資料３
Material 3

平成 26 年 1 月

（独）理化学研究所
研究担当理事　川合 眞紀

平成 25 年度実施 主任研究員の中間レビューの結果について

主任研究員制度設置規程(平成 25 年規程第 13 号)第 5 条に基づき主任研究員の中間レビューを実施し、評価結果は下記のとおりです。

１．評価対象： 高田構造科学研究室 高田 昌樹 主任研究員

１）評価体制

実施日：平成 25 年 12 月 3 日（火曜日）

4 名の所外有識者を評価委員とするヒアリングレビューを実施。

評価者：

Yoshiyuki AMEMIYA, Professor
Department of Advanced Materials Science,
The University of Tokyo, Japan

Sadamichi MAEKAWA, Director General
Advanced Science Research Center,
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２）評価結果の概要等

General comments:

【Reviewer 1】

Dr. M. Takata and his team have been carrying out the extensive study on the structural and electronic properties of materials by using X-ray generated by SPring-8 Synchrotron radiation facilities. The importance of the Synchrotron Radiation is increasing as a tool for the study on materials and biology. SPring-8 is the most powerful Synchrotron Radiation facilities in the world. It is expected for the facilities to be utilized by researchers in various fields. Dr. Takata and his team belong to both RIKEN and JASRI. RIKEN pursues pure sciences and JASRI arranges experiment in SPring-8. For Takata Lab., the synergy effect of RIKEN and JASRI is going well. In particular, based on

the collaboration with researchers in universities and other research institutes, the charge density in transition metal oxides, ferroelectrics and layered materials obtained by the MEM/Rietveld method is a very unique and interesting result. The members have the advantage that they can have the machine time more than others in SPring-8 and that they can enjoy the collaboration with researchers in universities and other research institutes in SPring-8.

Dr. Takata and his team are expected to extend the contribution to both basic sciences and the development of the Synchrotron Radiation facilities in SPring-8.

【Reviewer 2】

Professor Takata has clearly demonstrated to be one of the leaders in the area of x-ray scattering of materials where he and his colleagues have pushed the technique into new domains in the RIKEN Spring-8 center. What is in particular noticeable is the large degree of collaborations with other groups outside of RIKEN. This clearly demonstrates a high level of success of the Takata group attracting outstanding scientists to work with them.

The group has further developed the Maximum Entropy Method together with refinements in the measurements to a high level of sophistication in powder diffraction allowing for detailed mapping of real space charge densities in materials. I find this a unique and novel application of x-ray scattering to observe what the important valence electrons are doing. It is most illustrative to observe the difference in charge densities in the valence bonds between diamond and silicon. This should be a picture in chemistry textbooks demonstrating the change in spatial orbital overlap between atoms of different sizes that naturally also accounts for the difference in the band gaps. The group has further developed the method to derive an electrostatic potential to each atoms in the system to account for the charge densities and made some beautiful applications in manganite's, ferroelectric materials, polymers, structural changes due to hydrogen absorption and structural changes in electrode materials.

The group has taken a world lead in the usage of polarized x-ray diffraction to probe various magnetic materials. The magnetic scattering cross section is very weak and for a successful endeavor this requires highly sophisticated instrumentation to allow measurements with precision that clearly the Takata group has accomplished. They applied this to novel problems related to spin chirality in ferroelectrics, crystallographic discrimination or domain distributions. They have also solved the magnetic structure of iridium oxides where also resonant scattering was used to determine spin-orbit couplings.

The SACLA source opens up new opportunities for coherent scattering of nanoparticles that will be explored in the future by the Takata group. There is an extraordinary opportunity to further develop their world leading capabilities to derive charge densities to time resolved measurements probing breaking and formation of chemical bonds using

SACLA. This could be something completely unique in the future.

【Reviewer 3】

Professor Takata, Chief Scientist, has been developing a field of structural materials science, which is an interdisciplinary field between photon science and materials science. He and his team members have elucidated charge/orbital order of transition metal oxides, hidden structures of gas molecules and many complicated materials using some precise data acquisition techniques and Maximum Entropy Method (MEM). These scientific results are highly appreciated by the international community. They newly bring in electrostatic potential analysis based on the MEM to visualize subtle difference of the charge density in some functional materials. This method is an effective way to detect atomic level polarization. They have also developed magnetic scattering technique to study the magnetic structure. In particular, the spin chirality in multiferroic materials is elegantly detected using polarization switching of x-rays by a twofold phase retarder. The reviewer also highly appreciates the success of x-ray pinpoint structural measurement, which is Prof. Takata's CREST project. The result showed the power of synchrotron radiation to the industry.

In these excellent achievements they are taking advantage of SPring-8: high brilliance, low emittance, polarization properties, and stable top-up mode operation. Their research strategy in strong collaborations with outstanding researchers outside RIKEN is highly appreciated. The management of the laboratory is very good. The team members show their great facilities in their cutting-edge studies. Their future plans sound good and are enough competitive ones.

In summary, evry research object is very clear and their achievements are excellent and outstanding. I strongly recommend that RIKEN continues to support this research program.

【Reviewer 4】

Dr. Takata's laboratory and its members aim to make the best use of the highly brilliant x-rays available from SPring-8 for the advanced research in structure materials science.

Among their many research results, the followings are highly evaluated.

1) Electrostatic potential imaging with an atomic resolution based on the combination of in situ & precise powder diffractometry and MEM (Maximum Entropy Method). This method has been successfully applied to several materials. Further development of this method should be made to clarify the relation of the structure and the function of materials.

2) Establishment of a so-called "X-ray Pinpoint Structural Measurement", which permits to measure time-resolved structural change with an atomic resolution at a

spatially confined area of materials. Based on this method, they succeeded in observing the crystal-amorphous phase change with a 20 ns time-resolution for optical recording of DVD/RAM system.

They have also made collaborations with many researchers in materials science, and helped them produce valuable scientific results, which would not be possible without the methods they developed and the high-quality x-ray beam from SPring-8.

Dr. Takata' management of the laboratory is also highly evaluated. He trained the young researchers so that they have the scientific and technical skills enough for them to pursue their own scientific objectives.

Though it may be out of the scope, the contribution of Dr. Takata to the management of SPring-8 is worthwhile being highly evaluated.

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