

Metals & Alloys (M&A) Subcommittee Minutes
19 March 19 2014
Peter L. Wallace, Chairman

Upcoming M&A Working Group Meetings

1. **2014 Fall Meeting:** We will meet October 17-20, 2014 at ICDD Headquarters.
2. **2015 Spring Meeting:** We will meet in March 2015 the Friday through Monday before the ICDD annual meeting.

Agenda Nos. 1-3: Business Items

The meeting was called to order at 11:20 am. The [agenda](#) is on page 4, and the attendance list has been given to ICDD Headquarters for archiving. Terry Kahmer took meeting notes, and Pete Wallace wrote the minutes. The M&A Subcommittee minutes of March 2013 were approved as written.

4: Review of the M&A Mission Statement

The following is the current M&A 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, and
- (4) Extending the coverage and usefulness of the metals and alloys subfile.

Pete Wallace read through our current mission statement and asked for comments or suggested changes. There were none.

5: Board of Directors' Liaison Report

Because of our late start, no BOD Liaison Report was given. Also, there were no motions to report on from our last meeting.

6: Thanks to a Hard-Working Team

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

- Jeff Dann
- Cathy Foris
- Cam Hubbard
- Terry Kahmer
- Monika Kottenhahn
- Andy Roberts
- Earle Ryba

The work being reported here could not have been done without them and the ever-helpful staff at ICDD Headquarters.

7: Maintaining and Updating the M&A Web Page

Terry Kahmer and Pete Wallace have identified sources for all but one section (a tutorial) of the M&A Web Page. Terry now has this material and will work with Monika Kottenhahn to get it in place. Pete Wallace will supply the material for the missing section.

Once the needed material is in place, we hope to relocate the M&A web page to a more visible spot on the ICDD web site (possibly under the *Resources* tab). In addition, we will need to do some polishing of the M&A web page content. Many thanks to Terry and Monika for all their help in this endeavor.

8: The M&A Prototype Structure Table

The M&A Prototype Structure Table

- Has grown to contain over 6,000 entries (up from 5,000 entries a year ago) sorted by Pearson Symbol
- Contains cross-references to (a) previously used prototype structures, (b) M&A Strukturbericht symbols, and (c) mineral names for M&A prototype structures
- Contains (a) approved and a few provisional prototype structures, and (b) Wyckoff sequences when they are known
- Does not contain atom positions
- Is used in the assignment of M&A prototype structures to PDF entries
- Is available upon request and will soon be available on the M&A web page [Please contact Pete Wallace for a copy.]

9: M&A Working Group meetings

The M&A working group meets twice a year to conduct editorial reviews and discuss other business as required. Recent meetings were in October 2013, and in March 2014, just before the ICDD annual meeting. Our next meeting will be October 17-20, 2014 at ICDD Headquarters.

10: Status of the Pearson Symbol Code Index (PSCI-IV) editorial review

The PSCI-IV review of more than 140,000 entries is now about 50% complete. In this review, the M&A entries are sorted in ascending Pearson Symbol Code order, evaluated individually, and given (a) prototype structures, (b) Wyckoff sequences, (c) structurally-correct empirical formulae, and (d) Z's wherever needed. Then, a second (quality) check is performed on each section prior to submission to ICDD Headquarters. Completed sections are sent to the editorial team at ICDD Headquarters for incorporation in the PDF.

The volunteers listed in Section 6, above, are responsible for all the success of this project.

11: Review of current M&A patterns.

These reviews are performed on printed output sent to the PDF metals and alloys editor (P. Wallace). We currently are up-to-date.

12: M&A Tutorials

Three M&A tutorials (numbers 1, 3 and 6 on the master list) are in varying stages of development. They include problems on:

No.	Tutorial Goal	Status
1	Understanding Pearson symbols (PS), Pearson symbol codes (PSC), prototype structures, prototype structure profiles, and prototype structure nomenclature.	Written text is complete; oral presentation needs to be completed.
3	Estimating the Pearson symbol code given the unit cell, d / I list and hkl's. <u>Note</u> : Access to (a) the atomic-size table for close-packed-structures and (b) the table of general extinction conditions is needed for this tutorial.	To be started next. <u>Note</u> : The written text for this tutorial is needed to complete the M&A web page.
6	Constructing and using Pearson symbol code indexes. <u>Note</u> : Such an index is useful in looking for isotypical phases and in identifying possible prototype structures for a material of interest.	Both the written text and oral presentation materials are complete.

13: New/Old Business

13. a. M&A Motion

After a brief discussion regarding the need for the M&A editor to have access to Pearson's Crystal Data at home, A. Roberts made the following motion:

The Metals and Alloys (M&A) Subcommittee moves that one copy of Pearson's Crystal Data be made available for the use of the M&A Editor at home.

The motion was seconded by C. Hubbard. The motion was passed with:

9 in favor,
0 opposed, and
2 abstaining by name (P. Wallace and T. Fawcett)

13. b. M&A File Size

Pete Wallace reported that there are now 126,042 entries in the M&A subfile.

14: Adjournment

The meeting was adjourned at about 11:50 am.

REVISED AGENDA
Metals & Alloys Subcommittee Meeting
Wednesday, 19 March 2014
International Centre for Diffraction Data Headquarters
Conference Room A
11:00 a.m. - 12:00 noon
P. Wallace, Chairman

1. Call to Order P. Wallace
2. Appointment of Minutes Secretary
3. Approval of Minutes of March 2013
4. Review of Mission Statement. P. Wallace

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.
5. Board of Directors' Liaison Report. D. Balzar
6. Thanks to a Hard-Working Team. P. Wallace
7. Maintaining and updating the Metals & Alloys Web Page T. Kahmer
8. The M&A prototype structure table contains over 6,000 P. Wallace

entries, and is used to facilitate M&A reviews.
9. M&A Working Group meetings
10. Status of the Pearson Symbol Code Index (PSCI-IV) editorial review. P. Wallace
11. Review of current M&A patterns. P. Wallace
12. New/Old Business
13. Adjournment