Research Highlights

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Pair Distribution Function Analysis Offers New Insights into the Structure and Identity of Nanomaterials

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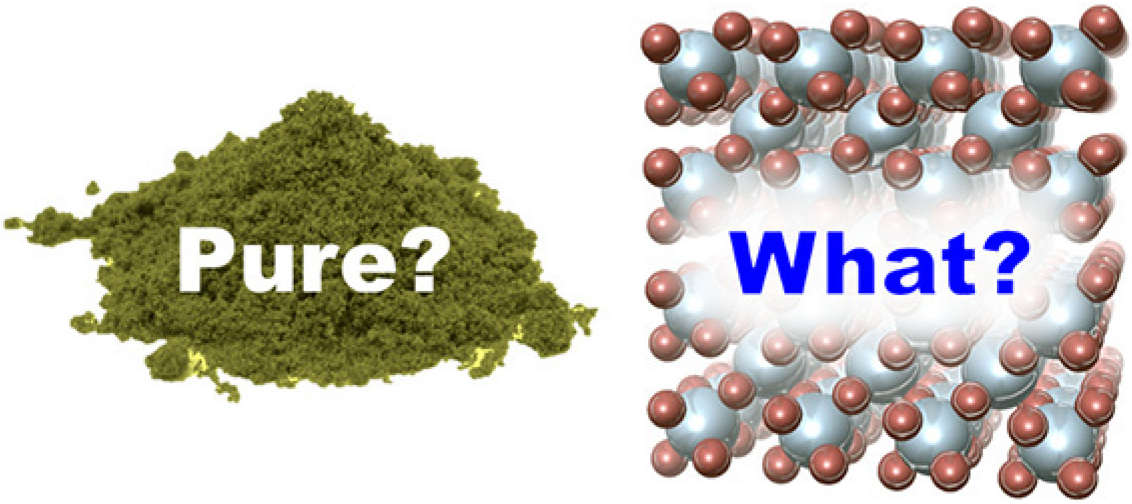

Figure: There is room for further research in identity and structures of nanomaterials, though these two are investigated naturally in conventional material research.

Satoshi Tominaka is a scientist at International Center for Materials Nanoarchitectonics (MANA) and internationally acknowledged for research on the applications of pair distribution functions (PDF) for the analysis of nanomaterials. “The structural analysis of nanomaterials is critical for understanding their basic properties from a fundamentals scientific perspective and for applications,” says Tominaka. “My approach to attain a deeper understanding of the purity and structural phases of nanomaterials is based on using PDFs. They offer powerful insights into the structural properties of nanomaterials and overcoming the limitations of X-ray diffraction analysis at the atomic scale.”

Although PDF based analysis has a long history in the analysis of amorphous materials, and more recently the analysis of crystalline structures with third generation synchrotron radiations sources, PDF analysis of nanomaterials is still in its infancy.

Concisely, PDF analysis yields detailed information about the physical relationships between distances of atom pairs—for example Au-Au in Au crystals—and the density of the pairs in the crystals. This information cannot be obtained by X-ray diffractometry (XRD) that only produce broad diffraction peaks because it is not suitable for extremely small crystals.

Tominaka is working with colleagues in Japan and Europe on the development of PDF analysis for nanomaterials research on two main topics. First, the analysis of the purity of nanomaterials. “In certain materials, our PDF analysis shows large concentrations of phases of low symmetry or smaller particle sizes,” says Tominaka. “The existence of mixtures of phases in nanomaterials is associated with the formation of nanomaterials under kinetically controlled conditions.”

Specific reports by Tominaka on this topic include the properties of reduced titanium oxide nanoparticles [1] and the observation of unique electrical conduction of mesoscopic cobalt phosphide—a mesoporous semimetallic conductor—due to the coexistence of Co2P phases found by PDF analysis [2].

The other area of research is exploiting the power of PDF analysis for identifying unknown structures have been uncovered by using X-ray PDFs. “Certain materials are only stable as nanosized structures,” says Tominaka. “Such materials cannot be identified based on data from bulk materials.”

Research on materials discovery using PDF includes new insights into heterojunctions made of inert materials for electrocatalysts where gold was covered with a two-dimensional corrugated carbon−nitrogen structure [3]; the determination of the structure of two-dimensional boron hydride sheets which show potential for hydrogen storage [4]; and the discovery of disordered catalytic activity of titanate phase with TiO6 octahedral connectivity [5].

“My research is ongoing and still in its youth,” says Tominaka. “There are still many issues to address including the development of algorisms for nanomaterials analysis.”

Reference

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Ken Sakaushi,et al.
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