

Utilization of informatics and database for x-ray analyses

Keywords: Model-free analysis, Objective analysis, Rapid analysis, Informatics

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Background

- Visualization and quantification of x-ray analysis are not easy
- The x-ray wavelength comparable to atomic size requires assumptions and models based on atomic physics
- Even after long time analysis, the result frequently shows a lack of objectivity
- Recent computer progress is compatible with informatics using big data in database

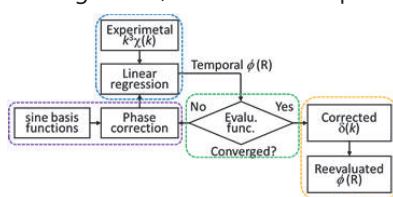
Aim

- Development of model-free analysis for x-ray absorption fine structure (XAFS)
- Proposal to rapid and objective x-ray diffraction (XRD) using big data in databases
- Robust analysis to deduce essential features from fluctuated data
- Informatics for measurements using statistics and databases

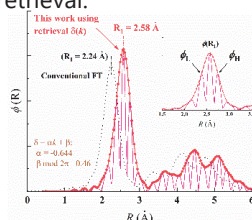
Advanced Research Topics

Informatics in x-ray absorption fine structure (XAFS):

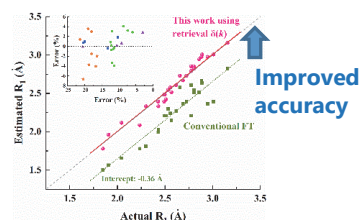
We do NOT use any structural assumption which is mandatory for conventional XAFS analyses. Under the severe limitation, we successfully determined atomic local structure precisely using a new algorithm, Self-consistent phase retrieval.



Algorithm for self-consistent phase retrieval



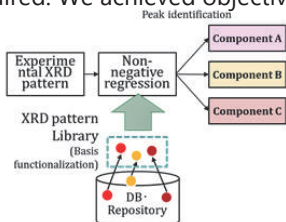
Radial function distribution obtained with the model-free analysis



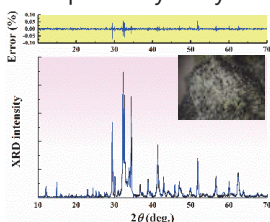
Predicted- vs. actual- bond lengths.

Informatics in x-ray diffraction (XRD):

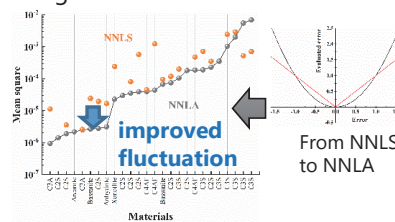
In conventional XRD analysis for mixed crystals, intuition, experience, and long analysis time are required. We achieved objective and rapid analysis by using storage data in database.



Algorithm for non-negative linear regression analysis



Objective and rapid analysis of mixture including minor crystals



Robust analysis to solve data fluctuation

Publications

- M. Ishii, OYO BUTURI, Vol. 85, p.p. 223-227 (2016).
- M. Ishii, The 17th International Conference on X-ray Absorption Fine Structure, 22-27 July 2018, Kraków, Poland.

Applied area and future prospects

- Local structure analysis of unknown materials
- Objective & rapid analysis of unknown materials
- Application to the other analytical techniques
- Combination of instruments and NIMS database: Realization of database combining with laboratories

Issues for technology transfer

- Brush up of usability of software. Preparation of user friendly interface
- Development of rapid search technique and cleansing of old data in crystal database
- Collaboration with hardware and software companies.