

Ceramics Subcommittee
March 25, 2009
ICDD Headquarters
Peter Zavalij, Chairman

Call to Order

Peter Zavalij called the meeting to order.

Appointment of Minutes Secretary

Amy Gindhart appointed minutes secretary.

Approval of Minutes from March 2008 Meeting

March 2008 meeting minutes approved.

Moved: John Faber

Second: Mark Rodriguez

7 For

0 Opposed

0 Abstained

Board of Directors' Liaison Report

Mark Rodriguez gave the Liaisons' Report since Evgeny Antipov was not able to be at the meeting. Motion was passed to allocate up to \$3,000 for the group to meet next Annual meeting 2010, to work on property subfiles.

Task group, Antipov, Misture and Kabekkodu to coordinate and present a plan at the board meeting in the fall. The first step is to tap into articles that we have in-house and extract the physical properties. The task group is still debating the types of data that they would like to extract. The size and project scope is still being determined.

Old Business

Development of Subfiles:

Ionic Conductors (V.B Nalbandyan, G. Subba Rao)

ION is one of the most complete subfiles for ceramics.

Set 59 was reviewed and 25 entries were marked as ION.

V.B. Nalbandyan helped by adding 30 property entries this year.

Superconductors (E. Antipov, W. Wong-Ng, L. Cook)

Critical temperatures (T_c) were added for SCM subfile in sets 1-51.

Set 59 was reviewed and 8 entries were marked as SCM.

T_c will be added for remaining sets by L. Cook.

R. Shpanchenko proposed to add new, heavily studied HTSC materials such as arsenides and similar compounds, e.g. RFe_2As_2 .

Microwave Materials (W. Wong-Ng)

W. Wong-Ng next presented some of her work done for classifying Microwave materials.

976 inorganic patterns from Set 59 were studied and 64 were marked as MIC.

She presented the list of those materials that are being marked in the database and presented some of the current work she is doing on Microwave Dielectrics with her group. These materials are important due to increasing need for miniaturization of circuits.

Thermoelectric Materials (W. Wong-Ng)

W. Wong-Ng presented some of her work done with her colleagues on thermoelectric materials. 6 new entries from Set 59 were marked as TEM.

There is a great need to develop alternative energy capabilities over the next 20 years. Power generation from waste heat to electricity is ideal to further this field.

W. Wong-Ng presented a plan for the future of the thermoelectric subfile.

- Recruit task group members
 - Task group members include:
 - Joshua Martin (NIST): Chalcogenides, complex pentatellurides, clathrates
 - Winnie Wong-Ng (NIST): Oxides, half heusler, metal silicides
 - Claudia Rawn (Oak Ridge): Skutterudites
 - Evan Thomas (NIST): Pnictides, Others
- Define thermoelectric materials in PDF
- Categorize thermoelectric materials into different groups according to structure type or chemistry.
- Each member is responsible for one or more categories of materials
- Each member will perform two subtasks
 - Perform literature search
 - collect detailed thermoelectric properties
 - determine if reference pattern is available in PDF
 - if available, fill in information
 - if not available, give information to grants-in-aid recipients for sample and pattern preparation
 - Select thermoelectric phases from historical datasets that are potential thermoelectric materials based on structure type or chemistry
 - each task group member will be given data from the metal/alloy or ceramic subfiles
 - information includes formulas, lattice parameters, detailed structure, and references
- Create subfile mark 'TEM' once about 100 patterns have been identified

High T_c superconductor task group (W. Wong-Ng, J. Kaduk, Z. Yang, G. Liu, T. Lou)

W. Wong-Ng presented work done by the High T_c superconductor task group on coated conductors. She presented several multi component phase diagrams.

A collaboration between W. Wong-Ng and J. Kaduk to synthesize and analyze these materials has been ongoing.

Semiconductors (SEM) (A. Davydov, M. Delgado)

Set 59 was reviewed and 75 new entries were marked as SEM.

Of the 75 new entries, 4 were marked SEM/CER (e.g. Cu_3TaSe_4).

A. Davydov presented a brief overview of SEM subfile.

He presented a flow chart representing the different elemental and compound SEM materials.

He presented some needs for the SEM subfile:

- Add new entries to the database (only 6 industrially important phases identified out of 161 SEMs/1975 total-entries)
 - alloys (AlGaN, ZnCdSe, CdHgTe)
 - high-temperature/high-pressure phases (cubic GaN)
 - metastable forms of important compounds (c-GaN/GaAs)
- Review/add data:
 - Structural data:
 - Include lattice parameters for stress-free vs. strained material
 - Indicate what form: bulk, films, nanoparticles/nanowires
 - Phase diagrams
 - Electronic properties (Eg)
 - Transport properties (conductivity type, carrier mobility)

Battery Materials (P. Zavalij)

The BAT subfile is practically complete.

Set 59 was reviewed and 1 new material was marked for MH electrode materials by the editorial department.

BAT subfile currently has 35 property entries.

Properties for some materials are still missing (*mono*-LiMnO₂, Nb₂O₅, CuFeS₂).

Bioceramics (S. Misture, J. Reid)

J. Reid is currently working on revising the content and re-reviewing the information for the Bioceramics subfile.

A new definition was proposed for the Bioceramics subfile by J. Reid with input from S. Kabekkodu and S. Misture.

Old Definition:

Ceramic materials - calcium phosphates, alumina, zirconia, etc., used for biomedical applications - prosthesis, dental restoration and bone implants.

New Definition:

Ceramic materials used for biomedical applications such as prosthetics, bone implants, implant coatings, joint replacement, dental restoration and tissue engineering, including (but not limited to) the following systems:

- calcium phosphates
- calcium sulfates
- bioactive glasses and glass ceramics
- titanium oxides
- alumina
- zirconia

The subfile content includes selected common precursor reactants and *in vivo* corrosion products.

Ferroelectrics (L. Cook, S. Ivanov, V. B. Nalbandyan)

Set 59 was reviewed by V. B. Nalbandyan and S. Ivanov and 38 new entries were marked as ferroelectrics.

No work on properties went on this past year, but L. Cook agrees to add/review properties of these materials.

Cements (L. Cook)

1150 patterns were flagged using an automated procedure.

There are still many that are left to be flagged.

We need to consider compounds reported in cement literature and get an idea of how many are actually there and how completely they are represented.

Proposed organization of cement phases' 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

Large percentage of primary cement systems flagged, but gaps remain.

Cements subfile does not adequately represent chemically modified cements.

Coverage can be improved by detailed survey of cement literature (e.g. JCCR).

Subfile can be made more useful for cement professionals by adding commonly used designations (“alite,” “belite,” “pleochroite”) and more detailed flagging and/or comments.

Link to NIST database of ~100 fitted patterns and structures of Portland cement phases will provide additional high quality data.

P. Zavalij proposed to add sorrel cements to the list.

Perovskites

Nothing was discussed formally about subfile.

Giant Magneto Resistance

Subfile is currently empty.

Piezoelectrics

S. Ivanov agreed to review incoming entries for possible future subfile.

Activity of Task Group

Task group meeting was Mar. 23, 2009.

The task group reviewed set 59.

Property data sheets:

- SCM – T_c for sets 52 & up will be added (L. Cook)
- THE – adding properties in progress (W. Wong-Ng)
- FER – currently assigned to S. Ivanov;
L. Cook agrees to add properties
- CEM – is being revised by L. Cook

Looking ahead to New Subfiles:

“Intermetallic Compounds for Hydrogen Storage” subfile:

- will include Pressure-Concentration-Temperature (PCT) diagrams
- including subset of electrochemical cycling and capacity plots for “Metal-Hydride Electrodes”, which should be also marked as Battery Materials.

Definition:

Intermetallic compounds with the capacity to absorb at least 0.5 H atoms per 1 metal atom (or weight H capacity of more than 1 wt.%).

Examples were introduced including IMC for hydrogen storage and Metal-hydride electrodes.

P. Zavalij: Definition will be improved as the work on property subfile starts.

It was proposed to invite representative from “Hydrogen storage” group for the ICDD annual meeting in 2010.

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 2010 ICDD Annual meeting to work on property subfiles with following activity report.

Move: John Faber

Second: Miguel Delgado

For: 8

Opposed: 0

Abstain: 0

Motion passed

Motion 2:

The Ceramic Subcommittee recommends to initiate work on “Intermetallic Compounds for Hydrogen Storage” property subfile.

Move: John Faber

Second: Frank Rotella

For: 7

Opposed: 1

Abstain: 0

Motion passed

Motion 3:

The Ceramic Subcommittee recommends to adopt revised definition of Bioceramics subfile.

Definition: Ceramic materials used for biomedical applications such as prosthetics, bone implants, implant coatings, joint replacement, dental restoration and tissue engineering, including (but not limited to) the following systems:

- calcium phosphates
- calcium sulfates
- bioactive glasses and glass ceramics
- titanium oxides
- alumina
- zirconia

The subfile content includes selected common precursor reactants and *in vivo* corrosion products.

Move: Tom Blanton

Second: Miguel Delgado

For: 7

Opposed: 0

Abstain: 0

Motion passed

Adjournment