

Metals & Alloys Subcommittee Meeting
Wednesday, 13 March 2019
P. Wallace, Chairman

1. Call to Order P. Wallace
The meeting was called to order at 11 am.
2. Appointment of Minutes Secretary M. Carr
3. Approval of Minutes of March 2018
Minutes approved.
4. Review of Mission Statement
The Metals and Alloys Subcommittee shall be responsible for (1) assuring that the metals and alloys subfile meets present and future needs of metallurgists and materials scientists, (2) developing and updating the metals and alloys subfile, (3) editing metals and alloys data and products to ensure a high standard of quality, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page to communicate with members and other materials scientists.
5. Board of Directors' Liaison Report A. Payzant
6. Update on the PDF Phase Diagram Capability J. Blanton
See presentation from Justin Blanton for further details on database updates.
ICDD 2020 Product Developments_M&A.pptx

Discussion point: Comment from A. Payzant-Color coding based on structure may be an option in the future. The improvements mentioned in Justin Blanton's presentation are not limited to metals and alloys. Comment from P. Wallace-Improvements detailed in Justin's presentation may be useful to ceramic scientists.
7. M&A Prototype Structure Profiles, an update P. Wallace
P. Wallace discussed failed motion from last year. Unable to make profiles available to general population because of proprietary information. It has been decided that the editorial staff and members who are contract employees are the only individuals permitted to know all information.
8. The M&A prototype structure tables contain 8,307 entries P. Wallace
up from 8,089 last year, and are on the M&A web page.
See P. Wallace presentation. M&A Subcommittee VGs 03-13-19.pptx
9. M&A Working Group Activities. P. Wallace
See P. Wallace presentation. M&A Subcommittee VGs 03-13-19.pptx
10. M&A Editor's report P. Wallace
See P. Wallace presentation. M&A Subcommittee VGs 03-13-19.pptx
11. Next M&A Working Group meeting is October 11-14, 2019. P. Wallace

The M&A Subcommittee moves to the Technical Committee that funding be provided for the Oct 11-14, 2019 meeting. Requests up to \$5,000.

Moved: P. Wallace, Second: J. Dann

Yes: 8, No: 0, Abstain: 0 – Motion passed.*

**The above motion ended up being unnecessary. It was approved shortly thereafter by the Chairman of the Technical Committee (M. Rodriguez).*

12. New/Old Business

P. Wallace

Motion:

The M&A Subcommittee recommends to the Technical committee that ICDD consider offering PDF® users the option of choosing the standard cell (Crystal Data or Parthe') that best suits the users' needs.

Notes:

- 1) Parthe' is now used as a standard cell by LPF, ICSD, and many experimenters*
- 2) The nearly completed M&A PSCI-IV review and the current PSCI-V review are adding Wyckoff sequences to the database that reflect the Parthe' setting.*
- 3) This motion if implemented after the requested consideration will require significant programming effort at the ICDD and should be considered in that light.*

Moved: P. Wallace, Second: J. Dann

Yes: 7, No: 0, Abstain:1 (Kabekkodu abstains by name) – Motion passed.

13. Adjournment

Metals and Alloys Subcommittee

Attendance Sheet

Wednesday, 13 March 2019

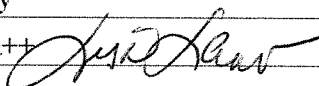
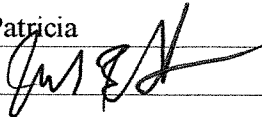
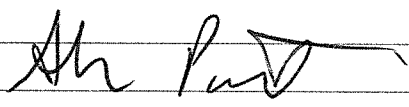
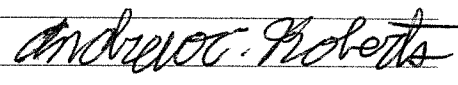
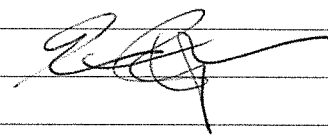
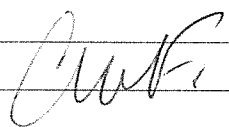
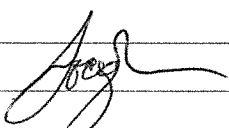
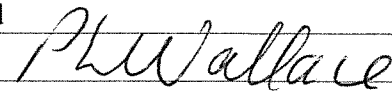
Time: 11:00 - 12:00 noon

Conference Room A

Peter Wallace, Chairman

Andy Payzant, Liaison

Soorya Kabekkodu, Staff Liaison

Name of Member	Signature	Name of Member	Signature
Ali, Ghulam (SA)		Kaduk, James	
Anibou, Noureddine		Kahmer, Theresa	
Antipov, Evgeny		Khan, Ashraf	
Balzar, Davor		Kimmel, Giora	
Belan, Bohdana		King, Danny	
Ben Hassen, Rached		Lanno, Lisa++	
Benard-Rocherulle, Patricia		Leoni, Matteo	
Blanton, Justin++		Lima, Milton	
Blanton, Tom		Mai, Zhenhong	
Blatov, Vladislav		Martin, Larry	
Bosnic, Vesna++		Martinez, Luis	
Boughzala, Habib		Mayo, William	
Bruma, Alina		Noyan, Ismail Cevdet	
Clark, Harlan		Payzant, Andrew	
Cui, Qingzhou		Proserpio, Davide	
DiNunno, Antonio		Reddy, M.V.	
Diouf, Saliou		Roberts, Andrew	
Ellouze, Mohamed		Rodriguez, Mark	
El-Meligi, Amin		Rogante, Massimo	
Ely, Thomas		Ruud, Clayton	
Fawcett, Timothy		Ryba, Earle	
Foris, C.		Sadangi, Rajendra	
Gates-Rector, Stacy++		Sagnella, Diane++	
Gilles, Ralph		Sharma, Yogendra Kumar	
Gindhart, Amy++		Shi, Lei	
Gourdon, Olivier		Sitepu, Husin	
Grzeta, Biserka		Sornadurai, Dhamardoss	
He, Wei		Squires, Leah	
Hubbard, Camden		Tran, Thanh Thao (SA)	
Jeitschko, Wolfgang		Ungar, Tamas	
Johnson, Jr., Gerald G.		Vasudevan, R.	
Jones, Howard		Velisavljevic, Nenad	
Kabekkodu, Soorya		Wallace, Peter	

(SA) Student Affiliate, Non-voting

** Associate Member, Non-voting

++ Staff Consultant - Non-voting

Metals and Alloys Subcommittee

Attendance Sheet

Wednesday, 13 March 2019

Time: 11:00 - 12:00 noon

Conference Room A

Peter Wallace, Chairman

Andy Payzant, Liaison

Soorya Kabekkodu, Staff Liaison

Name of Member	Signature	Name of Member	Signature
Wolska, Emilia			
Yuan, Wenxia			
Zavalij, Peter			
Zavaliy, Ihor			
Zeng, Lingmin			
Zhao, Yanming			
Zheng, Weitao			

Guests - Please sign on the next page.

Guest List Attendance Sheet

Name (Please print)	Signature
---------------------	-----------

Charles Weth	C. Weth
Ben Hish	Ben Hish
JANET GRANDE	
Jackie Hollencamp	
SOB HE	SOB HE
Chris Gilman	Chris Gilman
Takashi Ida	Takashi Ida
DAVID RAFAVA	DAVID RAFAVA
MICHAEL CARR	MICHAEL CARR
Miguel Delgado	Miguel Delgado
GRACIELA DIAZ DE DELGADO	GRACIELA DIAZ DE DELGADO
Nicola Ernst Boris	Nicola Ernst Boris

Name (Please print)	Signature
---------------------	-----------

MEMBER	Jeffrey H. Damm
--------	-----------------

New Features for Data Mining

The screenshot displays the CCDC search interface with the following sections:

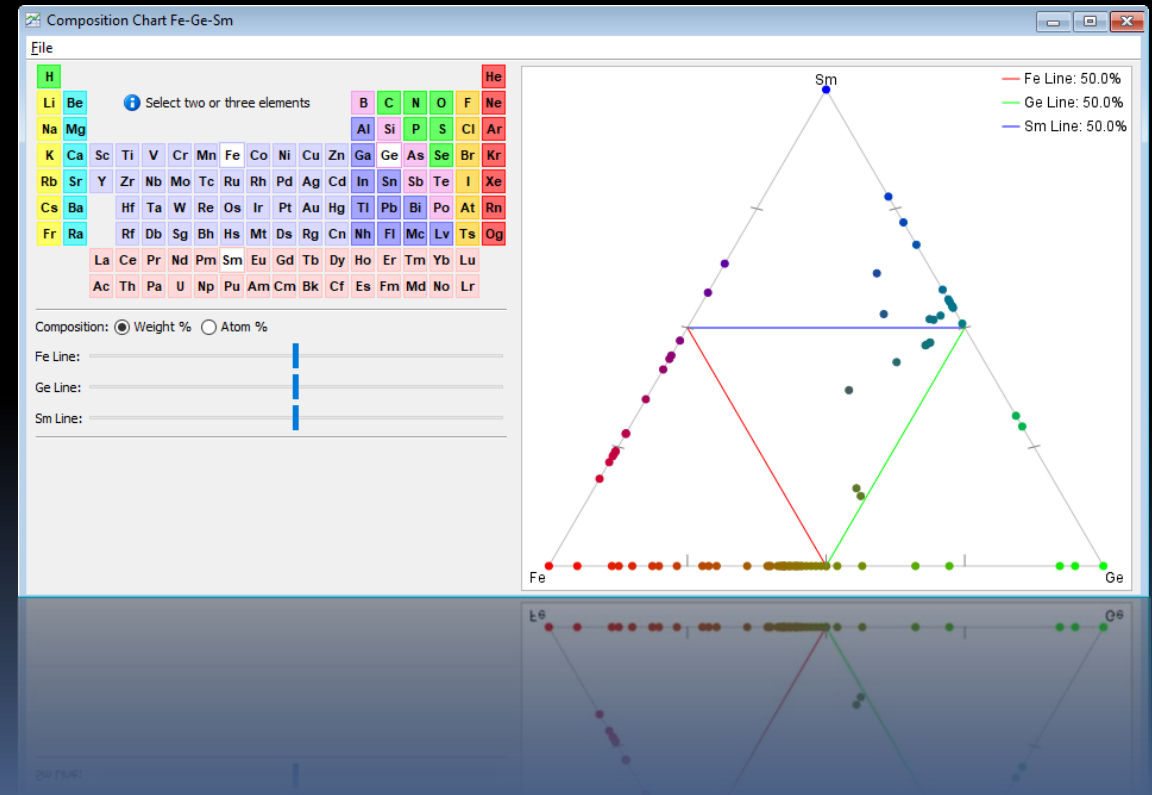
- Subfile:** Custom PDF Set, Alkaloid, Amino Acid, Peptide & Complex, Battery Material, Bioactive, No Subclass, Depressant, Narcotic, Pesticide & Antimicrobial.
- Environment:** Ambient, Non-ambient, Temp., Press., Temp. & Press., Atomic Coordinates, Raw Diffraction Data.
- Status:** Primary, Alternate, Deleted.
- Quality Mark:** Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision.
- Database:** ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05).
- Periodic Table:** A color-coded periodic table with elements highlighted in green, yellow, and red.
- Search Results:** A table with columns for Formula/Name, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The results are sorted by Empirical Formula and Hits.

- Quinary sorting of composition diagram lists (M&A subcommittee motion for 2018)

- A, B, C, D, and E compounds (pure elements)
- A-B compounds (sorted by A content)
- A-C compounds (sorted by A content)
- A-D compounds (sorted by A content)
- A-E compounds (sorted by A content)
- B-C compounds (sorted by B content)
- B-D compounds (sorted by B content)
- B-E compounds (sorted by B content)
- C-D compounds (sorted by C content)
- C-E compounds (sorted by C content)
- D-E compounds (sorted by D content)
- A-B-C compounds (sorted by A content)
- A-B-D compounds (sorted by A content)
- A-B-E compounds (sorted by A content)
- A-C-D compounds (sorted by A content)
- A-C-E compounds (sorted by A content)
- B-C-D compounds (sorted by B content)
- B-C-E compounds (sorted by B content)
- C-D-E compounds (sorted by C content)
- A-B-C-D compounds (sorted by A content)
- A-B-C-E compounds (sorted by A content)
- A-B-D-E compounds (sorted by A content)
- A-C-D-E compounds (sorted by A content)
- B-C-D-E compounds (sorted by B content)
- A-B-C-D-E compounds (sorted by A content)

New Features for Data Mining

- Composition graphs (M&A subcommittee motion for 2018)
 - Supports binary and ternary systems
 - Color-coded data points
 - Weight % or atomic %
 - User-defined divider lines
 - Tooltips show composition
 - Click to view PDF entries



Thanks to All M&A Working Group Members

- Jeff Dann
- Cathy Foris
- Cam Hubbard
- Howard Jones
- Suri Kabekkodu
- Terry Kahmer
- Monika Kottenhahn
- Andy Roberts
- Earle Ryba
- Rajendra Sadangi

M&A Subcommittee

Agenda – Items 1-5

1. Call to Order.
2. Appointment of Minutes Secretary (M. Carr).
3. Approval of Minutes of March 2018.
4. Review of Mission Statement.

The Metals and Alloys Subcommittee shall be responsible for (1) assuring that the metals and alloys subfile meets present and future needs of metallurgists and materials scientists, (2) developing and updating the metals and alloys subfile, (3) editing metals and alloys data and products to ensure a high standard of quality, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page on the ICDD site to communicate with members and other materials scientists.

5. Board of Directors' Liaison Report. (A. Payzant)

6.0 PDF Phase

Diagram Capability

an update --- J. Blanton

7.0 M&A Prototype

Structure Profiles, an update

M&A prototype structure profiles are based on the Crystal Data cell and contain observed ranges for the:

- Pearson Symbol Code,
- Lattice parameters, cell angles, and axial ratios,
- Atomic volumes,
- Calculated densities, and
- If possible, elements that are found in specific atomic positions of the structure.
- We are working with the ICDD on (a) how to make these profiles available and (b) to whom.

8.0 M&A Prototype Structure Table

- The M&A library of prototype structures now has more than 8,307 entries and cross-entries (up from 8,082).
- Each entry has a Wyckoff sequence and other useful information.
- Z-values have been added.
- This library is available on the M&A web page.

9.0 M&A Working Group Activities

- We met in October 2018 and March 2019, and each meeting covered four days.
- Primary tasks:
 - a. Concluding the fourth (Pearson Symbol Code Index or PSCI) Review, and beginning the fifth PSCI Review.
 - b. Updating the M&A web page and M&A tutorials as needed.
- A description of PSCI reviews and data from PSCI-IV follow.

9.1 The PSCI-IV Review, a nearly-final report

- The PSCI review of 141,423 M&A entries is about 96.1% complete.
- In this review, entries are
 1. Sorted by (a) Pearson Symbol Code, (b) SG No., and (c) axial ratio(s),
 2. Evaluated individually, and
 3. Given (a) prototype structures, (b) Wyckoff sequences, (c) *standard empirical formulae*, and (d) *standard Z's* whenever possible.

9.2 Anorthic entries

	Before Review		After Review	
	No.	%	No.	%
Total entries	990	100%	990	100.0%
No space group number	13	1.3%	8	0.8%
No M&A prototype structure	370	37.4%	110	11.1%
No LPF prototype structure	344	34.7%	113	11.4%
No Wyckoff sequence	394	39.8%	83	8.4%

9.3 Monoclinic entries

	<i>Before Review</i>		<i>After Review</i>	
	No.	%	No.	%
Total entries	9,475	100.0%	9,475	100.0%
No space group number	181	1.9%	156	1.6%
No M&A prototype structure	2,832	29.9%	444	4.7%
No LPF prototype structure	2,404	25.4%	499	5.3%
No Wyckoff sequence	3,225	34.0%	409	4.3%

9.4 Orthorhombic entries

	Before Review		After Review	
	No.	%	No.	%
Total entries	23,599	100.0%	23,599	100.0%
No space group number	337	1.4%	264	1.1%
No M&A prototype structure	6,621	28.1%	652	2.8%
No LPF prototype structure	5,946	25.2%	557	2.4%
No Wyckoff sequence	7,431	31.5%	584	2.5%

9.5 Tetragonal entries [except for 2,962]

	Before Review		After Review	
	No.	%	No.	%
Total entries	22,307	100.0%	22,307	100.0%
No space group number	175	0.8%	139	0.6%
No M&A prototype structure	3,146	14.1%	238	1.1%
No LPF prototype structure	5,177	23.2%	263	1.2%
No Wyckoff sequence	6,384	28.6%	273	1.2%

9.6 Hexagonal entries, [except for 2,617]

	Before Review		After Review	
	No.	%	No.	%
Total entries	34,759	100.0%	34,759	100.0%
No space group number	391	1.1%	248	0.7%
No M&A prototype structure	10,589	30.5%	490	1.4%
No LPF prototype structure	10,757	30.9%	369	1.1%
No Wyckoff sequence	10,239	29.5%	436	1.3%

9.7 Cubic Entries

	Before Review		After Review	
	No.	%	No.	%
Total entries	44,815	100.0%	44,815	100.0%
No space group number	215	0.5%	126	0.3%
No M&A prototype structure	23,729	52.9%	282	0.6%
No LPF prototype structure	16483	36.8%	198	0.4%
No Wyckoff sequence	12666	28.3%	218	0.5%

9.8 A Summary of All Entries (less 5,579)

	Before Review		After Review	
	No.	%	No.	%
Total entries	135,945	100.0%	135,945	100.0%
No space group number	1,312	1.0%	941	0.7%
No M&A prototype structure	47,287	34.8%	2,216	1.6%
No LPF prototype structure	41,111	30.2%	1,999	1.5%
No Wyckoff sequence	40,339	29.7%	2,003	1.5%

9.9 M&A Tutorials

- The M&A Subcommittee has created eight tutorials based on the M&A subfile.
- All are available on the M&A web page.
- Many thanks to Terry Kahmer and Monika Kottenhahn for making this happen.

10.0 M&A Editor's Report

- Secondary review of the latest M&A patterns is continuing.
- The review of the *M&A Prototype Structure File* including the addition of the Z-value for each entry is complete.
- A review of the *M&A Common Names Index* is continuing to ensure that:
 - (a) Each cited entry has the required M&A common name on it,
 - (b) Each cited entry is the best available entry, and
 - (c) Each prototype structure is in the LPF format.

The *M&A Prototype Structure File* and the *M&A Common Names Index* are available on the M&A web page.

11.0 New Business, An M&A Motion

The M&A Subcommittee moves to the Technical Committee that the ***ICDD consider offering PDF users the option of choosing the standard cell (Crystal Data or Parthe') that best suits the users' needs.***

Notes:

- (1) The Parthe' Cell is now used as a standard cell by the LPF, the ICSD, and many experimenters.
- (2) The nearly-completed M&A PSCI-IV review and the current PSCI-V review are adding Wyckoff sequences to the database that reflect the Parthe' setting.
- (3) This motion (if implemented after the requested consideration) will require significant programming effort at ICDD and should be considered in that light.

Final M&A Agenda Items

12.0 Other New Business.

13.0 An announcement: The next M&A Working Group meeting is October 11-14, 2019.

14.0 Adjournment.