Adaptive design of experiments for X-ray magnetic circular dichroism spectroscopy

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X-ray microscopy such as transmission X-ray microscopy (TXM) or scanning transmission X-ray microscopy (STXM) is a modern experimental technique to observe magnetic domains with several ten-nm spatial resolutions. Observation of magnetic domains with these techniques is based on X-ray magnetic circular dichroism (XMCD), a phenomenon that the the absorption coefficient at absorption edges of ferromagnetic materials differs for right- or left-handed circularly polarized X-rays.

We demonstrated the quantitative analysis of magnetic domains with XMCD-STXM [1]. STXM experiment was performed at the Photon Factory, High Energy Accelerator Research Organization [2]. STXM images around Sm $M_{4,5}$ absorption edges of $SmCo_5$ permanent magnet for right- and left-handed circularly polarized X-rays, respectively. X-ray absorption and XMCD spectra were obtained for an area of 2.7×1.4 μm^2 by 100 nm steps. Spatial distributions of spin and orbital magnetic moments were obtained by applying magneto-optical sum rules to pixel-by-pixel XAS and XMCD spectra.

Although XMCD-STXM is a powerful tool to analyze magnetic domains, the experimental throughput is a problem. Typically, it takes several hours to measure one data set. Experimental parameters for STXM are the number of spatial points (scanning area and steps on sample), the number of energy points (energy range and steps), and the dwell time at each point. To improve the efficiency of STXM, we conceived a reduction of energy points using a machine learning technique, Gaussian process regression. We developed an adaptive design of experiments (ADoE) that combines measurement, analysis and machine learning. It is demonstrated that the ADoE for $Sm_{4,5}$ XMCD spectra reduces the energy points to 20% of a conventional experimental design to obtain magnetic moments with satisfactory accuracy [3].

<u>Reference</u>

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3) T. Ueno, H. Hino, A. Hashimoto, Y. Takeichi, M. Sawada, and K. Ono, "Adaptive design of an X-ray magnetic circular dichroism spectroscopy experiment with Gaussian process modelling", npj Computational Materials **4**, 4 (2018).