

Dos Arroyos

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memorandum

To: Distribution
From: Peter L. Wallace
Phone/fax/e-mail: (520) 878-9884/plw_dae@juno.com
Filename: M&A Minutes 03-09.doc
Date: April 18, 2009

Subject: Metals & Alloys (M&A) Subcommittee Minutes for March 12, 2009

Business Items

The meeting was called to order at 11 am. The agenda is on page 6, and the attendance list has been sent to ICDD Headquarters for archiving. Andy Roberts took meeting notes, and Pete Wallace wrote the minutes. The M&A Subcommittee minutes of March 2008 were approved as written.

M&A Working Group Meetings

The M&A Working Group met for four days (August 2-5, 2008) before the 2008 Denver X-ray Conference (DXC) and March 21 and 23, 2009 prior to the ICDD Annual Meeting. The focus of both meetings was to continue the PSCI-III review.

Upcoming M&A Working Group Meetings

1. **2009 Fall Meeting:** October 24-27, 2009 at ICDD Headquarters.
2. **2010 Spring Meeting:** Will be held the four days before the ICDD annual meeting.
3. **2010 Fall Meeting:** Will be held the four days before the regular sessions of the DXC. Note: At the 2008 DXC we had an isolated meeting room with the computers, etc. that were needed, the ICDD Editor-in-Chief was in attendance, and there were no distractions. As a result, we had one of our most productive meetings ever. Thus we are planning a repeat meeting. (ICDD Headquarters has been notified of our intent to meet before the 2010 DXC.)

Board of Directors Liaison Report

Ray Goehner reported on Board of Directors actions regarding last year's M&A motions.

At our last meeting, the M&A Subcommittee passed the following motions:

1. The M&A Subcommittee recommends to the Technical Committee that the *M&A Common Names List* be made available as a part of ICDD electronic products.

2. The M&A Subcommittee recommends to the Technical Committee that four display fields be moved from the PDF-4+ product's *Miscellaneous* tab to the *Crystal* tab, if possible. The fields are (1) the Pearson Symbol, (2) the Pearson Symbol w/o H, (3) the Prototype Structure, and (4) the LPF Prototype Structure.

The ICDD Board of Directors passed the first motion. As a result, the M&A common names are being placed in the common names field. The latter field can be used to produce the M&A Common Names List (select the M&A subfile and list the common names in the preferences module). These names will be available in the editorial files for Release 2009.

The ICDD Board of Directors did not pass the second motion. Instead, ICDD Headquarters will explore other options (possibly including PDF-4+ design changes) and report back to the Board.

M&A Web Page

The M&A Subcommittee would like to open this web page to the public. In order to do this, the M&A Subcommittee needs to:

1. Have the web page reviewed by ICDD Headquarters for any sensitive issues or materials.
2. Protect any sensitive areas.
3. Gain final approval from the ICDD Executive Director.

Action: Pete Wallace will make a formal request to ICDD Headquarters that the three steps be carried out.

Calculated Pattern Round Robin

No activities were reported.

M&A Electronic Editors' Book

The M&A subcommittee is working with Suri Kabekkodu, Terry Kahmer, and Joel Reid at ICDD Headquarters to produce various electronic tables aimed at helping the M&A volunteers in their editing. Pete Wallace issued a final copy of the specifications for the tables on May 29, 2008. The key difference between these tables and those that can be generated in PDF-4+ is that these tables will contain all entries, even those that are still in the ICDD editorial process.

While the current PSCI review (see the next section) is not complete yet, it has progressed to the point where the need for the new review tables can be foreseen. In a meeting this week, Pete, Suri, Terry, and Joel discussed what we needed to do.

Pete noted that the *Pearson Symbol Code Index* (PSCI) is the most important table with the three prototype structure tables being next in importance. He also said that M&A volunteers hope to be able to see at least an alpha test version of the PSCI at their fall meeting in late October 2009. Suri agreed to do this and possibly have test versions of some other tables, too.

Action: Pete Wallace agreed to send copies of the specifications for the tables as well as the priorities to Suri, Terry, and Joel.

Note: Pete Wallace requested that the following non-agenda item be added to these minutes.

In the above meeting, Pete Wallace asked Suri (a) what the process was and (b) how long it took to incorporate M&A volunteers' PSCI review comments into the ICDD master database. Suri said that once they had the electronic file containing the comments, it took about two days. Suri does a quick review of the comments focusing on the volunteers' notes and then the comments are added to the database. Most of the comments concern ICDD and LPF prototype structure assignments.

Status of the Pearson Symbol Code Index (PSCI-III) Editorial Review

Introduction:

1. This review uses Pearson symbol code index tables created in 2005 after a very large increase in the population of the M&A subfile occurred.
2. This review is the first review where M&A volunteers are working directly on electronic files and submitting their recommendations in electronic form first to the M&A subcommittee chairman for a quality check and then to ICDD Headquarters for approval and implementation.
3. The ICDD is adding about 7,000 to 10,000 entries to the M&A subfile each year. So, we have our work cut out for us. Fortunately, we believe that the work we have done (and will do) establishes a basis for automatically assigning prototype structures based on established *prototype structure profiles*. ICDD Headquarters is working on this possibility now. A caveat: Computer-assigned prototype structures still will need a review until we have confidence that the assignment is done correctly.

Status:

1. The team of volunteers grew by one (Ryba) at this meeting and now includes Harlan Clark, Jeff Dann, Catharine Foris, Andy Roberts, Earle Ryba, and Pete Wallace (chair). Note: Pete is responsible for the quality reviews as well as some of the initial reviews.
2. The task requires the review of about 101,000 M&A entries focusing on the addition of prototype structures and correction of (generally minor) database errors.
3. Microsoft Excel files in PSCI format are used for the review.
4. We use a two step review process: (1) An M&A volunteer does the first, or primary, review. (2) Then the chairman performs the quality assurance review.
5. As of today, 18,136 entries have gone through both reviews and have been sent to ICDD Headquarters; 29,104 entries have had the primary review and are awaiting a quality check; 33,174 entries are going through the primary review (i.e., are in-process); and 20,352 have not been started. (Please see page 7 for more details.)
6. Results and Comments: To date, about 97% of the M&A entries have assigned prototype structures. Many small errors have been corrected. When we complete this review cycle, we will have established a baseline for subsequent reviews that should make the future assignment of prototype structures easier whether the assignment is done manually or automatically with manual oversight.

Review of Current M&A Patterns

This review involves from 100 to 200 experimental patterns a year. Most of these patterns are from Grant-in-Aid recipients. We are current in these reviews.

1. Labeling Polymorphic Phases

Jeff Dann led a discussion on how the ICDD database should label polymorphic phases for the M&A subfile. At present, there is no clear guidance on this, leading to a situation where Greek letters, spelled-out Greek letters, phase designations such as rt, ht, and hp, and other designations (e.g., 6H, etc.) are used. The lack of a standard can lead to confusion. For example, in the table below, Jeff has compared the published and LPF designations for the same phase. For the most part, the published designations are what is used in industry while the LPF designations have the advantage of simplicity. Further discussion of these examples, as well as those that differ, will be needed before this subcommittee can make recommendations

Published	LPF Designation	LPF Prototype Structure
Alpha-Pu	Pu rt	Pu,mP16,11
Beta-Pu	Pu ht1	Pu,mS34,12
Gamma-Pu	Pu ht2	Pu,oF8,70
Delta-Pu	Pu ht3	Cu,cF4,225
Delta prime-Pu	Pu ht4	In,tI2,139
Epsilon-Pu	Pu ht5	W,cI2,229
Pu	Pu hp1	Cs,oP4,62
Pu	Pu hp2	Pu,hP8,176
Alpha-U	U rt	U,oS4,63
Beta-U	U ht1	U,tP30,136
Beta-U	U ht1	U,tP30,118
Beta-U	U ht1	U,tP30,102
Gamma-U	U ht2	W,cI2,229
U	U stab	Cu,cF4,225

2. M&A Subfile Sections

Secretary's comments: The principal use of the partitioning discussed below appears to be reducing the size of files that are edited by volunteers and submitted to ICDD Headquarters for approval and implementation. To date, that has not been a problem for the volunteers, and in many cases, it has helped to have all the examples of a prototype structure together, something that would not happen if the editing was on one of the subsections discussed below.

Suri Kabekkodu continued the discussion begun at earlier subcommittee meetings on the possibility of identifying subsections of the M&A subfile. Possible subsections could be:

1. Pure metals and alloys
2. Intermetallic compounds
3. Related phases
 - a. Sulfides, selenides and tellurides
 - b. Arsenides borides, carbides, hydrides, nitrides, binary oxides, and phosphides
 - c. All other phases

No action was taken at this time.

Adjournment

The meeting was adjourned at about 11:30 am.

Reference: M&A Minutes 03-09.doc

The M&A Agenda for March 25,2009

- 1 Call to Order
- 2 Appointment of Secretary
- 3 Approval of Minutes
- 4 Board of Directors Liaison Report (Ray Goehner)
- 5 M&A Web Page (Camille Jones)
- 6 Calculated Pattern Round Robin (Jeff Dann)
- 7 M&A Electronic Tables for Editors (Pete Wallace)
- 8 Status of the Pearson Symbol Code Index (PSCI-III) Editorial Review
(Pete Wallace)
- 9 Review of Current M&A Patterns (Pete Wallace)
- 10 Report on the August 2008 M&A Working Group Meeting at the DXC
(Pete Wallace)
- 11 New/Old Business
- 12 Adjournment

Reference: M&A Agenda 03-09.doc

Status of the Metals and Alloys (M&A) Pearson Symbol Code Index (PSCI) Review, Third Pass (PSCI-III)

Last update: April 6, 2009

Filename: M&A PSCI-III Review Status.xls

Volunteer	Crystal System	Pearson Symbol Codes	Entries	Status	Completion Date	Date Quality Review Complete	Date Submitted to ICDD
Andy Roberts	Anorthic	aP ...	682	Complete.	07/16/07	07/16/07	ca. 10/27/07
Pete Wallace	Monoclinic	mC... + mP...	6599	Complete.	ca. 7/1/06	07/13/06	7/13/06
Harlan Clark	Orthorhombic	oC... + oP ...	13,973	In process; two of four parts are complete.			
Andy Roberts		oF...	620	Complete.	07/26/06	09/26/06	09/26/06
Andy Roberts		ol...	1,852	Complete.	07/26/06	09/26/06	09/26/06
Andy Roberts	Tetragonal	tl...	10,806	Complete. Need PLW QA review.	03/10/08		
Harlan Clark		tP...	3000	Complete.	07/21/07	3/24/09	
Harlan Clark		tP...	3929	Complete. Need PLW QA review.	03/12/08		
Andy Roberts	Hexagonal	hP...	20,588	In process.			
Jeff Dann		hR...	5,613	In process.			
Not assigned	Cubic	cF...	20,352	Test set of 2000 to C. Foris on 3/21/09.			
Jeff Dann		cl...	4,369	Complete. Need PLW QA review.	07/21/08		
Pete Wallace		cP...	8,383	Complete	12/17/08	12/17/08	12/17/08
Pete Wallace	All Systems	Complete Incomplete Pearson Symbols	(photocomps)	Have not been requested yet.			
			Approximate total	100,766	[Includes unpublished patterns.]		