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0.1 Scientific Advancements and Technological Developments of High P-T Neutron Diffraction at LANSCE

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In-situ high $P-T$ neutron diffraction experiments provide unique opportunities to study the crystal structure, hydrogen bonding, magnetism, and thermal parameters of light elements (*eg.* H, Li, B) and heavy elements (*eg.* Ta, U, Pu,), that are virtually impossible to determine with x-ray diffraction techniques. For example, thermoelasticity and Debye-Waller factor as function of pressure and temperature can be derived using *in-situ* high $P-T$ neutron diffraction techniques. These applications can also be extended to a much broader spectrum of scientific problems. For instance, puzzles in Earth science such as the carbon cycle and the role of hydrous minerals for water exchange between lithosphere and biosphere can be directly addressed. Moreover, by introducing *in-situ* shear, texture of metals and minerals accompanied with phase transitions at high $P-T$ conditions can also be studied by high $P-T$ neutron diffraction.

We have successfully conducted high $P-T$ neutron diffraction experiments at LANSCE and achieved simultaneous high pressures and temperatures of 10 GPa and 1500 K. With an average 3-6 hours of data collection, the diffraction data are of sufficiently high quality for the determination of structural parameters and thermal vibrations. We have studied hydrous mineral ($MgOD_2$), perovskite ($K_{.15}$,$Na_{.85}$)MgF_3, clathrate hydrates (CH_4-, CO_2-, and H_2-), metals (Mo, Al, Zr), and amorphous materials (carbon black, BMG). The aim of our research is to accurately map bond lengths, bond angles, neighboring atomic environments, and phase stability in $P-T-X$ space. Studies based on high-pressure neutron diffraction are important for multi-disciplinary science

and we welcome researchers from all fields to use this advanced technique.

We have developed a 500-ton toroidal press, TAP-98, to conduct simultaneous high $P-T$ neutron diffraction experiments inside of HIPPO (High-Pressure and Preferred-Orientation diffractometer). We have also developed a large gem-crystal anvil cell, ZAP-01, to conduct neutron diffraction experiments at high-P and low-T. The ZAP cell can be used for integrated experimental techniques of neutron diffraction, laser spectroscopy, and ultrasonic interferometery. We are conducting further developments of high $P-T$ technology with a new 2000-ton press, TAPLUS-2000, and a ZIA anvil package to achieve of pressure of 20 GPa and temperatures of 2000 K. The new design of a dedicated high pressure neutron beamline, LAPTRON, is also underway for simultaneous high P-T neutron diffraction, radiography, and tomography studies. We seek strong community support for this new development.