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バロン物質ダイナミクス研究室　研究業績レビュー報告
Materials Dynamics Laboratory Periodical Review

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場所 Venue：播磨研究所　上坪講堂ほか　RIKEN Harima Institute (SPring-8)
レビュアーReviewers：

Dr. John Peter Hill (Brookhaven National Laboratory)
Dr. Kazuyoshi Yamada / 山田 和芳（KEK）
Dr. Hidetoshi Fukuyama / 福山 秀敏（Tokyo University of Science）

評価結果の概要 Abstract of the reports：

1. General comments

This Laboratory (MDL) was founded in April, 2006. Research activities so far have been carried out on BL35. Funding for the new beamline (BL43) started in 2009, which is now under commissioning, and some test measurements are under way including investigation and improvement of the analyzers.

1.1 Research objectives

The research objectives of the MDL are explorations of elementary excitations in a wide range of both momentum and energy. These are crucially important for understanding of the properties of condensed matter. For the past few years MDL efforts have centered on the development of the new IXS beamline (BL43XU). In this BL, Baron has identified a scientific need and an opportunity that plays to two of the key strengths of the SPring-8 facility, namely the high electron energy and the extremely long straights. As a result, this BL will be a truly unique facility, with the highest flux in the world at high-resolution. It will offer unprecedented opportunities to exploit the strengths of IXS to address key scientific questions. The BL is currently undergoing early commissioning and with the exception of the analyzers appears to be working well. We congratulate Baron on what is clearly a remarkable BL, with novel solutions to the challenges of creating and working with the intense beam from 3 x 5m undulators. We feel confident that he will ultimately understand and solve the issues associated with the mass production of analyzer crystals with a new vendor at which point the BL will then be a very exciting facility indeed. The future goals of the MDL (at BL43XU) are to carry out momentum-resolved studies of;

i) Electronic excitations (including orbitons) with unprecedented energy resolution,
ii) Weak, high-energy phonons in high-Z compounds,
iii) High-pressures studies of geologically (and other) relevant materials,
iv) Liquid dynamics, including surface dynamics

In addition, on a longer time scale, he also seeks to develop the use of an analyzer based on nuclear resonance

effects to achieve improved energy resolution.

Each of these represents interesting directions for research. We recommend that Baron carefully prioritize between these to ensure that the highest impact science is done in the early stages of the new facility, paying particular attention to what he can learn that cannot be learned through existing techniques such as neutron scattering, RIXS and ARPES.

1.2 Research results

High energy-resolution non-resonant type of x-ray inelastic scattering (NRXIS) spectrometers have been constructed at several major synchrotron facilities around the world and have been providing high quality data on lattice dynamics. The NRXIS spectrometer at BL35 developed by MDL is the best machine in the world. With this BL, Baron has a track record of carrying out high quality research over the past few years. His most highly cited papers are split roughly 50:50 between instrumentation and science. Scientific highlights include the work on MgB2, cuprates and B-doped diamonds. More recently he has been working on the phonons in the so-called 1111 iron-arsenide (FeAs) superconductors (39 citations). Since NRXIS does not require large single crystals, the MDL has succeeded in performing timely experiments on the above superconductors and in taking high quality phonon data. These studies have attracted attention from many material scientists who have confirmed the high potential and the complementarity of NRXIS compared to neutron scattering spectroscopy. The SCSS Test Accelerator test facility has been delivering UVU light to the users since 2007 in collaboration with laser research group in RIKEN, which would have positive impact for VUV sciences as well as preparing the future x-ray users of the SPring-8 XFEL. The success of the innovative accelerator ideas employed for the SCSS Test Accelerator system has been noticed worldwide by the accelerator community and would influence plans for future light source facilities.

Baron has identified research on cuprates and FeAs superconductors as areas he wants to continue to work on. In particular, the oxygen phonon modes should be significantly more intense at BL43XU (a factor of 10 relative to the earlier work) allowing him to accurately explore the phenomena, something that is not possible with the present BL. In the case of the iron-arsenides, he is taking a new approach to analyzing the phonon spectra, attempting to simultaneously fit intensities and positions, including two-phonon contributions, to a few thousand spectra. If successful (and it should be), this could reveal new information on the phonon behavior and should be widely applicable. It does require large amounts of computing power, however, and we encourage him to be proactive is seeking these resources.

1.3 Management of the laboratory

The group appears to be happy and hardworking, working well together on the instrumentation aspects of IXS. It is clear that the members of the laboratory respect Baron and he allows them to pursue their own research agendas, providing the necessary support and interacting with them scientifically when needed. The group's scientific interests are diverse and this can lead to an environment in which individuals can be a bit scientifically isolated. This in turn can have a negative effect on scientific productivity and on the impact of the research if it lacks

context. We encourage Baron to take steps for a more frequent exchange of information or discussion with scientists both inside and outside the RIKEN group. This can be achieved through group meetings in which each discusses their own research, focused workshops on science questions, and an expanded visitor program in which relevant scientists (including theorists) spend a more extended time in the group, interacting with group members and perhaps even acting as science coordinator or consultant according to the scientific subjects. Since young scientists in the MDL are trying to find an academic or a research position outside of RIKEN or JASRI, emphasis should also be placed on writing more papers in a timely fashion.

Moreover entering into the new phase with two BLs operational, there are several issues related to the management of the MDL.
(i) Simultaneous operation of two beam lines BL35 and BL43 definitely requires more manpower (this is true even though the JASRI staffs will help operate the former beam line and support user experiments).
(ii) Since the new spectrometer is not open to the public users, in contrast to the BL35, the MDL needs to setup a strategic plan to perform experiments effectively and to produce number of scientific papers and outputs with high impact.

1.4 Future research plan

Future scientific research plans of MDL have already been discussed partly in (1) above. Since the performance of the newly constructed NRXIS spectrometer at BL43 is much higher than that of BL35, we hope the new spectrometer will expand the research field of NRXIS by measuring new excitations, including correlated electronic excitations and orbital-lattice coupled excitations. Furthermore lattice dynamical studies under extreme conditions such as high pressure (~100GP), high/low temperature and high magnetic field will provide indispensable information not only on the mechanism of novel properties such as multiferroics and superconductors but also on earth's interior, as proposed by the MDL.

The installation of two types of spectrometer on BL43; (a) high energy-resolution and (b) high-intensity with medium resolution, is appropriate to proceed with the proposed experiments. In order to pursue more challenging experiments, however, continuous development of the spectrometer is necessary. In this context, Baron has identified two particularly novel approaches to solving the problem of next generation analyzers which require high energy resolution whilst at the same time maintaining a large angular acceptance. The first of these, silicon crystals with induced temperature gradients to match the required Bragg angle is a wonderful idea and is currently being implemented at BL43XU. We congratulate Baron on this innovation. The second idea proposes the use of nuclear resonances in Fe foils to provide extremely high energy resolution. This would certainly work but at a great price in count rates. It is not clear that there is a scientific question well suited to this analyzer.

1.5 Overall assessment

The MDL has built a world-leading BL and, with a good research track record, and stands ready to do some exciting science. There are a few changes that can be made to maximize the scientific productivity and impact of the MDL, the most important of which is that a new position be created for BL scientist at BL43XU as soon as

possible. This will ultimately free up Baron’s time to focus more on science research rather than running the BL and providing user support. It is important that this person be hired as soon as possible so that they can work with Baron during the commissioning phase currently underway.

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