

Dos Arroyos

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memorandum

To: Distribution
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Filename: M&A Minutes 03-13.doc
Date: May 16, 2013

Subject: Metals & Alloys (M&A) Subcommittee minutes for March 13, 2013

Upcoming M&A Working Group Meetings

1. **2013 Fall Meeting:** We will meet October 26-29, 2013 at ICDD Headquarters.
2. **2013 Spring Meeting:** We will meet in March 2014 just before the ICDD annual meeting.

Agenda Nos. 1-3: Business Items

The meeting was called to order at 11:15 am. The agenda is Attachment 1, and the attendance list has been sent to ICDD Headquarters for archiving. Jeff Dann took meeting notes, and Pete Wallace wrote the minutes. The M&A Subcommittee minutes of March 2012 were approved as written.

4: Review of the 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 changes. There were none.

5: Board of Directors' Liaison Report

Davor Balzar reported that M&A Subcommittee had had no motions from 2012, but he did mention that creation of a phase-diagram button in PDF++ now seems possible (this in response to a M&A proposal to the ICDD Lon Range Planning Committee). More work needs to be done, but this is an area of great interest to the M&A Subcommittee. (See also Section 13.)

6: New M&A members

We are pleased to announce that Terry Kahmer (she retires from the ICDD in June) and Joel Reid are joining our subcommittee. We plan to put Terry to work in three areas: M&A web page content

(see the next item), M&A tutorial problems (item 12b.), and communication with overseas M&A members. We hope that Joel can be involved with our editorial efforts (items 9 and 10), but that depends on his work schedule.

7: Completing and updating M&A Web Page content

The M&A web page is open to the public, but lacks content in many areas. Thus, the following assignments have been made.

- Terry Kahmer and Pete Wallace are responsible for the content, and
- Monika Kottenhahn will continue to maintain the web site.

8: The M&A *Prototype Structure Table*

The M&A *Prototype Structure Table*

- Contains over 5,000 entries 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, and
- Is available upon request. [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 (for example, see Section 10, below), and discuss other business as required. Recent meetings were in August 2012 before the DXC, and in March 2013 just before the ICDD annual meeting. Our next meeting will be October 26-29, 2013 at ICDD Headquarters.

10: Pearson Symbol Code Index (PSCI-IV) editorial review status

The six volunteers working on this project have made significant progress as the four completed sections of the PSCI-IV review show (please see Attachments 2-5).

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 are up-to-date except for the package received just before this meeting. (Secretary's note: This package was completed and sent to ICDD Headquarters on April 2, 2013.)

12: Informational Items

- a. M&A common names index is available upon request; eventually we hope to make it available on M&A website (Andy Roberts and Pete Wallace).
- b. M&A tutorial problems are being developed. The first two are nearly done and will be submitted to ICDD Headquarters for comment.
- c. In the near future, we hope to discuss some PDF-4+ ideas with ICDD Headquarters:
 - Adding the ability to convert authors' cell and hkl's values to the Crystal Data cell,
 - Adding the CD-cell Wyckoff sequence to the structural data,
 - Revising the M&A drop-down formats for PSCI and AFI tables, and
 - Adding the LPF prototype structure column to the S/M results table. (Secretary's note: This project is already in progress at ICDD Headquarters.)

13: New/Old Business

- a. Pete Wallace led a discussion about PDF phase diagram functionality along with some ideas for its implementation. The ideas have been passed on to ICDD Headquarters for possible implementation.
- b. Earle Ryba led a discussion on how to make PDF optical information regarding metallic materials clearer for the user. No motions were made.
- c. Jim Kaduk discussed a proposal he planned to make in the Minerals Subcommittee regarding space groups and proposed links between them. No motions were made.
- d. Pete Wallace reported that there were now 125,974 entries in the M&A subfile.

14: Adjournment

The meeting was adjourned at 11:55 am.

Attachment 1: M&A Subcommittee Agenda for March 13, 2013

1. Call to Order P. Wallace
2. Appointment of Minutes Secretary
3. Approval of Minutes of March 2012
4. Review of Mission Statement.
5. Board of Directors' Liaison Report D. Balzar
6. Volunteer needed to update and maintain the M&A web page.
7. The M&A prototype structure table contains over 5,000 entries and is used to facilitate M&A reviews. P. Wallace
8. Pearson Symbol Code Index (PSCI-IV) editorial review status P. Wallace
9. Review of current M&A patterns P. Wallace
10. Report on the August 2012 M&A Working Group meeting P. Wallace
11. Metals & Alloys Working Group will meet in late October 2013 for 4 days at ICDD Headquarters.
12. New/Old Business
13. Adjournment

Attachment 2: A comparison of aPn entries before and after PSCI-IV review.

	<i>Before Review</i>		<i>After Review</i>	
	No.	%	No.	%
Total entries	990	100%	990	100%
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%

Attachment 3: A comparison of mPn entries before and after PSCI-IV review.

	<i>Before Review</i>		<i>After Review</i>	
	No.	%	No.	%
Total entries	4,400	100%	4,400	100%
No space group number	159	3.6%	135	3.1%
No M&A prototype structure	1,443	32.8%	283	6.4%
No LPF prototype structure	1307	29.7%	349	7.9%
No Wyckoff sequence	1629	37.0%	285	6.5%

Attachment 4: A comparison of oFn entries before and after PSCI-IV review.

Total entries	836
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	<i>Before review</i>	<i>After review</i>
No space group	4 0.5%	4 0.5%
No M&A prototype structure	390 46.7%	34 4.1%
No LPF prototype structure	436 52.2%	34 4.1%
No Wyckoff sequence	273 32.7%	13 1.6%

Attachment 5: A comparison of tIn entries before and after PSCI-IV review.

Total entries	15307
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	<i>Before review</i>	<i>After review</i>
No space group	39 0.3%	27 0.2%
No M&A prototype structure	2005 13.1%	102 0.7%
No LPF prototype structure	3428 22.4%	146 1.0%
No Wyckoff sequence	4201 27.4%	85 0.6%