Meeting of the COMPTECH TAB of Jan 15 2015

Participants of the meeting included:

- Jay Bass (COMPRES, University of Illinois)
- Quentin Williams (University of California, Santa Cruz)
- Guoin Shen (Carnegie Institution of Washington)
- Yanbin Wang (University of Chicago)
- Lars Ehm (Stony Brook University)
- Robert Downs (University of Arizona)
- Przemyslaw Dera (University of Hawaii)
- Jin Zhang (University of Hawaii)

Dera presented a short summary of the COMPTECH activities in 2013 and introduces the new COMPTECH Technology Officer, Jin Zhang.

Zhang presented a plan of proposed activities for 2015. Two major development projects and two experimental technology improvement side projects have been described:

Thermal Diffuse Scattering (TDS) for measuring single-crystal elasticity:

X-ray thermal diffuse scattering (TDS) is caused by lattice thermal vibrations (phonons). In contrast to sharp Bragg diffraction peaks, TDS is diffusely distributed, due to the continuous distribution of phonon modes in the reciprocal space. It has been used for determining phonon dispersion relation of materials under ambient condition, but its application to high-pressure mineral physics has not been widely recognized.

Suggestions from TAB include:

- 1. Investigation of temperature (T) effects to TDS signal is important. Evaluation of the high T limit of this technique is necessary.
- 2. Establishment of robust data acquisition and analysis procedure is important.
- 3. Benchmark experiment is necessary. It's better to start with well-defined samples, for example, MgO, which is a well-defined pressure standard and its high-pressure single-crystal elastic properties have been measured using other techniques (e.g. Brillouin).
- 3. Organize future workshops on TDS, not only for teaching and training purpose, but also for seeking assistance.
- 4. HPCAT has tried TDS at high pressures before, seeking advice and collaboration with HPCAT should benefit the project.
- 5. For real samples, we need to consider separating effects other than TDS, e.g. signals from local ordering, defects etc.

Multigrain Analysis (MGA)

Reliable analysis of data from high-pressure experiments that involve samples in-between the single crystal and powder state has been very high on the wish list of mineral physics researchers for several years. Typical high-pressure samples synthesized within diamond anvil cell contain multiple homogeneous single crystal grains on a micrometer scale with mixture of phases present (e.g. untransformed starting material). Structure and properties (e.g. oxidation state) of these grains can be evaluated using multigrain diffraction (monochromatic or Laue).

Suggestions from TAB include:

1. Collaboration with HPCAT will be beneficial, not only with software development, but also sample synthesis procedures.

2. Software development with professional software engineers is possible.

Universal membrane cap for DAC pressure remote control:

Membrane-driven DACs are ideal for synchrotron experiments. With membrane caps, each conventional screw-driven DAC is transformed into a membrane-driven DAC, and pressure inside DACs could be controlled remotely. However, each type of DACs would require a specifically designed membrane cap. Having a universal membrane cap that fits most DACs could benefit the whole COMPRES community. This project is a side project related to the proposed two major development projects: TDS and MGA.

Suggestions from TAB include:

- 1. It is essentially a side project; we have to make sure it will not be a time sink.
- 2. The use of universal membrane cap can be good for high-pressure user facilities hosting users, e.g. high-pressure beam lines at APS, ALS, NSLS-II.

Cost-effective Heater for DAC:

Traditional Pt-ceramic heaters for DACs are very expensive, in general not reusable and their performance is not sufficiently reproducible. Commercial W-Al₂O₃ heaters sealed within evacuated ceramic capsules can reach 1000 K within 30 s and are very stable. Power curves of such heaters are reproducible between different heaters in different runs. Our plan is to redesign the commercial W-Al₂O₃ heaters for low-medium temperature (300-900K) high-PT DAC experiments.

Suggestions from TAB include:

- 1. For preliminary testing, all data has to be well documented.
- 2. It is better for us to explicit on what T range we plan to work on.
- 3. It is also possible to consider working on graphite heater and collaborating with ALS in the future if higher temperatures are desired.
- 4. Similar to Membrane project, we have to make sure it will not occupy too much time.

In addition to the above projects Zhang also presented plan for update and expansion of the content of the COMPTECH website, which mainly related to updates in the "tools" session. Including a relatively complete list of software tools for high-pressure mineral physics study would be very helpful for researchers, especially for beginning graduate students.

Suggestions from TAB include:

- 1. For COMPTECH website, we could consider adding new sections, and making advertisement for possible future techniques, and the progress of the techniques under development.
- 2. Advertise COMPTECH webpage more, e.g. on COMPRES homepage.

The members of the TAB expressed their opinions and advice about the proposed plan, which were generally very positive, and approved the proposal without vote.

Notes taken by J. Zhang and P. Dera.