

MINUTES
X-RAY METHODS SUBCOMMITTEE
2011 March Meeting of the ICDD
Scott Misture, interim Chair

1. Approved minutes from last meeting - unanimous

2. Old Business: Reports from the Task Groups:

2-D diffraction (D. Balzar): *No report*

3. New Business

Discussion of topics relevant to the PDF-4 and PD3

A. Extracting reference patterns from Rietveld refinements for multiphase specimens.

Questions:

- Reporting of full patterns from multi-phase mixtures
- Editorial issues in quality marks, given that overall sample chemistry is not representative of the phase of interest. Can this be addressed by use of microprobe analysis or by reliance on knowledge of additional phases present?

Discussion centered on whether Rietveld analyses are acceptable for patterns for mixtures extracted from the literature, the LPF, CSD, etc. However, the group agreed that the Grant-in-Aid program would continue to insist upon data only from single-phase samples (where single-phase is considered as having less than approximately 5% impurity).

B. PD3 full pattern database and total scattering analysis.

Questions:

Linking experimental data with structural models from PDF analysis or other physical data (SAS)

Discussion did not lead to any recommendations or suggestions for further investigation.

Although polymers are generally handled well by the community, what about inorganic nanomaterials? Oxide and metallic glasses? Do these materials require a different approach than polymers?

Nanomaterials, glasses, and other materials that are well described by PDF analysis should be handled in a manner that mirrors the ICDD approach to polymers: focus on industrially-relevant materials and store full patterns where possible.

Business from the floor:

- *M. Leoni suggested that we should consider materials with 5-fold symmetry that are not modulated structures (i.e., those with icosohedral symmetry).*
- *J. Kaduk suggested that the Subcommittee consider developing guidelines for accurate measurements. Additional discussion then led to the idea of having basic tutorials on the ICDD website for various kinds of analysis – polymers, amorphous/nano, and of course traditional powder XRD. The idea is to enable technicians who have limited XRD background to get a quick introduction to the techniques. For example, a tutorial might contain 20 slides. Misture, as the SC chair, will e-mail the SC list and solicit volunteers.*

Respectfully submitted by S. Misture, April 21, 2011.