



Film structure modeling and refinement software: FilmInsight

A novel modeling and refinement software designed to analyze the detailed structure of thin films using X-ray diffraction data.

IP Status: Copyrighted

Applications

- Conduct layer-by-layer structural refinement of thin films on substrates, capturing subtle depth variations with 0.01 angstrom spatial resolution*
- Perform quantitative assessment of surface roughness and substrate-film interface by discerning changes in film layers within these regions relative to the bulk of the films*
- In-operando study of thin film devices, evaluating structural changes during device operation
- Simulate and fit laboratory high-resolution X-ray diffraction data
- The novel phase-retrieval algorithm can be adapted to other diffraction techniques, including neutron scattering

* Resolving detailed layer-by-layer structure requires high-quality X-ray diffraction data, such as those from synchrotron X-ray diffraction. However, simple film modeling and data fitting are applicable to lower-quality laboratory X-ray diffraction data.

Key Benefits & Differentiators

- **Broadly applicable:** Uncover depth profiles of film structures with significantly reduced diffraction data requirements compared to current phase retrieval methods. This capability is invaluable in scenarios where samples degrade during prolonged data acquisitions or when prolonged measurements are impractical

Technology Overview

Investigating the structure of thin films on a substrate is important for producing materials with novel properties for modern devices. However, achieving atomic resolution depth profiling of the structure, particularly during device operation, presents considerable challenges. While X-ray diffraction (XRD) combined with phase retrieval methods enables imaging of the thin film's atomic structure layer by layer, existing approaches are costly and time-consuming. The necessity for substantial synchrotron X-ray diffraction data significantly restricts their practical application.

Researchers at the University of Minnesota have developed a structure modeling and refinement software to compute the film structure using a novel algorithm. It employs an innovative constrained phase retrieval algorithm to resolve depth variations within thin film structures. This enables researchers to unravel intricate layer-by-layer details of thin film structures with a minimal amount of diffraction data, overcoming the limitations posed by

Technology ID

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Category

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stringent data requirements in traditional phase retrieval methods.

If you are interested in commercial use of this software or access to the source code, please contact us.

Phase of Development

TRL: 6-7

The software has been shown to be effective in a research setting. A more user-friendly interface is being developed.

Desired Partnerships

This technology is now available for:

- License
- Sponsored research
- Co-development

Please contact our office to share your business' needs and learn more.

Researchers

- [Guichuan Yu, PhD](#) Characterization Facility Staff Scientist, Material Science Imaging Analyst and Consultant