Extraction of Physical Parameters from X-ray Spectromicroscopy Data Using Machine Learning

Yuta Suzuki[1,4], Hideitsu Hino[2], Tetsuro Ueno[3], Yasuo Takeichi[4], Masato Kotsugi[1], Kanta Ono[4,*]

1. Tokyo University of Science, Tokyo, Japan., 2. The Institute of Statistical Mathematics, Tokyo, Japan.,
3. National Institutes for Quantum and Radiological Science and Technology, Hyogo, Japan., 4. High Energy Accelerator Research Organization, Ibaraki, Japan.

Introduction

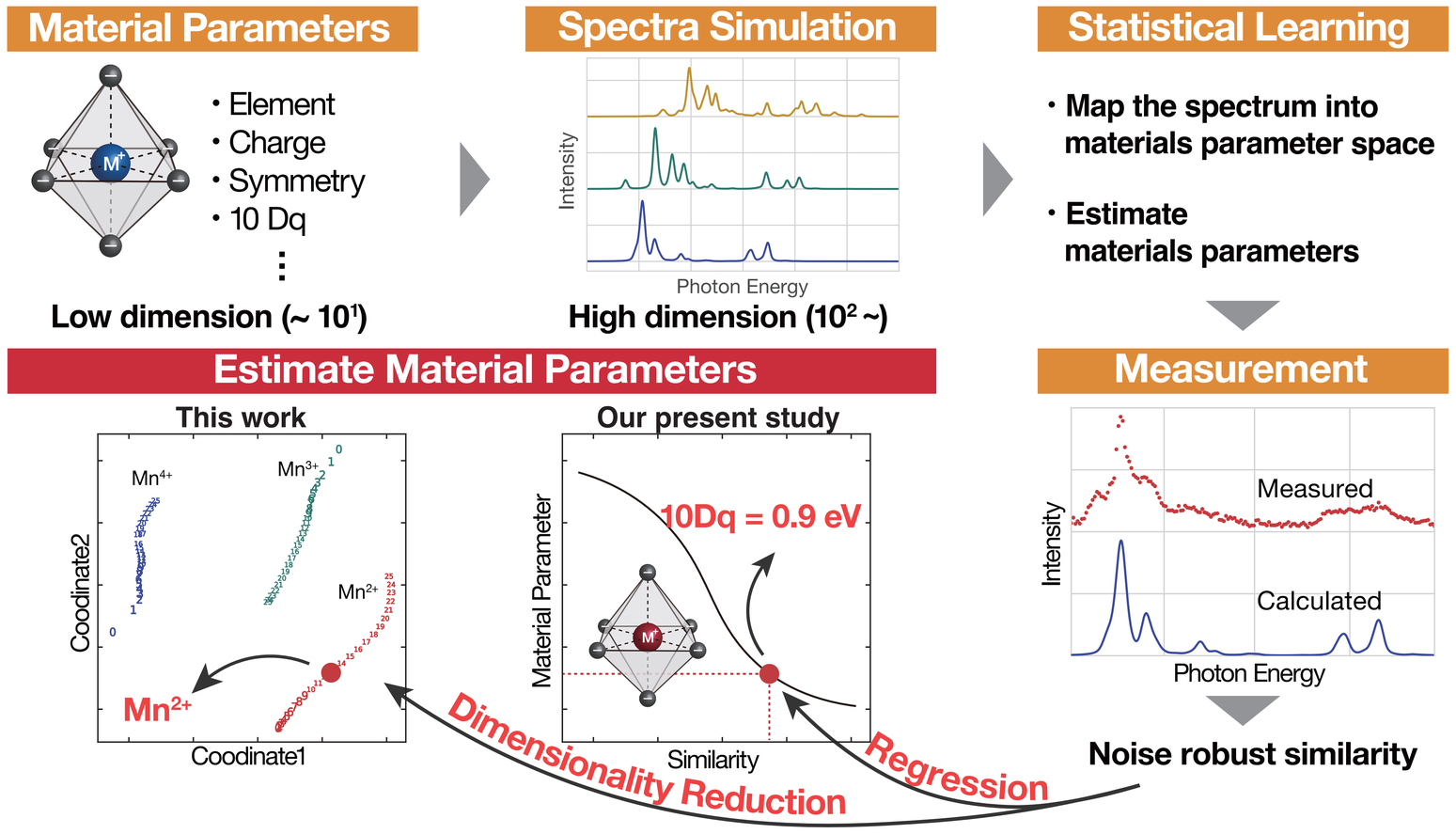
■ **Materials Informatics (MI)**
Acceleration of materials discovery and obtaining knowledge by statistical learning of materials data.

■ **Key of accelerate materials development**
1. Combinatorial systhesys of materials
2. High-throughput experiments
3. On-the-fly data analysis

■ **X-ray Absorption Spectroscopy (XAS)** is a typical technique for materials characterization. But, **the coventional analysis is achieved by hand**, it could be a **bottleneck** of research workflow.

■ **XAS data has hundreds of datapoint.**
It will make a difficulty in comparison of XAS spectra. **Dimensionality reduction, such as Manifold Learning** technique should help us to handle such *"high-dimensional"* data**.**

Our strategy



Objectives

■ Easy understandable visualisation of many spectra as with dimensionality reduction.

■ Based on the similarity of spectra, the material parameter by dimensionality reduction is estimated.

■ We try to determine the charge and crystal field parameter from 2p XAS of Mn compownds.

■ We are aiming to accelererate materials discovery by integtare the high-throughput experiments and on-the-fly data analysis.

Manifold Learning

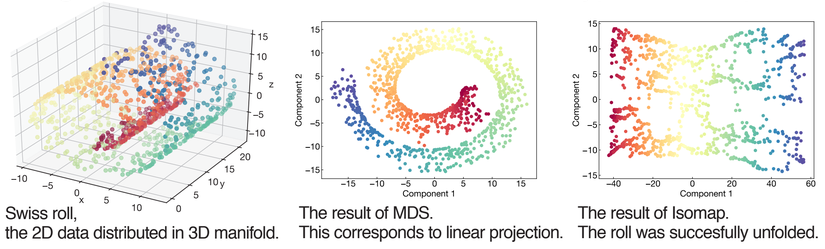
■ **Projection of high-dimensional data into few-dimensional feature space retaining the relevant information.**

■ **Manifold hypothesis**
Most of data are distributed on a relatively lower-dimensional manifold, even though it is apparently high-dimensional data. Swiss roll is the typical example.

■ **Popular algorithms**
Multi-dimensional-scaling (MDS):
Find a lower-dimensional representation y_i that keeps the distance in the original space $d_0(x_i - x_j)$. It can be solved as an eigenvalue problem.

$$\min\{y_i\} \ (d_0(x_i - x_j) - ||y_i - y_j||_2)^2$$

Isomap:
Nonlinearly expansion of MDS. K-neighborhood graph of each data point in original space are used as distance instead of $d_0(x_i - x_j)$.



Swiss roll, the 2D data distributed in 3D manifold.

The result of MDS. This corresponds to linear projection.

The result of Isomap. The roll was succesfully unfolded.

Results and Discussion

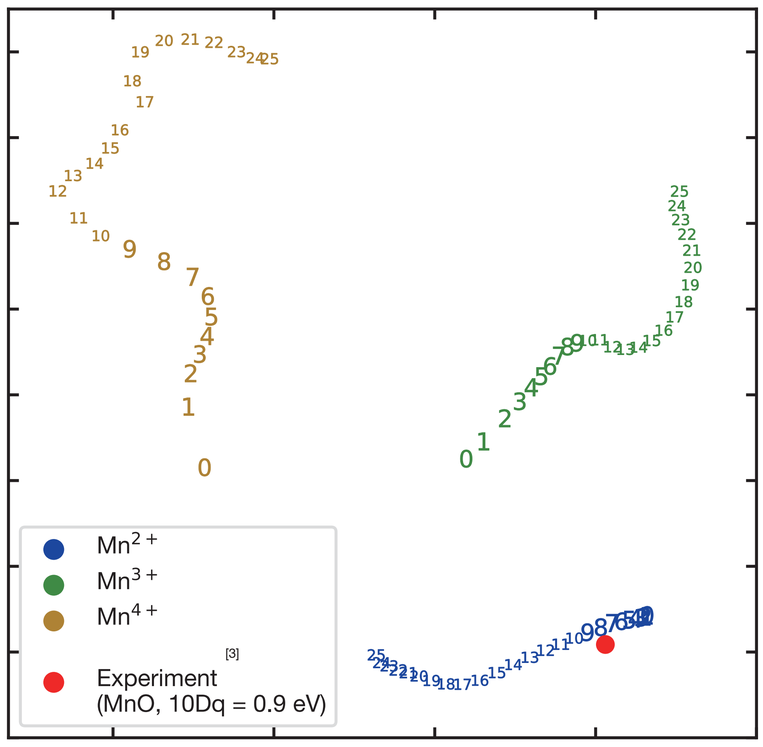


Fig.1 The result of dimensionality reduction of Mn 2p XAS spectra using MDS. This is the visualization of similarity of each XAS spectrum. The numbers in this figure correspond to 10Dq (eV) multiplied by 10.

Fig.2 The comparison of measured XAS spectrum and calculated XAS spectrum. The calculated XAS corresponds to the estimated parameter. The estimated parameters (charge and crystal field parameter 10Dq) was in accord with determined by human professional.

■ Dimensionality reduction has been carried out with MDS, calculated 79 XAS spectra were represented in two-dimension in Fig.1.

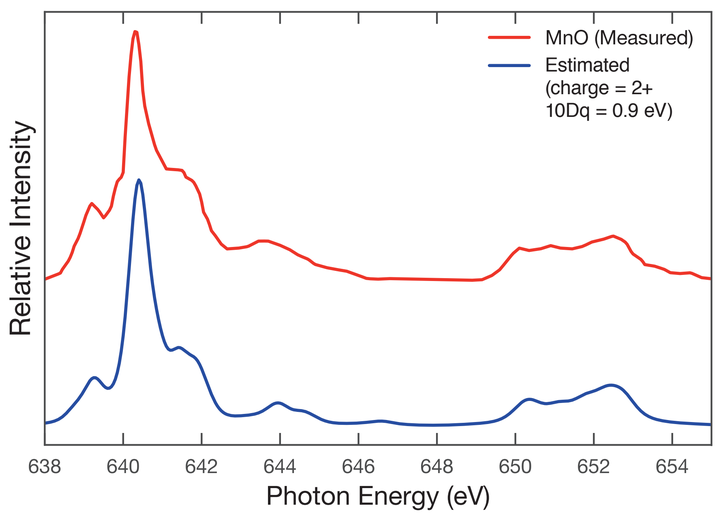
■ **The distance of each XAS spectra in MDS visualization is corresponding to their material parameters (Fig.1).**

■ **Experiment XAS spectrum is located at appropriate position corresponded to its charge and 10Dq.**
The same result was obtained with Isomap.

■ This result suggest that visualization of similarity of spectra with dimensionality reduction helps us to understand complex materials property.

■ This methodology can be applied to any kind of data, such as an image or 3D data.

■ The computation time was with in a minute for laptop PC. It can be achieved on-the-fly with a high-throughput measurement.



Summary

■ **We applied dimensionality reduction to XAS spectra, and demonstrated that the material parameters (i.e., charge, 10Dq) can be determined from similarity of spectra.**

■ **This methodology helps us to obtain the knowledge from complex materials data. That can be applied to other kind of data, such as 2D or 3D image.**

■ **We will study this method on more sophisticated first-principle XAS simulation with 600,000 materials database.**

Methods

■ Mn 2p XAS dataset for comparison was prepared by simulation with CTM4XAS [1] [2]. The charge and 10Dq were set to 2+, 3+, 4+, 0-2.5 eV, respectively.
The crystal field symmetry was set to octahedral.

■ Experimentally measured XAS of MnO was used for validation. The parameter was determined by human as 10Dq = 0.9 eV, octahedral symmetry[3].

Resources

■ Please visit our GitHub and website for download this poster and contact us.

github.com/resnant/XRM2018

resnant.github.io

1. de Groot, F. M. F., Fuggle, J. C., Thole, B. T. & Sawatzky, G. A. Phys. Rev. B 42, 5459–5468 (1990).
2. Stavitski, E. & de Groot, F. M. F. Micron 41, 687–694 (2010).
3. de Groot, F. & Kotani, A. Core Level Spectroscopy of Solids. (CRC Press, 2008).