

## Minutes of the March 2009 ICDD Non-Ambient Diffraction Subcommittee Meeting

Meeting was called to order by Andrew Payzant. Joel Reid agreed to record the minutes.

The minutes of last meeting (March 2008) were read by A. Payzant, and accepted.

ICDD Board of Directors Liaison (J. Kaduk) reported on the motion from 2008 regarding "...development of non-ambient data from important materials in increments appropriate for the non-ambient behaviour of the material." As reported by J. Kaduk, the response from the Publication Department was: "S. Kabekkodu added technologically important materials to the grantee wish list. A. Payzant is working on a list to include also." Discussion followed. A. Payzant's list has not yet been completed/submitted to ICDD. Further, S. Kabekkodu's list could not be located by J. Kaduk, and the current grantee cycle does not include ANY non-ambient series.

There was consensus that there was a need to draft some recommendations regarding calibration of non-ambient systems.

The Chair reviewed the subcommittee membership, mission statement, and noted the increase in non-ambient entries in the PDF. Upcoming activities include a phase transformations session at the ACA 2009 Meeting, and (so far) a single time-resolved high-temperature XRD paper at DXC 2009. It was also noted that the number of "non-ambient" entries in the PDF has increased by an order of magnitude from PDF-4+ 2007 to PDF-4+ 2008.

A suggestion to pursue a special issue of Powder Diffraction dedicated to non-ambient XRD met a positive response from all in attendance. The possibility of a "feature paper" possibly coming out of the workshop and sessions from the last DXC 2008 was also discussed. The importance of capturing and disseminating information from the ACA 2008 and DXC 2008 meetings was discussed, and it was suggested that the ICDD website might facilitate this.

The importance of capturing thermal expansion data (where available) in the comment field of the PDF was discussed. Some discussion of how best to incorporate new useful non-ambient data into the PDF followed, coupled with a concern to avoid incorporation of unnecessary data. The need for high-temperature patterns to facilitate search-match was clear, but as in past years, there was concern about overloading the file with closely similar patterns. There was discussion of distinguishing ambient data on non-ambient phases from data collected under non-ambient conditions.

B. Toby suggested there was a need to add another dimension to the relational database to accommodate multiple data for temperature, pressure, etc., in a single card. M. Bennett pointed out that in addition to T, P, other parameters may need to be considered – examples being atmosphere and humidity.

P. Wallace would like to see thermal expansion curves (equations and scanned plots) included in the PDF when available.

New motions proposed for consideration by the Board:

- Any pattern not collected under ambient conditions or that cannot be made (or be reasonable stable) at ambient conditions be flagged as non-ambient.  
Motion made by J. Cline. Second by M. Rodriguez.  
Motion subsequently withdrawn following discussion.
- **The ICDD is requested to explore the concept of a new dimension on a card to link a series of experimental patterns at different temperatures and/or pressures. This might permit non-ambient data to be captured without the need to add unique cards.**  
**Motion made by J Cline. Second by M. Rodriguez.**  
**Motion unanimously approved.**

A recommendation was made to form a Task Group under the Technical Subcommittee Chair (A. Payzant). This Task Group will identify and recommend to the ICDD clarifications on what is meant by non-ambient data versus non-ambient materials, e.g. quenched samples, metastable phases, etc. Members of this task group have not been assigned at this time.

Motion to adjourn followed.