

Dos Arroyos

ENTERPRISES

memorandum

To: Distribution
From: Peter L. Wallace
Phone/fax/e-mail: (520) 878-9884/plw_dae@q.com
Filename: M&A Minutes 03-15.doc
Date: March 30, 2015

Subject: Metals and Alloys (M&A) Subcommittee minutes for March 25, 2015

Upcoming M&A Working Group Meetings

1. **2015 Fall Meeting:** We will meet October 23-26, 2015 at ICDD Headquarters.
2. **2016 Spring Meeting:** We will meet in March 2016 the Friday through Monday before the ICDD annual meeting.

Agenda Nos. 1-3: Business Items

The meeting was called to order at 11:00 am. The agenda is on page 5, and the attendance list is on page 6. Jeff Dann took meeting notes, and Pete Wallace wrote the minutes. The Metals and Alloys Subcommittee minutes of March 2014 were approved (5-0-0) as written.

4: Review of the Metals and Alloys Mission Statement

The following is the current Metals and Alloys Subcommittee 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

Jeffrey Dann gave the report for Davor Balzar.

6: The M&A Working Group

a. The Workers

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

b. The Metals & Alloys Web Page

Pete Wallace gave a brief update on description and content of the Metals and Alloys webpage:

- Monika Kottenhahn maintains it.
- Terry Kahmer and Pete provide the content.
- Your comments and input are always welcome.
- It will be renamed *Metals and Alloys Resources* (currently it is called the *Metals and Alloys Subcommittee Area*).
- For now, it can be found under Membership/Technical Subcommittees
- And in the future, it will also be found under *Resources*.

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

Note: As of March 26, 2015, the webpage has been renamed and all remaining tasks are completed. Readers are encouraged to look at the webpage and provide feedback. The information will be posted to: <http://www.icdd.com/subcommittees/metalsalloys/index.htm>.

c. The M&A prototype structure table

- Contain over 6,000 entries,
- Are used to facilitate M&A reviews, and
- Are available on the M&A webpage or by request
- *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.

d. Status of the Pearson Symbol Code Index (PSCI-IV) editorial review

- This is the fourth iteration, covers 141,423 entries, and is about 63% complete.
- Entries are sorted to place materials with similar PSCs, space groups, and axial ratios [a(0) for cubic materials] side-by-side.
- The reviewer evaluates each entry to be sure (when possible) that it has a complete PSC, a space group, and both LPF and M&A prototype structures.
- New in this iteration is the addition (when possible) of an *M&A Standard empirical formula* and *Z* that match the assigned prototype structure, as well as the *Wyckoff sequence* for that structure.

e. The Working Group's next meeting

Metals and Alloys Working Group will meet next at headquarters October 23 - 26, 2015.

7. M&A motions

There were two motions submitted and passed by the Metals and Alloys Subcommittee. [Note: Both motions were subsequently passed by the ICDD Technical Committee.]

Motion 1: The M&A Subcommittee recommends to the Technical Committee that the *M&A Standard empirical formula, space group, Z, 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.

Moved: Pete Wallace Second: Cam Hubbard Vote: 6-0-0

Motion 2: The M&A Subcommittee recommends to the Technical Committee that structural information (e.g., prototype structure and Pearson Symbols) located under the *Miscellaneous* tab of PDF-4+ be relocated to the *Structure* or a new *Structure-II* tab when possible.

Moved: Pete Wallace Second: Cam Hubbard Vote: 7-0-0

8. Review of current M&A patterns

Pete Wallace is up-to-date on reviewing new M&A entries submitted to the ICDD.

9. New/Old Business

The following items were discussed, but no motions were made.

- a. Should there be Subclasses for the 140,000 entries in M&A Subfile? Should they be based on chemistry, uses, or properties? Answer: Subclasses are not needed based on chemistry because a Periodical Table search can be performed.
- b. The guide for assigning prototype structures is currently based on the Pearson Crystal Data (PCD). Another database (the ICSD) is now also providing prototype structures, which may be different from the PCD. How should these differences be handled? Answer: We will use the PCD prototype structures.
- c. Should there be another structure field, similar to ANX (which is based on the valences of elements), but based just on chemical formula? An example would be AB₂O₄ for spinels. No conclusions were reached here.

10. Adjournment

The meeting was adjourned at 11:55 am.

Attachment 1: AGENDA
Metals and Alloys Subcommittee Meeting
Wednesday, 25 March 2015
International Centre 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 2014
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, and (4) extending the coverage and usefulness of the metals and alloys subfile.

5. Board of Directors' Liaison Report. D. Balzar
6. The M&A Working Group. P. Wallace
 - a. The Workers.
 - b. The Metals and Alloys Web Page.
 - c. The Metals and Alloys prototype structure tables
 - (1) Contain over 6,000 entries,
 - (2) Are used to facilitate M&A reviews, and
 - (3) Are available on the M&A webpage or by request.
 - d. Status of the Pearson Symbol Code Index (PSCI-IV) editorial review.
 - e. M&A motions.
 - f. Review of current Metals and Alloys patterns.
 - g. Metals and Alloys Working Group will meet (TBD).
7. New/Old Business
 - a.
 - b.
8. Adjournment

Attachment 2

Metals and Alloys Subcommittee

Attendance Sheet

Wednesday, 25 March 2015

Time: 11:00 - 12:00 noon

Conference Room A

Peter Wallace, Chairman

Davor Balzar, BoD Liaison

Suri Kabekkodu, Staff Liaison

Name of Member	Signature	Name of Member	Signature
Abrar, Muhammad (SA)		Jones, Howard	
Al-Dajane, Maher		Kabekkodu, Soorya	<i>Soorya Kabekkodu</i>
Ali, Ghulam (SA)		Kaduk, James	<i>James Kaduk</i>
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++		Levin, Eduard (SA)	
Blanton, Tom		Lima, Milton	
Bosnic, Vesna++ <i>Vesna Bosnic</i>		Mai, Zhenhong	
Cernatescu, Iuliana Dragomir		Martin, Larry	
Clark, Harlan		Martinez, Luis	
Cui, Qingzhou		Mayo, William	
Dann, Jeffrey <i>Jeffrey H Dann</i>		Misture, Scott	
DiNunno, Antonio		Noyan, Ismail Cevdet	
Ellouze, Mohamed		Reddy, M.V.	
El-Meligi, Amin		Roberts, Andrew <i>Andrew C. Roberts</i>	
Ely, Thomas		Rogante, Massimo	
Fawcett, Timothy		Rotkina, Lolita	
Foris, C.		Ruud, Clayton	
Gates, Stacy++		Ryba, Earle <i>Earle Ryba</i>	
Gilles, Ralph		Sagnella, Diane++	
Gindhart, Amy++		Saparov, Bayrammurad (SA)	
Goehner, Raymond		Sharma, Yogendra Kumar	
Gourdon, Olivier		Shi, Lei	
Grzeta, Biserka		Sitepu, Husin	
Han, Ibrahim		Sornadurai, Dhamardoss	
He, Wei		Squires, Leah	
Hubbard, Camden <i>CR Hubbard</i>		Tran, Thanh Thao (SA)	
Jeitschko, Wolfgang		Ungar, Tamas	
Johnson, Jr., Gerald G.		Vasudevan, R.	

(SA) Student Affiliate, Non-voting

** Associate Member, Non-voting

++ Staff Consultant - Non-voting

Metals and Alloys Subcommittee

Attendance Sheet

Wednesday, 25 March 2015

Time: 11:00 - 12:00 noon


Conference Room A

Peter Wallace, Chairman

Davor Balzar, BoD Liaison

Suri Kabekkodu, Staff Liaison

Name of Member	Signature	Name of Member	Signature
Velisavljevic, Nenad			
Wallace, Peter			
Wolska, Emilia			
Yang, Heng (SA)			
Yuan, Wenxia			
Zavalij, Peter			
Zavaliy, Ihor			
Zeng, Lingmin			
Zhao, Yanming			
Zheng, Weitao			
Zhong, Kai++			

Lizhi Liu  Guests - Please sign on the next page.

Bob He

John Falco

Jack Hollencamp

Janet Grande

Joseph Jeyaraj

Richard Dupont

Chris Gilmore

Andrew Payzant