The Syllabary

Issue 2, January 2017

This is a brief newsletter distributed by email to update SEQUOIA users and enthusiasts regarding the status of the instrument, Spallation Neutron Source beam line 17. We would like to share with the SEQUOIA user community ongoing upgrades occurring at the instrument, science highlights, and peer-reviewed publications and theses resulting from measurements at SEQUOIA.

Please also feel free to share feedback with the user office or your local contact regarding your experience as a user at the SNS and HFIR facilities. This feedback can be shared through the survey forms sent out by the user office after experiments, or by contacting your local contact or the user office directly. Please do not hesitate to contact the beamline instrument scientists for any assistance in preparing beam-time proposals or if you are having difficulties with data reduction or analysis.

Experiments And Publications

The 2016-A and 2016-B run cycles are now complete. We ran approximately 50 experiments in 2016 at the SEQUOIA beam line. The accelerator has had excellent reliability this past year with power outputs at approximately 1200 kW. We successfully used the new 8 Tesla vertical field cryomagnet for the first time at SEQUOIA in 2016, and several pressure cells made their SEQUOIA debut in 2016 as well, including a gas pressure cell working up to 4.8 kbar.

SEQUOIA's publication output was also high in 2016. Since last year's newsletter, 19 peer- reviewed publications were accepted, including several high profile publications from the beam line. Congratulations to all the authors. SEQUOIA results are also included in a PhD dissertation and a master's thesis, both published within the last year. Many students have been to the beam line and are working hard to finish their research projects. The American Physical Society (APS) March 2016 meeting and the 2016 American Conference on Neutron Scattering (ACNS) also had many presentations that featured SEQUOIA results. Other publications are currently in review, and we expect 2017 to be another productive year for the instrument.

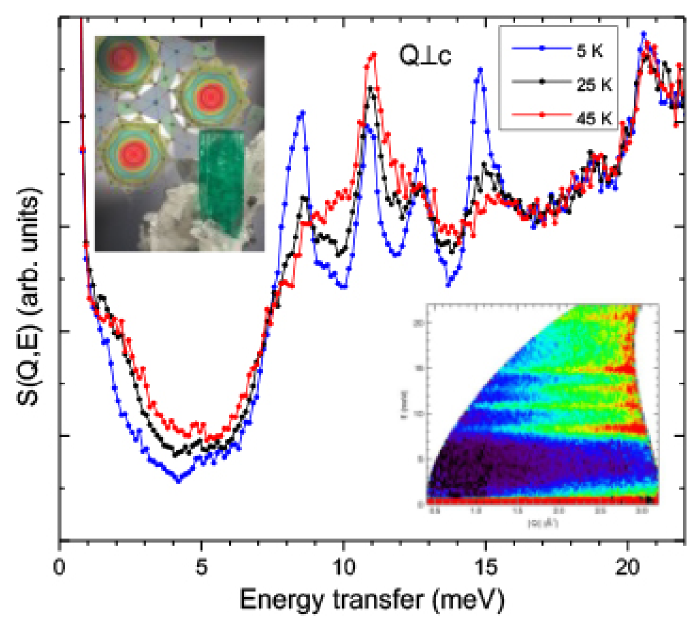
A list of SEQUOIA publications is available at http://neutrons.ornl.gov/sequoia/publications and in the PuSH database available at http://neutrons.ornl.gov/publications. We have also listed these publications at the end of this newsletter. Publications that include SEQUOIA results must be accounted for by ORNL and our sponsors. Please let us know if your SEQUOIA publication or thesis is not listed.

Science Cross-Section

The following SEQUOIA publications received significant attention in 2016. The experiments for these publications span two of the instrument's missions: measuring magnetic excitations and hydrogen excitations in condensed matter systems.

Quantum tunneling of water in beryl – by Alexander (Sasha) I. Kolesnikov

Water is commonly known in its gas, liquid, and solid states. Using neutron scattering and ab initio simulations, we discovered a new "quantum tunneling state" of the water molecule confined in 5 Å channels in the mineral beryl, characterized by extended proton and electron delocalization. We observed a number of peaks in the inelastic neutron scattering spectra, which were uniquely assigned to water molecules tunneling between six symmetrically equivalent positions around the c-axis quantum mechanically. In addition, the water proton momentum distribution was measured with deep inelastic neutron scattering, which directly revealed coherent delocalization of the protons. The average kinetic energy of the water protons was found to be ~30% less than it is in bulk gas, liquid or solid water. Due to the observation of tunneling peaks and large coherent delocalization of protons in the neutron scattering experiments, we consider that tunneling water can be called "a new state of the water molecule."



INS spectra of water in beryl measured at SEQUOIA with Ei=25 meV. The top-left insert shows the proton charge density map in the ab-plane of beryl overlain on the beryl structure. A macroscopic green beryl crystal (emerald) is also shown. Data are from Kolesnikov et al. *Physical Review Letters* **116**, 167802 (2016).

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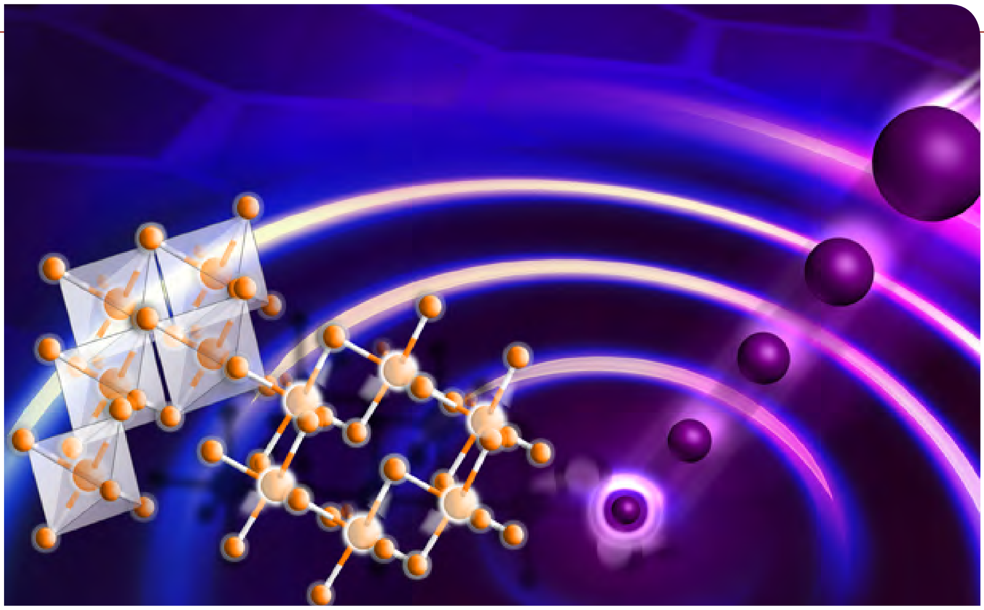

Image illustrating neutron scattering from the quantum spin liquid state observed in α-$RuCl_3$. These measurements are further described in Banarjee et al. (Ref. 11 in the newsletter).

Upgrades

SEQUOIA is fully upgraded to the new EPICS-based data acquisition system (DAS) used at SNS. Improvements to the detector array's firmware and electronics resulted in a robust DAS throughout 2016.

The vacuum upgrade project has been ongoing throughout the 2016 outages. A turbo-pump was installed on the sample chamber and integrated into the vacuum system. Two large turbo-pumps will also be installed on the detector chamber in January 2017. These pumps provide redundancy in case of cryopump failures. They also allow for more accurate leak checking of the vacuum systems. This upgrade will improve the reliability, safety, and performance of the vacuum system with a new controls system and hardware that adheres to facility standards. Changes will include rewiring the control system to remove high voltage lines from the control racks and switching to a standard roughing pump for the sample.

We currently operate with two Fermi choppers installed, most often the 100 meV fine chopper and the 700meV "sloppy" chopper. We are still pursuing the addition of a third Fermi chopper to the "chopper pit" after receiving permission to provide space by removing a concrete block. Once we prove that this concrete block does not modify our or our neighbor's neutronic background, we can proceed with designing a larger chopper translation mount.

We are making changes to the SEQUOIA workhorse bottom loading closed cycle refrigerator, CCR-22. This CCR is used for single crystal measurements and also shifted off-axis for use with a sample changer for three powder samples. Changing this configuration requires hours of detailed work near the cold-finger of the CCR, sometimes resulting in broken wires or sensors. With the help of the sample environment team, we have redesigned the sample changer to make changing CCR configurations an easier and faster process. This sample changer will be built and assembled in 2017. We also plan to purchase a low-background top-loading CCR with faster cool-down times. This CCR will be shared with ARCS, SNS beam line 18, and will allow simpler sample changes during experiments and should provide more time for measurements.

Other SEQUOIA upgrades being considered include a scattered beam radial collimator to reduce the background from complicated sample environments, an incident collimator to reduce the beam divergence for experiments looking for signal at very low scattering angles, and detectors to begin populating the top and bottom rows of the detector bank. SEQUOIA is also considering placing detectors within the beam-stop of the instrument. These detectors would be useful for measurements at very small scattering angles, but would likely require an incident beam collimator to reduce the beam divergence. Please do not hesitate to share suggestions for instrument upgrades that would improve the measurements for research programs with the SEQUOIA team.

Quantum spin liquid excitations in α-$RuCl_3$ – by Matthew Stone

Measurements of the proximate quantum spin liquid system α-$RuCl_3$ were performed at the SEQUOIA spectrometer (see Banerjee et al., Ref. 11). A quantum spin liquid consists of magnetic moments that interact but do not develop long-range order down to zero temperature. One hallmark of quantum spin liquids is the possibility of fractionalized spin excitations. The exactly solvable spin ½ Kitaev model on a honeycomb lattice is a particularly interesting example where anisotropic Ising interactions result in fractionalized Majorana fermion excitations, that theoretically could be used as thermally stable, topologically protected qubits for quantum computing. The microscopic Hamiltonian describing the magnetic interactions in α-$RuCl_3$ is believed to contain Kitaev terms. The SEQUOIA chopper spectrometer allowed for the measurement of the magnetic excitations, taking full advantage of the low-angle detector coverage and energy resolution of the thermal chopper spectrometer. Remarkably, the neutron scattering response function measured at SEQUOIA shows strong evidence for high energy excitations resembling magnetic Majorana fermions, and future research promises to reveal much more about the unique excitations in this material.

Future Experiments

Thanks for making 2016 another great year at SEQUOIA. The next proposal call for run cycle 2017-B beam time will close on April 12, 2017. Please do not hesitate to discuss your proposals with beam line staff before submission.

Staff

Victor Fanelli joined the SEQUOIA team in 2016 as a new Scientific Associate (SA). Victor received his PhD in condensed matter physics and previously worked at the Lujan Center located at the Department of Energy's Los Alamos National Laboratory. Victor has quickly gotten involved in supporting efforts at SEQUOIA, and he is being cross-trained at the ARCS instrument. The SA from ARCS, Lacy Jones, has also been cross-training at SEQUOIA and managing the SEQUOIA vacuum upgrade project.

2016 SEQUOIA Publications

1| J. A. M. Paddison, M. Daum, Z. Dun, G. Ehlers, Y. Liu, M. B. Stone, H. Zhou, M. Mourigal, "Continuous excitations of the triangular-lattice quantum spin liquid $YbMgGaO_4$." Nature Physics (2016).

2| C. A. Majerrison, C. M. Thompson, G. Sala, D. D. Maharaj, E. Kermarrec, Y. Cai, A. M. Hallas, M. N. Wilson, T. J. S. Munsie, G. E. Granroth, R. Flacau, J. E. Greedan, B. D. Gaulin, and G. M. Luke, "Cubic Re^{6+} (5d1) double perovskites, Ba_2MgReO_6, Ba_2ZnReO_6 and $Ba_2Y_{2/3}ReO_6$: magnetism, heat capacity, μSR, and neutron scattering studies and comparison with theory." Inorganic Chemistry 55, 10701 (2016).

3| A. I. Kolesnikov, A. Podlesnyak, R. A. Sadykov, V. E. Antonov, M. A. Kuzovnikov, G. Ehlers, and G. E. Granroth, "Pressure effect on hydrogen tunneling and vibrational spectrum in α-Mn." Physical Review B 94, 134301 (2016).

4| R. Morrow, A. E. Taylor, D. J. Singh, J. Xiong, S. Rodan, A. U. B. Wolter, S. Wurmehl, B. Büchner, M. B. Stone, A. I. Kolesnikov, A. A. Aczel, A. D. Christianson, P. M. Woodward, "Spin-orbit coupling control of anisotropy, ground state and frustration in 5d2 Sr_2MgOsO_6." Nature-Scientific Reports 6, 32462 (2016).

5| A.E. Taylor, R. Morrow, R.S. Fishman, S. Calder, A.I. Kolesnikov, M.D. Lumsden, P.M. Woodward, and A.D. Christianson, "Spin-orbit coupling controlled ground state in Sr_2ScOsO_6." Physical Review B 93, 220408 (R) (2016), Rapid Communication and Editor's Suggestion.

6| S. K. Mishra, M. K. Gupta, R. Mittal, A. I. Kolesnikov, and S. L. Chaplot, "Spin-phonon coupling and high-pressure phase transitions of $RMnO_3$ (R = Ca and Pr): An inelastic neutron scattering and first-principles study." Physical Review B 93, 214306 (2016).

7| S. V. Carr, C. Zhang, Y. Song, G. Tan, D. Abernathy, M. B. Stone, G. Granroth, T. G. Perring, and Pencheng Dai, "Electron doping evolution of the magnetic excitations in $NaFe_{1-x}Co_xAs$." Physical Review B 93, 214506 (2016). Editor's Suggestion.

8| A.I. Kolesnikov, G.F. Reiter, N. Choudhury, T.R. Prisk, E. Mamontov, A. Podlesnyak , G. Ehlers, A. Seel, D.J. Wesolowski, and L.M. Anovitz, "Quantum Tunneling of Water in Beryl: A New State of the Water Molecule", Physical Review Letters 116, 167802 (2016). Editor's Suggestion, and featured in 40 news outlets including Physics Focus.

9| O. Mashtalir, M. R. Lukatskaya, A. I. Kolesnikov, E. Raymundo-Pinero, M. Naguib, M. W. Barsoum, and Y. Gogotsi, "The effect of hydrazine intercalation on the structure and capacitance of 2D titanium carbide (MXene)." Nanoscale 8, 9128 (2016).

10| A. M. Hallas, J. Gaudet, M. N. Wilson, T. J. Munsie, A. A. Aczel, M. B. Stone, R. S. Freitas, A. M. Arevalo-Lopez, J. P. Attfield, M. Tachibana, C. R. Wiebe, G. M. Luke, and B. D. Gaulin, "XY antiferromagnetic ground state in the effective S=1/2 pyrochlore $Yb_2Ge_2O_7$." Physical Review B 93, 104405 (2016).

11| A. Banerjee, C. A. Bridges, J-Q. Yan, A. A. Aczel, L. Li, M. B. Stone, G. E. Granroth, M. D. Lumsden, J. Knolle, S. Bhattacharjee, Y. Yiu, R. Moessner, D. A. Tennant, D. G. Mandrus, and S. E. Nagler, "Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet." Nature Materials 15, 733 (2016). Featured in more than 70 news outlets. Cover image for the publication.

12| J. J. Wagman, J. P. Carlo, J. Gaudet, G. Van Gastel, D. L. Abernathy, M. B. Stone, G. E. Granroth, A. I. Kolesnikov, A. T. Savici, Y. J. Kim, H. Zhang, D. Ellis, Y. Zhao, L. Clark, A. B. Kallin, E. Mazurek, H. A. Dabkowska and B. D. Gaulin, "Neutron scattering studies of spin-phonon hybridization and superconducting spin gaps in the high temperature superconductor $La_{2-x}(Sr, Ba)_xCuO_4$." Physical Review B 93, 94416 (2016).

13| . Y. Yiu, A. A. Aczel, G. E. Granroth, D. L. Abernathy, M. B. Stone, W. J. L. Buyers, J. Y. Y. Lin, G. D. Samolyuk, G. M. Stocks and S. E. Nagler, "Light atom quantum oscillations in UC and US." Physical Review B 93, 014306 (2016).

14| J. Y. Lin, H. Smith, G. E. Granroth, D. L. Abernathy, M. D. Lumsden, B. Winn, A. A. Aczel, M. Alvazis, and B. Fultz, "MCVine – An object oriented Monte Carlo neutron ray tracing simulation package." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 810, 86 (2016).

15| K.W. Plumb, K. Hwang, Y. Qiu, L.W. Harriger, G.E. Granroth, A.I. Kolesnikov, G.J. Shu, F.C. Chou, Ch. Rüegg, Y.B. Kim, and Y.-J. Kim. "Quasiparticle-continuum level repulsion in a quantum magnet", Nature Physics 12, 224 (2016).

16| C. M. Thompson, C. A. Majerrison, A. Z. Sharma, C. R. Wiebe, D. D. Maharaj, G. Sala, R. Flacau, A. M. Hallas, Y. Cai, B. D. Gaulin, G. M. Luke, and J E. Greedan, "Frustrated magnetism in the double perovskite La2LiOsO6: A comparison with La2LiRuO6." Physical Review B 93, 14431 (2016).

17| Z. Xu, J. A. Schlneelock, J. Wen, E. S. Bozin, G. E. Granroth, B. L. Winn, M. Feygenson, R. J. Birgeneau, G. Gu, I. A. Zaliznyak, J. M. Tranquada, and G. Xu, "Thermal evolution of antiferromagnetic correlations and tetrahedral bond angles in superconducting $FeTe_{1-x}Se_x$." Physical Review B 93, 104517 (2016).

18| A. Banerjee, G. Ehlers, B. Winn, A. A. Aczel, G. E. Granroth, S. E. Nagler, J. Q. Yan, and Z. L. Dun, "Spin and orbital excitations in rare-earth vanadates." in IAEA 5th Conference on Neutron Scattering (2015).

19| S. Calder, J. H. Lee, M. B. Stone, M. D. Lumsden, J. C. Lang, M. Feygenson, Z. Zhao, J.-Q. Yan, Y. G. Shi, Y. S. Sun, Y. Tsujimoto, K. Yamaura, and A. D. Christianson, "Enhanced spin-phonon-electronic coupling in a 5d oxide." Nature Communications 6, 8916 (2015).

2016 SEQUOIA theses

1| G. Dellea, "Collective excitations in high temperature superconducting cuprates studied by resonant inelastic soft x-ray scattering." Ph.D. Dissertation, Polytechnic University of Milan (January 2016).

2| C. A. Marjerrison, "Investigation of Frustrated Magnetism in Double Perovskites." Masters Thesis, McMaster University (2016).

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