Dos Arroyos
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memorandum

To: Distribution
From: Peter L. Wallace
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Filename: M&A Minutes 03-11.doc
Date: April 2, 2011

Subject: Metals & Alloys (M&A) Subcommittee minutes for March 16, 2011

Business Items

Before and as an introduction to the M&A meeting, Pete Wallace thanked the many volunteers and Headquarters staff members for their help over the years in the editing of the M&A subfile. Please see Figure 1 for a list of (hopefully) all who have helped.

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 2010 were approved as written.

Upcoming M&A Working Group Meetings

1. **2011 Fall Meeting**: Tentatively, we will meet on October 23-26, 2011.
2. **2012 Spring Meeting**: Will be held during the four days before the ICDD annual meeting.

Board of Directors' Liaison Report

Jeff Dann reported on ICDD actions regarding three motions passed at the last M&A meeting. The text of those motions along with the ICDD response follows.

Motion 1: The Metals and Alloys Subcommittee recommends to the Technical Committee that for M&A phases Greek-letter formula modifiers (e.g., alpha-Al2O3, beta-Pu, alpha-Ti, etc.) as well as other commonly-used formula modifiers (e.g., 6H, 12R, etc.) (a) be added to the database and (b) be searchable. For the other commonly-used formula modifiers, M&A volunteers would create the needed list beginning with SiC, SiO2, and other similar phases and expand it as appropriate.

Response from the Science Department: Plans are to include Greek character searching capabilities in the 2011 release of DDView and DDView+.

Motion 2: The Metals and Alloys Subcommittee recommends to the Technical Committee that the Crystal Data cell axial ratios are made available in PDF-4+ through *Preferences*.

Response from the Science Department: Implemented in 2010 product.

Motion 3: The Metals & Alloy Subcommittee moves that the Technical Committee either:

1 Allow the Prototype Structure field to have multiple entries so that former prototype designations and Strukturbericht symbols can be added, *or*

2 Create a field called Other Prototype Structures that allow multiple entries.

Response from the Publication Department: Structure type formula table has been modified in the editorial database to incorporate multiple structure prototypes and their source. This will enable searching structure types, like "All Names Search," for compound names.

M&A Web Page

All needed documents have been supplied to ICDD Headquarters. The last step remaining to open this page to the public is a formal request to Headquarters and Pete Wallace did this recently.

M&A Electronic Editors' Book

The M&A Subcommittee is working with Suri Kabekkodu at ICDD Headquarters to produce various electronic tables aimed at helping the M&A volunteers in their editing. Suri has completed initial versions of these tables and has sent them to Pete Wallace to review, distribute and comment on as appropriate.

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

Introduction:

This review uses Pearson symbol code index tables created in 2006 after a very large increase in the population of the M&A subfile occurred. 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. 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 will still need a review until we have confidence that the assignment is done correctly.

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. Microsoft Excel files in PSCI format are used for the review. 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. Current M&A volunteers include Jeff Dann, Catharine Foris, Andy Roberts, Earle Ryba, and Pete Wallace (chair).

Status:

We are more than 90% done with the PSCI-III review, and the details are in Figures 2-10. About 95% (or more) of the reviewed M&A entries have assigned prototype structures, and many small errors have been corrected. As would be expected, the success rate is highest for the highest symmetry crystal systems.

When we complete the PSCI-III review in the Fall of 2011, 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.

As a part of this review, we are looking at the development of prototype structure profiles, and Figure 11 shows a portion of the table for tetragonal prototypes. The full table would also contain the range in lattice parameters and chemistry as well as the range in axial ratios. Lastly, Figure 12 shows our plans for future reviews and the increasing scope of them. It is clear that we have a lot to do.

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 currently reviewing the latest package.

Report on the August 2010 and March 2011 M&A Working Group Meetings

The M&A Working Group met both before the 2011 DXC meeting and just before this meeting. Work continued on the PSCI-III review with the results shown in Figures 2-10.

New/Old Business

1. Overseas M&A members:

Pete Wallace asked the audience and in particular the Regional Co-Chairs how this subcommittee might get more involvement from overseas M&A members. After a lively discussion, the following suggestions and comments were received.

- Use teleconferencing if practical.
- Use member surveys carried out by Headquarters. (We supply the questions. For example, do M&A members know about what data and features our editorial efforts have added to the database?)
- Use a newsletter to highlight new features, data, and uses of the M&A subfile.
- Contact the ASM again to see if they have an interest in becoming a cooperating society.
- See if other ICDD subcommittees and task groups want to collaborate with us. (The Battery Materials Task Group may be interested.)
- Initiate a general discussion on involving overseas members at an upcoming Technical Committee meeting

2. New M&A Working Group Member

The M&A working group is pleased to add Cam Hubbard as a member. Cam will be added to our e-mail list and will be welcome at our next meeting in October 2011.

Adjournment

The meeting was adjourned at about 12:00 pm.

Reference: M&A Minutes 03-10.doc

Attachment 1: The M&A Agenda for March 16, 2011

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 (Pete Wallace)
6 M&A Electronic Tables for Editors / Prototype Structure Profiles (Pete Wallace and Suri Kabekkodu)
7 Status of the Pearson Symbol Code Index (PSCI-III) Editorial Review
8 Review of Current M&A Patterns
9 Report on the August 2010 M&A Working Group Meeting
10 M&A Working Group meets next at ICDD Headquarters in October 2011
11 New/Old Business
12 Adjournment

Reference: M&A Agenda 03-11.doc

Figure 1 **lists the many people and groups that have helped in PSCI reviews. We thank all of you!**

M&A Subcommittee	**Headquarters**
Mike Bennett	Vesna Bosnic
Larry Calvert	The DXC staff who have met our every need, every time.
Harlan Clark	Janet Grande
Jeff Dann (*)	Mark Holomany
Cathy Foris (*)	Suri Kabekkodu (*)
Ludo Frevel	Terry Kahmer
Ting Huang	Monika Kottenhahn
Jerry Johnson	Lisa Lanno
Camille Jones	Frank McClune (*)
Howard Jones	Joel Reid (*)
Mel Mueller	Joe Sunzeri
Andy Roberts (*)	Chuck Weth
Earle Ryba (*)	
Pete Wallace (*)	

(*) Currently active in PSCI reviews

***Figure 2* shows a summary of all work on M&A entries.**

All Crystal Systems	Pearson Symbol Codes	Entries
Totals	90.2%	90,860

(*) Of a total of 100,777

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
1,148	57,927	41,483
1.3%	63.8%	45.7%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
1,001	2,297	3,319
1.1%	2.5%	3.7%

***Figure 3* shows a summary for the M&A anorthic entries.**

Crystal System	Pearson Symbol Codes	Entries
Anorthic	aPn	682

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
3	348	352
0.4%	51.0%	51.6%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
4	123	186
0.6%	18.0%	27.3%

***Figure 4* shows a summary for the M&A monoclinic entries.**

Crystal System	Pearson Symbol Codes	Entries
Monoclinic	mPn and mCn	6,599

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
200	3,288	2,848
3.0%	49.8%	43.2%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
147	595	985
2.2%	9.0%	14.9%

***Figure 5* shows a summary for the M&A orthorhombic entries.**

Crystal System	Pearson Symbol Codes	Entries
Orthorhombic	oPn, oCn, oIn and oFn	16,445

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
260	10,215	8,690
1.6%	62.1%	52.8%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
233	543	758
1.4%	3.3%	4.6%

***Figure 6* shows a summary for the M&A tetragonal entries.**

Crystal System	Pearson Symbol Codes	Entries
Tetragonal	tPn and tIn	17735

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
245	10,960	8,228
1.4%	61.8%	46.4%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
219	336	501
1.2%	1.9%	2.8%

***Figure 7* shows a summary for the M&A hexagonal-primitive entries.**

Crystal System	Pearson Symbol Codes	Entries
Hexagonal	hPn	20,588

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
275	13,429	9,239
1.3%	65.2%	44.9%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
241	380	460
1.2%	1.8%	2.2%

***Figure 8* shows a partial summary for the M&A hexagonal-rhombohedral entries. The work on these entries should be complete by the Fall of 2011.**

Crystal System	Pearson Symbol Codes	Entries
Hexagonal	hR17 to hR700	2,059

(*) Of a total of 5,613

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
22	1,250	1,210
1.1%	60.7%	58.8%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
23	73	159
1.1%	3.5%	7.7%

***Figure 9* shows a partial summary for the M&A cubic F-centered entries. The work on these entries should be complete by the Fall of 2011.**

Crystal System	Pearson Symbol Codes	Entries
Cubic	cF3 to 8; cF8 to 56	14,000

(*) Of a total of 20,355

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
11	9,852	5,572
0.1%	70.4%	39.8%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
7	27	31
0.1%	0.2%	0.2%

***Figure 10* shows a summary for the M&A cubic primitive and I-centered entries.**

Crystal System	Pearson Symbol Codes	Entries
Cubic	cPn and cIn	12,752

Before		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
132	8,585	5,344
1.0%	67.3%	41.9%

After		
No space group	**No M&A prototype structure**	**No LPF prototype structure**
127	220	239
1.0%	1.7%	1.9%

Figure 11 **shows some examples of prototype structure profiles. M&A volunteers are working with ICDD editors to produce expanded versions of this table covering all prototype structures used in the M&A subfile.**

LPF formula	PS	SG	Examples	c/a (low)	c/a (high)
U Ge Te	tI12	139	115	3.63	4.362
Cu Al2	tI12	140	370	0.738	0.891
Th Si2	tI12	141	309	3.09	3.652

In *Figure 12* we discuss the next step in our ongoing review and quality upgrade of the M&A subfile.

The fourth iteration (PSCI-IV) of the PSCI reviews is next.

It will cover many more entries than the 100,777 entries in the current review, because
(a) many of those entries have been replaced by LPF entries, and
(b) we have been adding new entries at a rapid rate.

Bottom line: There is a lot for us to do.

Notes:

1. Suri is producing the PSCI-IV listings for us now.
2. Because each review is a snapshot in time of the M&A file, there will be subsequent PSCI reviews.