

Introduction

In this presentation, we show progress made in the modeling of off-specular neutron reflectometry data. The attributes of the formalism are defined and explained in terms of how they contribute to the representation of measured data. Measurements were taken on a sample of Au pillars in a square lattice. Data was obtained using a position sensitive detector (PSD) on Advanced Neutron Diffractometer/Reflectometer (AND/R) at the NIST Center for Neutron Research (NCNR) facility is presented. Data measurements were modeled using a parallelized version of the Substrate Modified Born Approximation (SMBA) which is one step toward the full Distorted Wave Born Approximation (DWBA).

Motivation

While some theory has been developed in the area of off-specular neutron reflectometry, its widespread use as a characterization technique has yet to be fully realized. This is partially due to the lack of complete, user friendly, and broadly distributed modeling software package. The University of Maryland, along with NCNR, and the NSF funded DANSE project, are currently developing a software component for fitting multilayer two dimensionally structured samples, thereby making off-specular neutron reflectometry accessible to a broader scientific community.

Data and Modeling

i. Experimental

Au/Cr/Si Sample Fabrication

The Au parallelepiped features were produced by sputter deposition of ~20Å of Cr followed by ~600Å of Au onto a Si substrate using a Denton Discovery 22 sputtering system. The Au was patterned using standard lithography techniques with a Suss Microtec MA8 Front Side Aligner. The Au was etched using room temperature dilute Aqua Regia (HNO₃:3HCl:20H₂O) until the Cr was visible.

Au Neutron Measurements

The sample shown below was created to provide a simple non-magnetic scattering data set that could be used to validate the models.

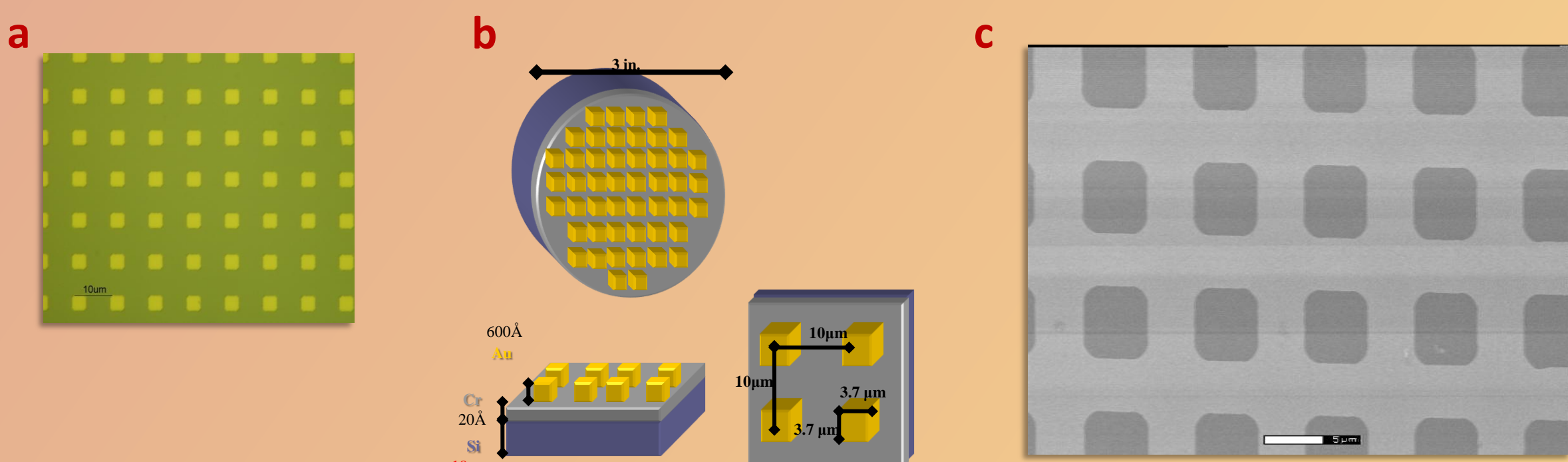


Figure 1: a) Optical image of the Au sample to show morphology b) Schematic representation of Au sample c) Scanning Electron Microscopy image of the Au showing rounded corners due to over-etching.

ii. Computational and Theoretical Properties

Aliasing

Low sampling rates in Q space calculations can cause artifacts in the model. To eliminate these artifacts, the integral between q points divide by the q range is solved for.

$$S = \frac{\sin(MqD/2)}{\sin(qD/2)}$$

$$S = \int_{q_{n-1}}^{q_n} \frac{\sin(MqD/2)}{\sin(qD/2)} dq / \Delta q$$

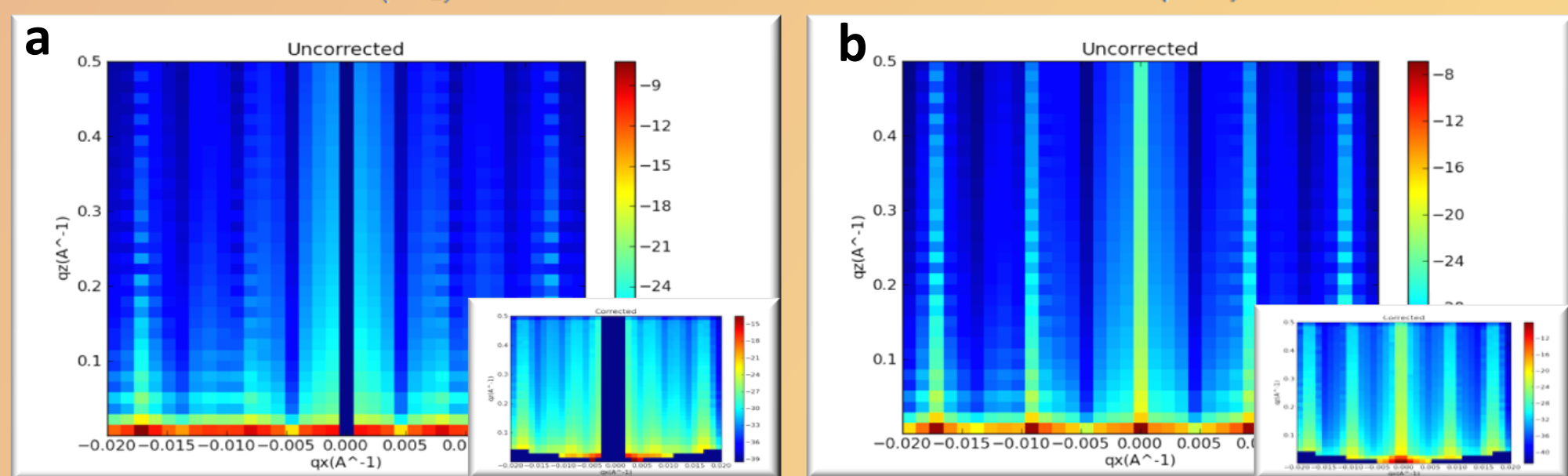


Figure 2: a) The scattering results for a low resolution scattering calculation. Errors are seen at the specular (totally eliminated) and the first diffraction peak (lower intensity than the second order peak). b) The integrated solution. Artifacts are eliminated.

Coherence Length

The coherence length of the neutron beam contributes significantly to the off-specular scattering. The Gaussian shape of the beam coherence length convoluted with the delta function diffraction peak gives an accurate representation of the scattering. Below is a comparison of scattering models with and without coherence length.

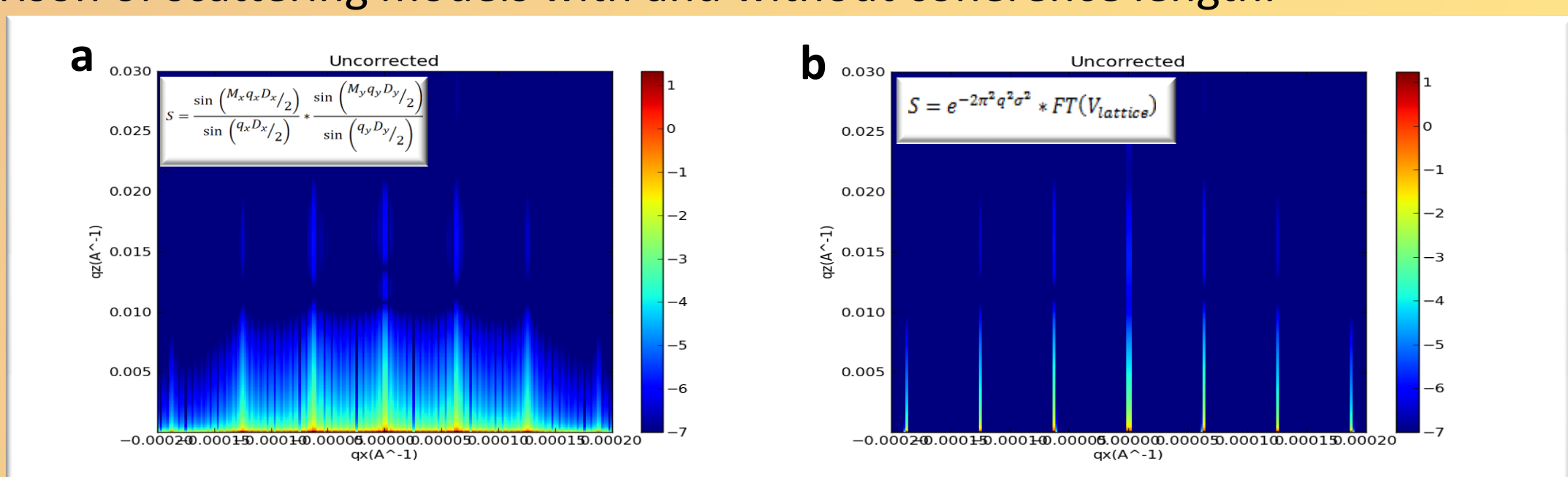


Figure 3: a) Uses structure factor which does not include the coherence length of the neutron beam. b) Uses a structure factor that includes the Gaussian coherence length of the beam provides a more accurate result.

Resolution Correction

The resolution of the neutron beam has a dramatic effect on the off-specular scattering. Specifically, the corrections included in the models presented here are for wavelength and θ_{in} divergence.

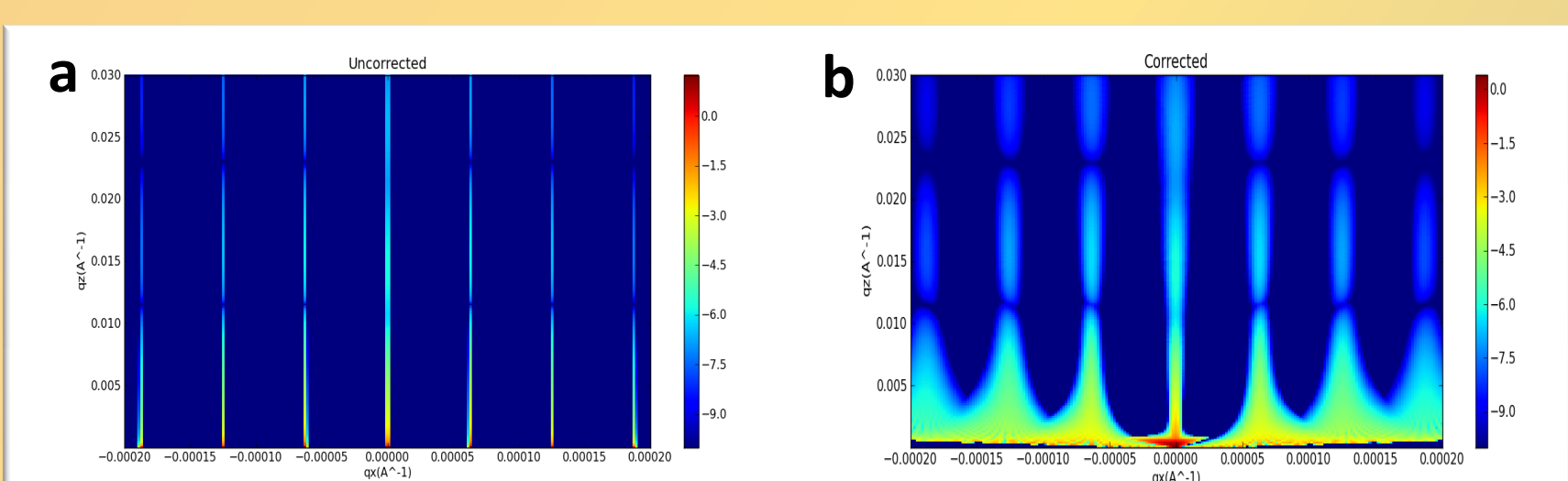


Figure 4: a) Born Approximation without resolution correction. b) Born Approximation with resolution correction.

Substrate Refraction

When the neutron beam enters or leaves the substrate at an angle close to normal (in reflectometry, when the beam enters or leaves the side of the substrate) the beam refracts.

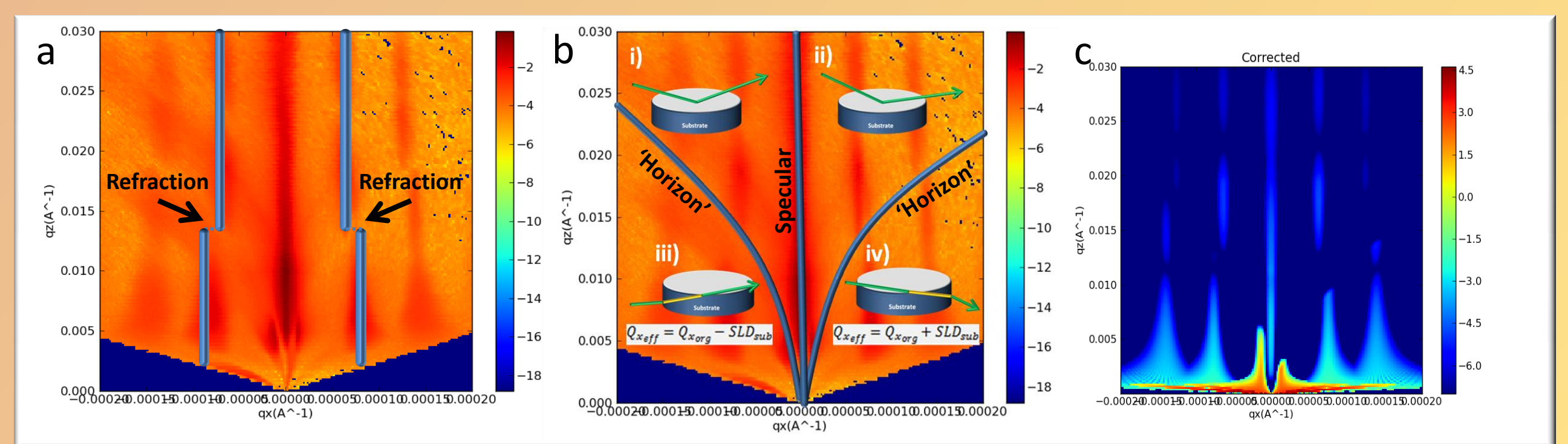


Figure 5: a) Au feature scattering data with lines indicating the shift of the diffraction peak below the 'horizon'. b) Schematic indicating the geometry which is causing the scattering: i) $\theta_{out} > \theta_{in}$ ii) $\theta_{out} < \theta_{in}$ iii) $\theta_{in} < 0$ iv) $\theta_{out} < 0$. c) model with refraction effects included.

Substrate Modified Born Approximation

While many factors contribute to dynamical scattering in neutron reflectometry, there is a substantial contribution from the substrate/incident media interface. By distorting the Born Approximation scattering by the solution to the wavefunction for the incident media and the substrate, some dynamical effects can be captured.

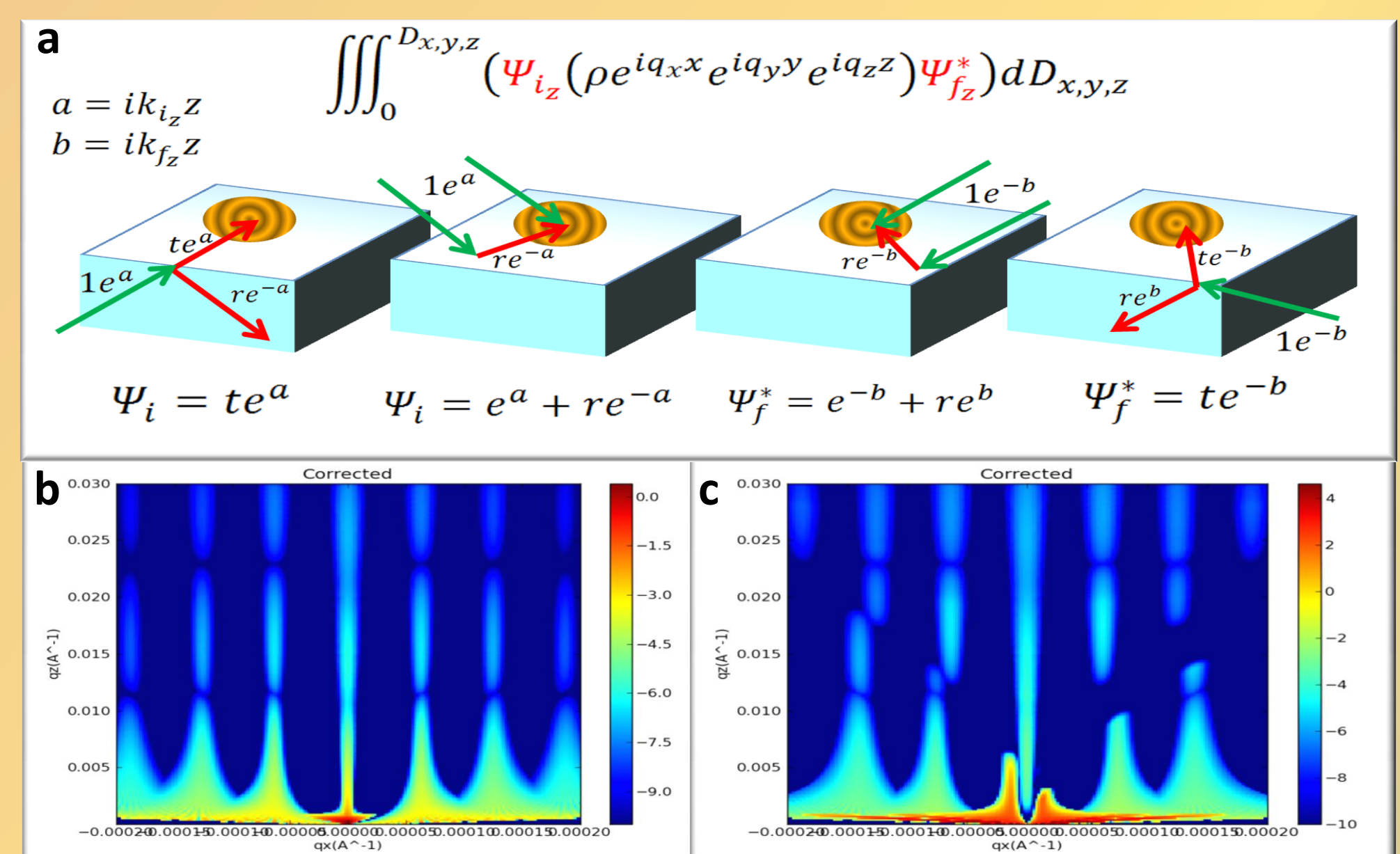


Figure 6: a) Schematic of the wavefunction calculation for the SMBA. Shows the contributing components based on incoming and outgoing beam angle. b) Resolution corrected BA. c) Resolution corrected SMBA. Note the 'horizons' are captured in the model.

Parallelization

As the approximations become more complicated, the ability to use mathematical techniques which improve computation time (ie. fft, czt) becomes limited. As a result, models can take hours to compute. To decrease this time, a version of the models have been written using C++/Cuda to allow for parallelization of the calculation.

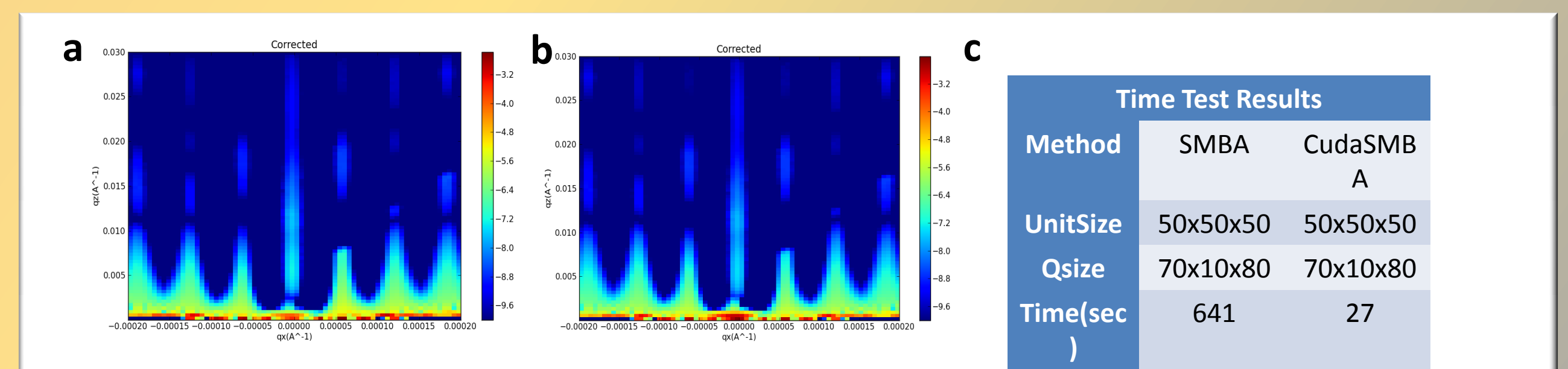


Figure 7: a) Model using a Python implementation of the SMBA. b) Model using a C++/Cuda implementation of the SMBA. c) Table of time test information.

iii. Modeling

Using the math developed in the previous section, a model of the data can be produced. This is shown below. It is important to note that the model can still not capture scattering near the 'horizons' accurately and still has the inaccuracies associated with the Born Approximation.

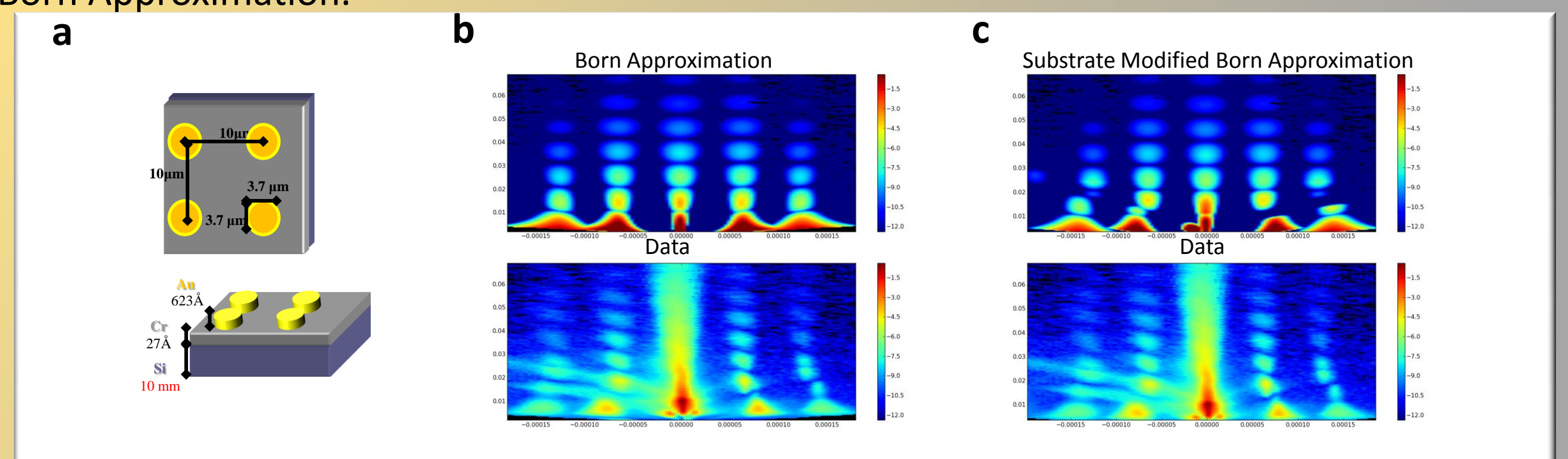


Figure 8: a) Au parallelepiped system. b) Born Approximation c) Substrate Modified Born Approximation.

Conclusions and Future Work

Although many features of off-specular scattering have been captured by our models, disparities still exist. To capture these effects a more complete Distorted Wave Born Approximation which takes into account the wave-sample interactions between every interface rather than just the incident media-substrate interface is still needed. Also, parameters for a description of the disorder in the sample is still required. Because magnetic sensitivity is an important attribute of neutron scattering, the modeling software will also need support for the modeling of magnetic samples.

References

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- [3] Dura, J. A., Pierce, D. J., Majkrzak, C.F., Maliszewskyj, N. C., McGillivray, D. J., Losche, M., O'Donovan, K.V., Mihailescu, M., Perez-Salas, U., Worcester, D. L., White, H., *Rev. Sci. Instrum.* (2006), 77, 074301

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