Ceramics Subcommittee Meeting Minutes
Wednesday, 15 March 2017
International Centre Headquarters
Conference Room A
1:00 p.m. – 2:00 p.m.
W. Wong-Ng, Chairman

1. Call to Order
   The meeting was called to order at 1:00 pm by W. Wong-Ng.

2. Appointment of Minutes Secretary
   G. Kazimierczak was appointed as the minutes' secretary. Attendance List on record at headquarters.

3. Approval of March 2016 Minutes
   W. Wong-Ng projected the minutes from March 2016, and the minutes were approved by consent.

4. Review of Mission Statement
   The Ceramics Subcommittee shall be responsible for (1) identifying ceramic compounds in the PDF, 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.

5. Board of Directors Liaison Report
   S. Misture reported that there were no motions made by the Ceramics Subcommittee to bring to the board.
   A special note that the Board of Directors are happy with the Subfile work that adds value to the PDF.

6. Technical Presentation
   Cement Materials – **L.P. Cook**
   - A brief Space-Time Tour of Cements
   - Cement Processing
   - Cement and the Environment
   - Cements in the PDF

   Cements Subfile-Current Status -~1360

   Possible More Detailed Organization of Cement Subfile

   A. Cements (primary flag)
   Type of Cement (second level flag)
   1. Portland
   2. Calcium Aluminate
   3. Slag, Pozzolan, Flyash, or Silica Fume -Containing
   4. Halide, Sulfate, Phosphate or Borate –Modified or -Based
   5. Organic Polymer –Modified or –Based
   6. Other (unspecified, specialty cements, etc.)

   Cement Component (third level flag)
   1. Raw Material
   2. Clinker
   3. Addition or Admixture
   4. Pre-Setting Product
   5. Post-Setting Product
   6. Corrosion Product
   7. Unspecified

   Is a more detailed organization of the cements subfile desirable?
   -Would it be of benefit to the users?
   -Is it doable?

   What, if any, should be the role of the following?
   -Calculated Patterns?
   -Amorphous Phases?
   -Well-Characterized Mixtures?
   -Properties Sheets?

7. Task Group Reports

(a) Semiconductors M. Delgado/A. Davydov

- Update –**Specialty Set 67:** 158 new entries.
  - Property sheets: 39 entries, some are due to Yucheng Lan
  - Identify industrially important semiconductors (~60 compounds)
  - Add physical properties and information:
    - Structural data:
    - Electronic properties (Eg)
    - Transport properties (carrier mobility, etc.)
    - Phase diagrams, etc.
- Plan for next year:
  - 40 I III V2 and II IV V2 compounds: $CuInS_2$, $CuGaS_2$, etc.
  - 20 I2 II IV VI4 compounds: $Cu_2FeSnSe_4$, $Cu_2ZnSnSe_4$, etc.

(b) Solar Materials Y.C. Lan/N. King

Task Group Report on Solar Materials

Energy Consumption Sources

- Fossil fuels
- Nuclear power
- Renewable energy

Solar Materials 2015

The order of the compounds listed below were given by the task group chair.

1) Hexagonal Selenium (Se)
2) Cubic Cuprous Oxide (Cu_2O)
3) Cubic Silicon (Si)
4) Cubic Gallium Arssenide (GaAs)
5) Cubic Indium Phosphide (InP)
6) Tetrahedral Copper Indium Gallium diSelenide, CIGS ($CuInxGa1-xSe_2$)
7) Cubic Cadmium Telluride (CdTe)
8) Cubic Gallium Antimonide (GaSb)
9) Cubic Germanium (Ge)
10) Tetragonal Copper Indium diSelenide, CIS ($CuInSe_2$)

Properties and Datasheet of Photovoltaic Se

Solar Materials 2016

11) Cadmium Selenide (CdSe)
12) Cadmium Sulfide (CdS)
13) Indium Gallium Phosphide (InGaP)
14) Copper Zinc Tin Sulfide (CZTS)
15) Boron Nitride (BN)

Solar Materials 2017

16) Aluminium Nitride (AlN)
17) Gallium Nitride (GaN)
18) Indium Nitride (InN)
19) Boron Phosphide (BP)
20) Aluminum Phosphide (AlP)
21) Gallium Phosphide (GaP)
22) Boron Arsenide (BAs)
23) Aluminum Arsenide (AlAs)
24) Indium Arsenide (InAs)
25) Boron Antimony (BSb)
26) Aluminium Antimonide (AlSb)
27) Indium Antimonide (InSb)
28) Indium Bismuth Alloy (InBi)
29) Aluminium Gallium Phosphide (AlGaP)
30) Indium Gallium Arsenide (InGaAs)
31) Aluminium Gallium Arsenide (AlGaAs)
32) Indium Gallium Nitride (InGaN)
33) Aluminium Gallium Nitride (AlGaN)
34) Aluminium Gallium Antimonide (AlGaSb)
35) Gallium Indium Antimonide (GaInSb)

36) Diamond (C)
37) Graphene (C)
38) Sulfur (α-S8)
39) α-Tin (α-Sn)
40) Tellurium (Te)

Solar Materials Expected in 2018

Oxides:
(Cu_2O)
FeO
FeOOH
CoO
peroskite: ABO_3

Sulfides:
(CuZnSnS)
(CdS)
Cu_2S
Bi_2S_3

(c) Thermoelectric Materials W. Wong-Ng/Y. Yan

How we judge how well the Thermoelectric Material in Figures of Merits (ZT); look for high ZT.

Patterns prepared CaO--Eu_2O_3-CoO_x

Samples/Patterns for Thermoelectric-related Materials

- $Ba_{12}Nb_{8-x}Ta_xCo_4O_{36}$ (x=1,2,4,5,7)
- $(Ca_{2.7}Gd_{0.3})Co_2O_6$
- $(Ca_{1.1}Gd_{0.9})Co\ O_3$
- Sr_2RNbO_6 (R= Nd, Sm, Gd, Dy, Ho, Y, Tm, and Lu)
- $Ni_{1-x}Zn_xCoNb_4O_{12}$(x= 0.2, 0.4, 0.6, 0.8)
- $Bi_{1-x}Ca_xCuSeO$ ((*x*=0, 0.05, 0.075, 0.1, 0.2 and 0.3)
- $Bi_{1-x}Ba_xCuSeO$ (*x*= 0.05, 0.075, 0.1, 0.2)

Set 67 Jack Yan (45)*

ICDD Thermoelectric Property Data List*

(Y. Yan, Wuhan University of Technology, 2016)

(d) Battery Materials E. Pomerantseva

Update –**Specialty Set 67**(837 entries):

- **13** compounds assigned to **BAT**:
  e.g., $Li_2Fe(P_2O_7)$, $LiVP_2O_7$, $Li_{0.33}Ti_2O_4$, $Na_3(VOPO_4)_2F$
- **8** of which are electrode materials for lithium-ion batteries
- **3** of which are electrode materials for sodium-ion batteries
- **2** of which is a electrolyte material for solid-state lithium-ion batteries

Highlights in New Battery Materials*

New electrode materials reported:

- '$Li_4Mn_2O_5$' prepared by direct mechanochemical synthesis at room temperature. This rock-salt-type nanostructured material shows a discharge capacity of 355 mAh g^{-1}, which is the highest yet reported among the known lithium manganese oxide electrode materials. According to the magnetic measurements, this exceptional capacity results from the electrochemical activity of the Mn^{3}+/Mn^{4+} and O^{2-}/O^{-} redox couples, and, importantly, of the Mn^{4+}/Mn^{5+} couple also [Freire et al., A new active Li-Mn-O compound for high energy density Li-ion batteries, Nature Materials 15 (2016) 173].
- Transition-metal carbodlimides, **MNCN (M = Cu, Zn, Mn, Fe, Co and Ni)**, are electrochemically active materials for electrochemical energy-storage systems. They exhibit high reversible capacities (200-800 mAh $g^{-1)}$ for lithium and sodium ion batteries, stored by means of conversion reactions [Eguia-Barrio et al., Carbodiimides: new materials applied as anode electrodes for sodium and lithium ion batteries, J. Mater. Chem. A 4 (2016) 1608].
- Transition metal carbides, nitrides and carbonitrides (Mxenes): To date, numerous MXenes have been synthesized, including Ti2C, **V_2C, Nb_2C, Ti_3C_2, $(Ti_{0.5},Nb_{0.5})_2C$, $(V_{0.5},Cr_{0.5})_3C_2$, $T_{i3}CN$, Ta_4C_3, Nb_4C_3 and Mo_2TiC_2**, and dozens more predicted.

* Reference list was presented in Wong-Ng's presentation (available by request to HQ).

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

1) V. B. Nalbandyan and G. Subba Rao, reviewed the list of entries for set 67. 16 FER and 9 ION Marks have been added. 31 previous ION marks have been marked wrong or dubious and reasons for this briefly explained.
   Several corrections of chemical formulas have been suggested.
2) New data sheets on structure and chemical properties of ionic conductors have been compiled and submitted to the ICDD. These were for only 20 of the planned 30 entries.

Lithium Ion Conductors*
- Stuffed Garnet type
- Tetrahedral Structures
- Antiperovskites

Fluoride Ion Conductors

(f) Perovskites* — L. Vasylechko

- Set 67 was reviewed and 179 patterns of the perovskite phases were identified;
- Organisation and plenary lecture on ICDD Workshop, September 23-24, Lviv, Ukraine
- Regular submission of experimental patterns through Grant-in-Aid Program.
  620 experimental patterns since 2002
  ≈ 550 patterns are of the perovskite and perovskite-related phases.
- Property sheet project (30)

(g) Superconductors — E. Antipov

- Identified 4 SCM materials:
  a. Tetragonal FeS (Tc = 5K)
  b. $LiTi_2O_4$ (Tc = 11K)
  c. Ta_5GeB_2 (Tc = 3.8K)
  d. LuV_2Al_{20} (Tc = 0.57K)
- Disapprove the SCM flag for 5 phases from Set 67.
- Need to have more information from the ICDD
- Why the SCM flag was assigned to those phases?

(h) Hydrogen Storage Materials* — I. Zavaliy

- "Grant-in-aid N^O 03-05 "X-ray and Neutron Diffraction Data for Intermetallic Compounds and their Hydrides"
  25 XRD patterns and the crystal structure data of the intermetallic compounds and their hydrides were submitted to ICDD database. XRD patterns and crystal structure of new Nd_2 MG Co_9 hydride was presented as an example.
- 30 property files of the intermetallic compounds and their hydrides were prepared. Property sheet with PcT diagram as a main characteristic for the TiBe2 hydride is presented as a sample.

(i) Ferroelectrics & Antiferroelectrics — S. Ivanov/V. Nalbandyan/G.S. Rao
No presentation

(i) Subfiles and Data Sheet — S. Kabekkodu
No presentation

8. New business:

New Members Ceramics Subcommittee:

Sophie Beckett
Charlene Greenwood
Indrajit (Indy) Dutta

Interested in studying bio ceramics/magnetic material.

9. Motions: None

10. Adjournment: 2:00p.m., W. Wong-Ng

* Reference list was presented in Wong-Ng's presentation (available by request to HQ).