xrd_simulator: Towards a PyTorch-based framework for FEM simulation of crystalline materials and diffraction experiments

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X-ray powder diffraction, particularly synchrotron-based techniques, is a powerful tool for characterizing crystalline materials. However, conventional diffraction analysis often relies on collapsing diffraction signals into one-dimensional profiles for fitting, which eliminates critical information related to crystallographic texture and local strain fields. This limitation hinders the extraction of spatially resolved microstructural details essential for advanced materials characterization [1].

To address this challenge, the open-source Python package *xrd_simulator* enables the simulation of monochromatic X-ray diffraction experiments directly from finite element method (FEM)-based meshes [2]. By incorporating crystal deformation and polarization effects, *xrd_simulator* facilitates realistic diffraction simulations of deformed microstructures obtained from prior FEM calculations. Figure 1 presents a schematic representation of the primary reference systems used in an xrd_simulator experiment.

This work focuses on an ongoing effort to accelerate diffraction simulations by reimplementing *xrd_simulator* in PyTorch with GPU acceleration. This transition significantly enhances computational efficiency, enabling simulations of FEM meshes containing up to one million tetrahedral elements within seconds, compared to the tens of hours required by CPU-based methods. Figure 2 illustrates the results of an *xrd_simulator* experiment and a potential application of the tool in testing 3D reconstruction techniques such as XRD-CT [3].

Beyond simulation, the framework is intended to be extended into a direct analysis tool by leveraging the PyTorch forward model for inverse problem-solving. By minimizing the difference between experimental and simulated diffraction patterns, this approach aims to refine microstructural parameters such as crystal orientations and phase distributions within the sample, providing a pathway toward automated, high-throughput diffraction data analysis [4].

References

[1] Frewein, M. P. K., et al., *Materials and Computation*, 11 (2024) 809-820.
[2] Henningsson, A., and S. A. Hall., *Journal of Applied Crystallography* 56.1 (2023) 282-292.
[3] Artioli, Gilberto, et al., *Analytical and Bioanalytical Chemistry*, 397 (2010) 2131-2136.
[4] Raventós, Marc, et al., *Scientific reports*, 9.1 (2019) 4798.

Figures

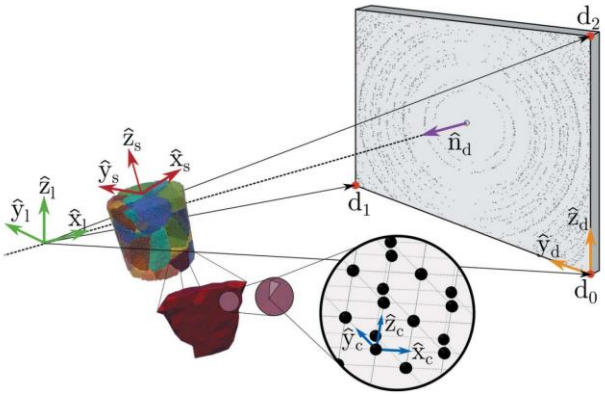

Figure 1. Scheme of all four reference systems used in *xrd_simulator*: Laboratory (green), detector (yellow), sample (red), crystal (blue). Adapted from [1] with permission.

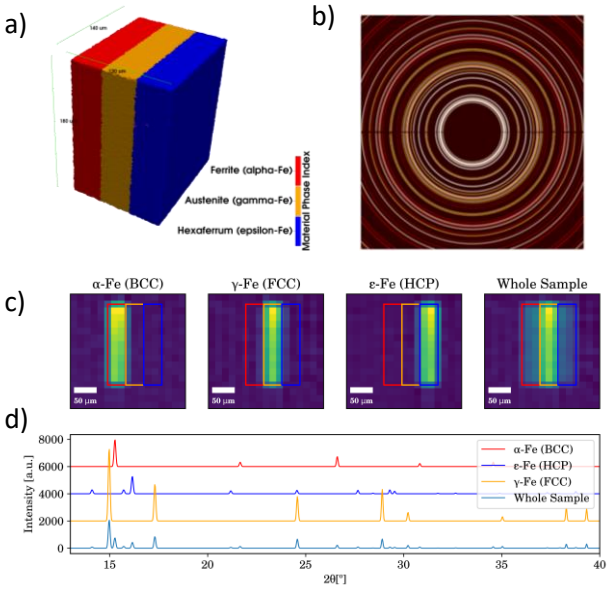

Figure 2. Example of an *xrd_simulator* experiment. a) Tetrahedral mesh composed of three iron allotropes (α, γ, and ε phases), visualized with ParaView. b) Diffraction resulting from the simulation under 23keV X-rays with a Pilatus6M detector. c) Slice of a Diffractive Contrast Tomography (DCT) reconstructed from simulated data.