

Dos Arroyos

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memorandum

To: Distribution
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Subject: Metals and Alloys (M&A) Subcommittee Minutes for March 16, 2016

Upcoming M&A Working Group Meetings

1. **2016 Fall Meeting:** We will meet October 14-17, 2016 at ICDD Headquarters.
2. **2016 Spring Meeting:** We will meet in March 2016 the Friday through Monday before the ICDD annual meeting.

Nos. 1.0-3.0 Business Items

The meeting was called to order at 11:00 am. The agenda is the last page of this document. Jeff Dann took meeting notes, and Pete Wallace wrote the minutes. The Metals and Alloys Subcommittee minutes of March 2015 were approved (8-0-0) as written.

4.0 Review of the Metals and Alloys Mission Statement

The current Metals and Alloys Subcommittee mission statement is:

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; and (4) extending the coverage and usefulness of the Metals and Alloys subfile.

After a short discussion, Pete Wallace proposed and Cam Hubbard seconded the following motion:

Motion 1: The M&A Subcommittee recommends to the Technical Committee that the M&A mission statement be changed as follows (the proposed change is part 5):

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.

The motion passed 9-0-0.

5.0 Board of Directors' Liaison Report

Jeff Dann gave the report for Davor Balzar. A M&A motion from the March 2015 annual meeting has not been implemented because of priority issues. The text of this motion and the ICDD response are shown in the box below.

BoD 315-17E(2)(b) 7

Leoni recommended to the Board of Directors that the M&A Standard empirical formula, space group, Z, and Wyckoff sequence be made available to PDF-4+ users. Note: M&A Standards are based upon the accepted Linus Pauling File (LPF) prototype structure for each material.

Response: Database Department - Access to these items is available to the M&A task groups today. For the general PDF-4 user, we would need to build specialty tables for this information and make them available for display using special "Preferences" options. We have questions in deciding the priority of putting these tables in the PDF-4 database.

After a discussion stressing the very high priority the M&A Subcommittee places on this motion, Pete Wallace moved and Cam Hubbard seconded the following motion.

Motion 2: The M&A Subcommittee recommends to the Technical Committee that the Board of Directors approve the previous BoD Motion 315-17E(2)(b), and that the changes be implemented in the 2017 product.

The motion passed 12-0-0.

6.0 The M&A Prototype Structure Table

The M&A prototype structure table:

- contains over 7,175 entries,
- is used to facilitate M&A reviews,
- is available on the M&A webpage or by request, and

- *Wyckoff sequences* and *Pearson Symbol Codes* (PSCs) are new additions to this table. The latter occur only when the PSC differs significantly from the Pearson Symbol due to vacancies or other reasons.

7.0 Prototype Structure Profiles and Their Utility

The two prototype structure definitions of interest both use a *standard formula*, *Z*, *crystallographic setting*, and *cell*.

- 1) ***Linus Pauling File (LPF) Prototype Structures*** – These prototype structures are based on a rigorous analysis of each atom’s environment, and rely on the experimenter having similar data about their material’s atomic environments. The Parthe’ standard cell is used.
- 2) ***M&A Observationally-Based Prototype Structures*** – These prototype structures are derived from M&A entries in the *Powder Diffraction File*. The Crystal Data standard cell is used.

M&A observationally-based prototype structures 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. Examples of site-specific elements might include:
 - (a) sulfur, selenium, and tellurium,
 - (b) tin and lead, or
 - (c) rare earths and actinides.

Either type of prototype may be used when assigning a prototype structure to a material that does not have one, depending on how much detail is known about the material of interest.

8.0 M&A Editor’s Report

Two projects are in process:

- secondary review of the latest M&A patterns, and
- the *M&A Common Names Index* (see the M&A web page) is being reviewed 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.

9.0 M&A Working Group Activities

Pete Wallace gave thanks and recognition to the members of the M&A Working Group:

- Jeff Dann,
- Cathy Foris,
- Cam Hubbard,
- Howard Jones,
- Terry Kahmer,
- Monika Kottenhan,
- Andy Roberts, and
- Earle Ryba.

The work reported in the following sections could not have been done without them, and the ever-helpful staff at ICDD Headquarters.

The M&A Working Group met in October 2015 and March 2016, and each meeting covered four days. The primary tasks were:

- continuing the Pearson Symbol Code Index (PSCI) Review,
- updating the M&A web page, and
- developing and updating M&A tutorials.

9.1 The Fourth M&A Pearson Symbol Code Index Review (PSCI-IV)

This is the fourth iteration of M&A PSCI reviews. It covers 141,423 entries, and is more than 80% complete. In these reviews, entries are:

- sorted by (a) Pearson Symbol Code, (b) SG No., and (c) axial ratio(s) in that order, (Note: This sorting places crystallographically similar entries side-by-side.)
- evaluated individually, and
- given (a) prototype structures, (b) Wyckoff sequences, (c) *standard empirical formulae*, and (d) *standard Z's* whenever possible.

9.2 PSCI-IV Review Sections

This table shows the number of entries in each PSCI section.

PSC	Entries	Percent
aPn	990	0.7%
mPn	4,400	3.1%
mCn	5,075	3.6%
oPn	13,742	9.7%
oCn	6,317	4.5%
oIn	2,704	1.9%
oFn	836	0.6%
tPn	9,961	7.0%
tIn	15,307	10.8%
hPn	29,581	20.9%
hRn	7,795	5.5%
cPn	11,666	8.2%
cIn	6,062	4.3%
cFn	26,987	19.1%
Total	141,423	

9.3 Some Recent PSCI-IV Results

All PSCI-IV results are summarized in *before-and-after* tables. See below.

A comparison of hP38.3 to hP64 entries before and after PSCI-IV review.				
	Before Review		After Review	
	No.	%	No.	%
Total entries	1,005	100%	1,005	100%
No space group number	19	1.9%	14	1.4%
No M&A prototype structure	496	49.4%	39	3.9%
No LPF prototype structure	366	36.4%	26	2.6%
No Wyckoff sequence	333	33.1%	49	4.9%

9.4 The Metals & Alloys Web Page

M&A web page (<http://www.icdd.com/subcommittees/metalsalloys/index.htm>) is available on the ICDD website. This web page is used to keep M&A Subcommittee members up-to-date, and each member has been notified about it. A 2016 review/update will be complete soon. Many thanks to Terry Kahmer and Monika Kottenhahn for making this happen.

The content includes sections on:

- the M&A Subcommittee and its mission.
- meetings, Membership, and Minutes.
- the M&A Working Group.
- Pearson Symbols.
- M&A Tutorials.
- M&A Products (largely a historical section).
- references and reference tables (for example, prototype lists, atomic volumes for close-packed structures, etc.)
- links to related sites.

Readers are encouraged to look at the webpage and provide feedback.

9.5 M&A Tutorials

The M&A Subcommittee has created four tutorials based on the M&A subfile. All are available on the M&A web page. A fifth, based on our poster presentation, is to be added soon. Many thanks to Terry Kahmer for making this happen.

9.6 The Next Meeting

The next meeting of the M&A Working Group will be October 14-17, 2016 at ICDD Headquarters.

10.0 New/Old Business

- Tom Blanton, Chris Gilmore, Cam Hubbard, Earle Ryba and Pete Wallace will be looking into uses of Cluster Analysis on the M&A subfile.
- Headquarters will be looking for examples of M&A problems to be used for teaching. Jim Kaduk offered some examples involving tin foil. Pete Wallace will query the M&A membership about this as well.
- Jim Kaduk gave a short discussion of three-dimensional (3D) pattern recognition involving patterns with all same atoms to see the effect on the structure.

- Longer Range: M&A will work with ICDD Headquarters to see if all the patterns for a given phase diagram could be retrieved with a minimum of key strokes. For example, enter two (or three) elements, and get all the polymorphs of each metal plus all their intermetallic compounds in a logical order.

11.0 Adjournment

The meeting was adjourned at 11:55 am.

AGENDA

Metals & Alloys Subcommittee Meeting
Wednesday, 16 March 2016
International Centre Headquarters
Conference Room A
11:00 a.m. - 12:00 noon
P. Wallace, Chairman

- 1.0 Call to Order. P. Wallace
- 2.0 Appointment of Minutes Secretary.
- 3.0 Approval of Minutes of March 2015.
- 4.0 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.
- 5.0 Board of Directors' Liaison Report. J. Dann
- 6.0 The M&A prototype structure tables now contain 7,175 entries, and these are used to facilitate M&A reviews. P. Wallace
- 7.0 Prototype structure profiles and their utility. P. Wallace
- 8.0 M&A Editor's report. P. Wallace
- 9.0 M&A Working Group Activities. P. Wallace
 - 9.1 The Pearson Symbol Code Index (PSCI-IV) Review.
 - 9.2 PSCI-IV Review Sections.
 - 9.3 Some recent PSCI-IV results.
 - 9.4 The M&A Web Page.
 - 9.5 The M&A Tutorials.
 - 9.6 The Next Meeting.
- 10.0 New/Old Business.
- 11.0 Adjournment.