【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Chemistry)

Title of Project : Visualizing ultrafast dynamics of molecular structure with femtosecond X-ray solution scattering

Shin-ichi Adachi
(High Energy Accelerator Research Organization, Institute of Materials Structure Science, Professor)

Research Project Number : 17H06141 Researcher Number : 60260220
Research Area : Synchrotron Radiation Science, Physical Chemistry
Keyword : Ultrafast Dynamics, Structure Science

【Purpose and Background of the Research】

One of the fundamental goals in physical chemistry is to describe how a chemical reaction proceeds from reactants to products via intermediates, if they exist, at the atomic and molecular levels. In particular, solution-phase reaction dynamics are of much interest since many chemical and biologically relevant reactions occur in solution. Time-resolved X-ray solution scattering provides direct information of the transient molecular structures, because scattering signals are sensitive to all chemical species present in the sample and can be compared with the theoretical scattering signal calculated from 3-D atomic coordinates of the chemical species involved. In this project, we capture ultrafast structural dynamics of molecules by time-resolved X-ray solution scattering technique with femtosecond X-ray pulses.

【Research Methods】

The major limitation of time-resolved X-ray solution scattering was the limited temporal resolution from the duration of the available X-ray pulses, which is ~100 picoseconds from synchrotron storage rings. However, the limitation of the X-ray pulse width has been improved into the femtosecond regime with the advent of X-ray free electron lasers (XFELs). We applied time-resolved X-ray solution scattering technique to Au-Au bond formation reaction of $Au(CN)_2^-$ oligomers in liquid phase by using both synchrotron storage ring and XFEL facilities, and successfully elucidated the ultrafast structural dynamics of the Au-Au bond formation process at the atomic level (Fig. 1).

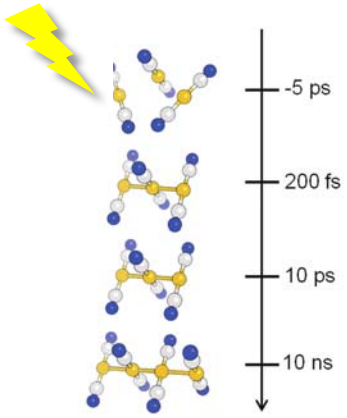

Fig. 1 Ultrafast structural dynamics of Au-Au bond formation of $Au(CN)_2^-$ oligomers.

【Expected Research Achievements and Scientific Significance】

Based on the previous work, this project is aiming to directly detect ultrafast vibrational motion of molecules by femtosecond time-resolved X-ray solution scattering technique. This experimental technique will hopefully open a new research field of fundamental chemistry as “ultrafast molecular structure science in the liquid phase”.

【Publications Relevant to the Project】

"Direct observation of bond formation in solution with femtosecond X-ray scattering”
Kim, Kim, Nozawa, Sato, Ihee, & Adachi *et al.* ***Nature***, 518, 385-389 (2015).

”Synchrotron-Based Time-Resolved X-ray Solution Scattering (Liquidography)”
S. Adachi, J. Kim, & H. Ihee
Advances in Lasers and Electro Optics, Nelson Costa and Adolfo Cartaxo Ed., (2010) ISBN: 978-953-307-088-9, INTECH.

【Term of Project】

FY2017-2021

【Budget Allocation】

154,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www2.kek.jp/imss/pf/
shinichi.adachi@kek.jp