XRD Enhanced-Characterization of Steel Through Computational Methods

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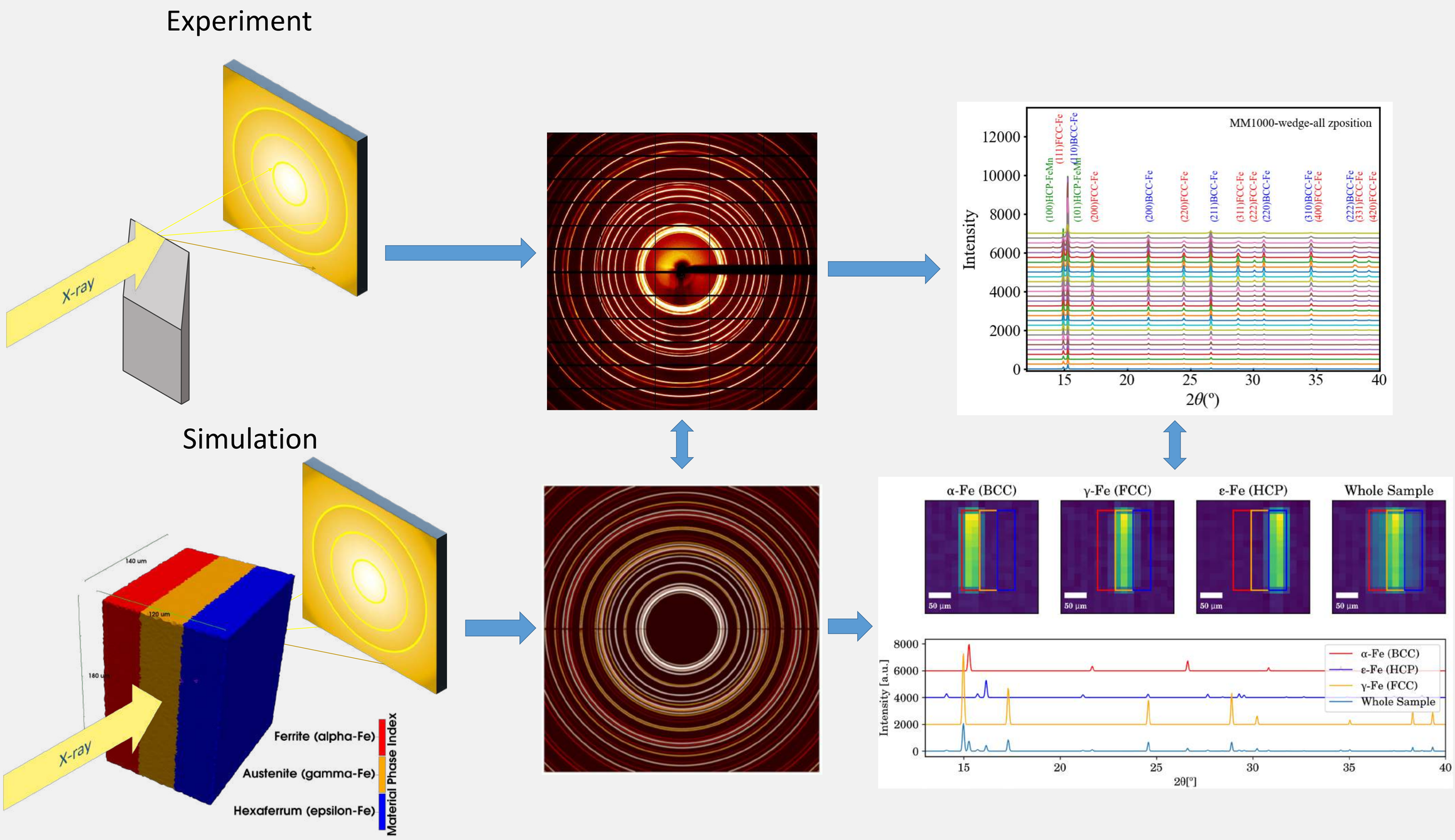
Introduction

Third-generation steels rely on the precise distribution of different crystallographic phases to provide higher tensile strength and ductility than previous steels. However, the relationship between the crystalline lattice and microstructure and the emergent superior mechanical properties is not yet completely understood. To better understand this relationship, we are working on an finite-element x-ray diffraction forward model (xrd_simulator) to assist on the 3D retrieval of the phase distribution, texture and lattice parameters.

Experimental results

The experimental data was acquired at the NOTOS beamline of the ALBA synchrotron with an energy of 23KeV and a Pilatus6M 2D area detector. The sample is a steel extracted from an 1.5mm thick industrial rolled sheet of medium-Mn alloy, well known for its transformation-induced-plasticity (TRIP) properties. The sample was scanned in the vertical direction with 10um steps to evaluate the difference in composition through the sample. The identified phases from the Rietveld-refinement in the bulk yielded a 40% retained Austenite (FCC), 59% of Ferrite (BCC) and a 1% of so-called Hexaferrum (HCP). These phases were then used as an input for the diffraction forward model.



Simulation results

An ‘ice-cream’ sample with dimensions 120x180x140 um^3 and an average grain size of $1um^3$ (~3 million grains) was created, having the three distinct phases clearly separated and each occupying one third of the sample’s volume. A raster scan with a 15um pitch and beam width was perform for the whole sample width over 180º with steps of 1º, than the diffraction patterns were reconstructed for the brightest peak of each phase to retrieve the shapes. The comparison between the experimental and simulated patterns are shown on the right, while the three phases have been identified based on their diffraction patterns.

Conclusions and further work

We have shown how our forward model can simulate the diffraction patterns of real samples, and how it is helping us develop advanced tomography reconstruction algorithms for powder diffraction experiments. Our next steps involve the development of an iterative approach for the refinement of the texture and lattice of real data, as well as the creation of large labeled diffraction datasets to train a convolutional neural network for quick phase classification of real data.

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