High Pressure Neutron Scattering at the Spallation Neutron Source

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In situ high pressure neutron scattering is very useful for the characterization of materials and their behaviors under extreme conditions. Neutron diffraction can be used to determine elemental stoichiometries and atomic positions of light elements and can also be used to directly determine magnetic structures. Neutron spectroscopy can measure dynamics and can, for example, determine phonon dispersions or phonon density of states. Exploiting these capabilities for *in situ* high pressure studies s has, however, previously been limited in maximum pressures due to large sample volumes required. Recent developments at the Spallation Neutron Source (SNS) aim to overcome these limitations and I will highlight several ongoing developments here.

Neutron scattering is widely used to probe the phase behavior of quantum materials under ultra-low temperature (ULT) conditions down. Combining ULT conditions with high pressure has in the past been mainly limited to the use of piston-cylinder type cells (so-called clamped cells) that are limited to ~2 GPa in pressure. At the SNS we are addressing this pressure limit through coupling a large-volume neutron diamond anvil cell (DAC) equipped with polycrystalline anvils [1] with a dilution refrigerator. Here, I will detail *in situ* neutron diffraction experiments on Yb_2O_3 conducted at 6 GPa and 170 mK on SNS's SNAP high pressure diffractometer.

Next, I will detail high pressure neutron spectroscopy performed at the ARCS spectrometer in a Paris-Edinburgh cell up to 16 GPa. This will include insights into the necessary normalization steps required for meaningful data analysis. Interesting insights into the pressure-induced metallization of germanium and the subsequent formation of a useful metastable polymorph with desirable electronic properties are discussed.

Finally, I will highlight the recent developments of a new neutron diamond anvil cell that has finally enabled studies above the Mbar [2] as well as its application to graphite [2] and hydrogen-containing materials [3]. I will also provide an outlook on necessary future developments for simultaneous extreme conditions such as, for example, high pressure, high temperature in a laser-heated neutron diamond cell [4].

References:

[1] B. Haberl, *et al.*, Review of Scientific Instruments **89**, 092902 (2018).
[2] B. Haberl, M. Guthrie, R. Boehler, Scientific Reports **13**, 4741 (2023).
[3] B. Haberl, M.E. Donnelly, J.J. Molaison, M. Guthrie, R. Boehler, Journal of Applied Physics **130**, 215901 (2021).
[4] B. Haberl, D.G. Quirinale, C.W. Li, G. E. Granroth, H. Nojiri, M.-E. Donnelly, S.V. Ushakov, R. Boehler, B.L. Winn, Review of Scientific Instruments **93**, 083907 (2022).

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