

**Ceramics Subcommittee Meeting Minutes**  
**March 13, 2013**  
**ICDD Headquarters**  
**Peter Zavalij, Chairman**

**Call to Order**

Winnie Wong-Ng called the meeting to order.

**Appointment of Minutes Secretary**

Bridget Gavaghan appointed minutes secretary.

**Approval of Minutes from March 2012 Meeting**

March 2012 meeting minutes approved.

**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 need 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 2013 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.*

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

*Response: Suggested changes were made.*

**Old Business**

**(a) Development of Subfiles-current status (P. Zavalij – not present)**

*Presentation was given by Winnie Wong-Ng.* 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 63 was reviewed and 48 new patterns were flagged including the new HTSC subclass. Three new HTSC materials were added. E. Antipov said some flagged as superconductors are not superconductors. He suggested that there should be justification for why the mark was assigned. For example, a comment of  $T_c$  or how superconductivity is induced should be added.

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

*Presentation was given by Winnie Wong-Ng.* She reviewed applications of thermoelectric materials, definitions, types, and the different ways we can review the materials. ICDD and ASM databases have been surveyed for TE half-Heusler materials. Half-Heusler materials were described. Survey was done to figure out what TE materials are missing and add physical property information. Materials were divided into 5 categories. 306 potential XYZ compounds were identified. 234 are in PDF. 84 of these are half-Heusler compounds. 70 are missing patterns. J. Yan and W. Wong-Ng reviewed Set 63 and found 38 potential TE materials. Task members Xian-Li Su, Jack Yan, and Josh Martin have been adding TE properties to list of TE materials for the past 4 years. 30 per year have been added for a total of 120.

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

Set 63 was reviewed and 26 new patterns were marked as semiconductors. Property sheets are being reviewed and added.

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

Set 63 was reviewed and 6 patterns were marked as metal hydride electrodes. Property descriptions were submitted for 30 patterns, with 120 total done. With this rate, it will take 5-8 years to finish. Experimental patterns from GiA program have been added. There is no formal subfile for hydrogen storage materials. A motion was presented to the Technical Committee to create this subfile.

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

ION is one of the most complete subfiles including properties. Set 63 was reviewed and 5 new entries were marked ION. 17 were removed from auto assignment.

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

Set 63 was reviewed and 6 new entries were marked FER. No property entries were made.

**(h) Cements (V. Peterson-not present)**

Set 63 was reviewed and 4 entries were marked as CEM. No property entries were made.

**(i) Battery Materials (P. Zavalij/S. Upreti)**

Set 63 was reviewed and 21 new patterns were marked as BAT. In the BAT subfile, there are 37 cathode materials.

**(j) Bioceramics**

Nikolaos Kourkoumelis and Lauro Bucio agreed to co-chair Bioceramics task group.

**(k) Perovskites (L. Vasylechko – not present)**

L. Vasylechko has been adding property descriptions to perovskites (approximately 30/year).

**New Business**

New task groups will be formed for piezoelectrics, multiferroics, and giant magneto-resistant materials.

**Activity of Task Group**

Set 63 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 2014 ICDD Annual meeting /2013 Denver X-ray Conference to work on property subfiles with following activity report.

**Move:** Winnie Wong-Ng

**Second:** David Taylor

**For:** 12

**Opposed:** 0

**Abstain:** 0

**Motion passed**

**Motion 2:**

The Ceramic Subcommittee recommends to the Technical Committee that a hydrogen storage material subfile be created.

Definition of hydrogen storage materials: Hydrides of intermetallic compounds and metals (e.g.  $MgH_2$ ,  $LaNi_5$ ,  $TiFeH_2$ ), complex hydrides (e.g.  $NaAlH_4$ ,  $LiAlH_4$ ,  $Mg(BH_4)_2$ ) as well as any other chemical compounds, which can be used as a storage medium for hydrogen, often reversibly. The capacity - at least 0.5 H atoms per 1 atom (or weight H capacity of more than 1 wt.%).

**Move:** John Faber

**Second:** Miguel Delgado

**For:** 10

**Opposed:** 0

**Abstain:** 0

**Motion passed**

**Adjournment**