Integration of X-ray measurement and analysis and data science

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Advanced characterization using quantum beams is used in many natural science fields, from condensed matter physics to life sciences, and has become an indispensable tool in scientific research. However, there are problems in measurement and analysis using quantum beams, such as the effective use of limited beamtime in synchrotron and neutron facilities. Solving these problems is necessary for further progress in scientific research. We are promoting efficient, automated, and autonomous X-ray measurement and analysis using data science to solve these problems.

These research fields are called measurement informatics and are being developed through advances in data science, as well as recent advances in computational resources, and are expected to:

1. enable measurements that previously required synchrotron radiation and neutron facilities to be made with the laboratory source.
2. enable the optimization and improvement of the efficiency of X-ray measurement and analysis.
3. enable observation of previously unobservable phenomena through data sciences.

The research and development of measurement informatics related to quantum beams will make it possible to realize advanced measurements by data science without significant hardware upgrades. The key to the next generation of quantum beam measurement will be using data science to achieve advanced measurements. Autonomous measurement and data analysis will be essential for the next generation of quantum beam measurement.

We will introduce the following topics by integrating x-ray measurement, analysis, and data science.

1) Automatic design of an optimal x-ray experiment [1].
2) When should x-ray experiments stop [2]?
3) Speed up x-ray measurements with data science [3]?
4) Automating x-ray data analysis: crystallography and spectroscopy [4,5,6].
5) Decision-making in x-ray data analysis [7].
6) Cartography of inorganic materials using crystal structure [8].