

**Polymers Subcommittee Meeting Minutes**  
**Wednesday, 15 March 2017**  
**International Centre Headquarters**  
**Conference Room D**  
**1:00 p.m. – 2:00 p.m.**  
**L. Liu, Chairman**

1. Call to Order and Opening Remarks L. Liu
2. Appointment of Minutes Secretary Stephanie Jennings
3. Roll Call and Attendance

Attendance sheet is on file at ICDD Headquarters.

4. Review of Mission Statement

Enable the polymer scattering/diffraction community to make the best use of diffraction/scattering data for analyzing polymeric materials. This includes producing databases, promoting best practices for data analysis, campaigning the national laboratories and instrument manufacturers for polymer-friendly instrumentation and software, and educating the diffraction community about issues that have a special impact on polymer characterization, and the polymer community on the significance of careful and thorough evaluation of the diffraction data.

5. Approval of the 2016 Meeting Minutes

Misprint – Jeff Dann needs to be changed to Jeff Deschamps in two places in paragraph four, under “Status of Polymer Activity and Discussion”. Stephanie Jennings will submit change to Linda Shertz.

Approved – 7-0-0

6. Report of Board Liaison

J. Kaduk

J. Kaduk reports that in the current release of the database, there is an orientation distribution function for the calculation of 2D patterns that showed up in the new release. J. Kaduk has used it a few times and it seems to work well. It leads to the next logical step, which would be to calculate a fiber pattern. J. Kaduk asked the group if they knew of a decent program to use to calculate a fiber pattern. L. Liu said he knows of someone at Stonybrook that does a lot of work in simulation. L. Liu said he could get in touch with him to see what software he uses to calculate a fiber pattern. Discussion followed about different settings you can use in order to calculate the pattern.

7. Status of Polymer Activity

L. Liu

S. Gates-Rector displayed a chart with each of the 14 new polymers by PDFID, and name. L. Liu asked T. Blanton if he saw any difference between PEG, when compared to PEO. T. Blanton reported that with the PEG, it was a low molecular weight material that depending upon how you were handling it, it did not take much until it turns to liquid. You have to get the molecular weight up a little bit before you see a crystalline pattern.

T. Blanton reported that all of the new polymer information was collected on ICDD’s new D2 Phaser that is in ICDD’s lab now.

J. Deschamps asked T. Blanton if he is thinking about collecting field objects to put in the diffractometer. T. stated that we are not currently set up to do that now, but we would like to in the future.

L. Liu began a report on the Evaluation of Principle Residual Stress in Rigid Semicrystalline

Polymers. He said it is an important issue for engineering polymer applications. It has challenges though, including, a large fraction of amorphous phase diffraction at low angle range. You cannot simply borrow the method for metallic plates. Currently, you have to use the hole drilling method. Residual stress in a crystal region can be much larger than in an amorphous region. A rigid crystal network is then formed in the material. Strain in the crystal region is all we can get from X-ray diffraction. For uniaxially oriented PP film, the crystal orientation correlates well with the direction of maximum principal residual stress. For principal Residual Stress in Bi-axially Oriented PP film, both the modulus and the shrinkage of the films show a good correlation with principal residual stress obtained with our approach. Shrinkage: The principle stress is preferably aligned toward TD direction (final stretching).

J. Kaduk reported that they are getting ready to start production on Volume H of the International Tables of Crystallography. The online and book version will not have a chapter on polymers because the information they received was not accepted. J. Kaduk asked for recommendations for an author to write a chapter for the next edition.

## 8. Future Focus

T. Blanton reported that ICDD Staff is going to continue working on adding high volume polymers into the database. S. Gates-Rector will continue to work on the 2D Detector project to collect polymer data to add to the database.

## 9. Adjournment

Meeting adjourned at 2:05pm