Ceramics Subcommittee Meeting Minutes
Wednesday, 13 March 2019
1:00 p.m. – 2:00 p.m.
W. Wong-Ng, Chairman

1. Call to Order — W. Wong-Ng
   The meeting was called to order at 1:05 pm by Wong-Ng

2. Appointment of Minutes Secretary - G. Kazimierczak was appointed as the minutes' secretary. Attendance list below.

3. Approval of March 2018 Minutes

   Wong-Ng moved the minutes from March 2018, and the minutes were approved.
   Thomas Ely seconded.
   Unanimous - Motion passed.

4. Review of Mission Statement

   The Ceramics Subcommittee shall be responsible for identifying ceramic compounds in the PDF, organizing the ceramic subfile into minifiles according to their functions and properties, and assuring the relevance and quality of the present & future data to meet the need of the users.

   No change to the Mission Statement.

5. Board of Directors Liaison Report — Scott Misture

   There were two motions to add entries to various subfiles, BOD advised the Subcommittee to figure it out business as usual. One motion was being rejected related to the superconductor file. The Subcommittee will revisit the motion and report next year.

6. Technical presentation
   Atomically-Thin Photovoltaics: Promise and Outlook — Deep Jariwala
   (Presentation is not available.)
   Wong-Ng introduced Deep Jariwala, and recommended he apply for membership. He will work with Y.C. Lan in the Solar Materials Task group.

7. Task Group Reports
   (a) Semiconductors (link presentation) — A. Davydov/M. Delgado

   (b) Solar Materials — Y.C. Lan/N. King
   See page 9 of Wong-Ng's presentation.
   Reviewed/Identified Set 69 with 18 new additions.

   (c) Negative thermal expansion materials — Cora Lind-Kovacs
   A discussion had occurred the previous day as to what we declare as Negative expansion materials.

   Materials for a database that contains crystallographic data; single phase material that shows a contraction of at least one unit cell dimension, and we arbitrarily picked over at least 50K temperature range has to be the crystallographic property, magnetic phase transition charge transfer with a slow gradual change in symmetry, single phase material.

   Feedback on the definition is welcome.

   Recruit help: Flag materials, code work, review older datasets, modify definition.
   Need a second set of eyes. Peterson may be able to help.

   (d) Thermoelectric Materials — Y. Yan/W. Wong-Ng
   See pages 4 – 9 of Wong-Ng's presentation.

   (e) Battery Materials — E. Ponomarantseva
   See page 11 of Wong-Ng's presentation.

Pomerantseva is stepping down as Chair of the Battery Materials task group. Davydov suggested his colleague at NIST, Vladimir Oleschko, may be willing to serve as Chair.

(f) Bioceramic Materials — Charlene Greenwood
See page 10 of Wong-Ng's presentation.

(g) Superconductors — E. Antipov

(h) Ionic Conductors — V.B. Nalbandyan
See page 12 of Wong-Ng's presentation.

(i) Perovskites — L. Vasylechko
See page 13 of Wong-Ng's presentation.

(j) Hydrogen Storage Materials — I. Zavaliy
See page 14 of Wong-Ng's presentation.

(k) Ferroelectrics & Antiferroelectric materials — S. Ivanov/V. Nalbandyan
See pages 16-19 of Wong-Ng's presentation.

(l) Cements — B. Scheetz

8. New business

Magnetic materials — Yu-Qi Yan

Theo Siegrist, professor at Florida State University, is very interested in becoming the Chair of Magnetic materials task group. Also a guest at NIST, Yi-Qi Yang a physicist from China, has volunteered.

9. Motions
No motions.

10. Adjournment

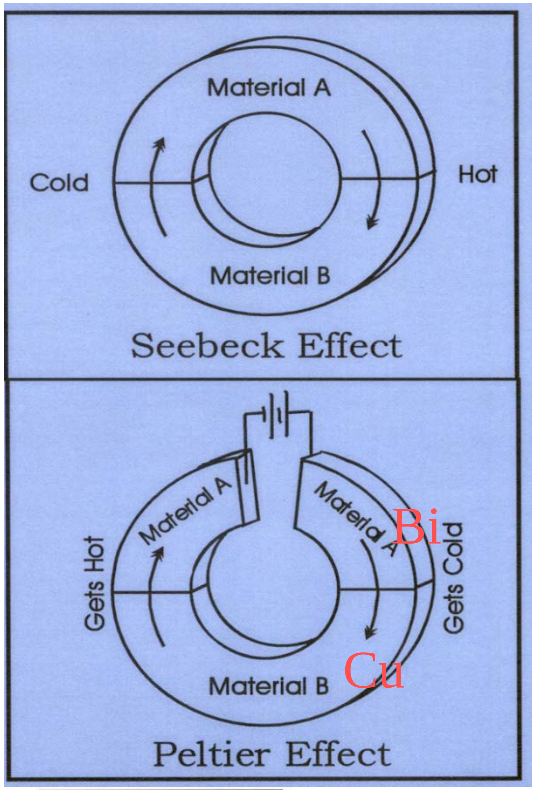
Agenda

1. Call to order	W. Wong-Ng
2. Appointment of minutes secretary	Georgia Kazimierczak
3. Approval of the last meeting minutes	
4. Review of Mission Statement	
5. Board of Directors' Liaison Report	Scott Misture
6. Technical Presentation	
Atomically-Thin Photovoltaics: Promise and Outlook	Deep Jariwala
7. Task Group Reports:	
(a) Semiconductors	A. Davydov/M. Delgado
(b) Solar Materials	Y.C. Lan/N. King
(c) Negative thermal expansion materials	Cora Lind-Kovacs
(d) Thermoelectric Materials	Y. Yan/W. Wong-Ng
(e) Bioceramics	Charlene Greenwood
(f) Battery materials	E. Ponomarantseva
(g) Superconductors	E. Antipov
(h) Ionic Conductors	V.B. Nalbandyan
(i) Perovskites	L. Vasylechko
(j) Hydrogen Storage Materials	I. Zavaliy
(k) Ferroelectrics & Antiferroelectrics	S. Ivanov/V. Nalbandyan
8. New business	
Magnetic materials	Yu-Qi Yang, T. Siegrist
New members (Yu-Qi Yan, JiangXi Univ of Science & Technology Yi Feng Han, Sun Yat-Sen University, China)	
9. Adjournment	

Thermoelectric Materials Task Group Members

Y. Yan	Wu Han University, China
W. Wong-Ng	NIST
J. A. Kaduk	Illinois Institute of Technology
J. Martin	NIST
G.Y. Liu	China University of Geosciences
S. H. Lapidus	APS, ANL
Q. Huang	NIST
Y. Yang	JiangXi Univ of Sci. & Tech., China
W. Liu	Tianjin University, China
J. Ifeduba	Howard University
Nacole King	NIST/NRC post-doc
G. Nguyen	NIST

Thermoelectric Materials



Thomas Johann Seebeck (1770-1831)

John-Charles-Athanase Peltier (1785-1834)

Figure of Merits (ZT)

$$ZT = \left(\frac{\sigma S^2}{K_e + K_l} \right) T$$

- ZT = Normalized Thermoelectric Eff.
- σ = electrical Conductivity
- S = Seebeck Coefficient
- K_e = Thermal Conductivity (Electronic)
- K_l = Thermal Conductivity (Lattice)
- T = Temperature

$S = -V_{12}/\Delta T_{12}$ S-Seebeck Coeff

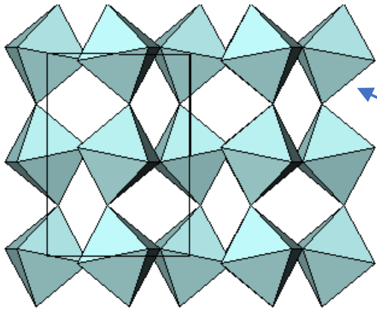
$Q = \Pi \cdot I$ Π - Peltier Coeff

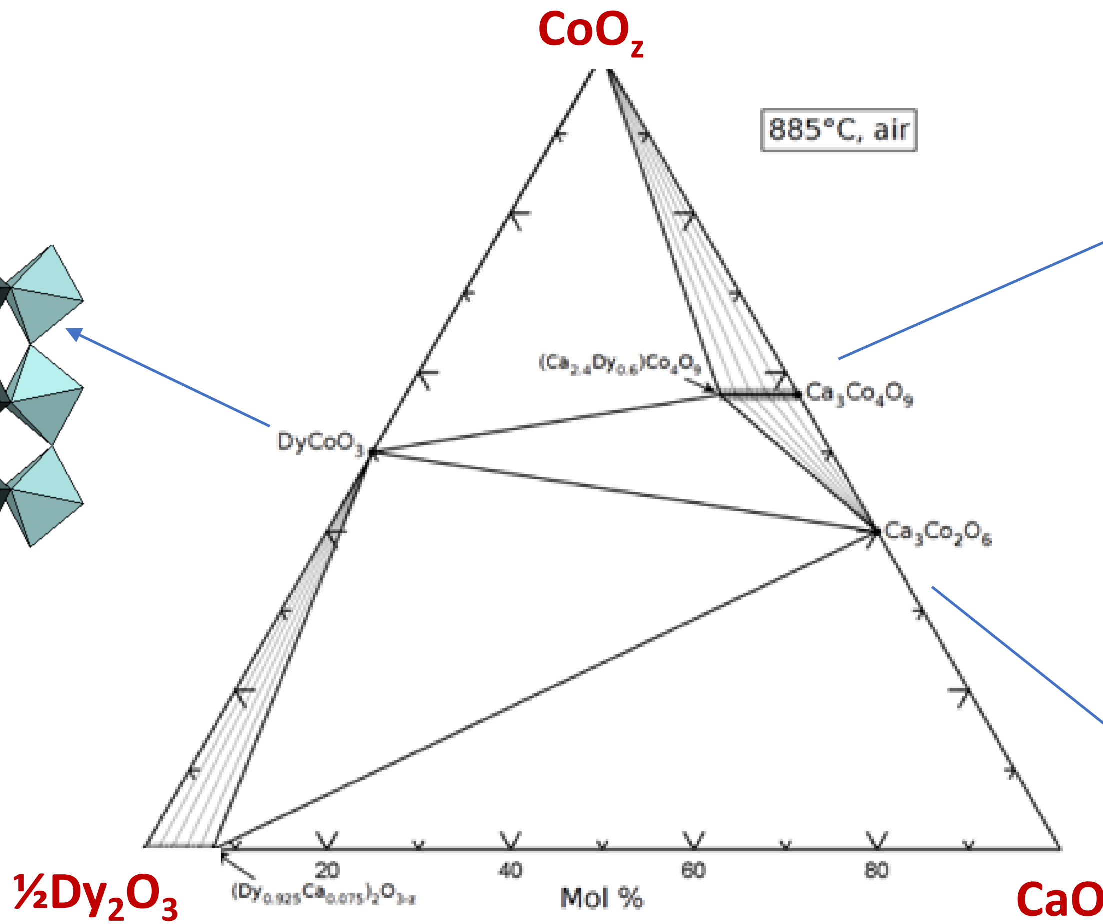
Seebeck Effect & Peltier Effect

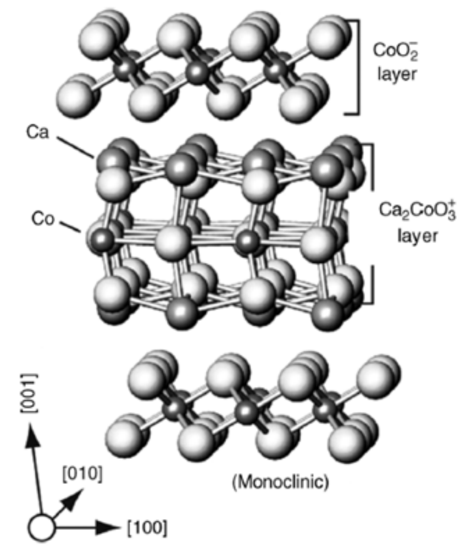
Thermoelectric materials (TEM)

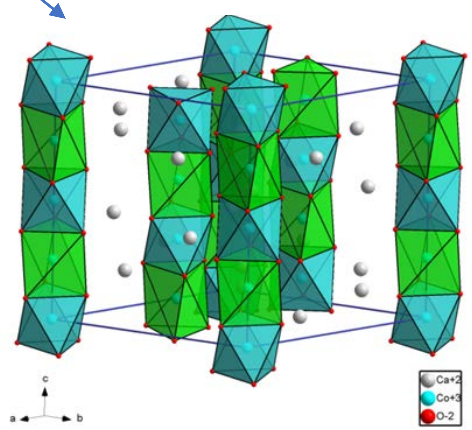
Thermoelectric materials (TEM: Commercially used thermoelectric materials (mostly semiconductors) are materials that have high Figures of Merit (ZT; materials with high Seebeck coefficient, high electrical conductivity and low thermal conductivity). The TEM code in the PDF will be used to represent thermoelectric materials that fall in a number of categories (Half-Heulsers, skutterudite, clathrates, pentatellurides, Di-chalcogenides, and layered-oxides, etc.). These materials have some or all of the associated properties (Seebeck coefficient, electrical conductivity or resistivity, thermal conductivity and figure of merit (ZT) available.)

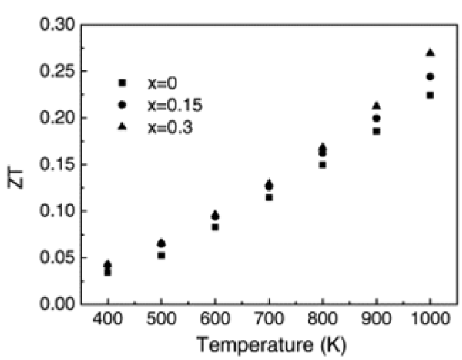
Patterns prepared $CaO\text{-}Dy_2O_3\text{-} CoO_x$











Samples/Patterns for Thermoelectric-related Materials & Others

Kaduk, Liu, Derbeshi, Anike, Yan, Liu, and Wong-Ng

SrR_2NbO_6, (R= Nd, Sm, Gd, Dy, Ho, Y, Tm, and Lu)

$Ba(Pb_{1-x}Sr_x)O_{3-z}$

$(Ba_{1-x}Sr_x)_2CoWO_6$ (0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9)

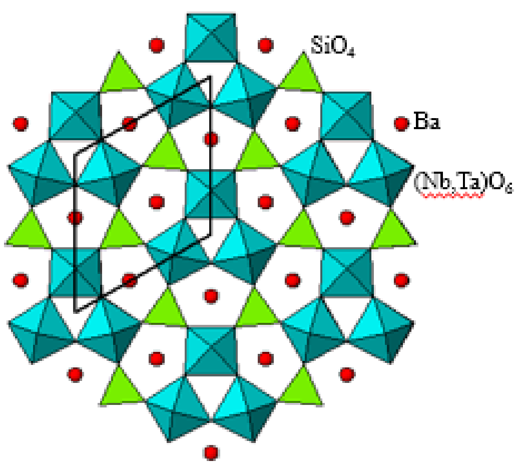
$Ni_{1-x}Zn_xCoNb_4O_{12}$ (x= 0.2, 0.4, 0.6, 0.8)

$Ba_3(Ta_{6-x}Nb_x)Si_4O_{26}$ (x=0.6, 1.2, 2.4, 3.6, 4.8)

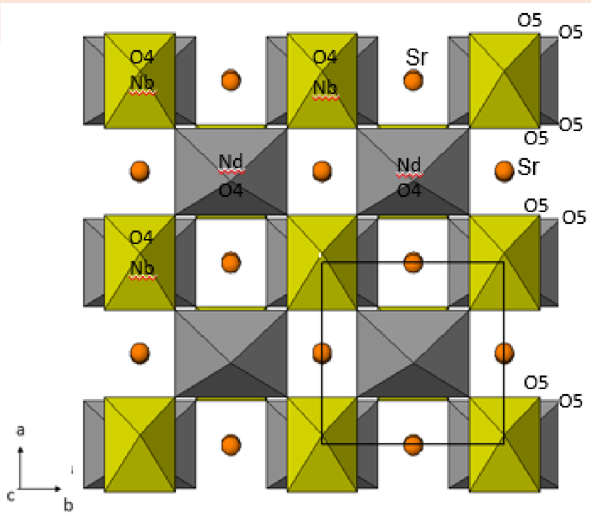
$Ba(Co_{1-x}Zn_x)SiO_4$ (x=0.2, 0.4, 0.6, 0.8)

$Zn(Fe_{2-x}In_x)O_4$ (x=0.2)

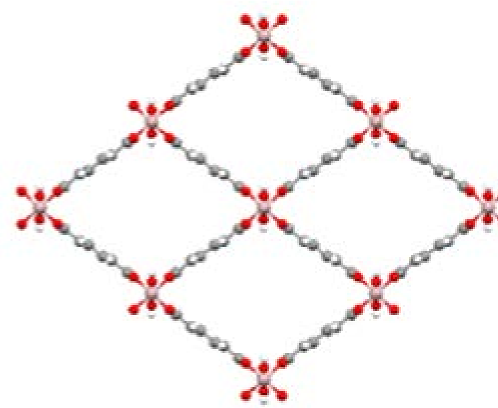
MIL-53 (Al) ($Al(OH)[O_2C\text{-}C_6H_4\text{-}CO_2]$) (HT form)



$Ba_3(Ta_{6-x}Nb_x)Si_4O_{26}$



SrR_2NbO_6



MIL-53 (Al)

Set 69 (Jack Yan)

New addition (18)

$Cu_{0.5}(Ga_{0.375}In_{0.125})_5Se_4$
$CaCuS_2$
$SrCo_{0.95}Mo_{0.05}O_3$
$SrCo_{0.925}Mo_{0.75}O_3$
$Cu_{10}Hg_2Sb_4Se_{13}$
$CuFe_2S_4$
$SnAg_{0.01}In_{0.01}Te_{1.02}$
Au_3TlTe_2
$KCuFeTe_2$
$Cd_{0.50}Cu_{0.25}In_{0.25}Te$
$Cu_{0.25}In_{0.25}SeZn_{0.50}$
$Cu_{0.25}In_{0.25}TeZn_{0.50}$
Sb_2Te_3
$Rb(LiFe)Se_2$
$PdAg_2S$
$CuSbSe_2$
$CaTiO_3$
$RbFe_4Se_4$

Bioceramic Task Group

Charlene Greenwood

Keele University, UK.

- **Bioceramic Definition:** A ceramic used as a biomaterial. Biomaterials are substances, synthetic or natural in origin, which can be used as whole or as part of a system to treat, augment, or replace any tissue, organ, or function within the body. These inorganic, solid, crystalline materials must be highly biocompatible and antithrombogenic. They are used in prosthetics, bone implants, implant coatings, joint replacement, dental restoration and tissue engineering, including (but not limited to) the following systems: calcium phosphates (synthetic and natural); calcium sulfates; bioactive glasses and glass ceramics; titanium oxides; alumina; zirconia.

- Set69: 8 Bioceramic materials identified (Inorganic subfile)

- Three individuals should be submitting membership applications this year:
  - Emily Arnold
  - Samantha Davies
  - Sarah Gosling

Ekaterina Ponomarantseva

Update - **SpecialtySet69** (1108 entries):

- **24** compounds assigned to **BAT**:
  e.g., Li_xCoO_2; $Li_xCo_{0.85}Ni_{0.15}O_2$ ($x \geq 1$);
  $Na_{0.67}V_{0.71}Ti_{0.29}O_2$; $Li_{6.5}La_3Hg_{1.5}O_{12}$
  (**2016: 26** compounds;
  2017: 13 compounds;
  2018: 10 compound)
- **16** of which are electrode materials for lithium-ion batteries or pseudo-capacitors
- **5** of which is an electrode material for sodium-ion batteries
- **3** of which is a electrolyte material for solid-state lithium-ion batteries

Ionic Conductors

Vladimir B. Nalbandyan

As annually, the list of entries for the new PDF issue, Set 69, has been reviewed.

- 4 new ION entries, 7 new FER entries and 10 new BAT entries have been identified and marked, in addition to those marked earlier. Besides, some errors or misprints have been found.

- Several earlier ION marks have been deleted due to considerable electronic conductivity:

La2 Ni O4.133
La2 Ni O4.16
K Cu Fe Te2
Ca Fe0.083 Ti0.459 Mn0.458 O2.92
Ca Fe0.167 Ti0.417 Mn0.416 O2.96

- The following formulae for the apatite-type silicates contain extra cations that cannot be accommodated in the structure:

I07439 La9.83 Sr Si6 Al O26+x
I07440 La9.38 Sr0.45 Si6 Al O26+x

- The following formulae are not charge-Balanced and, thus, impossible:

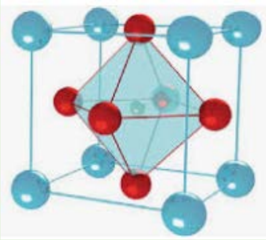
Ba0.5 Na0.5 Ti O3
Na0.47 Bi0.41 Ba0.11 Ti O3
Bi0.5 Fe0.5 Mn0.45 Ti0.05 O3
Sr11 Mo3 Ti O23
Sr11 Mo3.5 Ti0.5 O23
Sr11 Mo3 Nb O23
Sr11 Mo3.5 Nb0.5 O23
Ca5 Co0.224 O13 P3
Na0.47 Bi0.44 Ba0.29 Ti O3 (Sum of A cations is 1.2, impossible in perovskite)

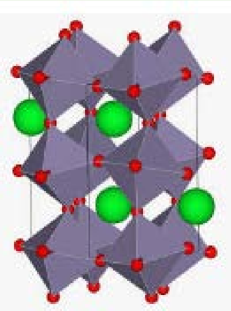
- Incorrect chemical names: ending –ide is only used for a nonmetal in its negative oxidation state

ID	Formula	Present	Should be
I07690	Na5 K2 Ca (Al6 Si6 O24) (S5) (S H)	...Sulfide Hydride	...Pentasulfide Hydrosulfide
I07864	Li Ni P O4	...Oxide Phosphide	...Phosphate
I08285	Ca5 Co0.224 O13 P3	...Oxide Phosphide	...Phosphate

Perovskites (Leonid Vasylechko)

- Set 69 was reviewed and 152 patterns of the perovskite phases were identified
- Regular submission of experimental patterns through Grant-in-Aid Program. More than 740 patterns were submitted since 2002 (about 600 patterns of the perovskite and perovskite-related phases).
- 30 property sheets were submitted. Project "*Thermal Expansion Properties of Perovskite Materials for Fuel Cell Applications*"





- Perovskite oxide materials for cathodes, in particular, "pure" and mixed cobaltites $NdCoO_3$, $SmCoO_3$, $Pr_{.3}Dy_{.7}CoO_3$, $Pr_{0.8}Y_{0.2}CoO_3$, $Nd_{.8}Gd_{.2}CoO_3$, $Nd_{0.3}Tb_{0.7}CoO_3$, $Sm_{0.8}Dy_{0.2}CoO_3$, $Eu_{0.5}Gd_{0.5}CoO_3$, $Gd_{0.8}Tb_{0.2}CoO_3$, $La_{1-x}Sr_xCoO_{3-y}$ (x=0.3, 0.4)
- Ferrites, ferrites-cobaltites and ferrites-nickelates $YFeO_3$, $La_{1-x}Sr_xFeO_3$ (x=0.1, 0.2), $NdFe_{0.7}Co_{0.3}O_3$, $GdFe_{0.7}Co_{0.3}O_3$, $TbFe_{0.3}Co_{0.7}O_3$, $LaFe_{0.4}Ni_{0.6}O_{3-\delta}$
- Manganites $NdMnO_3$, $YMnO_3$, $ScMnO_3$, $La_{0.7}Sr_{0.3}MnO_{3-\delta}$, $Sr_{0.8}Ce_{0.2}MnO_3$, $La_{2/3}Ba_{1/3}MnO_3$, $Sr_{0.9}Ba_{0.1}MnO_3$, $Sr_{0.7}Ce_{0.3}Mn_{1-x}Al_xO_3$ (x=0.1, 0.2)
- Mixed chromites of rare earth and Sr(Ca) for anode and interconnect materials: $HoCrO_3$, $La_{1-x}Sr_xCrO_3$ (x=0.1-0.3), $ErCr_{0.5}Co_{0.5}O_3$
- Double perovskite $A_2BB'O_6$ and brownmillerite $A_2B_2O_5$ electrode materials: Sr_2CoMoO_6, $Sr_2Fe_2O_5$, $Ca_2Fe_2O_5$

Hydrogen storage materials

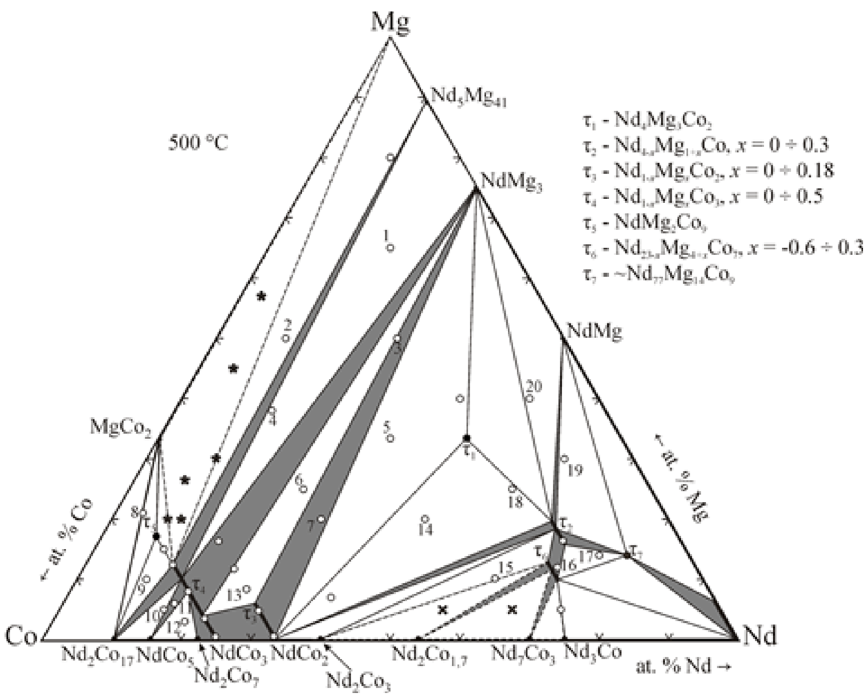
Prof. Ihor Yu. Zavaliy

Physico-Mechanical Institute, National Academy of Sciences of Ukraine

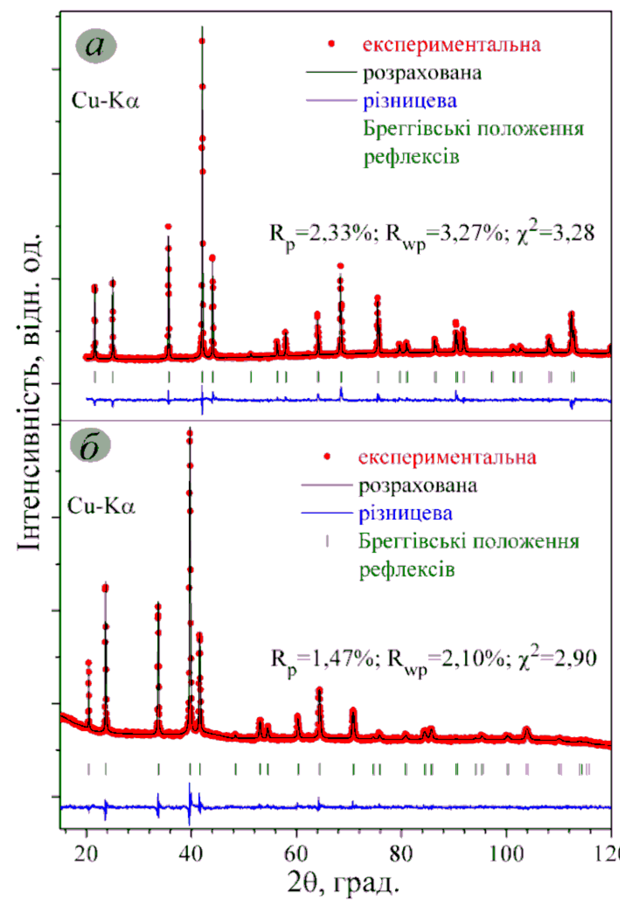
Grant № 03-05 "XRD Reference Patterns of Intermetallic Compounds and Their Hydrides".

45 XRD patterns and the crystal structure data of the intermetallic compounds and their hydrides were submitted to ICDD database in 2018.

The studied phase diagram of the Nd-Mg-Co system is presented as a basis for search of novel compounds or solid solution alloys.



The reference XRD patterns for the $NdMgNi_2Co_2$ (*a*) and its hydride (*b*) are presented below.



V. Shtender, V. Pavlyuk, R. Denys, I. Zavaliy et al. **Phase equilibria in the Nd–Mg–Co system at 300 and 500 °C, crystal structure and hydrogenation behavior of selected compounds.** ***Intermetallics*, 87 (2017) 61–69.**

Property files for Intermetallic Compounds and Their Hydrides

30 property files of the intermetallic compounds and their hydrides were prepared. Property sheet with capacity decay curves as a main characteristic for MH electrode materials is presented as an example →

List of Selected Property files:

P-c-T diagrams for IMC-H_2 systems:

1) $CeY_2Ni_9+H_2$
2) $LaMg_2Ni_4Cu_5+H_2$
3) Hf_2Fe+H_2
4) $HfNi+H_2$
5) $HfCo+H_2$
6) $HoNi_4Al+H_2$
7) $Zr_{0.7}Ti_{0.3}Mn_2+H_2$
8) $Zr_{0.9}Ti_{0.1}Mn_2+H_2$

Hydrogen sorption-desorption properties of IMC:

9) $Zr_4Fe_2O_{0.6}H_x$ – Hydrogen desorption
10) $Pr_{0.5}La_{0.5}MgNi_4$ – Hydrogenation
11) $Pr_{0.5}La_{0.5}MgNi_3Co$ – Hydrogenation
12) $Pr_{0.5}La_{0.5}MgNi_2Co_2$– Hydrogenation

Electrochemical properties of MH-electrodes:

13) $Pr_{0.5}La_{0.5}MgNi_4$
14) $Pr_{0.5}La_{0.5}MgNi_3Co$
15) $Pr_{0.5}Nd_{0.5}MgNi_4$
16) $Pr_{0.5}Nd_{0.5}MgNi_3Co$
17-30) *others*

Electrochemical hydrogenation properties of $La_{0.5}Pr_{0.5}Mg(Ni,Co)_4$

Parent Compound:
Chemical name: Lanthanum Praseodymium Magnesium Nickel
Chemical formula: $La_{0.5}Pr_{0.5}MgNi_4$
Crystal structure: *F-43m; a* = 7.1435(4) Å

Hydride:
Chemical name: Lanthanum Praseodymium Magnesium Nickel Hydride
Chemical formula: $La_{0.5}Pr_{0.5}MgNi_4H_{\sim 6}$ and $La_{0.5}Pr_{0.5}MgNi_4H_{\sim 4}$
Crystal structure: *F-43m; a*= 7.6051(7) Å for $La_{0.5}Pr_{0.5}MgNi_4H_{\sim 6}$ and *Pmn2₁*; *a*= 5.134(1), *b* = 5.504(1), *c* =7.464(2) for $La_{0.5}Pr_{0.5}MgNi_4$

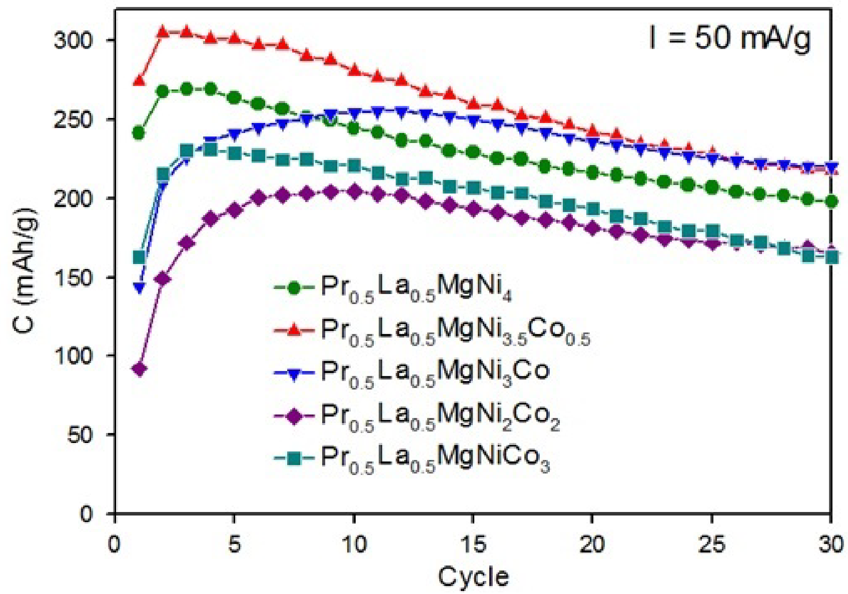


Fig. Cyclic stability of $Pr_{0.5}La_{0.5}MgNi_{4-x}Co_x$ electrodes; discharge current density I = 50 mAh/g.

Sergey Ivanov

Ferroelectric materials ICDD 2018

- 48 new patterns were added to PDF-4
- New ferroelectric family appeared (corundum-related structure Co3-xZnxTeO6)
- 22 new double perovskites
- 14 new phases with tungsten bronze structure
- 6 pyrochlores
- 7 phases with ilmenite-related structure

Ferroelectric materials in PDF4: problems

- ***Only*** 32% of phases with * estimation.
- ***Only*** 38% of patterns with experimentally confirmed chemical composition.
- ***In 65% of files*** for Pb-based perovskites the content of Pb and O is unknown.
- ***70%*** of cif files are without information about main ferroelectric properties.
- ***15%*** of patterns are without any information about sample preparation.

Ferroelectric materials in PDF database : new possible subfiles

Several classes of ceramic materials are still without a logic classification in PDF !

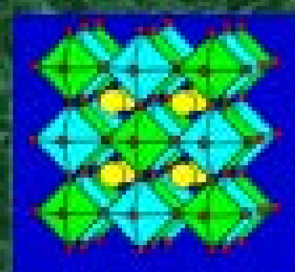
- Magnetic materials
- Polar dielectrics
- Relaxors
- Ferroelastics
- Multiferroics

Ferroelectric materials in PDF database : new touches to the old face

Multiferroics

Polar dielectrics

- Ferroelectrics
- Ferroelastics
- Antiferroelectrics
- Relaxors



Magnets

- Ferromagnetics
- Antiferromagnetics
- Ferrimagnetics