

Ceramics Subcommittee
March 21, 2012
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 2011 Meeting

March 2011 meeting minutes approved.

Motions: Peter Zavalij

Second: Evgeny Antipov

2 For, 0 Opposed, 0 Abstained

Review of Mission Statement

The Ceramics Subcommittee shall be responsible for (1) identifying ceramic compounds in the PDF, (2) organizing the ceramic subfile into minifiles according to their functions and properties, and (3) assuring the relevance and quality of the present and future data to meet the needs of the user community.

Board of Directors' Liaison Report

W. Wong-Ng gave the Liaisons Report.

The Motion was to allocate \$3,000 for the group to meet at the next Annual meeting/DXC in 2012 to work on property subfiles.

Response: Business Department – Approved funds were allocated in the Technical Committee R&D Fund. The task group did not meet at DXC and are not scheduled to meet during the annual meeting.

Old Business

(a) Development of Subfiles-current status (P. Zavalij)

Peter Zavalij proposed to the group to work on perovskites subfile this year. It's currently populated based on the structure and he would like to see what properties can be attached to each entry. Peter mentioned the procedure for developing the subfiles/classes.

(b) Superconductors (E. Antipov)

Set 62 was reviewed and 15 new patterns were flagged including the new HTSC subclass. 49 were looked at in total and 34 were removed as not being relevant. Last year, ~20 new HTSC were added.

Presentation was given by Sergey Kazakov. He talked about Iron oxypnictides and chalcogenides as new superconductors. $\text{LaFeAsO}_{1-x}\text{F}_x$ and $\text{Sr}_{1-x}\text{La}_x\text{FeAs}$ amongst others were presented. He mentioned that there are a lot of opportunities to chemically optimize and obtain new structures.

(c) Thermoelectric Materials (W. Wong-Ng)

Presentation was given by Winnie Wong-Ng. She talked about thermoelectric materials and the different ways we can review the materials. Some of the materials she synthesized during the past year include BaRCO_4O_7 (R=lanthanides),

$\text{Ba}_{6-x}(\text{Sr,Ca})_x\text{R}_2\text{Co}_4\text{O}_{15}$ (R=lanthanides) and various Skutterudites. She mentioned that Jack Yan has identified a lot of phases in Set 62 that can be flagged as TEM. He also worked to formulate property data lists for materials already in the PDF. He added 30 new data sheets. So far, we have 90 total in the database. She believes there are probably about another 100 to go. She also mentioned two Metal-Organic-Framework compounds she made of MOF-74 as well as tailored materials for CO_2 capture applications. Winnie will talk with Terry Kahmer about submitting a list of TEM materials for the Grant-in-Aid program.

(d) Semiconductors (M. Delgado/ A. Davydov)

Set 62 was reviewed and 32 new patterns were marked as semiconductors, including some with property sheets.

(e) Metal Hydride Electrodes (I. Zavalij-not present)

Property descriptions were submitted for 30 patterns, with 90 total done. With this rate, it will take 8-10 years to finish. P. Zavalij mentioned increasing the number of entries per year. He will talk with Terry Kahmer to see how to best do that.

(f) Ionic Conductors (V.B. Nalbandyan/G. Subba Rao)

ION is one of the most complete subfiles including properties. Set 62 was reviewed and 14 new entries were marked ION. 3 were removed from auto assignment.

(g) Ferroelectrics (V.B. Nalbandyan/S. Ivanov)

Set 62 was reviewed and 11 new entries were marked FER. No property entries were made.

(h) Cements (V. Peterson)

Set 62 was reviewed and 9 entries were marked as CEM. It was mentioned that the committee could invite a specialist to come to a meeting to discuss the way to organize the cements subfile. Andrew Payzant will give P. Zavalij a list of potential names.

(i) Battery Materials (P. Zavalij/Shailesh Upreti)

Set 62 was reviewed and 37 new patterns were marked as BAT. W. Wong-Ng suggested Evgeny Antipov help generate property sheets for this file. He said he will help.

(j) Bioceramics (J. Reid)

Peter was not sure if this subfile was looked at for Set 62. Joel looked at Set 62 and no new entries were flagged.

(k) Other Subfiles

Proposed: Piezoelectrics, multiferroics, Giant Magneto-resistant materials

Existing: Bioceramics, perovskites

Experts are needed for these subfiles.

New Business

L. Valyslechko has agreed to work on the perovskites properties including thermal expansion in these materials.

E. Antipov wanted to know what types of perovskites to put these properties in for. He recommended narrowing to fuel-cell or a specific category to start with.

Activity of Task Group

Set 62 was reviewed.

Property data sheets were added for TEM (30) and Hydrogen storage materials (30), with more in the works.

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 2013 ICDD Annual meeting / Denver X-ray Conference to work on property subfiles with following activity report.

Move: Peter Zavalij

Second: Evgeny Antipov

For: 5

Opposed: 0

Abstain: 0

Motion passed

Motion 2: Was motioned directly at the Technical Committee meeting.

The Ceramic Subcommittee recommends to the Technical Committee that headquarters look into placement of the properties sheet on PDF entries.

Move: Peter Zavalij

Second: Tom Blanton

For: 25

Opposed: 3

Abstain: 5

Adjournment