X-ray Fluorescence Subcommittee Meeting Minutes

Wednesday, 14 March 2018
International Centre Headquarters
Conference Room D
10:00 a.m. – 11:00 a.m.
Mark Rodriguez, Chairman

1. **Call to Order**
   Chairman, **Mark Rodriguez**, called the meeting to order and the attendance list was distributed for signatures; list is on file at headquarters.

2. **Approval of 2017 Minutes**
   2017 minutes were reviewed. A motion to approve was made by **Mark Rodriguez**. The motion was seconded by Tim Fawcett, and a vote was taken:
   Yes-6 No-0, abstain-0-. The minutes were approved unanimously.

3. **Appointment of Minutes Secretary**
   D. Zulli was appointed as Minutes Secretary.

4. **Review of Mission Statement**
   M. Rodriguez read the mission statement to the committee:

   The X-ray Fluorescence Subcommittee will provide recommendations for X-ray Fluorescence to be a complement to both the PDF and ICDD. This entails synergistic interchange between data collected from XRD and XRF:

   - Use of chemical composition to support powder diffraction analysis
   - Ability to improve chemical composition by use of the powder diffraction
   - To ultimately obtain simulated XRF data as a means of material analysis validation such as refinement of data from multiple analytical methods

   In addition, the subcommittee shall develop new educational opportunities for ICDD and offer guidance on addressing elemental composition issues which are of strategic interest to ICDD.

   The committee had no changes to the mission statement.

5. **Board of Directors' Liaison Report**
   Xialong Chen reported that no motions were made last year.

6. **Discussion Regarding Import of Data**
   Dave Taylor, Tim Fawcett and **Mark Rodriguez** discussed what import ideas should be sent to the Technical Committee. Discussions led to the conclusion that the simulation idea is difficult, and that importing data through *.csv is already possible. You can already input from an excel spreadsheet with a simple cut and paste.

   Tim F. gave a summary to the committee of what has been done in the past two years. Justin has created an algorithm that has been tested against the Smithsonian standard sets and it worked out beautifully.

   There are some practical limitations, one is light elements, and light element detection. Another limit is the practical nature of the experimental data that we're using both on the XRF side and what's in our references. Overall, that process is pretty good. One of the goals was to figure out what the limit is. If you follow the rule of not mixing your formats (either entering all oxides or all elements but not both), you'll get great results. But those rules aren't obvious so you may or may not have success. Tim has written a paper on the necessary rules to achieve great results and will send copies to members of the committee.

   The end goal is to marry XRD and XRF results. You want the microanalysis to somehow communicate with the database. **Justin Blanton** informed the committee what the user can currently do to attain both results. Mark commented that the product is already half way to where we are going.

   Tim gave a PDF-4^{+} demonstration on the screen.

7. **New Features/Changes**
   Dave Taylor asked, what are the major changes from 2018 to 2019? **Justin Blanton** described the new features, including customized display fields on the search results. Cyrus Crowder asked for clarification regarding the current single phase and the steps to attain multi-phase. Tim supplied an explanation.

8. Motion

MOTION:

The Chairman of the XRF Subcommittee recommends to the Chair of the Technical Committee the following motion:

Merge the search match method in Sieve on XRD data with the chemical analysis data read into the database via a *.csv file. Report back to the subcommittee in one year concerning the effectiveness of using this multidimensional search procedure. Consider a light element filter for data collected systems that have limited chemical diagnosis (XRF). We desire a multiphase search/match capability for combined XRD/XRF by the release of the 2020 product.

Motion made by **Mark Rodriguez**, second by **Dave Taylor**, Vote: Yes- unanimous

Stacy Gates-Rector will act as the staff liaison to the committee.

9. New Business

Time did not permit the discussion of new business.

10. Adjournment