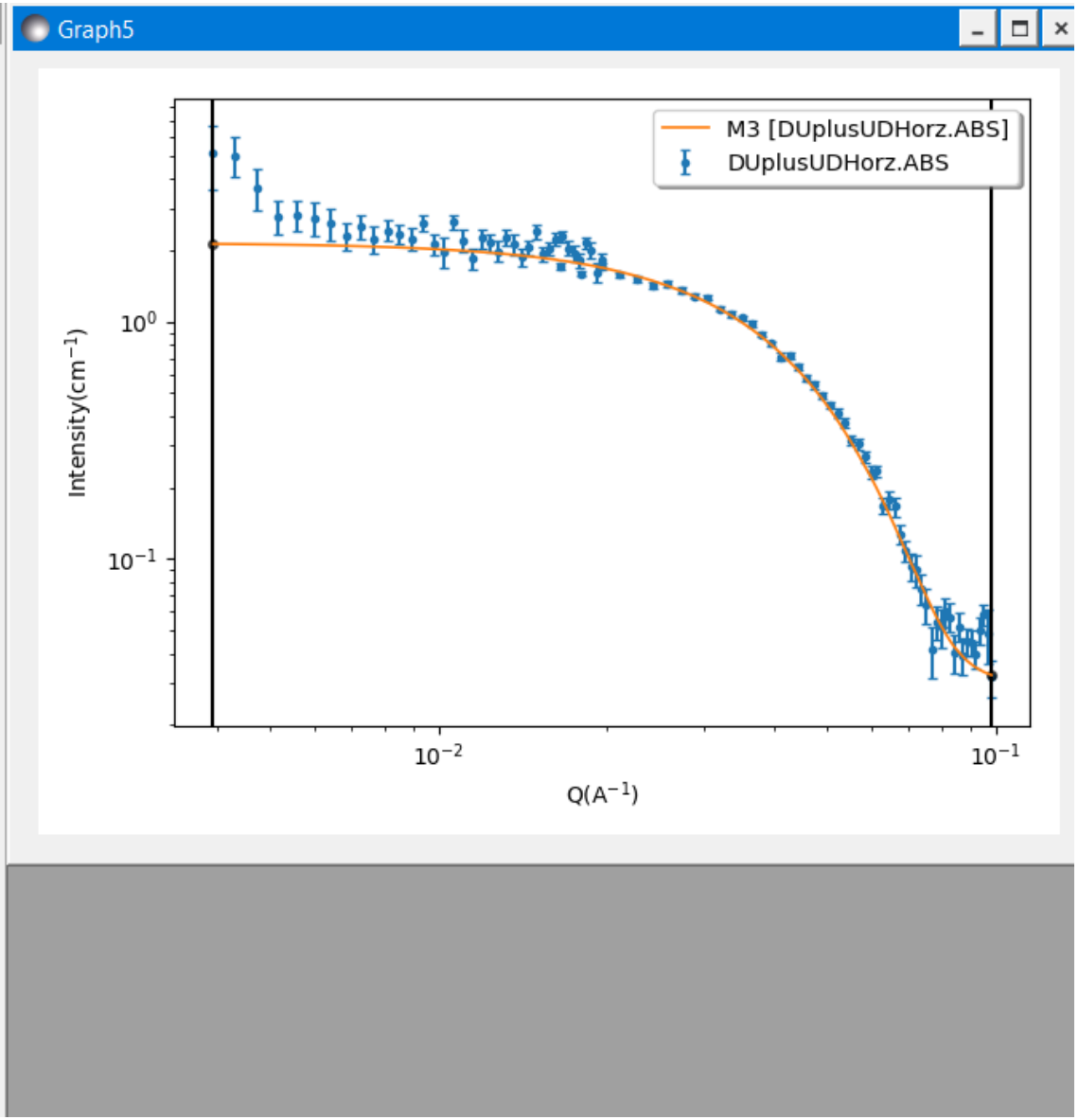
Parameter	Value	Min	Max
scale	0.2	0.0	∞
backgro...	0.02	-∞	∞
fcc_paracr...			
dnn	146	-∞	∞
d_factor	0.13	-∞	∞
radius	46	0.0	∞
sld	1	-∞	∞
sld_solv...	0	-∞	∞



1.0/1.42 = 70%

M_{Perp}^2 from DUplusUDHorz.ABS (GlassyCoFe2O410KHF_Ng7SANSData)





1.0/1.42 + 0.42/1.42 = 100% of magnetization accounted for!

The VSANS data map (300 K, 1.5 T) onto the XTAL sample:
Dnn = 146, more magnetization preserved.