ICDD Workshop
New Generation of XRD Databases:
Capabilities and Applications, Problem-Solving Techniques

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Session I: Editorial Efforts, Standardization, Classification (Tim Fawcett)

Purpose: The Powder Diffraction File contains data that are extensively reviewed and statistically analyzed. The new organization of the database allows every data field to be searched, sorted and custom organized to allow scientists full access. The author's original data is ***always changed*** by the ICDD's standardization and quality review processes and many materials properties are added based on calculation or additional bibliographic review. Teams of volunteer members and interested scientists, who are field experts, peer review the data and organize the data based on material and structural classifications. The purpose of the data changes, organizations and additions is to facilitate a user's ability to rapidly search and identify materials using the database. This workshop will explain the classifications, review procedures and the scientific basis for the property calculations to enable users to more effectively use the power of the database.

Session II: Novel new features in PDF-4+, a new user-interface, problem-solving, data-mining (J. Faber)

Purpose: The goal of many of the structural and material classifications used in the Powder Diffraction File is to facilitate the rapid identification of materials from an experimental diffraction pattern. Frequently material identification is just the first step in solving a problem. The Powder Diffraction File contains many problem solving tools that help in understanding material and structural chemistry. The PDF contains material knowledge of field experts, provided by members and editors. Novices can use this expertise, or experts in one field can apply the expertise to other fields. In this session, we explore the expertise built into the database and how this can be used to solve problems. The comprehensive nature of the database can now be used to study large groups of materials expanding our material knowledge

Session III: Problem Solving (Jim Kaduk)

Purpose: In this session, we want to ask the question: What do you do when the entry you are looking for is not apparently in the database? What if the structural data is incomplete or absent? There are many paths that can be followed to solve a problem and thus lead to materials characterization. This session will lead us along several of these paths.

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Session I: Editorial Efforts, Standardization, Classification

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Session I. Outline

I. Data Entry and Standardization

- Sources of Data and Conversion
- Entry Checks
  NBS Aids, other checks, warnings and errors
  Evolution to RDB and SQL Aids
- Formula and Nomenclature
- Diffraction Patterns
- Cell checks

II. Calculated Parameters

- Diffraction Patterns
- Densities
- Molecular Weight
- I/Ic

III. Quality Measures and Evaluations

- Quality Checks and Review
- Quality Figures of Merit and Definitions
  - Delta two theta
  - Densities – Observed, Calculated
  - Electron Density Calculations
  - Smith-Snyder Figure of Merit
  - R-Factors
  - Quality Marks

IV. Editorial Classifications

- Prototyping – New prototyping methods for all inorganics

- Mineral Classification System – Groups, Supergroups, Subgroups
- Zeolite Classification System
- Metals and Alloys – Pearson Symbols
- Atomic Environments
- ANX Formulation
- Peer reviewed subfiles
- Material classification subfiles

Session II: Novel new features in PDF-4+, a new user-interface, problem-solving, data-mining

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Session II. Outline

V. Searches

- Display Tools
- Basics of pattern simulations
- Electron, neutron or x-ray diffraction
- Simulating sample characteristics
- Simulated instrument profiles

VI. Problem solving examples

VII. Search and Identification Tools

- Preferences – Sort and Display
- Creating custom files within the PDF
- Using Display table and forms

VIII. Search Methods

- Hanawalt
- Fink
- Long 8
- Future Directions
- Identification and Match Evaluation
    - Search Window
    - Goodness of Merit
    - Digital Displays – visual matching
    - Sample and Instrument Simulations
    - Reference Intensity Ratio

IX. Prototype simulations

- Using electron, neutron or synchrotron data, EBSD data, TEM
- Studying semicrystalline and nanomaterials

X. Data Mining

- Exploring well characterized systems
- Polymorphism
- Phase Changes
- Non-ambient studies
- Solid solution studies

XI. Import/Export for advanced analyses

- Reference Intensity Ratio
- Pattern Fitting
- Rietveld Refinement

Session III: Problem Solving

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Session III. Outline

XII. When the initial search/match does not yield the complete answer
chemical unreasonableness/reasonableness/lattice similarity - bag filter deposit from refinery

- one strong peak + mineral - filling station filter deposit
- polymer subfile - PET wall deposit
- single peaks + “just” - vanadium phosphate catalyst
- spectroscopy + XRD + chemistry - valve deposit from piston aviation engine
- single peaks + mineral - anaerobic waste treatment granules
- long line + organic - amoxicillin
- when experimental pattern helps figure out what’s wrong with calculated patterns - Mo_5O_{14} in an over-calcined catalyst
- “Just” + Rietveld difference plot
- multivitamin
- commercial stain remover/oxygen bleach

XIII. PDF-4+ plus other databases

- separation + lattice match + chemical similarity - $[Fe(H_2O)_6](CF_3SO_3)_2$
- ANX + primary literature - $Al_4H_2(SO_4)_7(H_2O)_{24}$
- when the authors got their chemistry wrong - $(NH_4)Fe(CO_3)(OH)_2$
- smell + spectroscopy + chemical similarity - $(NH_4)Fe_2S_3$
- lattice match + chemistry - “$Fe_2F_5(H_2O)_7$”