

Dos Arroyos

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memorandum

To: Distribution
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Filename: M&A Minutes 03-12.doc
Date: April 14, 2012

Subject: Metals & Alloys (M&A) Subcommittee minutes for March 21, 2012

Business Items

The meeting was called to order at 11 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 2011 were approved as written.

Upcoming M&A Working Group Meetings

1. **2012 Fall Meeting:** We will meet August 4-7, 2012 in Denver, Colorado just before the 2012 Denver X-ray Conference. (Our thanks to Tim Fawcett, Terry Maguire and her DXC staff, Terry Kahmer, and Suri Kabekkodu for making this possible.)
2. **2013 Spring Meeting:** We will meet March 9-11, 2013 just before the ICDD annual meeting.

Board of Directors Liaison Report (Ray Goehner)

There were no Board of Directors actions to report on.

M&A Web Area (Howard Jones and Pete Wallace)

Note: With pleasure we welcome Howard Jones back to the M&A Subcommittee.

The M&A Web Area is up and open to the public. But, there are a number of sections that currently have no content, and we are working to fill them in. Headquarters staff will be assisting us in reviewing and then entering the information. Your comments on the M&A Web Area are always welcome.

Note: To get to the M&A Web Area, go to ICDD.com, click on [Membership](#), click on [ICDD Technical Committees](#), and then click on [Metals and Alloys Web Area](#).

The first section of the M&A Electronic Tables for Editors has been produced, and it includes Prototype Structure Profiles (PSPs). (Pete Wallace and Suri Kabekkodu)

The M&A electronic tables for editors comprise four tables: (a) an alphabetical formula index (AFI) for all M&A entries, (b) a prototype structure code index (PSCI) also for all entries, (c) an AFI for prototype structures, and (d) a PSCI for prototype structures. Suri has recently produced the latter table (the prototype structure PSCI) based on the PSCI-III review. The index is made up of what we have chosen to call prototype structure profiles (PSPs).

Each PSP describes the observed range of

- (1) Pearson-symbol-code integers,
- (2) Lattice parameters,
- (3) Axial ratios, and
- (4) Chemistry seen in PDF examples.

PSPs will eventually be used to suggest (subject to editorial review) prototype structures for new materials.

Review of Current M&A Patterns (Pete Wallace)

We are up-to-date except for the March 2012 package.

Report on M&A Working Group Meetings (Pete Wallace)

We met last October for four days at ICDD Headquarters and began the PSCI-IV review using data files supplied by Suri (thank you, Suri). We also met the three days before the 2012 annual meeting to continue the PSCI-IV review. The results of these meetings are described in more detail in the *Status of the Pearson Symbol Code Index (PSCI-IV) Editorial Review* section, below. Our next meetings will be just before the 2012 DXC and just before the 2013 ICDD annual meeting (please see the box, above).

Status of the Pearson Symbol Code Index (PSCI-IV) Editorial Review (Pete Wallace)

Note: Jeff Dann, Cathy Foris, Cam Hubbard, Andy Roberts, Earle Ryba, and Pete Wallace are all working on this review

We are reviewing 141,000 M&A entries to assign prototype structures and Wyckoff sequences and correct any observed problems. We have reviewed about 25,500 entries to date. The next step is a quality check, and of the 25,500 entries, about 15,300 entries are in this phase. After the quality check, the review files are sent to Suri for his review and concurrence.

New/Old Business

A. M&A Test Problems (Cam Hubbard, Howard Jones and Pete Wallace)

We have been asked to develop M&A problems that are representative of what metallurgists might meet. These problems then would be used in ICDD courses and materials. At a recent meeting, we

- (a) have identified several possible M&A problem areas,
- (b) need to define/refine our ideas into problems, and
- (c) need to submit the problems to ICDD Headquarters for approval and use.

M&A members are encouraged to send their thoughts and ideas regarding M&A test problems (or for that matter any other agenda item) to Pete Wallace.

B. Additional editorial database locations for PSCI reviews

To facilitate this PSCI review and future reviews, we are working with Suri to have two additional editorial database locations for each entry:

- One will be an M&A empirical formula, and
- The other will be an M&A Z (number of formula units/unit cell).

When the entry has an assigned prototype structure, the M&A empirical formula will reflect the prototype structure's stoichiometry, and the M&A Z will equal the prototype structure's Z.

When a prototype structure cannot be assigned, the M&A empirical structure and Z will be the same as those editorial database's usual empirical formula and Z. At this time, neither of these new locations will be available in ICDD products.

C. Phase Descriptors (Suri Kabekkodu)

Suri requested that the usage of phase descriptors (e.g., Greek letters, etc.) be uniform.

Adjournment

The meeting was adjourned at about 11:30 am.

Attachment 1: The M&A Agenda for March 21, 2012

- 1 Call to Order
- 2 Appointment of Secretary
- 3 Approval of Minutes
- 4 Board of Directors Liaison Report (Ray Goehner)
- 5 M&A Web Area (Howard Jones and Pete Wallace)
- 6 The first edition of the M&A Electronic Tables for Editors has been produced, and it includes Prototype Structure Profiles. (Pete Wallace and Suri Kabekkodu)
- 7 Status of the Pearson Symbol Code Index (PSCI-IV) Editorial Review (Pete Wallace)
- 8 Review of Current M&A Patterns (Pete Wallace)
- 9 Report on the October 2011 M&A Working Group Meeting (Pete Wallace)
- 10 The M&A Working Group meets next before the 2012 DXC
- 11 New/Old Business
- 12 Adjournment