The Journal of Open Source Software

cdsaxs: A model fitting package for CD-SAXS data analysis

Nischal Dhungana [1], **Guillaume Freychet** [1], and **Matthew Bryan** [1]

1 CEA, Leti, F-38000 Grenoble, France

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor: Sarath Menon

Reviewers:

- @benjaminbolling
- @marcocamma

Submitted: 22 September 2024
Published: unpublished

Summary

Miniaturizing transistors, the fundamental components of integrated circuits, poses significant challenges for the semiconductor industry. Accurate measurements of these features during production is essential to ensure the creation of high-quality chips. However, conventional in-line metrology techniques are approaching their limitations. To address these challenges, the industry is turning to advanced X-ray-based metrology (D. Sunday et al., 2015).

CD-SAXS (Critical Dimension Small Angle X-ray Scattering) is an emerging and promising technique in this field. Studies conducted by (D. Sunday et al., 2015) have demonstrated the effectiveness of CD-SAXS in accurately characterizing the shape and spacing of nanometer-scale patterns. The cdsaxs package is designed to offer comprehensive simulation and fitting tools for CD-SAXS synchrotron data, supporting researchers in advancing this innovative technology.

Statement of need

CD-SAXS is a powerful and developing technique for characterization of nano-components in the semiconductor industry. Efforts by the community were done to explore different combination of algorithms to model CD-SAXS data, as described by (Hannon et al., 2016) (D. F. Sunday et al., 2016). However, there is a lack of open-source software for comprehensive data analysis. Xi-cam (Pandolfi et al., 2018) is the only publicly available python package that contains CD-SAXS data analysis albeit the code is no longer maintained. While there are a few other proprietary softwares, they are not freely accessible to the community. Thus, development of model and its analysis for CD-SAXS requires researchers to develop their own solutions for simulating and fitting. Moreover, the diversity of samples analyzed using CD-SAXS requires versatile software that can accommodate different types of models and experimental conditions.

The cdsaxs package is designed to address this critical gap by providing a modular, open-source solution tailored for CD-SAXS data analysis. It includes two robust models for simulating CD-SAXS data, while also allowing researchers to integrate their own models. This flexibility is crucial for testing and validating models against experimental data, making the development process more streamlined and accessible.

A key feature of this package is its separation of the simulation and fitting processes, enabling users to concentrate on model development and data analysis without being encumbered by technical complexities. The package is optimized for performance, with support for vectorised fitting on both CPUs and GPUs, significantly enhancing the speed and efficiency of data processing. The fitting process in cdsaxs is powered by the CMAES (Covariance Matrix Adaptation Evolutionary Strategy) algorithm, known for its rapid convergence for x-ray fitting (Hannon et al., 2016). This efficiency allows for real-time data fitting during experiments, empowering researchers to dynamically adjust experimental parameters based on immediate feedback from the analysis.

Additionally, it incorporates uncertainty estimation in the fitted parameters using the MCMC (Monte Carlo Markov Chain) inverse algorithm, providing researchers with more reliable and nuanced results (D. F. Sunday et al., 2016).

By aiming to fill the current void in CD-SAXS data analysis tools, cdsaxs targets to speed up research workflows and to make advanced analytical techniques more accessible.

Description

The `cdsaxs` package provides a comprehensive framework for analyzing CD-SAXS data, focusing on the systematic workflow of candidate generation, evaluation, and uncertainty estimation. It is also flexible enough to accommodate user-defined models, making it a versatile tool for researchers working with diverse nanostructures.

1. **Candidate Generation and Evaluation**:
    - The core of the `cdsaxs` fitting process begins with generating a series of candidate parameters. Each set of parameters represents a possible nanostructure configuration, defined by a set of features (e.g., widths, heights, etc.).
    - These candidate models are then transformed into the reciprocal space through a Fourier Transform, allowing direct comparison with the experimental CD-SAXS data.
    - The package utilizes an optimization algorithm, specifically the Covariance Matrix Adaptation Evolutionary Strategy (CMAES), to iteratively refine the model parameters. This algorithm excels in high-dimensional optimization, rapidly converging on a solution that minimizes the error between the simulated and experimental scattering intensities.
2. **Simulation and Comparison**:
    - The simulation process can also function independently, generating CD-SAXS data based on user-defined parameters without the need for experimental data. This is particularly useful for testing and validating models in a controlled setting.
    - In addition to the two built-in models, users can define their own models, allowing for a wide range of nanostructure configurations to be tested.
    - When experimental data is available, the package simulates scattering profiles for each candidate model and calculates a goodness-of-fit metric by comparing the simulated data with the experimental measurements. The optimization algorithm adjusts the model parameters to minimize this metric, ensuring the best possible match.
3. **Uncertainty Estimation**:
    - After determining the best-fit model, `cdsaxs` employs a Monte Carlo Markov Chain (MCMC) algorithm to estimate the uncertainties associated with the model parameters. This step is crucial for understanding the robustness of the fit and identifying potential alternative structures that could produce similar scattering data.
    - The MCMC method generates a distribution of possible parameter sets, from which the package calculates confidence intervals, providing a quantitative measure of uncertainty for each parameter.

The following diagram illustrates the overall workflow of the CMAES algorithm in the `cdsaxs` package:

The Journal of Open Source Software

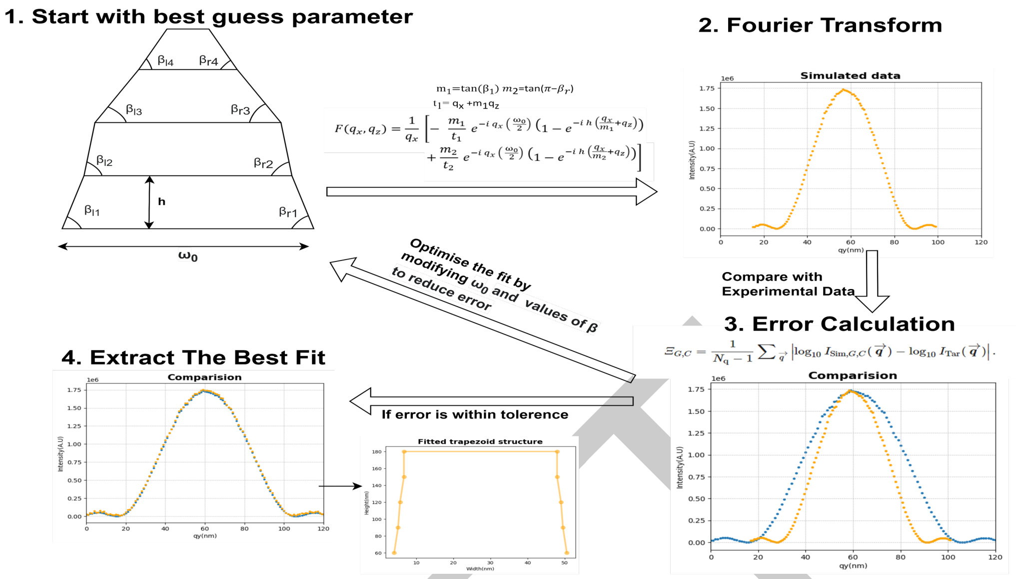

Figure 1: Workflow of the CMAES algorithm in the cdsaxs package.

The overall workflow of the MCMC algorithm:

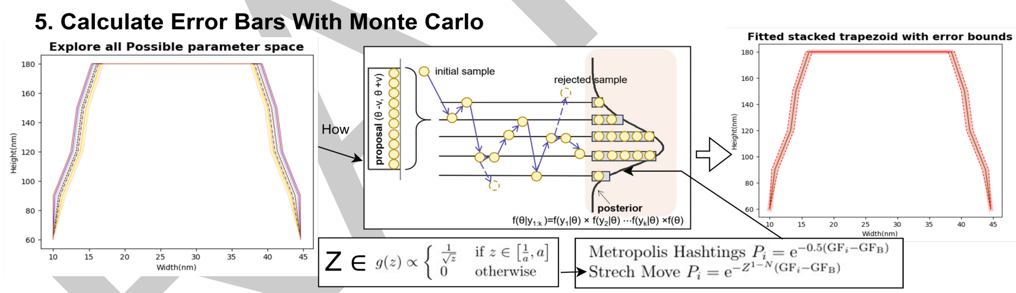

Figure 2: Workflow of the MCMC algorithm in the cdsaxs package.

This workflow ensures that the `cdsaxs` package not only identifies the optimal model configuration but also quantifies the confidence in the results, making it a powerful tool for CD-SAXS data analysis in both research and industrial applications.

Comparison

Xi-cam (Pandolfi et al., 2018) is the open source software that was used for CD-SAXS simulations described by Choisnet et al. (Choisnet et al., 2024). Notably they use a six stacked trapezoid model and a rounded trapezoid model to do the simulation. The experimental dataset used by Choisnet et al. for their study was used here to test our model. We also fitted the dataset with a six stacked trapezoid model, enabling a direct comparison between Xi-cam and this package. The results are shown in the figure below:

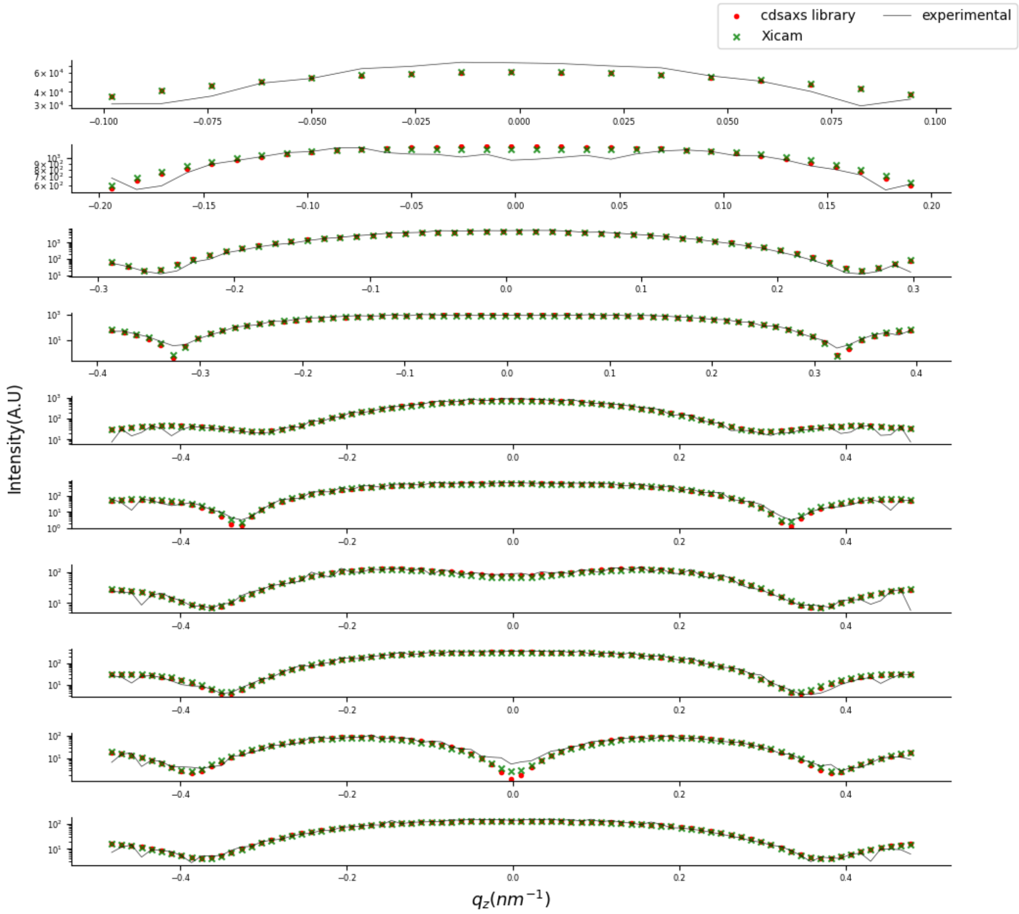

Figure 3: Comparison of fits obtained by Xi-cam and the cdsaxs package in fourier space. Results obtained experimentally are also plotted.

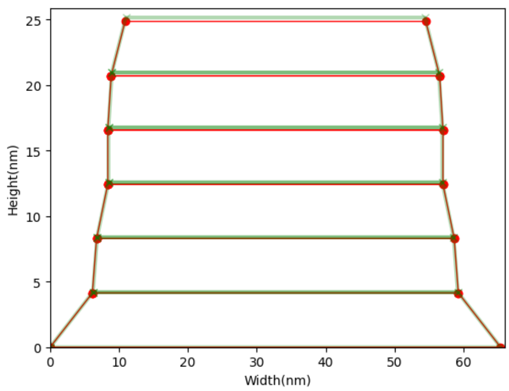

Figure 4: Comparison of fits obtained by Xi-cam and the cdsaxs package in real space.

For the same initial conditions and search criteria, we were able to demonstrate that the fits are remarkably similar and therefore demonstrate the accuracy of our modeling.

Similarly, with the same dataset the time taken to execute the program was measured. The number of generations was kept constant at 100 and different population sizes were tested. The test was performed on an Ubuntu server with 64 logical processors of model Intel(R)

Xeon(R) Platinum 8362 CPU @ 2.80GHz and the GPU used was NVIDIA A100 80GB PCIe.

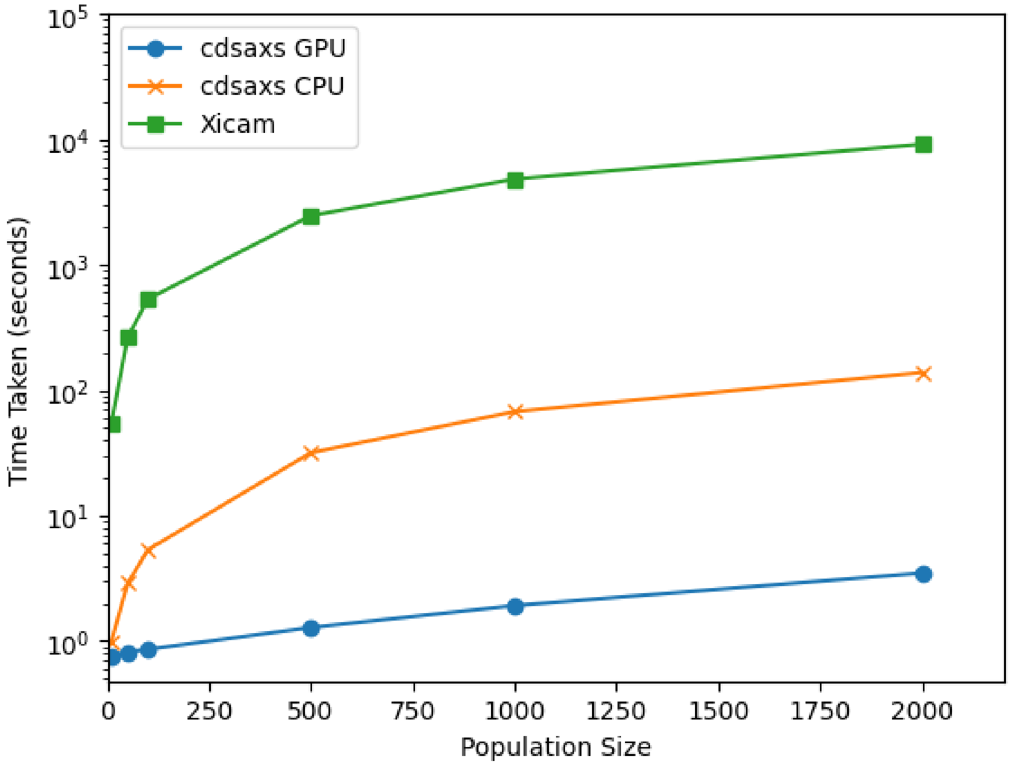

Figure 5: Execution time for the two versions of the code (CPU and GPU performance comparison).

We can observe that the cdsaxs package has significant improvement in execution time (more than 10 times for CPU execution and 100 times for GPU execution) over old code.

Conclusion

In this work, we presented the cdsaxs package, a comprehensive and modular open-source framework for CD-SAXS data analysis. By integrating CMAES for fast optimization and MCMC for robust uncertainty estimation, the package offers both speed and reliability for fitting synchrotron data. Benchmark comparisons demonstrate its significant improvements over previous tools, both in accuracy and execution time. We believe cdsaxs will accelerate research workflows in the semiconductor industry and provide a foundation for future developments in X-ray-based metrology.

Acknowledgements

This work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the "Recherche Technologique de Base" and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR).

References

Choisnet, T., Hammouti, A., Gagneur, V., Reche, J., Rademaker, G., Freychet, G., Jullien, G., Ducoté, J., Gergaud, P., & Cunff, D. L. (2024). Cross-evaluation of critical dimension measurement techniques. *Journal of Micro/Nanopatterning, Materials, and Metrology*, *23*(1), 014002. https://doi.org/10.1117/1.JMM.23.1.014002

Hannon, A. F., Sunday, D. F., Windover, D., & Kline, R. J. (2016). Advancing x-ray scattering metrology using inverse genetic algorithms. *Journal of Micro/Nanolithography, MEMS, and MOEMS : JM3*, *15*(3), 034001. https://doi.org/10.1117/1.JMM.15.3.034001

Pandolfi, R. J., Allan, D. B., Arenholz, E., Barroso-Luque, L., Campbell, S. I., Caswell, T. A., Blair, A., De Carlo, F., Fackler, S., Fournier, A. P., Freychet, G., Fukuto, M., Gürsoy, D., Jiang, Z., Krishnan, H., Kumar, D., Kline, R. J., Li, R., Liman, C., … Hexemer, A. (2018). *Xi-cam*: a versatile interface for data visualization and analysis. *Journal of Synchrotron Radiation*, *25*(4), 1261–1270. https://doi.org/10.1107/S1600577518005787

Sunday, D. F., List, S., Chawla, J. S., & Kline, R. J. (2016). Evaluation of the effect of data quality on the profile uncertainty of critical dimension small angle x-ray scattering. *Journal of Micro/Nanolithography, MEMS, and MOEMS*, *15*(1), 014001. https://doi.org/10.1117/1.JMM.15.1.014001

Sunday, D., List, S., Chawla, J., & Kline, R. (2015). Determining the shape and periodicity of nanostructures using small-angle x-ray scattering. *Journal of Applied Crystallography*, *48*. https://doi.org/10.1107/S1600576715013369