2020 Review of the Instrument Suite for Materials under Pressure, neutron Imaging, and Engineering applications (PIE)

Sean Agnew
Professor of Materials Science and Engineering at the University of Virginia,
user of Vulcan and NRSF2, and chair of the committee

Yan Gao
Senior Scientist, GE Global Research Center, and user of Vulcan and NRSF2

Stefan Klotz
Senior Professor at Sorbonne University, France and
past president of the European High-Pressure Research Group

Darren Pagan
Asst. Professor of Materials Science and Engineering and Mechanical Engineering and
previous lead instrument scientist for the Forming and Shaping Technology Beamline (FAST) at
the Cornell High Energy Synchrotron Source (CHESS).

Burkhard Schillinger
instrument scientist for neutron imaging at ANTARES,
Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II),
Technische Universität München, Germany

Introduction

The purpose of this report is to provide the Associate Laboratory Director, Paul Langan, and the broader management of the Neutron Sciences Directorate (NScD), including Hans Christen, with a review of the instrument suite for pressure, imaging, and engineering (PIE) science at SNS and HFIR. The committee considered the recent accomplishments, current capabilities, and future needs of the US for the types of materials research and analyses which this instrument suite presently enables and could enable with proposed upgrades.

The team of reviewers was comprised of members who are intimately familiar with neutron and synchrotron beamline experiments of the types performed by this instrument suite. Some members have been long-term users of the facilities at SNS and HFIR, while others were truly at-arms-length reviewers drawn from the international community of university and government laboratory researchers.

Before getting into details, the committee would like to commend the management on their creation of the PIE instrument suite. It is not initially intuitive, but the assembled team was able to clearly articulate why this eclectic band of condensed matter physicists, materials scientists, and engineers are well-served to be co-organized. Although the scientific topics of greatest interest on each of the beamlines are distinct, the way in which the experiments are performed is similar. They are frequently "one-off" experiments, with sample environments that are crafted by (or on behalf of) the users or instrument team, rather than drawing from the core facilities. We encourage the team to interact broadly, so that the anticipated synergies can be realized. HIDRA (strain mapping) and VULCAN (in-situ loading) are providing good, complementary diffraction-based capabilities. Imaging and high-pressure teams are doing an excellent job collaborating on the SNAP instrument. We encourage even more collaboration between imaging and the Vulcan team, perhaps building upon the recent pin-hole diffraction work of the latter.

The rest of the report is organized as follows. We provide detailed feedback on each of the 4 instrument suites in the following order: SNAP, Imaging, HIDRA, and Vulcan beamlines. Our review considered the following five elements:

1. Instrument technical capabilities, considering the wider instrument suite at SNS and HFIR (especially overlaps within and between instrument capabilities) and comparison of performance and productivity with those at other national and international neutron facilities
2. The ability of each beamline to meet the day-to-day needs of users for data collection, reduction, and analysis and future software planning
3. The current portfolio of science and business case for each instrument in the suite (e.g. demand; breadth of scientific use; overall impact; mission needs and agency support; and/or industrial use)
4. The future development and use of the suite of instruments, and of materials engineering and high-pressure science at SNS and HFIR.
5. Evaluation of the strategic visions of the beamlines, alignment with ORNL and DOE missions and effectiveness of process to implement vision

The report is then concluded with a short list of commendations, critiques, and recommendations for the suite as a whole. A short Appendix is included which lists data acquisition, reduction and analysis software which is referred to in the body text.

SNAP (Spallation Neutrons And Pressure diffractometer)

SNAP is a medium-resolution diffractometer dedicated entirely to high pressure experiments up to the Mbar range. SNAP has full portfolio of high-pressure devices capable to serve various communities from soft condensed matter to the earth sciences. Efforts have been made to combine high pressure with low temperatures, which now pay off by attracting more and more groups from the magnetism community.

SNAP is one of three existing dedicated high-pressure neutron beamlines, along with PEARL (ISIS, U.K.) and PLANET (MLF, J-PARC, Japan). It has gained considerable international visibility due to its strong program using diamond anvils cells (DACs) for neutron scattering which opens the way to carry out diffraction measurements to almost a Mbar. It is the ONLY one of the three dedicated beamlines which offers this possibility in its user program. In comparison other dedicated beamlines, SNAP is versatile and very flexible, mainly due to the possibility to rapidly change detector positions and therefore address different Q-ranges, adapt to different scattering geometries, and deal with both powders and single crystals.

SNAP is run by three permanent staff which form a solid and coherent team. The team relies heavily on a few associates and/or close collaborators (R. Boehler, B. Haberl, M. Guthrie) for cell development and handling of more complex and demanding setups. Over the years, the team has fostered collaboration with groups worldwide and has actively publicized the possibilities and capabilities of SNAP in very diverse science communities (Physics/Chemistry, Materials and Earth Sciences, soft condensed matter physics). *The fact that 50% of the institutions applying for beam time are foreign testifies the strong international visibility of SNAP*. For all these reasons, SNAP is considered clearly world class.

The strengths of SNAP are also its biggest threats. For example, the current predominance of DAC related experiments (~50%) which reduces considerably the time available for "low pressure" requests, which might nevertheless be scientifically highly valuable. Whilst the DAC program helps the instrument, team, and ORNL gain visibility, the success rate is considerably lower than for more standard high-pressure techniques. Hence, *the scientific output in terms of publications is rather low*. On top of that, the DAC data correction necessary to apply Rietveld methods is non-trivial and still not fully reliable, at least for standard users. Therefore, there is a strong risk that good data will "remain in the drawer" awaiting better correction procedures.

Thus, the committee feels that care must be taken to develop a healthy balance between the allocated DAC proposals and more standard lower pressure projects. A possible way forward could be an in-depth evaluation of the expected signal level of potential DAC proposals well before a proposal is submitted. It is easy to simulate the expected diffraction intensities knowing the structure and sample volume. A comparison with the signal from a reference sample will immediately tell if the signal is sufficient, or if it will be "drowned in the background". Such a procedure would allow focusing only on experiments which have a realistic chance of success, open up time for more standard high-pressure experiments and increase the overall output in terms of publications.

The DAC program relies entirely on the availability of large and high-quality CVD diamonds. Unfortunately, the number of providers is very limited. (According to the SNAP team presentation, there is currently only one company.) The team is aware of this potential threat and the committee recommends to take all possible precautions to insure a sustainable access to such material.

SNAP has gone through major upgrades recently which saw the replacement of the detectors and new guides. These should lead to a considerable decrease in background and an overall improvement in the data quality, as well as enabling more rapid change-out between experimental setups. Also, the committee applauds recent improvements in software which have made data handling much more user friendly. The full breath of benefits from these recent improvements could not yet be evaluated in detail due to Covid-19 related delays.

Considering Covid-19 related issues more generally, high pressure experiments have never been and will never be "push button" experiments where a user might simply send a sample and the beamline team runs the measurement. SNAP is therefore extremely vulnerable to newly introduced procedures related to COVID-19, if they continue to be applied for a long time. Obviously, the SNAP team is aware of this. The committee recommends that the specificity of SNAP should be recognized by the SNS management. It recommends to the SNAP team an in-depth reflection how high-pressure experiments could be run in the future with a minimum involvement of external users. Possible ways forward could include procedures where, for example, the loading of samples into the various cells is done externally, for example in the home institute of the user, or, if this is too complicated in a nearby facility which is more easily accessed. Standardization of pressure equipment and the use of "loading clamps" could make life easier in this respect.

Finally, it is well known that certain high-pressure diffraction measurements are better done on a reactor source. For this reason, the committee encourages the SNAP team stay abreast of the high-pressure diffraction capabilities at HFIR (e.g., at HB-3A and CG-4D, IMAGINE) and consider potential synergies which could develop through even closer collaboration.

Imaging

The imaging suite is comprised of current capabilities at CG1-1D, SNAP (~10% of available beamtime is being shared by the pressure team discussed above), and the future VENUS instrument, which is scheduled to come online late in 2022 or early 2023. The VENUS development timeline is recognized as a good, ambitious schedule. We hope that complications associated with COVID-19 do not lead to delays in this development.

During the previous triennial review in 2017, reviewers highlighted imaging as the area with greatest opportunity because of "the potential of the techniques far beyond physics and engineering to include archeology, geology, life sciences, paleontology, anthropology, cultural heritage, etc." Particularly for those committee members who had served on that committee, it was good to see that many of our recommendations had been effectively acted upon, especially as concerns the use and planning of the SNS beamlines and software developments. We encourage them to continue striving to implement the remaining suggestions in that report as we still see imaging as an area with great promise.

We want to recall the commendation of the review in 2017, "Scientifically, the performance of the imaging group is more than surprising. No other imaging group has so many complex research projects requiring complex experimental setups and sample environments, going deeply in other fields of science, per number of group members, and no other group can show such extensive software development as the ORNL group. Furthermore, the developed software and "notebooks" concept are outstanding and unique in the neutron imaging world…They tried to implement nearly all available imaging technologies at once on a still experimental and provisional beam line which was formerly a test beam line, and did so with amazing success [under less than ideal conditions]."

The current committee is impressed by the innovative and highly collaborative works in the area of energy-resolved (time-of-flight) neutron imaging that the team is performing on SNAP, including Bragg-edge neutron radiography and neutron resonance radiography (techniques which had previously been demonstrated at other accelerator-based facilities: J-PARC, ISIS, GELINA, and LANSCE, but not SNS). The open-source software developments that occurred along with these demonstrations is also a positive. In fact, the committee is largely impressed with the extensive array of software that is being developed to support imaging, which other facilities do not presently enjoy. The team is encouraged to capitalize on this capability as they continue developing their collaborative network. Shortly after the August 2020 review meeting, the four neutron imaging groups from the facilities at ORNL, INL, FRM II and ILL (with scientists of HZB involved) founded a new collaborative network with personal contacts and bi-weekly online meetings that concentrate on detector, scintillation screen and software development, but also experimental methods. In the final quarter of 2020, it turned out that many problems within one group had already found a solution in another group, which was happily shared. All facilities are collaborating on increasing spatial resolution of screens and detectors, and scientists from ORNL and FRM II have already begun very successful collaboration on the further development of evaluation software for grating interferometry, which will eventually be shared world-wide, and support the implementation of the necessary experimental hardware at ORNL.

Given these successes, it was disappointing to learn from the team that ORNL plans to eliminate imaging from the CG1-1D and repurpose that beamline for another single-crystal spectrometer. We admit that imaging capabilities at the CG1-1D beamline at HFIR had reached a bit of ceiling, requiring a major upgrade in order to see further improvement. However, it is still disappointing because CG1-1D represents the best position available for imaging at HFIR. Furthermore, this decision is hard for the present committee to understand, given the potential and given the large number of neutron spectrometers that already exist at ORNL. Imaging is always seen as a specific single instrument along a suite of scattering instruments, while imaging methods are today so manifold that they would justify building at least half a dozen specialized imaging instruments for different methods, just as there are many specialized scattering instruments. Since so many imaging methods must be realized in just one instrument, it should be given the highest priority for best conditions over all other neighbouring instruments, since it must cover alone what all others do together in terms of versatility.

Concerning other specific development plans that the imaging team shared with the reviewers, it is recommended that some more exploratory measurements be performed before further developing the Cupid concept, even though a beam position has been identified within the cold beam hall. Similarly, the concept of Mercury (thermal neutrons) was met with some skepticism. Questions regarding epithermal neutrons and about a thorough consideration over beam tube vs. beam guide (20-year plan) were raised. A neutron imaging instrument on a thermal guide would be very limited in beam size and spectral homogeneity (due to lower reflection angles for spreading the beam out). In the absence of the cold spectrum part that is interesting for Bragg edges and scattering effects, the slightly better penetration of the thermal beam alone does not really justify an additional imaging instrument, while a thermal imaging instrument on a flight tube would not be limited by energy-dependent reflections in a neutron guide, and provide a spectrum extended to higher energies that would allow for cadmium-filtered epithermal neutron imaging, and maybe even the use of fast fission neutrons remaining in the spectrum. Imaging with higher neutron energies at continuous sources is just beginning to be properly explored at INL and FRM II, where flight tube facilities are available, and a third partner facility at ORNL would be most welcome.

Concerns were raised by the committee about the need to have a plan for long term staffing and talent retention, but this concern did not seem to be shared by the imaging team. The reviewers would like to highlight that other instrument teams seem to have developed a pipeline, in terms of graduate student users who may become postdoctoral researchers who may become faculty or scientific researchers that help to populate the future user community. Similarly, the team was challenged to think hard about expanding the user community, *beyond the expert user*. We believe there are many potential users within the communities of the ASNT, ASM, and TMS societies. Again, the team expressed reluctance to build out the community at this time because of the huge time commitment required to analyze the data and the presently limited beamline capacity for imaging. With the new instrument coming on-line in about 2 years, it seems appropriate to begin planning and building up the user base now.

The need for improved spatial resolution is emphasized, since the user community is begging for it, and the neutron imaging community is falling further behind. However, not every user can clearly articulate why they need better resolution and what they would do with it. The ORNL team, with its eclectic scientific background and networking with other divisions within ORNL, seems very well positioned to help answer this question and make impactful demonstrations of what can be achieved with the highest resolution neutron imaging capabilities available. For example, the ORNL team has a clear understanding of technologically important issues related to Li-ion batteries. They may not be able to offer resolution sufficient to answer cutting-edge scientific questions related to nanoscale mechanisms. However, they will very likely be able to offer sufficient resolution to have a critical impact upon engineering applications related to processing and service conditions. To this end, the imaging team is encouraged to increase collaborations with other instrument teams, like the one at Grenoble, which has presently demonstrated a world-leading position with 4 µm resolution. Although this demonstration was performed with a Gd edge and likely of limited use in computed tomography, there may be opportunities for battery and fuel cell applications of interest to the ORNL team. They are also encouraged to consider reaching out to the earth science community, which can have tens of thousands of attendees at their conferences.

In summary, we were encouraged by the progress which has been made by the imaging team (both at the CG-1D imaging beamline and the time-of-flight imaging experiments on SNAP and progress towards the SNS). For committee members who had served on the last triennial review, it was good to see that our recommendations had been and continue to be effectively acted upon. The fact that a new-founded four-institute collaboration has already produced leaps for each facility involved is viewed very positively.

HIDRA (formerly NRSF2)

The HIDRA instrument team has produced a number of important publications including an award-winning paper on the impact of cooling on residual stress reduction for dissimilar welds, conferred in late 2017. Its industrial program has provided a number of highlights for BES to showcase the importance of the DOE's user facility for the US manufacturing industries. As HIDRA provides unique capabilities for the materials science and engineering community, the demands for beam time has always been higher than what the beamline can accommodate.

Based on the proposals submitted to HIDRA (one of the review committee members recently served on the proposal review committee), the quality of the user program on average is *good*. Being short of extraordinary or excellent reflects the fact that many users are probably from engineering or materials science background and may not have sufficient working acknowledge about residual stress measurement to articulate their science or technology needs eloquently for the proposed work. The beamline scientists are encouraged to educate their less experienced users to write better proposals. Such comments were also made in the 2017 review, and we appreciate the efforts the team is making through rapid access programs, etc. This is an issue which will continue to be important.

HIDRA has undergone significant upgrade from last review, including 2D detector, beamline optics, DAC control, new software tool (Cuboid) for sample manipulation, and new Python based software for data analysis and visualization. A good benchmarking paper for the vintage NRSF2 capability was published in 2018 (https://doi.org/10.1063/1.5037593). *It is now time to issue a similar study based upon the new capability.*

HIDRA has a sound development plan. It is under consideration to have a robot installed at the beamline, following the successful example at SRESS-SPEC, a similar beamline at FRM-II in Munich. The 2017 review panel noted the importance of this capability in their report, and we would like to join our voice with theirs. This is not simply an issue of engineers wanting a new toy. Use of such a robot arm, *especially if it is partnered with a laser coordinate measurement machine (CMM)*, will allow accurate positioning of samples with complex geometry with respect to the beam, obtaining strain components in multiple orientations (e.g., more than three (hopefully) principal directions), and texture measurement. Again, such a capability is especially important for components with complex shapes such as aeroengine and combined-cycle gas turbine blades and other complex shapes made possible by additive manufacturing. This is essential for ORNL to remain at the cutting edge of this field.

We applaud the HIDRA team for securing LDRD support to develop the Creep Electrostatic Levitator (CRESL) capability. If successful, this will be a truly heroic achievement, and the design team looks as likely as any to pull it off. We like the fact that it is being designed with multiple beamlines in mind, both within and outside the PIE instrument suite ($WAND^2$, IMAGING, GP-SANS, Vulcan, etc.). The immediate plans to make sure the chamber can be used in the adjacent instruments HIDRA and $WAND^2$ is a good first step in this direction.

HIDRA is a unique instrument for non-destructive residual stress mapping for bulk samples or large industrial components. The only other beamline in the US with comparable capability is BT-8 at NIST Center for Neutron Research. This beamline, however, is not really in the user program at present. HIDRA has a strong industrial access program. The beamline scientists, Jeff Bunn and Andrew Payzant, have combined youth enthusiasm and in-depth expertise in residual analysis, powder diffraction, structural engineering, and materials science in general. The stress-free d-spacing is among the most critical parameters for residual stress analysis. One way to relieve stress is to machine a small piece of the material from the sample after the measurement. At present, this is not possible due to radioactivity from the samples after neutron irradiation. Due to the importance of having stress-free d-spacing for residual stress analysis, we suggest the management work with health physics personnel for possible solutions.

Considering the importance of residual stress measurement for additive manufacturing, the beamline scientists, Jeff and Andrew who are both active in the ASM subcommittee for residual stress measurement, are encouraged to play more active roles to reach out to the broad materials and engineering community, providing guidance for the best practice in residual stress analysis. An additional scientific opportunity for HIDRA (as well as VULCAN) is combined texture and residual stress analysis, as even alloys with simple cubic structure are not isotropic in mechanical properties after processing. The use of the aforementioned robot would make such combined analysis feasible. We encourage both HIDRA and VULCAN to play even more active roles in the manufacturing community by providing high fidelity measurement and analysis, as well as guidance for best practices. Recognizing the limited capacity at both beamlines, it is important for the manufacturing industry to understand the complementary nature of different techniques for residual stress measurements, including non-destructive high-energy synchrotron diffraction, and destructive methods such as in-house XRD, contour and hole drilling. For bulk materials at ~mm spatial resolution, neutron diffraction technique may be considered most reliable.

Vulcan

The capabilities of Vulcan are comparable to or exceed other neutron instruments in terms of performance and breadth of available sample environments. Vulcan has a wide array of sample environment capabilities that enable users to study a huge array of thermomechanical loading conditions and renders the instrument competitive with other best-in-class facilities world-wide. However, immediate investments are required to maintain this status in the world community. In addition, care needs to be taken to contextualize Vulcan developments and capabilities in comparison to synchrotron sources. This information also needs to be put in the hands of potential users, to help them make the case for neutrons over x-rays within their research programs and in their beamtime proposals. The Vulcan team members have a clear, articulated vision and approach for tackling structural and energy materials challenges for which neutron characterization is the best choice. Obviously, major benefits for neutrons include larger sample volumes, which may include large crystallite sizes, and variations of scattering cross sections between chemical constituents.

Productivity is good, and the instrument is consistently oversubscribed. Significant effort is dedicated to maximizing the number of users given beamtime. Reduction in instrument turnaround time from 4-5 days to 2-3 days is laudable. Workflows are mature and the data processing is streamlined. This strength allows for researchers to rapidly reduce their data and get science out to publication. User program quality is good as evidenced by the healthy publication record. The increasing diversity of science supported by the beamline is also evidence of long-term health of the instrument. It is good to see that prior investments in new sample environments are fully utilized by the user program. Going forward, it is acknowledged that structural materials characterization is increasingly multimodal. To remain relevant, the team should strive to develop workstreams which leverage capabilities inside and outside of ORNL to perform complimentary characterizations at Vulcan (microscopy, destructive residual stress characterizations). This is a point which was also raised by the 2017 reviewers. We also believe that the COVID-19 pandemic may be instigating a paradigm shift in user service at large scale facilities. Planning should begin for the possibility that remote operations become standard. With streamlined workflows, Vulcan is well-positioned to make this transition smoothly. It is recognized that staffing increases are likely necessary to make this possible.

One area that the 2017 review team highlighted as a deficiency was integration with computational modeling. We would like to restate this as a great *opportunity* for the team. We recommend continued efforts to expand the userbase to users more focused on modeling. These users can develop diffraction / modeling interface tools that can then be used by the community. We would like to again highlight the synergies which have been enjoyed by the LANL team around the SMARTS instrument. Don Brown is not a computational modeler and has no interest in becoming one, but he has benefited immensely from strategic partnerships with modelers like Carlos Tomé. Together, their studies and resulting publications have been far more impactful than they would have been independently. Obviously, people like Bjorn Clausen, who have one foot in both camps are tremendously helpful, because they can deeply understand the challenges and opportunities on both sides. Similarly, committee member Darren Pagan notes that Prof. Matt Miller's efforts to build up experimental capability at CHESS has benefitted immensely from strategic partnerships with Prof. Paul Dawson, even well into the latter's retirement. Again, there have been a number of Cornell students and postdocs who have worked at the intersection of modeling and experiment. Joel Bernier (presently at LLNL) is a prime example, and his understanding of both is precisely what has enabled him to be a world-wide leader in developing analysis software for grain-by-grain in-situ measurements of internal strains. We are pleased that the group is beginning to do more of this sort of work, and we want to encourage them to push even harder. Frequently, the biggest opportunities are at the intersections of fields, not in the center of one or another.

Similarly, we feel that the Vulcan instrument would benefit from further cultivation of 'super-users' who can also contribute new capabilities to beamline. Committee member, Darren Pagan, recalls super users at CHESS who have made a lasting impact upon the capabilities there. For example, Prof. Bob Suter (CMU) has developed the technique known as near field High Energy Diffraction Microscopy (HEDM) which has helped to keep APS (and CHESS) at the forefront of world-wide developments in the field. Paul Shade (AFRL, Wright Patterson AFB) has led the in-situ load frame development known as RAMS, which is central to the instrument at CHESS and

APS. Prof. Aaron Stebner (GaTech) has led the instrument team's foray into shape memory alloy (SMA) research. (Who are the super users, who are helping to keep Vulcan at the forefront?)

The team and management are commended for the present investment in dedicated computational staff associated with Vulcan. This model is unique and aligns excellently with all science thrusts. Vulcan's push forward to inclusion into the Instrument Suite's software efforts is viewed as a positive. As a relatively mature instrument, Vulcan needs to work hard to continue excelling in the development of software and streamlined data workflows for users. The instrument will benefit from use of new Computational Instrument Scientists to provide final polish to software capabilities and integration with other packages from the NScD.

On the other hand, the planned upgrades to the instrument seem to be little more than a continuation of the current directions. Moving forward, a better articulation of the new science or applied technology (not measurements) which will be possible with planned major detector and sample environment upgrades should be made. Restated, the future vision for *measurement capabilities* at Vulcan are clear, however, the *scientific vision* is less clear. Pushing forward, additive manufacturing and high-entropy alloys is not a unique goal in the structural materials community. Identifying and pursuing the scientific niche which Vulcan will occupy in the midterm should be a priority.

Measurement capabilities will be significantly enhanced by planned detector bank and sample environment upgrades. As food for thought, consider that larger reciprocal space access will enable Vulcan to compete with synchrotron capabilities for mapping of texture and orientation dependence of strain while probing much larger real space volume (often more permitting the exploration of sample sizes which are relevant to application). We appreciate off-line communications from the team which help to make the scientific case. Things such as ability to use in-situ deformation studies to discriminate between possible mechanisms is a broad scientific goal. (An example was given in which the current layout could not exclusively prove FCC twinning as opposed to martensitic phase transformation). Opportunities for single crystal measurement under force were highlighted and recent studies have highlighted that high angle detector can be used for dislocation density measurement, which is critical for benchmarking many new, internal state variable (ISV) based models of constitutive behavior.

The Vulcan team is making good use of LDRD funding to advance measurement technique capabilities (pinhole mapping technique, dubbed PIND). This development provides good evidence that NScD staff is being effectively used to improve impact and science capabilities of Vulcan instrument. It is highlighted that the PIND is a new development which is enabled by the 2D detectors. Publications on the PIND development on VULCAN present a few use cases which show that there are huge opportunities in materials engineering, such as high spatial resolution residual stress measurement including near surface case (the edge effect is greatly reduced), interfacial mechanical behaviors, grain behaviors, etc. It is acknowledged that good detectors are needed, such as ^{3}He modules. Along these lines, it is noted that structural and energy materials scientific challenges of interest are increasingly demanding of increased temporal resolution. Collection time for neutron measurements decrease the relevance for tackling these types of problems. Efforts should be continuously made to try to reduce collection times (acquiring new detectors, improving data analysis capabilities to handle poor signal-to-noise) to mitigate this threat, although it is recognized there is no easy answer to this problem.

The nature of NScD/NTD support for projects like detector buildouts at Vulcan are unclear to the committee, though we applaud the team on their branding efforts (Vulcan-X, where X means eXpansion and also 10, in honor of the 10-year anniversary). It would indeed be excellent to be announce the upgrade during the 10-year anniversary of VULCAN.

Concerning possible threats, it is mentioned that as longer beamlines are becoming available at synchrotrons world-wide, and hence, larger X-ray beams will be available to users. The natural advantage of larger diffraction volumes during neutron measurements is eroding and this should be carefully monitored. European and Japanese teams have begun developing neutron-based grain mapping techniques. This class of techniques is particularly high impact for the structural materials community (with associated papers in high impact journals:
https://www.nature.com/articles/s41598-017-09717-w and
https://www.nature.com/articles/s41598-020-60330-w).
Development of pinhole mapping techniques may provide a response to these international efforts, but exploration of the feasibility of these techniques at Vulcan may be warranted to remain 'state-of-the-art.' (This could also be an opportunity for interfacing with the Imaging team within the PIE suite.)

In summary, Vulcan is doing an excellent job maintaining a wide array of sample environments that enable users to study a huge array of thermomechanical loading conditions. The development of mature software and processing workflows is also a huge benefit to the user community and subsequent publication of science. The planned upgrades (detectors and sample environments/manipulation) will be a huge leap forward in measurement capabilities enabling competitive reciprocal space coverage to synchrotron measurements. Moving forward, clear articulation of the new science or applied technology that will be enabled by planned upgrades would be beneficial. Vulcan would benefit from further cultivation of 'super-users' who can contribute new capabilities to beamline. As interfacing with modeling efforts is still limited, efforts to expand the userbase to users more focused on modeling may be the greatest opportunity. These users can develop diffraction / modeling interface tools that can be used by the community.

Conclusions

The overall impression of the committee is that the PIE instrument suite and its support teams are on par with similar domestic and overseas capabilities. Benchmarking instruments of similar kinds is difficult due to lack of comprehensive data. "If you're the only one, you're always number one," as no two beamlines are exactly the same. This comment is applicable to many beamlines at DOE user facilities. As we imply throughout this report, the beamline capability and performance are not the only measures for user experiences and productivity. While a great deal of attention was given to instrument capability and performance, the most valuable asset of the user facility is its people. A beamline is as good as its beamline scientist, support staff and user community, not more or less. This is probably one of the most important aspects to pay attention to for the long-term health and growth of user facility beamlines.

Overall, the committee is impressed by the high caliper and international reputation of the beamline scientists of this suite of instruments. Due to multiple functional duties imposed on the beamline scientists, from user support, continuous upgrades, to user community outreach, and their own research, it could be very challenging for the NScD staff to keep up with engagement with users and external researchers in continued and consistent manner. A detrimental outcome could be an *operational fatigue* from endless cycles of user support, day by day and year by year. The concern is that it may become a chronical "disease" for the health of a user facility in multi fronts, from morale to talent retention, and from creativity to scientific output. While funding constraint is often a plausible root cause, the management is encouraged to come up with innovative ideas to give a "break" to key staff for periodic refresh, such as short "sabbatical" leaves to other ORNL divisions or external institutions, academic or industrial. An exchange with other international institutions may be beneficial, simply to share instrument operations for a week or two, or to do joint measurement campaigns. Generous proprietary beam time for the instrument staff to explore their own ideas must be maintained if not expanded. Concerning the leveraging expertise of instrument users including NScD staff and external researchers to improve the impact of the suite, we have highlighted specific opportunities for enhancements related to the people involved with each instrument team in the specific subsections above.

As the future science directions are changing with time, it is very important for the user facility to keep up with where the winds are blowing for the government sponsored research programs. For example, in the last decades, we have seen the ebbs and flows of the hydrogen economy, nanotechnology, renewable energy (especially Li-ion battery), Materials Genome Initiative, advanced manufacturing, and most recently Quantum Information Systems (QIS). By and large, the lead scientists for this suite of instruments, as well as the division leadership, are well connected with the national and international scientific community, and as a result, their plans for future development are both justified and assuring. As a very general comment, the division between neutron scattering (NScD) and technologies (NTD) divisions was unclear to members of the committee. The management may like to strive to clarify this "division" of responsibilities.

A major positive is that we see good leveraging across the capabilities and through the laboratory (including the on-site divisions and the off-site Materials Demonstration Facility (MDF)). Both visions and priorities for this suite of instruments are clearly presented and articulated, in the scope of three-source strategy for the neutron science directorate. The leadership shows clear understanding in balancing the long-term (additional beamlines at FTS) and mid-term investment (various upgrades) for enhancing the overall capabilities of this suite. One specific area for improvement which was highlighted earlier is the opportunity for continued growth in the connections with computational modelers at ORNL and elsewhere. Similarly, we encourage even more collaboration between imaging and the Vulcan team, perhaps building upon the recent pin-hole diffraction work of the latter.

Concerning the adequacy and reliability of software, sample environment and ancillary equipment, "adequate but never enough" is probably a fair evaluation, as we keep pushing the envelope of science and technology, for faster data analysis, better visualization, and more demanding sample environment. The committee is impressed by the presentations on software development and sample environments for high pressure and diffraction experiments. LDRD is being used effectively to support a novel sample levitator for in-situ diffraction measurements. The software development for imaging is making good progress toward seamless interactions between beamline scientists and the software developer, the first CIS role for the division.

Covid-19 has revealed that working from home can often be just as productive as working from the institutional office, and we can discuss many things over the internet, including this review, without meeting in person. The same ideas may be applied to performing neutron experiments remotely without setting foot on the ORNL campus. As an example, a recent online QIS workshop at ORNL had to be postponed because the overwhelmed number of registration (450 people) requiring more time to process according to the organizers. For industrial users, cost has always been a major barrier for employing user facilities, such as those at SNS/HFIR. The cost has not only limited the number of experiments, but also the scope of participation. As most industrial projects involve people from different parts of a company, from materials development to processing, and from testing to modeling, remote participate in the neutron experiment virtually would give the entire team a sense of involvement and this could be very important for continued engagement of this team for similar experiments in the future.

We recognize this remote experiment is not for every beamline and will never completely replace onsite experiments (e.g., considering the educational values for students to be onsite), the committee believes that a remote experiment pilot program should be explored. This could greatly expand the user base for neutron techniques by removing the travel requirement for many users. This is also more time efficient as users could spend their idle time, say during data collection, for other activities. Such programs are already prepared at FRM II and ILL, but have not yet been implemented in real experiments due to the closure because of the Covid-19 situation. Further exchange about implementations and also future experiences on an institute level is advised. As mentioned earlier, despite the special challenges of performing high-pressure experiments at SNAP, the team is well-positioned to be a pilot facility. Therefore, the committee recommends that the SNAP team perform an in-depth reflection how high-pressure experiments could be run in the future with a minimum involvement of external users.

Data Acquisition Software

beamline	location	present software	comments (past software, upgrades, needs)
IMAGING	CG-1D	EPICS/CSS for CCD, sCMOS, and MCP (with Pixelman functionality)	sCMOS integration with EPICS has some glitches and the MCP should be integrated into EPICS as well
HIDRA	HB-2B	EPICS/CSS	we utilize some tools purpose built within the framework of CSS/EPICS like the cuboid tool for planning (the cuboid tool visualization is built using python based vdk); users can utilize monitor.sns.gov allows for triggering of autoreduction and viewing scan progress
SNAP	BL-3	EPICS / CSS	
SNAP (Imaging)	BL-3	EPICS/CSS for MCP (with Pixelman functionality)	
VULCAN	BL-7	nEd system with EPICS/CSS. Commercial device control and DAQ software.	Commercial software GUI, and highly customized CSS are the ones user would encounter.

Data Reduction and Analysis Software

beamline	location	present software	comments (past software, upgrades, needs)
IMAGING	CG-1D	2D: Jupyter notebooks, imageJ; 3D: iMars3D (3D reconstruction), Amira-Avizo, some jupyter notebooks that supports 3D	ImageJ, iMars, VG studio were used in the past. CT reconstruction code is currently being fixed. Needs streamline the 3D analysis flow and provide tutorials.
HIDRA	HB-2B	PyRS	Python based open source software available at: https://github.com/neutrons/PyRS, This system replaces the previous VIEW software which was labview based; meta data tracking in ONCAT.ornl.gov based on proposals
SNAP	BL-3	Mantid / Existing algorythm and occasionally custom scripts	Simple platform exists to integrate data into powder patterns. Key routines are missing, or just in prototype form: Incident spectra diamond correction, 3 D masking of diamond reflections. Link to live data, in a usable form, is needed. Also needed is a more convenient way to setup automatic reduction parameters.
SNAP (Imaging)	BL-3	Not available yet (started this effort June 1, 2020)	6-12 months before Bragg edge (strain maps) software is available, resonance imaging will be tackled after Bragg edge capability is available.
VULCAN	BL-7	IDL based VDRIVE and GSAS for data slicing, single peak fit (lattice strain, intensity, and fwhm), texture, and Rietveld etc. Mantid auto reduction is available for single run GSAS files.	Future is to convert and improve VDRIVE to python based PyVDRIVE with GUI and bond with GSAS-II.