High-throughput experiment of X-ray magnetic circular dichroism spectroscopy with machine learning

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X-ray magnetic circular dichroism (XMCD) spectroscopy is a powerful experimental technique to directly probe electronic states and magnetic moments of magnetic materials. Recently, by combining XMCD with X-ray microscopy, it has been able to visualize magnetic domains and conduct spectroscopy experiment in several ten nanometers scale [1]. This method is useful because a specimen with the size of only several square micrometers can be measured. Therefore, one does not need to prepare large single crystal samples. The method is also useful for heterogeneous systems such as microstructures in permanent magnet materials. However, one must scan large area (several 10 μm^2) with fine steps for an application to heterogeneous systems. In the present experimental system [2], typical measurement time is about 2 hours for an area of ~10 μm^2 with 200 energy points. To reduce the measurement time, we examined reduction of the total measurement energy points with a machine learning approach. Gaussian process (GP) modeling [3] was applied to predict an XMCD spectrum from an experimental spectrum with limited energy points.

XMCD spectroscopy experiment was performed at the BL-13A of the Photon Factory, KEK, Japan. Sm $M_{4,5}$ X-ray absorption spectrum (XAS) and XMCD spectrum were measured for an $SmCo_5$ specimen. X-ray energy was scanned around the Sm $M_{4,5}$ edges with a total energy points of 216. GP modeling was performed to predict XAS and XMCD spectra by following way. First, initial 30 data points are sampled with equal separation along the energy axis. GP modeling predicts a spectrum with input of experimental data points. Next sampling point is determined by several methods. After the sampling, a spectrum is predicted again. Orbital and spin magnetic moments, and their ratio were evaluated for each prediction by using magneto-optical sum rules. Measurement is stopped with the convergence of magnetic moments.

We tried three methods to determine next sampling point; (1) energy point with maximum variance of the predicted spectrum, (2) random sampling, and (3) random sampling weighted by maximum variance. Orbital magnetic moment evaluated from predicted spectra converges to reference value in total data points of about 40 points by sampling with maximum variance. Other sampling methods need more data points to converge to reference value. Maximum variance sampling was revealed to be better than other sampling methods in GP modeling of XAS and XMCD spectra. Therefore, total measurement data points are reduced to 1/5 by GP modeling as compared to conventional method [4].

In conclusion, we demonstrated the reduction of the total measurement energy points of XMCD spectra with a machine learning approach. This method enhances efficiency of XMCD spectroscopy experiment.

Reference

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