

Non-Ambient Subcommittee Meeting Minutes
Wednesday, 14 March 2018

Chair: Andrew Payzant

Minutes Secretary: Rick Santangelo

Call to Order

Review of Subcommittee Mission Statement

Approval of 2017 minutes (A. Payzant/S. Misture/unanimous)

New Business

1. Discussion on the need to develop standards in terms of reference materials, SRM standards and or best practice guides for high temperature alignment calibrations. This subject is, and should be, a concern for the Non-Ambient Subcommittee. The challenge is that we typically get data recorded at a very high accuracy. Accuracy can be disputed because typically the temperature isn't good to anything near the number of significant figures quoted. The problem not only exists in X-ray, but it's even a larger problem in the neutron world. Non-ambient includes pressure and the same issues apply to pressure standards. **Question:** What reference materials and/or best practices for diamond anvils and other pressure cells? For those who have not done diamond anvil cell before, ruby is often used as a standard. The lattice parameter of a ruby is taken as representing the pressure which is good to +/- .00001 bar. The actual error bars in the non-ambient parameter are much larger than what is represented in the lattice parameter of X-ray data.
2. New chair for the Non-Ambient Subcommittee:
The timeline for appointing a new chair would be next year. No members offered to accept the appointment at this time.
3. Winnie Wong-Ng suggested adding a negative thermal expansion materials class to the PDF. **Questions:** How are we going to work with that? Are we accurately capturing the needed thermal expansion data in order to make that class meaningful? **Comment:** Typically, these materials are only negative thermal over a limited range of temperatures. There are all sorts of issues to consider. There are other materials that are zero expansion as opposed to negative expansion – include these? **Question:** What about non-ceramics that have this similar behavior? **Question:** What about meta-stability as a general category? **Comment:** Historically, the comments field has been used to capture this information. There are questions as to how helpful and visible this solution is for the user?
4. Denver X-ray Conference will include a workshop/session by Scott Misture. It was suggested that this workshop could be used to aid in the development of the standards (Item #1) by capturing aspects of the workshop in either a PDJ article or an ICDD-published guideline. **Motion #3:** The Non-Ambient Subcommittee recommends to the Technical Committee that ICDD provide financial support for a task group meeting at DXC2018 to organize writing of a PDJ review paper on non-ambient diffraction methods and best practices
5. A request was made to the committee members to submit an abstract by Friday, March 16th to DXC.
6. Discussion of meta-stability - It was suggested that parsing of this is systematic non-ambient vs. incidental non-ambient. It was noted that dehydration processes are not systematically controlled, that materials such as sodium phosphate dodecahydrate can be affected by the atmosphere in different parts of the country. Temperature, pressure and humidity can play a factor during the acquisition of data. An effort needs to be made to note these factors. Sometimes a gas may be introduced that brings about a different condition. In certain cases, X-ray and electron beams can trigger a transformation of the material from a metastable phase. There may be some "low hanging fruit" susceptible classes, such as the battery cell and hydrates. There may be materials such as oxides that are more stable than other classes of material and less susceptible to unintended transformation.

Question: Is there enough contribution in the database to take this up at this point?

Question: How do we capture radiation damage?

Answer: In principal, samples that have experienced radiation damage can be captured by putting a full sample description in the comments field. The problem is that this rarely happens. This is a larger problem with the Grant-in-Aid patterns.

Motion #1: The Non-Ambient Subcommittee recommends to the Technical Committee that Headquarters encourage including submission of new non-ambient data with complete details of procedures and conditions and that they be documented in the PDF.

Motion #2: The Non-Ambient Subcommittee recommends to the Technical Committee that Headquarters identify materials (including unstable and reactive materials) for which the diffraction data is deemed likely to be highly sensitive to measurement conditions such as ambient humidity, partial pressure of oxygen, etc. Once such materials are identified there is an opportunity to evaluate whether additional warnings need to be recorded in the PDF.

The meeting was adjourned at 4:33 PM