Ceramics Subcommittee Meeting Minutes
March 17, 2010
ICDD Headquarters
Peter Zavalij, Chairman

Call to Order
Peter Zavalij called the meeting to order.
Appointment of Minutes Secretary
Amy Gindhart appointed minute's secretary.
Approval of Minutes from March 2009 Meeting
March 2009 meeting minutes approved.
Motion moved by Peter Zavalij
Seconded by Miguel Delgado
6 For
0 Opposed
0 Abstained

Board of Directors' Liaison Report

S. Misture gave the Liaison's Report in lieu of E. Antipov. The first Motion was passed to allocate $3,000 for the group to meet at the next Annual Meeting in 2010 to work on property subfiles. The second motion was passed as well with a contract for the review of 30 hydrogen storage physical properties in place. The last motion passed was for a revised definition of the Bioceramics subfile and will be implemented in the 2010 PDF products with the help file update showing up in the 2011 products.

Old Business

Development of Subfiles/Minifiles

<u>To initiate a property minifile, it should have</u>:
- important properties (or class of compounds);
- exact definition and preferably general selection criteria for editorial;
- assigned expert(s), task group, editorial staff, etc.

<u>To add a minifile in PDF release</u>:
- it should be populated;
- it should have comments/property data for PRIMARY entry with links to alternative entries, structure (if known), etc.

<u>Population of the minifile</u> :
- review/organize existing entries;
- annually review new database entries.

<u>Scheme of adding new entries</u>:
1) mark candidates from list of entries (full list or filtered by the editorial, if general selection criteria exists);
2) review marked entries using full data (provided on request);
3) add property/comments/links in the database (editorial).

Superconductors (*E. Antipov*)
Critical temperatures (T_c) were added for SCM subfile in sets 1-51.
Set 60 was reviewed and 4 entries were marked as SCM.
T_c will be added for remaining sets 52 and up.
Add new, heavily studied HTSC materials such as arsenides and similar compounds, for example $Fe_{1+x}Te$ and *RF*e_2As_2.

New High T_c materials (*E. Antipov presented*)
Many new high T_c materials were added. Two of the materials presented were:
Sr2ScO3FeP, T_c=17K
Sr2VO3FeAs T_c=32K
Several other materials were listed to show the increased need for the subfile.

Ideas introduced to help with populating the subfile:
E. Antipov- Possibly have someone in the Grant-in-Aid Program take on new materials to help with populating the subfile.
T. Fawcett- Possibility of requesting faster movement of specific materials into the database from ICSD or LPF is available in the contract. Editorial staff can look into implementing this clause to help with populating the subfile. They need a specific list of compounds and author names to give to ICSD or LPF.

Thermoelectric materials (*W. Wong-Ng*)
Reviewed set 60 and marked 6 new patterns as TEM.
Work on the property entries is in progress and 30 new property sheets are being added from 2009.

Winnie Wong-Ng Presentation
W. Wong-Ng presented some of her work done with her colleagues on thermoelectric materials. She explained that there is a desperate need to develop alternative energy methods over the next 20 years. She would like to have Figures of Merit (ZT), Seebeck Effect, and Peltier Effect values added to the database. She presented several materials including $Ba_5CaLa_2Co_4O_{15}$ and $Ba_6Sm_2Co_4O_{15}$, among many others that have been prepared and processed within the task group and submitted to the database. Professor C. Uher from The University of Michigan went through set 60 and picked up several patterns to be added to the subfile as well. Joshua Martin went through the database and found 30 files where he thoroughly updated thermo-properties as well as the references where that information came from. She plans on continuing to have Joshua Martin add prototypes and properties to an additional 30-50 files a year.

Semiconductors (*A. Davydov/M. Delgado*)
Reviewed set 60 and 122 patterns were marked as SEM.
They will continue to review all existing entries and work on adding properties.

Bioceramics (*J. Reid*)
Reviewed set 60 and marked 12 patterns as BIO.
A review of past entries should be completed by end of year according to Joel Reid.

Intermetallic Compounds for Hydrogen Storage (*I. Zavaliy*)
This subfile is currently under development for addition to the Powder Diffraction File.
I. Zavaliy has submitted property descriptions for 30 systems and more are coming soon.
Examples of various Metal-Hydride Electrodes were shown including $La_xMg_{3-x}Ni_9H_y$ and $YNi_{2.67}Mn_{0.33}H_{3.9}$.

Ionic Conductors (*V.B. Nalbandyan, G. Subba Rao*)
ION is one of the most complete subfiles for ceramics.
Set 60 was reviewed and 22 entries were marked as ION.
The subfile is mainly complete.

Ferroelectric (*S. Ivanov/V.B. Nalbandyan*)
Reviewed set 60 and marked 26 new patterns as FER.
Property entries are still needed for this subfile.

Battery materials
Reviewed set 60 and there were no new patterns.
The properties for a few non-essential materials are missing (Nb_2O_5, $CuFeS_2$).
BAT subfile is complete and has 35 property entries.

Existing subfiles
Perovskites (PER) - contains numerous entries but still has to be sorted out.
Giant Magneto Resistant (GMR) - is abandoned.

Proposed subfiles
Piezoelectrics
Multiferroics
Superconducting Materials – update with new class of compounds

These possible subfiles need help from people in the subcommittee to further the processing of the materials.

Cements (*L. Cook presented*)

Proposed organization of cement phase's subfile:

- Cement Phases (primary flag) CEM
- Type of Cement in Which Phase Occurs (second level flag)
    - Portland PLD
    - Calcium Aluminate CLT
    - Slag, Pozzolana, Flyash, or Silica Fume–Containing SLG
    - Halide, Sulfate, Phosphate, or Borate–Modified, or–Based MOD
    - Unspecified UNS
- Cement Component in Which Phase Occurs (third level flag)
    - Raw Material RAW
    - Clinker CKR

- Addition or Admixture ADD
- Setting Product SET
- Corrosion Product COR
- Unspecified UNS

Growth of Cements Subfile (total in subfile by year):
2005 414
2006 418
2007 952
2008 1169
2009 1183
2010 1224
Continued growth of the subfile is happening which is shown by above numbers.

What physical properties should be considered for the cements?
Thermodynamic properties
Transport properties
Magnetic properties
Electrical/electronic properties
Optical properties
Mechanical properties
Acoustic properties

Activity of Ceramic Task Group
Task group meeting was Mar. 15, 2010.
The task group reviewed set 60.

Property data sheets:
SCM – needed T_c for sets 52 & up and to add new compounds
TEM – adding 30 properties, more are coming
CEM – is being revised by L. Cook
IHS, MHE – added 30 properties, more are coming

Properties included in 2010 release:
HIS/MHE, TEM – Included
ION, BAT – appear to still be missing some.

A comprehensive list of properties was prepared and presented by L. Cook.

Properties in DDView – Look into having a separate tab added for all properties including main numerical value, references and/or links to properties sheets

Motion 1:
The Ceramic Subcommittee recommends to the Technical Committee that
a sum of up to $3,000 be allocated for meeting of Ceramics task group members during

2011 ICDD Annual meeting /2010 Denver X-ray Conference to work on property subfiles with report following activity.

Moved by: Peter Zavalij
Seconded by: Peter Wallace
For: 8
Opposed: 0
Abstain: 0
Motion passed.

Motion 2: The Ceramics Subcommittee recommends to the Technical Committee that all property sheets generated be included in the next release.

Moved by: Peter Zavalij
Seconded by: John Faber
For: 8
Opposed: 0
Abstain: 0
Motion passed

Motion 3: The Ceramics Subcommittee recommends to the Technical Committee that all property present in the database entry to be listed in and accessible from a separate "property" tab.

Moved by: Peter Zavalij
Seconded by: Evgeny Antipov
For: 7
Opposed: 1
Abstain: 0
Motion passed

Motion 4: The Ceramic Subcommittee recommends to the Technical Committee that HQ modify SCM selection criteria to include new SCM and accelerate inclusion of these materials in the database providing the Ceramic Task Group will generate the list of such compounds.

Moved by: Peter Zavalij
Seconded by: Winnie Wong-Ng
For: 7
Opposed: 0
Abstain: 0
Motion passed

Adjournment