Meeting of the COMPTECH TAB of May 28 2015

Participants of the meeting included:

- Andy Campbell (University of Chicago)
- Quentin Williams (University of California, Santa Cruz)
- Guoin Shen (Carnegie Institution of Washington)
- Lars Ehm (Stony Brook University)
- Robert Downs (University of Arizona)
- Przemyslaw Dera (University of Hawaii)
- Jin Zhang (University of Hawaii)

Zhang presented the COMPTECH activities from Jan. 2015 to May, mainly focused on thermal diffused scattering for measuring single-crystal elasticity. Dera introduced the ongoing software development for multi-grain analysis.

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

Work finished during 01/2015-05/2015:

1. Finished TDS measurement of Si (100) (111) and MgO (100) plane under ambient condition
    a. Surface truncation scattering from ultra-fine surface of Si single crystals is observed in addition to the TDS signal
    b. TDS signal is even more sensitive to the crystal quality than single crystal X-ray diffraction
    c. MgO (100) crystal quality poor, the crystal mosacity is ~1.5°, therefore not suitable for TDS measurement.
2. Finished TDS measurement of Si (100) under high pressure (~1.4 GPa) and ambient temperature
    a. Bragg peaks are significantly broadened at high pressure
    b. Additional features near Bragg peaks shown up
    c. No single-crystal elasticity of Si were measured under high pressure, therefore no comparison could be made
3. Experimental setup
    a. Experiements using regular single crystal diffraction setup have been tested using Mar CCD detector, the data were collected for Si (100) plane, resolution is lower than Pilatus detector.
    b. Using flight path +Pilatus detector set up, which was used for surface scattering experiments, could decrease background and enhance signal resolution a lot. Dr. Dongzhou Zhang helped on build up a robust calibration procedure for the detector in 13BMC.
4. Software development
    a. Calculation of TDS signal based on known hkls:
        i. Micro-force-constant model : Fortran code developed by Dr. Ruqing Xu, material-dependent
        ii. Macro-single crystal elasticity model: Python code developed by Dr. Jin Zhang, material-independent
    b. Linear inversion of elasticity model based on known hkls and measured TDS signal: Python code developed by Dr. Jin Zhang
5. Preliminary testing result:
    a. Micro-force-constant model and macro-single crystal elasticity model yield to very similar Cijs, suggesting the two calculation approaches are equivalent to each other.

b. Uncertainly in determining sample orientation has a large effect on the final inversion result.
c. Only Cij ratios could be determined accurately.
d. The experimental uncertainty is within 5%.

Suggestions from TAB include:

1. Crystal quality could be enhanced with laser annealing; usually higher quality crystal could be obtained after laser heating.
2. MgO crystal quality could be a concern, from doing a benchmark experiment point of view, maybe other materials could be better, e.g. corundum, garnet, foresterite.
3. In order to get absolute values of Cijs, bulk modulus derived from equation of state could be helpful.
4. Softwares and updates will be posted on the COMPTECH website once it's finalized.
5. Advertise this technique more during the COMPRES annual meeting.

Multigrain Analysis (MGA)

Work finished during 01/2015-05/2015:

1. Experiments and methodology
   a. Conducted 2 GUP experiments (February and April) at HPCAT 16IDB involving elements of multigrain/time resolved techniques:
      i. oFs100 single crystal (ambient temperature + resistive heating)
      ii. oFs100 single crystal + multigrain
      iii. cFs100 single crystal
      iv. CaSiO3 wollastonite single crystal + multigrain (ambient temperature + laser heating)
   b. Worked on automated rastering technique in data collection
2. Software: fully automated data processing for single crystal X-ray data using GSE_ADA

Suggestions from TAB include:

1. Collaboration with HPCAT, a group discussion should be held once in a while.

Universal membrane cap for DAC pressure remote control:

Work finished during 01/2015-05/2015:

1. Initial design and modification after discussion with University of Hawaii HIGP machine shop
2. Ordered pressure controller from GE.

Suggestions from TAB include:

1. 1. Keep track of the timing and purchase.

Cost-effective Heater for DAC:

Work finished during 01/2015-05/2015:

1. Preliminary testing: Power curve on sample heaters with ID 4mm and 6-10 Ohm resistance.
2. Solved problem of uneven heating by stacking two heaters together.
3. All testing procedures and results were uploaded onto COMPTECH website.
4. Received the updated model with ID 6mm and 1-2 Ohm resistance.

Suggestions from TAB include:

1. Advertise more, probably during the annual meeting or through COMPRES mailing list.

2. More tests need to be made with DACs.

Website development:

Work finished during 01/2015-05/2015:

1. Reorganized most parts of the COMPTECH website, adding more pictures and sections, including two sections specifically related to new technical development and technical advisory board.
2. New software tools added to COMPTECH website.

Suggestions from TAB include:

1. Timeline of the COMPTECH project status is recommended to add to the website.

The members of the TAB expressed their opinions and advice, generally very positive, and the TAB chair Quentin suggested a gather-together meeting for the TAB members during the COMPRES annual meeting.

Notes taken by J. Zhang and P. Dera.