

Ceramics Subcommittee
March 16, 2011
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 2010 Meeting

March 2010 meeting minutes were approved.

Moved: Scott Misture

Second: Tim Fawcett

4 For

0 Opposed

0 Abstained

Motion passed.

Board of Directors' Liaison Report

W. Wong-Ng gave the Liaison Report.

The first Motion was passed to allocate \$3,000 for the group to meet at the next Annual meeting in 2011 to work on property subfiles.

The second motion response from the Science Department at headquarters was that the property tables were included for display in the 2010 product but are not searchable. The property sheets will be searchable in the 2011 product.

The third motion response from the Science Department at headquarters was that an icon exists at the top of each entry for viewing property sheets. This icon becomes active for any entry which contains a property sheet.

The last motion response from the Executive Director and the Publication Department was that the motion was discussed with MPDS, who agreed to accelerate processing and delivered the special request for Superconducting Materials and their properties for specific compounds. All entries (~20) have been processed and will appear in the 2011 Release.

Old Business

Development of Subfiles

To initiate a property mini-file: it should have important properties or be an important class of compounds, have an exact definition and an assigned expert, task group, etc. available to acquire the information.

To add a mini-file in the PDF: it should be populated and it should have comments/property data for the specific entries.

Population of the mini-file: the patterns need to be reviewed and organized annually for new database entries.

Scheme of adding new entries: The patterns can be marked from a list of entries and reviewed so that property/comments and links can be added to the database.

Cements

There were 6 entries that were marked as CEM in the new set.

There are 1344 entries in the 2011 release.

Vanessa Peterson mentioned that the subfile is of use for companies that manufacture cement because they need a database for QPA for phase monitoring of their products. She proposed that we separate main cement materials and exclude hydrated cements and other related compounds in separate subclasses. She also mentioned that good quality data from main cements are very important, but at the same time their patterns are complex and that it requires time and effort to select data sets of good quality (standards).

Vanessa Peterson has volunteered to create a definition for the Cements subfile that can be voted on in a future meeting of the subcommittee. She has also been suggested as a consulting editor for the subfile to help with properties and to further oversee the population and contents.

Superconductors

There were four new SCM patterns that were reviewed for Set 61.

20 new HTSC materials were flagged this year.

160 High T_c entries are in the 2011 release.

The editorial staff at headquarters needs a new list of compounds by September 1st for the HTSC materials flag. Evgeny Antipov believes that 7009 patterns in SCM is too large to be useful for a search. He wants only those materials that have been fully characterized and expressed in the database to be included in the subfile to help thin out the subfile.

Battery Materials

The BAT subfile contains property sheets for 37 cathode materials and more are needed.

Set 61 was reviewed.

1423 battery materials were marked in the 2011 release.

There were only 835 in the 2010 release.

Peter Zavalij believes we need to remove the incorrectly assigned entries and assign only one primary experimental pattern and not have several entries. He proposed a way to see the best property data from a set of BAT materials and believes this could be beneficial for the entire database. Each primary entry must have a property document if it exists and link to the best structure. Keep alternative entries but he believes that you should link from alternative to primary and not from primary to alternative.

Vesna Bosnic is going to correct incorrect links and put them with the correct entries for some specific materials.

Tim Fawcett wants the task group to look through the list of materials and tell the editorial team which they prefer to have as primary or alternative if more than one primary entry exists. If there is a consensus among the Ceramics Subcommittee then the editorial team can implement.

Suri Kabekkodu suggested having the subcommittee come up with new criteria to help improve the search the editorial team currently has in place.

Shailesh Upreti presented a talk called: "Recent Progress in Li-ion Battery Materials." He introduced some of the research currently happening in the manufacturing industry including those from machinery, medicine, military, automobile industry, etc. He introduced some of the advance cathode materials in five categories that are being researched worldwide including Lithium-Sulfur, Lithium-Air, LiMPO_4 , Li_2MnO_3 - $\text{Li}[\text{MnNiCo}]\text{O}_2$, and $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$.

Thermoelectric Materials

Set 61 was reviewed and 15 new patterns were flagged as TEM.

Winnie Wong-Ng worked on property entries and 30 property sheets were given in 2010. She continues to work on increasing that number.

Bioceramics

Set 61 was reviewed by Joel Reid.

Semiconductors

Set 61 was reviewed and 53 patterns were marked as SEM. The committee still needs to review all existing entries and work on properties.

Ionic Conductors

Set 61 was reviewed and 16 entries were marked as ION. Property files for these patterns are mainly complete.

Ferroelectrics

Set 61 was reviewed and 30 new patterns were marked as FER. Property entries are still needed.

Intermetallic Compounds for Hydrogen Storage

Set 61 was reviewed and five entries were marked. More are still coming.

Microwaves

The Ceramics Subcommittee is no longer supporting this subfile. Headquarters now needs to maintain.

Other Subfiles

Existing subfiles-

Perovskites (PER) contains numerous entries and needs to be sorted through.

Giant Magneto Resistant (GMR) – has been abandoned.

Proposed- volunteers are needed to help populate the subfiles.

Piezoelectrics

Multiferroics

Activity of the Ceramic Task Group

Task group meeting was March 16, 2010.

The task group reviewed set 61.

Property data sheets:

TEM – added 30 properties, more are coming

HS – added 30 properties, more are coming

Properties included in 2010 release:

HS, BAT, ION, TEM – Included

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 2012 ICDD Annual meeting / Denver X-ray Conference to work on property subfiles with following activity report.

Moved: Peter Zavalij

Second: John Faber

For: 8

Opposed: 0

Abstain: 0

Motion passed

Adjournment