

X-ray Fluorescence Subcommittee Meeting Minutes

Wednesday, 15 March 2017
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. Appointment of Minutes Secretary

D. Zulli was appointed as Minutes Secretary.

3. Approval of 2016 Minutes

2016 minutes were reviewed. A motion to approve was made by **D. Taylor**. The motion was seconded by **P. Ricou**, and a vote was taken: Yes-6, No-0, abstain-0. The minutes were approved unanimously.

4. Review of Mission Statement

M. Rodriguez read the mission statement to the committee, which was modified at the last meeting:

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.

5. Overview of XRF Subcommittee's Progress

M. Rodriguez reported on the progress of the subcommittee from the past two years. In 2015, the subcommittee had an idea: To try and do phase identification with XRF composition alone. **T. Fawcett** took that concept and worked on a functional prototype which was tested at last year's subcommittee meeting. This year, it will be introduced as a new product feature. Concept to product in two years' time, thanks to this subcommittee.

D. Taylor commented that the feature does need some tweaking, which everyone agreed. **T. Fawcett** commented that there are at least three phases to this project, and only phase 1 had been completed. **D. Taylor** suggested there are two things that he would like to see:

- A. Slider for the ESD, rather than a set number
- B. And a "Maybe" instead of the "X"

Regarding the "Maybe" and the "X", **T. Fawcett** had already asked **J. Blanton** (Manager of Engineering & Design Dept.) to add a second scoring algorithm because he found a weakness in the first one. If the second scoring algorithm works the way he thinks it will, the "Maybe" and the "X" will not be needed because the second algorithm will take care of elements that you don't see. If it doesn't, then something more sophisticated will need to be used. Originally, **T. Fawcett** was thinking that an instrument profile may need to be added, but he no longer thinks that is necessary if the algorithms are written clever enough, it will do that automatically.

6. Board of Directors' Liaison Report

M. Rodriguez reported on the two motions that were sent to the board last year (2016) from the subcommittee:

- A. **M. Rodriguez** moved that headquarters develop a figure of merit algorithm for XRF data to be used for phase identification.

***BoD Response:** Engineering & Design Department – XRF phase identification has been added to the scheduled list of new features and will be discussed at the new features meeting. Fawcett will provide the algorithm to the E&D Dept.*

Today's Update: This has been done. **T. Fawcett** had started vigorous testing about two weeks ago and found some holes in the algorithm, and is now working with **J. Blanton** on the second algorithm. Algorithm 1 still provides good data and should be kept as well. The work is good enough to release in the new product, present at Denver X-ray

Conference and publish in the proceedings, *Advances in X-ray Analysis*. Two more phases still need to be completed, which **T. Fawcett** will work on in his retirement.

- B. **M. Rodriguez** moved that a Fundamental Parameters (FP) database for XRF analysis be established using the currently existing “Elam FP database.” This newly created database would serve as a baseline repository to archive and incrementally enhance FP data for the purposes of improving quantification for XRF users, equipment manufacturers, and future ICDD projects requiring accurate FP tabulations.

***BoD Response:** Database Department – The ICDD Editor-in-Chief had a discussion with **T. Elam** at the Denver X-ray Conference regarding this request. **T. Elam** has provided the FP database test files for evaluation.*

Today’s Update: ICDD has been given the opportunity to obtain the Elam FP Database (the numerical values we need to simulate XRF data). There are many databases like this available, and one is held by **T. Elam**. The information is not copyrighted and **T. Elam** has offered it to ICDD for free. ICDD currently has the information and could potentially put this in the database for the purpose of simulating XRF patterns.

7. What is the next step for the Fundamental Parameters Database for XRF?

M. Rodriguez stated that he would like to use the information that ICDD now has in its’ database and take it to the next level. What we’re missing is each persons’ instrument parameter files that they would need to import into their system to be able to simulate. We would have to do this as a generic fluorescence pattern and then the question would be, is that of significant value or not? **T. Fawcett** responded that when discussing what we have today and this new concept, it’s actually two different thoughts. What we have today, we assume that the user is using someone else’s FP. **M. Rodriguez** stated that his ultimate vision would be to dump the raw data in from the PXRD and XRF and do the phase ID with both sets. Right now, we have something like a hybrid where raw data can be imported. It’s not a DI list, but effectively we have a DI list from the XRF which is a composition of elements, however, they’re not married, and do we know the steps to marrying it? **T. Fawcett** then gave a live hands-on demonstration of the new database features.

M. Rodriguez decided that making a motion at this time would be premature, which the subcommittee agreed. **T. Fawcett** volunteered to write a “white paper” proposal of the next one or two steps for the Subcommittee to review. The BoD will then receive the proposal to review at their Fall meeting.

No motions were made.

8. Adjournment