# Metals & Alloys Subcommittee Zoom Meeting - Minutes Wednesday, 20 January 2021

# 11:00 am - 12:00 pm

# P. Wallace, Chairman

#### 1. Call to Order P. Wallace

The meeting was called to order at 11 am.

# 2. Appointment of Minutes Secretary – Michael Carr

#### 3. Approval of Minutes of March 2019

Moved: P. Wallace Second: A. Roberts

Minutes were unanimously approved.

#### 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, (4) extending the coverage and usefulness of the metals and alloys subfile, and (5) maintaining a web page to communicate with members and other materials scientists.

#### 5. Board of Directors' Liaison Report

A. Payzant

The board liaison should remind the chair that in order for a motion to move forward, a task group (or leader) needs to be assigned and named within the motion.

### 6. Update on the PDF Phase Diagram Capability

Discussion on this postponed until group can meet in person.

#### 7. M&A Prototype Structure Profiles, an update

Please contact headquarters or P. Wallace for further detail on MA Subcom. VGs January 2021-R.pptx

#### 8. The M&A prototype structure tables contain 8,974 entries

up from 8,307 last year, and are on the M&A web page.

Please contact headquarters or P. Wallace for further detail on MA Subcom. VGs

January 2021-R.pptx

# 9. M&A Working Group Activities

Please contact headquarters or P. Wallace for further detail on MA Subcom. VGs January 2021-R.pptx

#### 10. M&A Editor's report

Please contact headquarters or P. Wallace for further detail on MA Subcom. VGs January 2021-R.pptx

#### 11. Old Business

Discussion took place regarding Parthe cell. S. Kabekkodu says the Parthe program is not commercially available. There is one program called Platon, but its use is limited when it comes to Parthe cell.

#### 12. New Business: Standard Z's and Formulae

P. Wallace

**Motion 1:** The M&A Subcommittee moves to the Technical Committee that the M&A Z and M&A Empirical Chemical Formula be relabeled as the Standard Z and Standard Empirical/Chemical Formula.

- (1) In the vast majority of cases, both the M&A Z's and M&A empirical/chemical formulae are based on critically-reviewed prototype structures, and we have adopted the Z and chemical/empirical formulae of the prototype structure.
- (2) In a very few cases, the Z and empirical/chemical formulae are based on atomic volumes, the authors' cell, and the authors' assigned crystal system.

**<u>Discussion:</u>** S. Kabekkodu says this already exists in Powder Diffraction File, but motion was put forth anyway. Motion may not be applicable with further exploration of database designation.

Moved: P.Wallace Second: J.Dann

Unanimously approved.

S. Kabekkodu mentioned that we are getting many prototype structures from ICSD and we need unified structure types for proper mapping to Linus Pauling File. Not for 2022 Release, but in a future release Suri would like parameters of this unification to be decided.

## 13. An announcement: Next Working Group meeting TBD

Cautiously optimistic for an in-person meeting in October.

#### 14. Adjournment