



Using Machine Learning to Interpret Neutron Reflectivity Data for Materials Discovery

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BACKGROUND

Neutron Reflectometry (NR) is used to study the internal structure of thin film materials. NR measures how neutrons reflect off a sample at different angles, resulting in a reflectivity curve $R(q)^{[1][2]}$. **However, this curve doesn't directly reveal the material's structure.**

To uncover it, we analyze the reflectivity data to obtain a **Scattering Length Density (SLD) profile**, which provides insight into layer thickness, roughness, and material distribution.

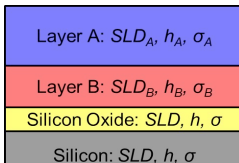


Figure 1. Liquids Reflectometer of ORNL

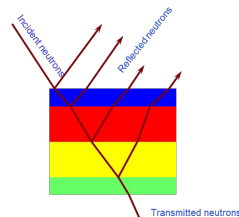


Figure 2. NR principle diagram(bottom) and SLD principle diagram(top)

PROBLEM STATEMENT

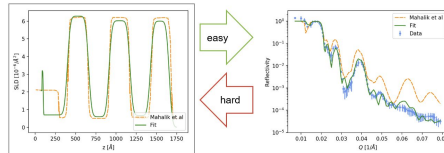


Figure 3. Going from SLD $\rightarrow$ NR has been made easy, going in opposite direction is still very hard. Both mappings are non-injective and as a result are non-invertible.

APPROACHES

1.Data Source: 100k simulated NR-SLD synthetic pairs were generated using *refl1d*^[3] fitting. Experimental NR-SLD data was provided by Oak Ridge National Laboratory.

2.Data Processing: Experimental NR curves were and reconstructed using an Autoencoder to extract latent features.

3.Training: An improved Convolutional Neural Network (CNN) was trained on the simulated NR-SLD dataset.

4.Pipeline Integration: All components are integrated into a PyPI package for streamlined use.

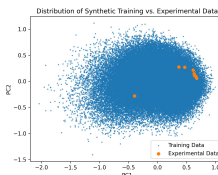


Figure 3. PCA analysis of synthetic data and experimental data. Cumulative explained variance 0.93.

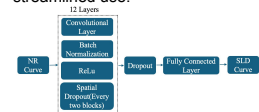


Figure 4. Architecture of the improved CNN model

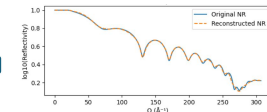


Figure 5. Comparison between AE-reconstructed NR and original NR

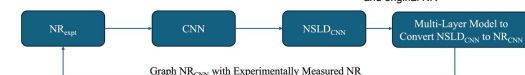


Figure 6. Synthetic NR data from Refl1d is fed into the CNN, which predicts the NSLD. The MSE between predicted and synthetic NSLD guides model training.

RESULTS

The improved CNN model, with dropout and architectural enhancements, yields more accurate SLD profiles from AE-reconstructed experimental NR data. It outperforms the previous model, aligning better with manual fit SLDs. As shown in Figure 8, R^2 improves by **8.7%** for NR and **12.0%** for SLD on experimental data.

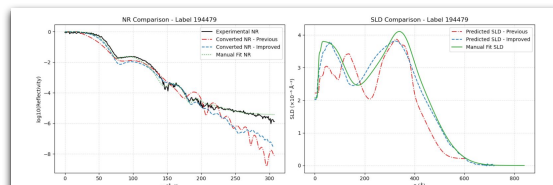


Figure 7. NR Curve and SLD Profile Comparisons for Sample 194479

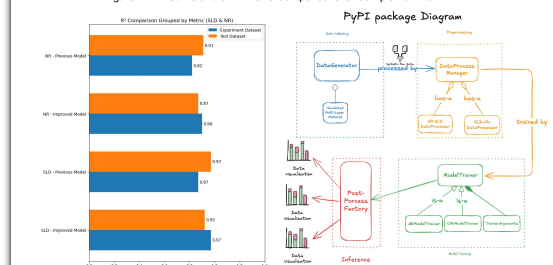


Figure 8. Comparison of NR and SLD R^2 Between Models

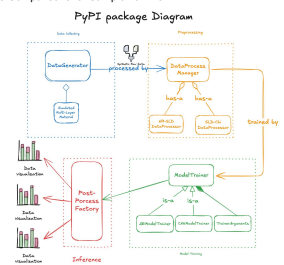


Figure 9. Python Package Design Diagram

CONCLUSIONS

The previous model worked but struggled with noisy data due to overfitting. Adding dropout and spatial dropout improved robustness and led to better predictions for both NR and SLD profiles.

REFERENCES

- [1] Dustin Ely, Miguel Fuentes-Cabrera, Rajeev Kumar et al., *Extraction of interaction parameters from specular neutron reflectivity in thin films of diblock copolymers: an "inverse problem"*, Nanoscale, 16(16), 7280-7291 (2023).
- [2] Brian Qu, Miguel Fuentes-Cabrera, Rajeev Kumar et al., *Learning continuous scattering length density profiles from neutron reflectivities using convolutional neural networks*, Mach. Learn.: Sci. Technol., 5(5), 050605 (2024).
- [3] Maraville B. B., Kenzie P., Sheridan R., Doucet M., Nelson A., Hoogenheide D. P., Book A. and Ghose R. 2020 (available at: <https://github.com/reflectometry/refl1d>)