SIMPLIFIED AND IMPROVED MODEL SMOOTHING IN REFLECTOMETRY FITTING

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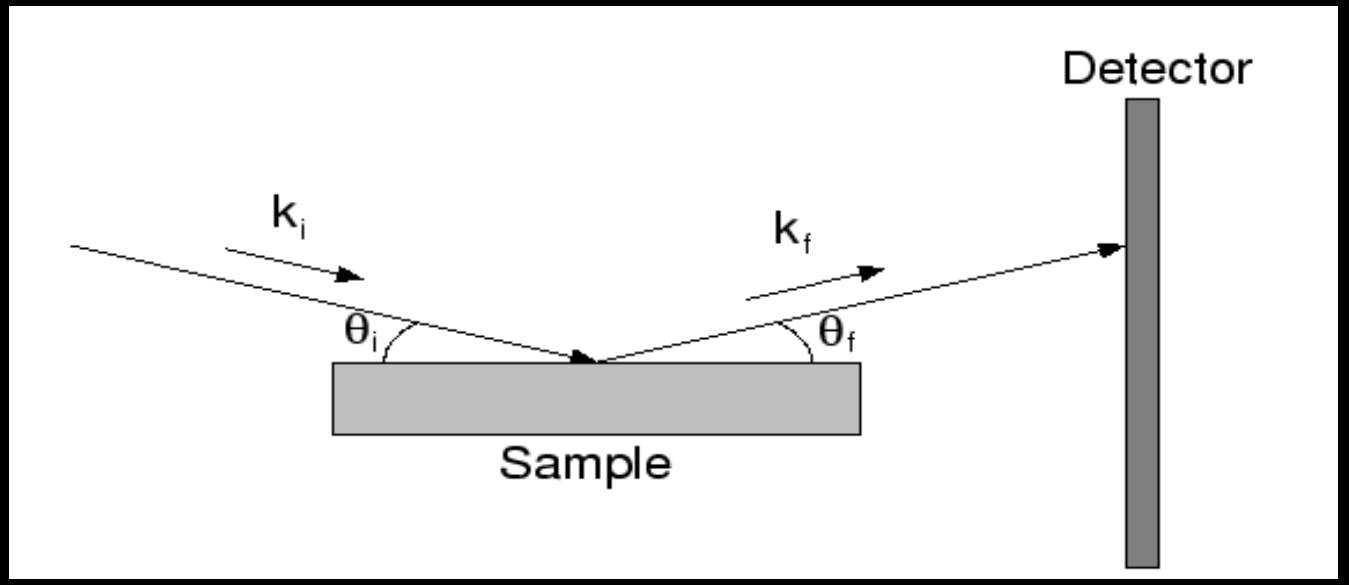
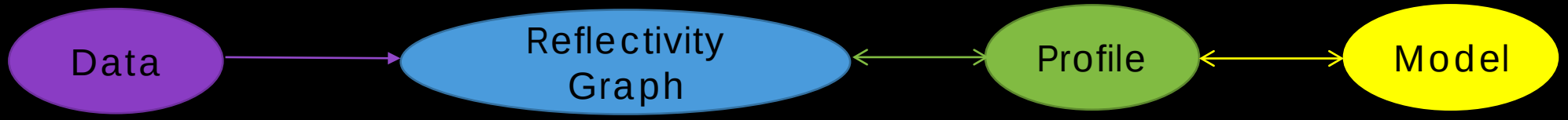
NEUTRON REFLECTOMETRY

- Neutrons are shot at thin films in order to determine structure
- Neutrons are sensitive to different isotopes of elements



MODELS AND FITTING

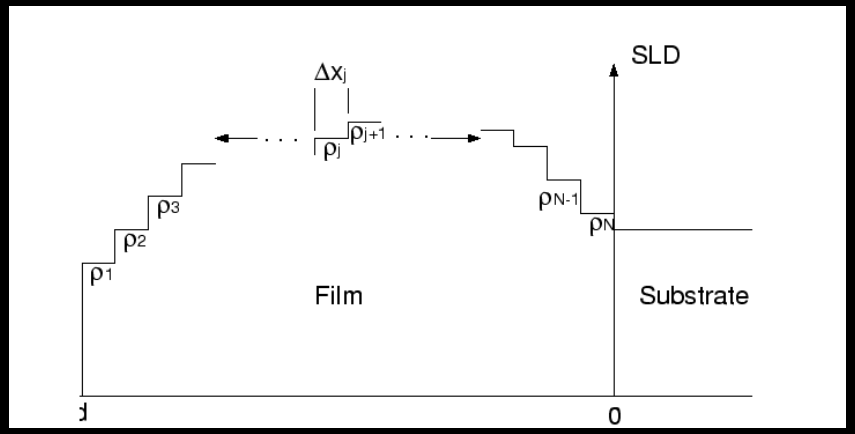
- Refl1D is the program we use to fit data to models



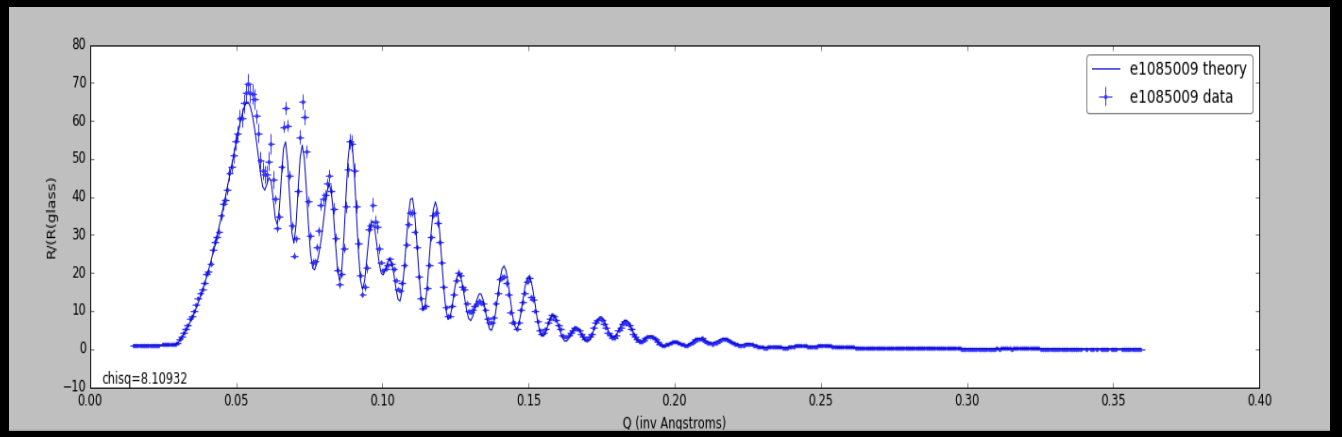
Hard to Interpret

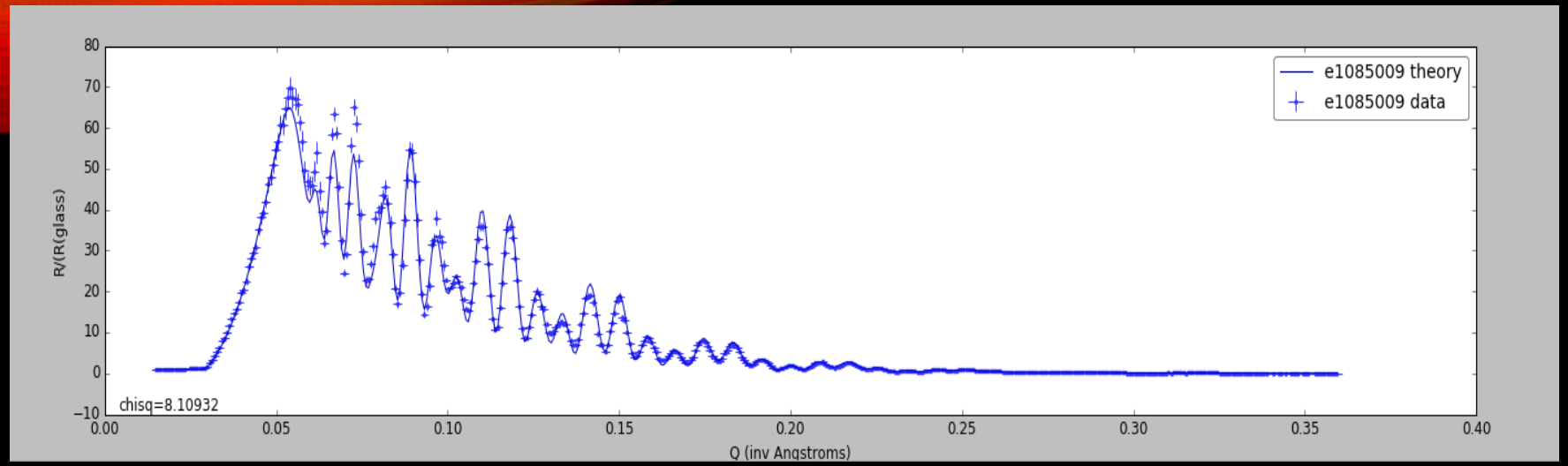
Easy to Interpret

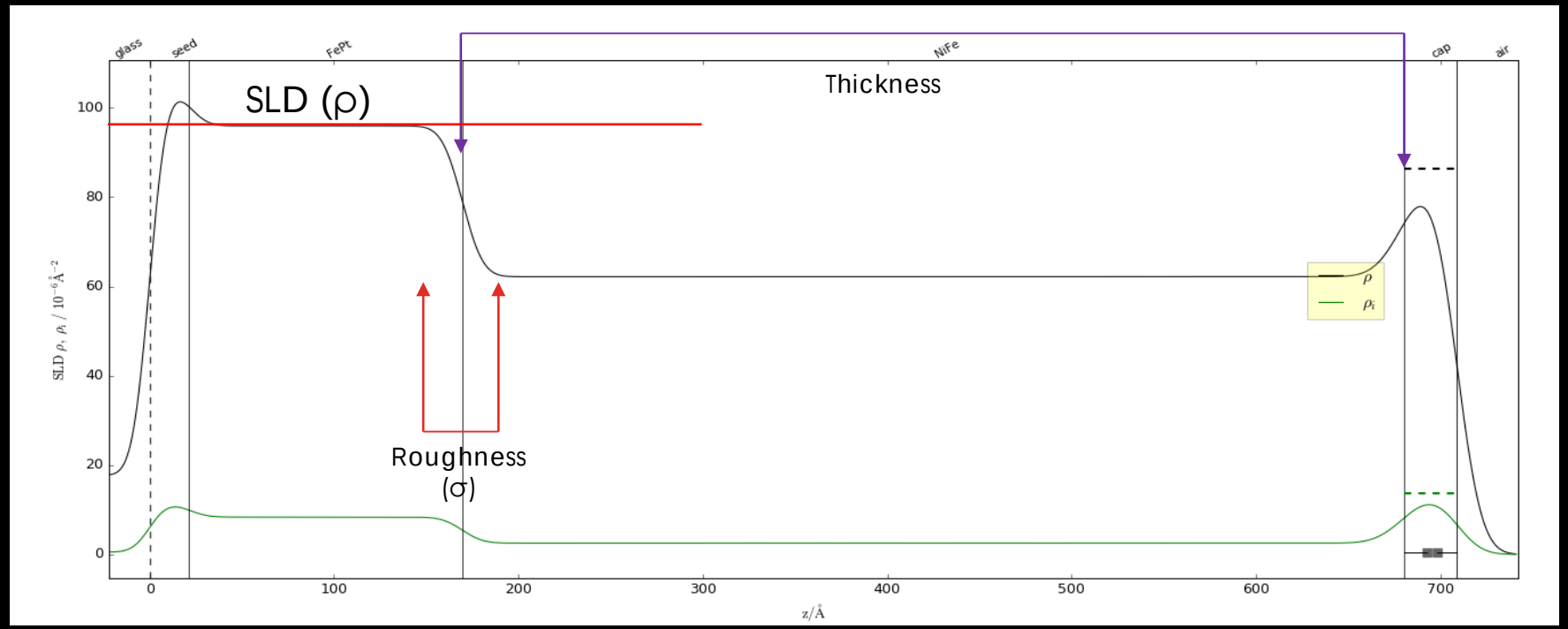
Non-Smooth Profile created from model



Model closely fitted to data points, reflectivity as a function of Q



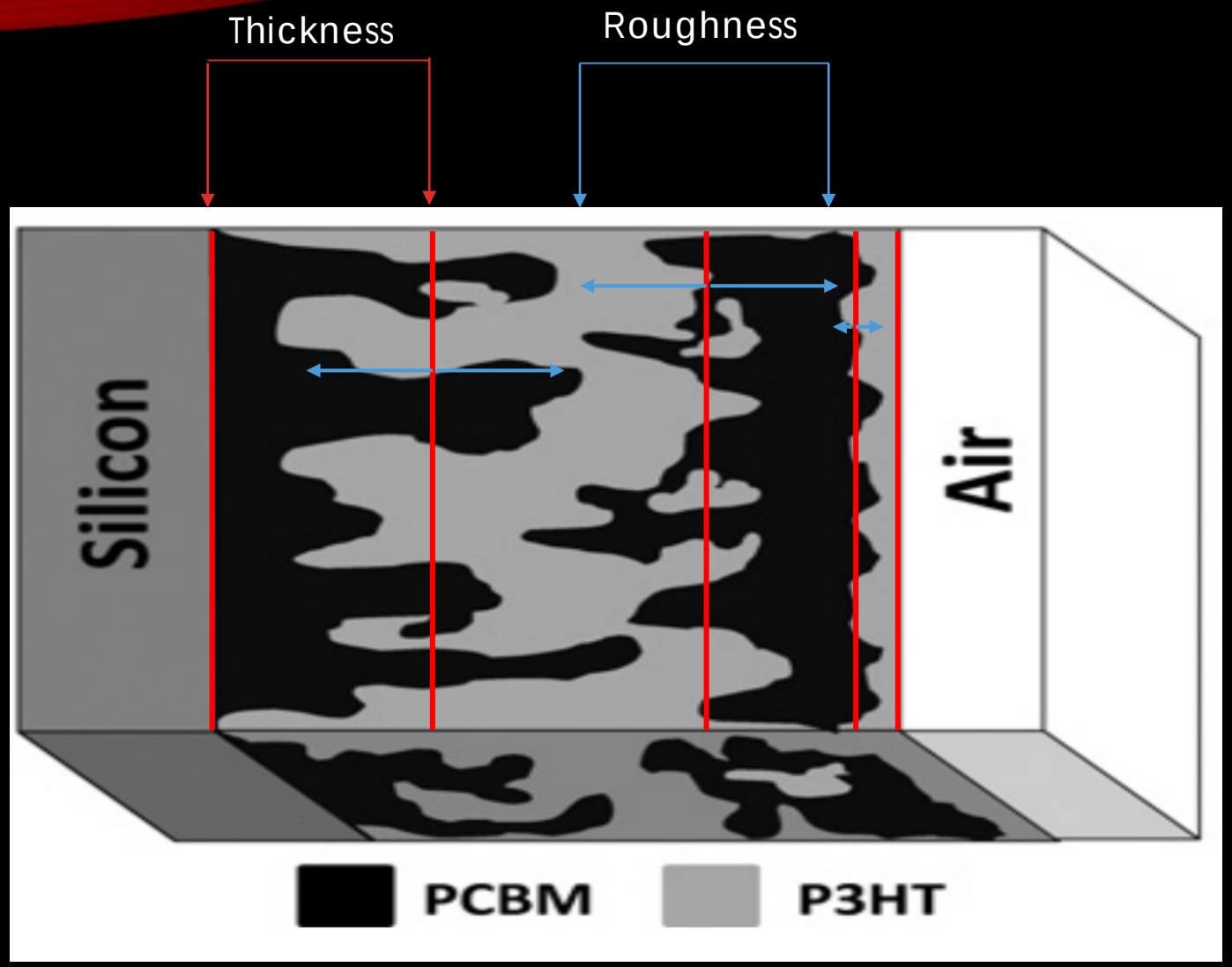




PROFILE OF MODEL TO GENERATE FIT

The model is composed of layers that each have thickness (width) and roughness (amount of blend between layers)

MODEL



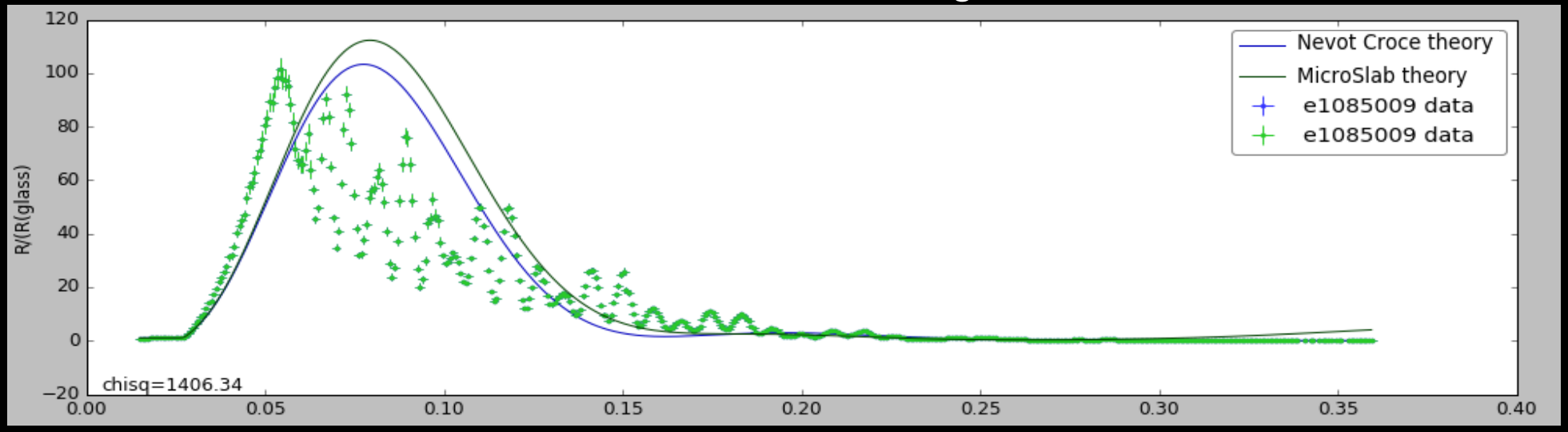
Silicon, PCBM, P3HT, and Air all have different SLD's

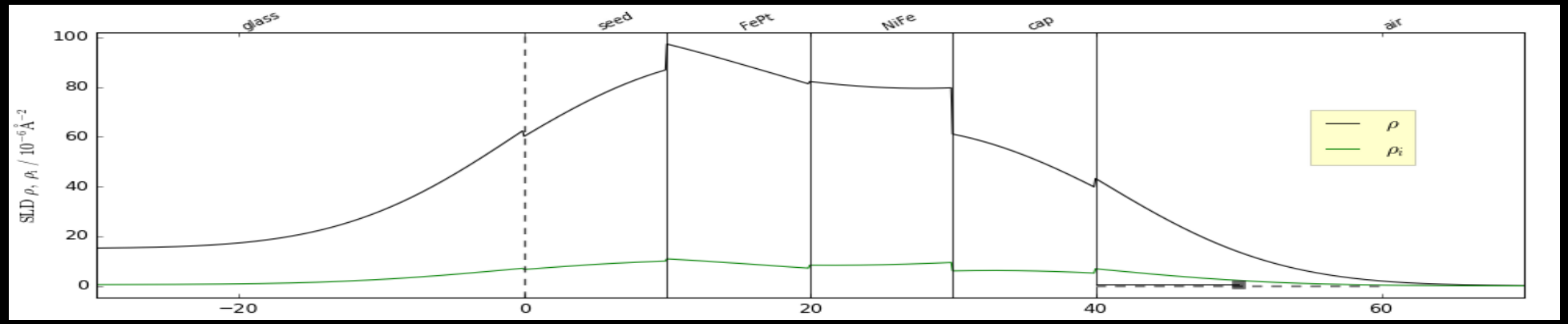
PROBLEM

- Models with layers that are very thin with large roughness are incorrectly calculated and smoothed out, which causes fits to be calculated wrong

Thickness = 10Å per layer

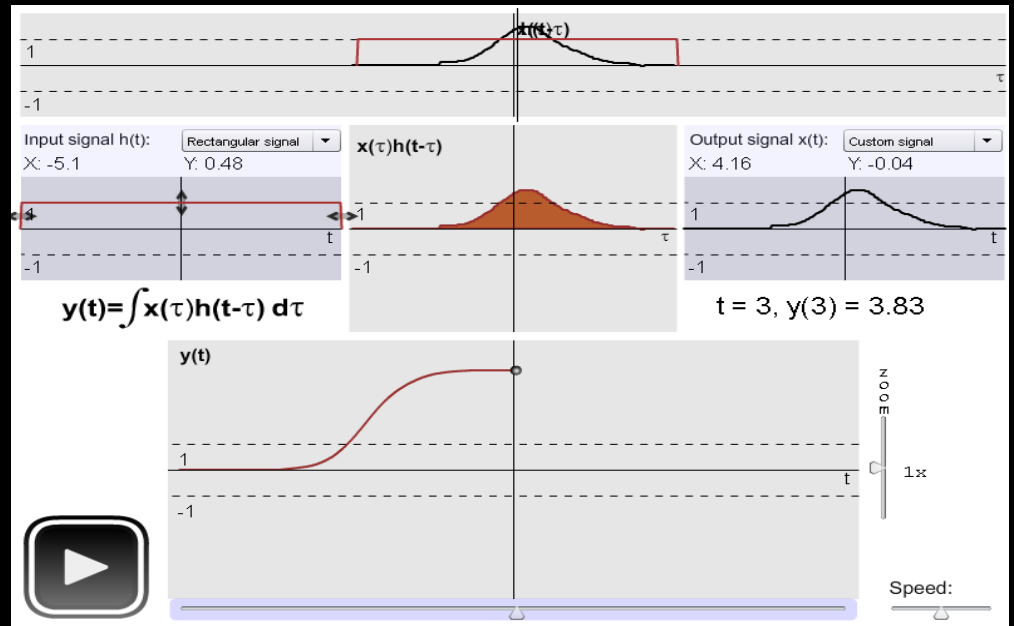
Roughness = 10Å per layer





SMOOTHING/BLENDING PROCESS

- Use Convolution of Gaussian and Step Function
  - Gaussian represents roughness
  - Steps represent difference in value of layers
- However, convolutions are very hard on the computer, so we use error functions to represent convolutions

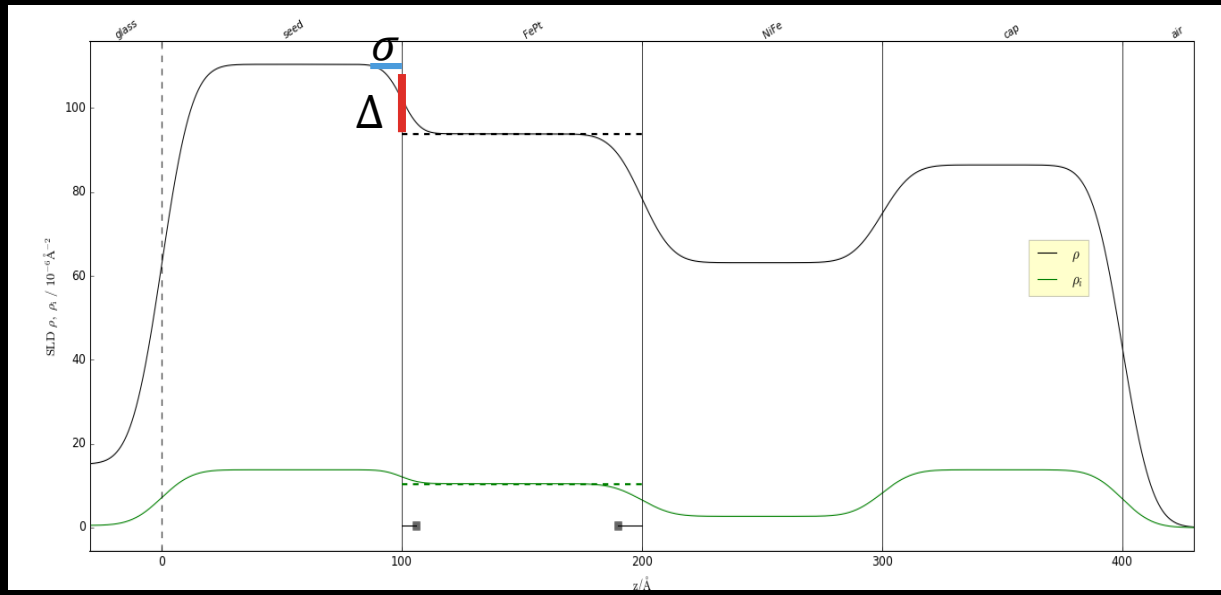


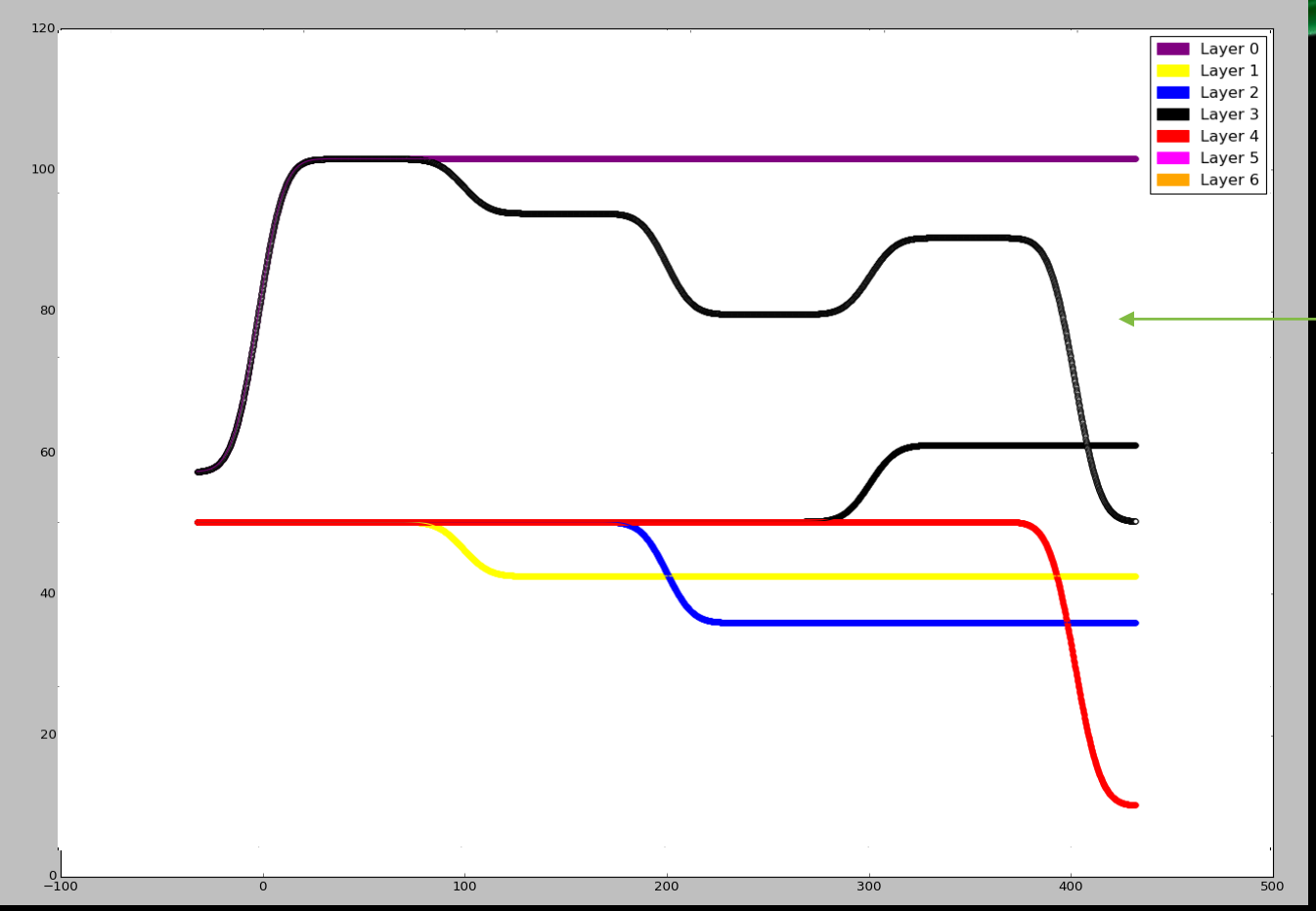
STEPS OF MY ALGORITHM

1) Calculate difference (Δ) in SLD of two layers
2) Find roughness (σ) of interface between layers
3) Create error function based on these numbers

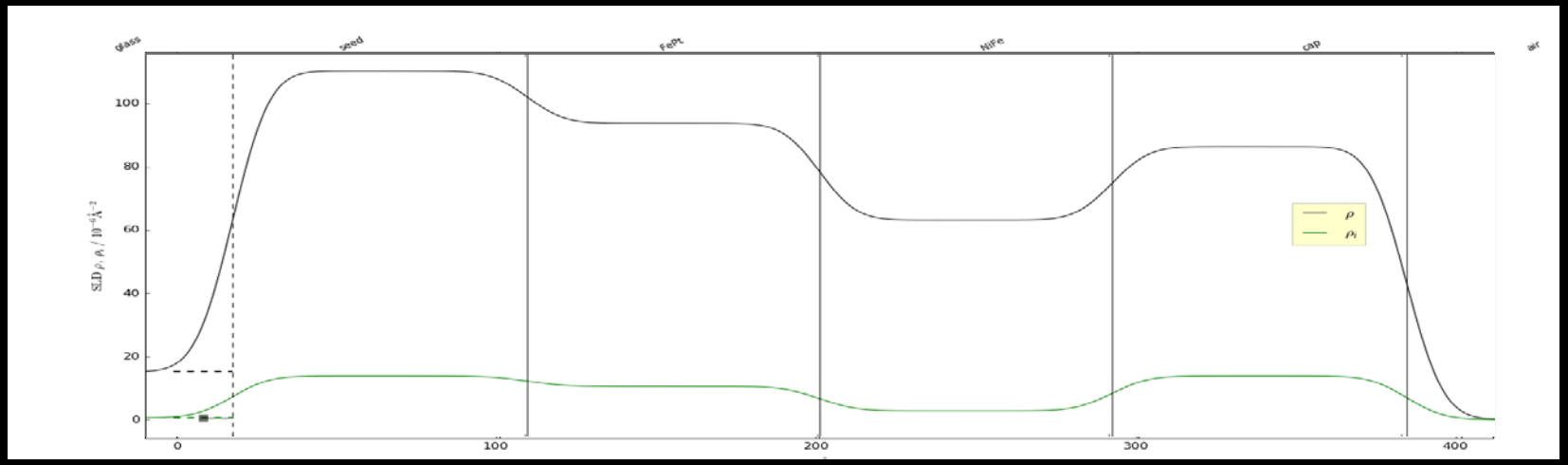
$$1) f(t) = \frac{\Delta}{\sqrt{\pi}} \int_0^z e^{-\frac{t}{\sigma\sqrt{2}}\text{^}2} dt$$

t is distance away from interface



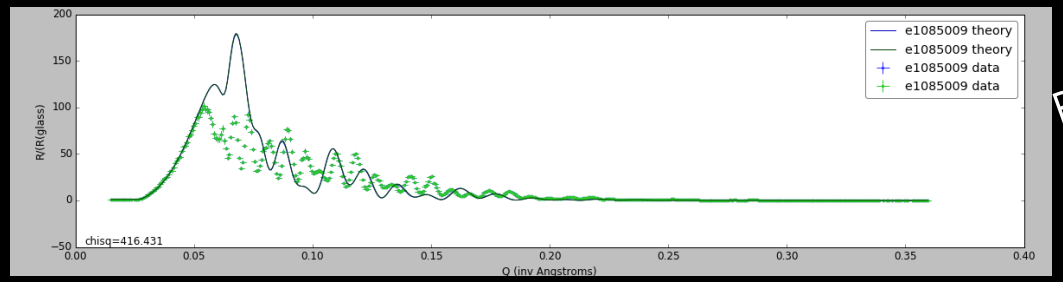


Result
(sum of interfaces)

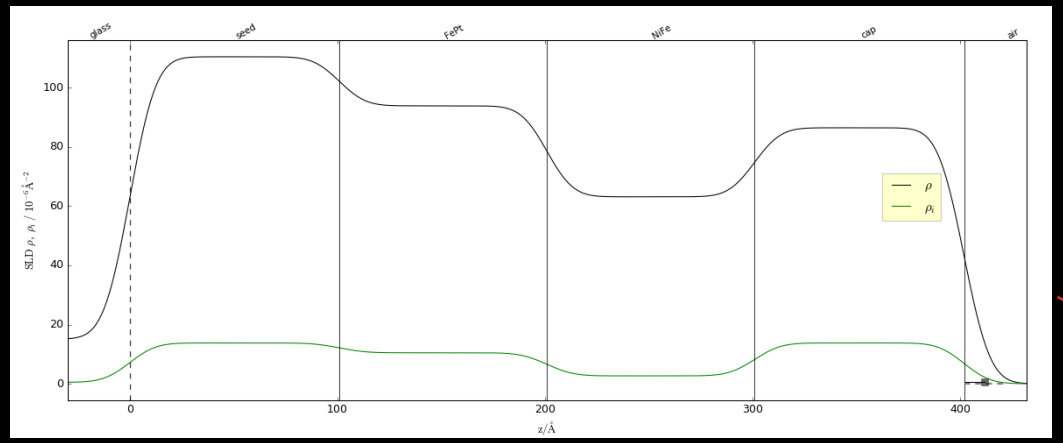


Expected

Mine

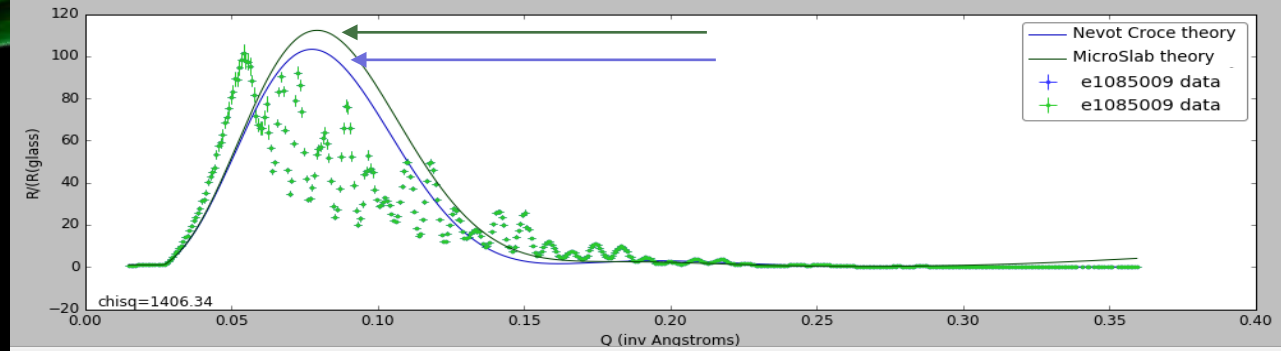


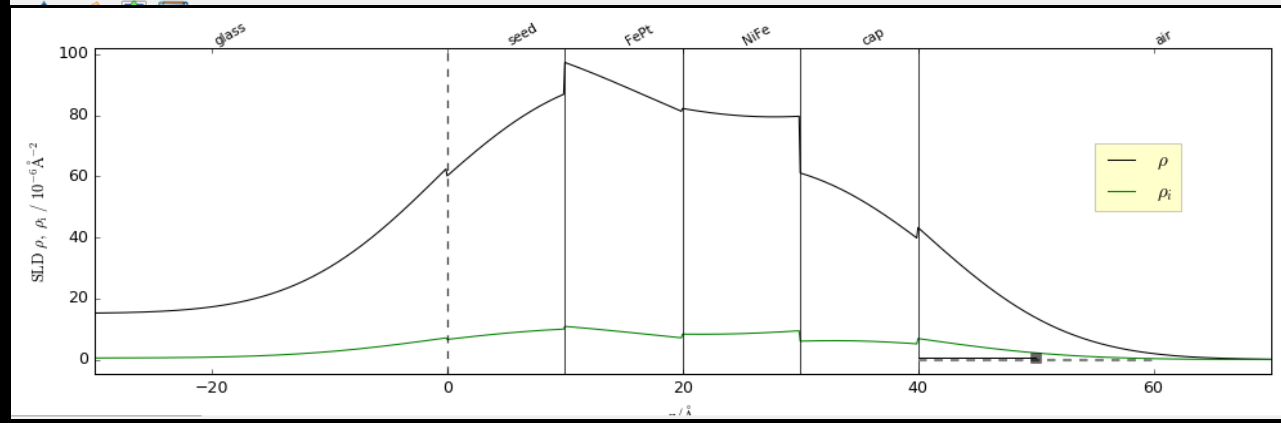
Before

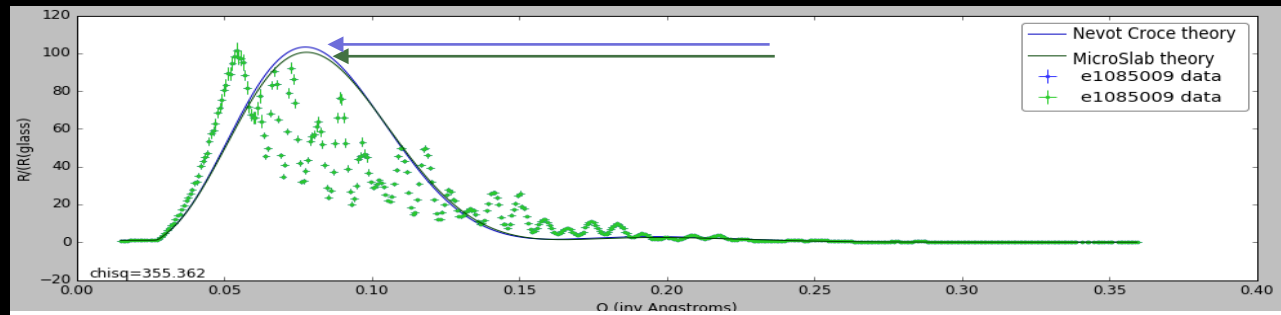


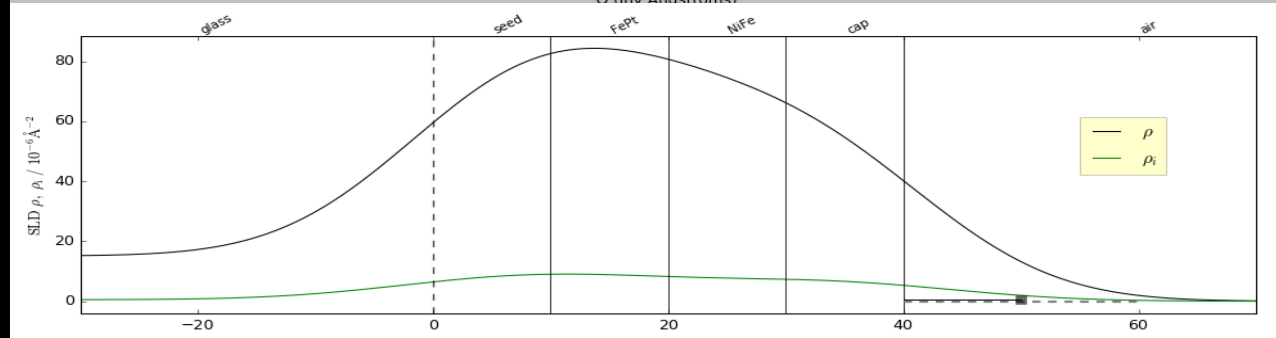
After

Same Model, but with thickness of layers decreased from 100Å to 10Å







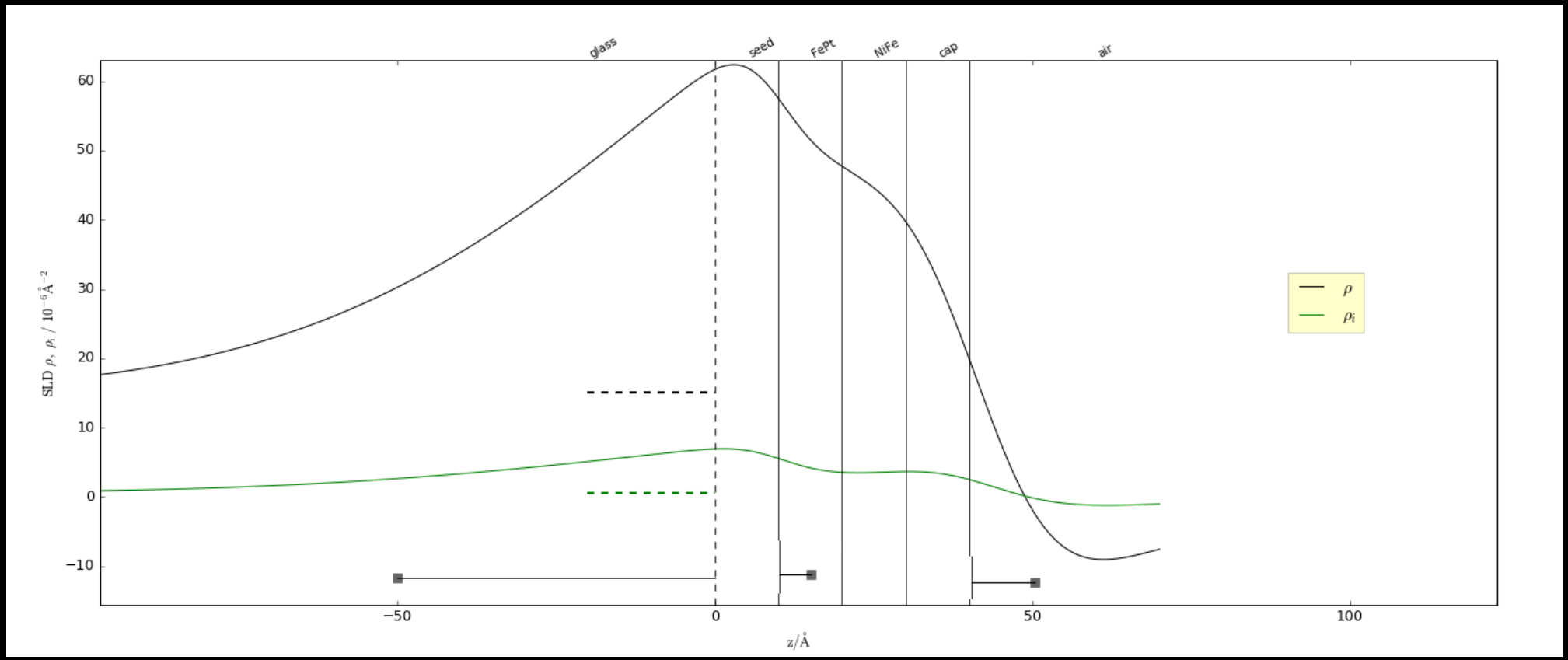


OUTCOME: MY ALGORITHM IS

- Faster than previous
- More accurate than previous
- Applicable to many reflectivity situations
  - Cell Membranes
  - Solar Cells

PROBLEMS

- Strange results in cases where roughness are unequal and large



IN ORDER TO MINIMIZE ISSUES (FOR NOW)

- Keep roughness equal in cases with large roughness and small thickness
- When roughness are unequal, roughness should be no more than the length of the next layer

THANKS!

- My Mentor, Brian Maranville
- SHIP Directors, Yamali Hernandez and Julie Borchers
- Paul Kienzle, one of the creators of Bumps and Refl1D
- CHRNS and NCNR