

2014年度指定パートナーユーザー事後評価報告 - 3 -

公益財団法人高輝度光科学研究センター
利用推進部

パートナーユーザー制度は、SPRING-8の共同利用ビームラインの更なる高度化および優れた成果の創出を推進するために、2014年度より運用しています。パートナーユーザー（以下「PU」という）は、公募・審査を経て指定されます。

PUの事後評価は、PU審査委員会において、あらかじめ提出されたPU活動終了報告書に基づいたPUによる発表と質疑応答により行われます。事後評価の着目点は、PUとしての(1)目標達成度、(2)活動成果（装置整備・高度化への協力、科学技術的価値および波及効果、ユーザー開拓および支援、情報発信）です。今回は、2014年度指定のPU1名（指定期間：2014年4月1日から2019年3月31日まで）について、事後評価（2019年12月4日開催）を行いました。

以下にPU審査委員会がとりまとめた評価結果等を示します。研究内容については本誌の「最近の研究から」にPUによる紹介記事を掲載しています。

1. Bo Iversen (University of Aarhus)

(1) 実施内容

研究テーマ：Application of synchrotron radiation in materials crystallography

高度化：Structural dynamics infrastructure development and its leading use

利用研究支援：Help and support to the users using upgraded beamline facilities

(2) ビームライン：BL02B1

(3) 評価コメント

This project set three goals. 1) Establishment of BL02B1 (single crystal structure analysis) to deliver high-quality and high-resolution diffraction data of the utmost quality for the purpose of charge density (CD) refinement and its application to novel materials. 2) Development of pico-second time-resolved data collection system for precise structural analysis at

charge density level. 3) Improvement of the usability of the system for users.

As for the Facility Upgrade, this group implemented a photon-counting pixelated CdTe detector Pilatus3 X 1M. They found that the both very strong and very weak data were suffered from systematic errors. They have developed an algorithm to correct the errors and succeeded in charge density refinement by using the detector. The achievement is highly esteemed. This detector system will be useful for collecting diffuse scattering data, for example, because the long reading and erasing time of about 7 minutes of the present imaging plate system prevents from collecting the data with a very thin slicing for omega rotation. They also introduced an x-ray chopper at the upstream side of the slit for the time-resolved data collection. They have succeeded in capturing the change in crystal structure of BaTiO₃ during the polarization reversal by the pump-probe method using the chopped pulse x-rays of 30 keV from the train bunch in the D-mode operation with the temporal resolution of 685 ns and a repetition rate of 1 kHz. The chopped SR pulse x-rays from the single bunch in the H-mode operation with the temporal resolution of 50 ps was also successfully obtained. They also tried to develop low-temperature high-pressure x-ray structure analysis.

The upgraded system was applied to the charge density refinement of many materials like rubrene, SnTe, CsCl, H₃Co(CN)₆, and TiS. The results provide valuable information about the chemical bonding and thermal vibration. The achievements were published in high-impact journals.

This group supported 18 proposals for 5 years. Although the outreach activity was rather limited, some of the proposals including time-resolved diffraction of quartz in 30-MHz electric field were successfully performed to produce a good achievement.

In summary, this PU project is highly evaluated from the viewpoint of beamline upgrade and its application. The committee recommends that the obtained knowledge about the CdTe detector system should be widely shared.