refellips: Ellipsometry data analysis in Python

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Ellipsometry is a widely employed, non-destructive optical technique used in thin film metrology, allowing users to characterise the physical properties of thin films, such as composition, thickness and roughness. Since its inception in the late 19th century, ellipsometry has evolved to become a ubiquitous and fundamental technique throughout surface science.[1] Many proprietary software packages are available to users for ellipsometry data analysis; however, these are frequently tied to specific hardware, not easily incorporated in to pipelines for data handling and reproducible research, and cannot be combined with packages for other techniques.

Here we present a simple method for the analysis, modelling, and optimisation of ellipsometry data: *refellips*.[2] *refellips* is an open-source software package written in Python 3 and is designed to be used in a Jupyter notebook environment; ultimately facilitating reproducible research. The software aims to assist users with all levels of ellipsometry data analysis and employs the range of local and global minimisers offered by the *scipy* package to fit data. Of note, *refellips* is integrated with the popular neutron (NR) and X-ray reflectometry (XRR) software package, *refnx*,[3] making both model sharing and the co-refinement of data across ellipsometry, NR and XRR possible. The collaboration of these three techniques enables better characterisation of complex interfaces in condensed matter films. Importantly, *refellips* allows for the facile batch processing of large ellipsometry datasets, such as areal maps of a surface, exploration of phase transitions in tethered polymer films, and time series data. These ellipsometry results can then be used to inform NR and XRR experiments and analysis. The modular design of *refellips* means that users can implement simple models (e.g., slabs) or create their own complex mathematical optical models to describe an interface. *refellips* is able to read a range of file types from common ellipsometers and is distributed with dispersion curves for frequently used materials.

[1] H. G. Tompkins, E. A. Irene, *Handbook of Ellipsometry*, William Andrew, 1st ed., **2005**, pp. 1–870.

[2] H. Robertson, I. J. Gresham, A. R. J. Nelson, *refellips*, `https://github.com/refnx/refellips`.

[3] A. R. J. Nelson, S. W. Prescott, *J. Appl. Crystallogr* **2019**, *52*, 193–200.