Multilayer structure of PbS/EuS nanocrystals revealed by combining of synchrotron small-angle X-ray scattering method and energy dispersive X-ray spectroscopy

<u>Hiroyasu Masunaga</u>, Hiroki Ogawa, Sono Sasaki, Takaaki Hikima, Masaki Takata, Takuya Nakashima, Tsuyoshi Kawaid

Japan Synchrotron Radiation Research Institute(JASRI) 1-1-1, Sayo, Sayo, Hyogo, 679-5198, Japan

Multilayer nanostructure analysis has been carried out for core-shell PbS/EuS NCs by the combination of the synchrotron SAXS measurement and EDS-TEM observation. Structure information on the PbS/EuS NCs was obtained from EDS-TEM images to construct their initial structure models for SAXS intensity analyses. With statistically high precision, structure of the PbS/EuS NCs was successfully analyzed using a trilayer-cubic core-shell structure model by combining different techniques of SAXS and EDS-TEM. SAXS measurement of NCs carried out at BL45XU in the SPring-8 (RIKEN SPring-8 Center, Japan). Fig. 1a shows a transmission electron microscopic (TEM) image of PbS NCs, which is core particles. It was found that the shape of the PbS NCs was a quasi-cube with a narrow size distribution. An electron density profile, $\rho(\mathbf{r})$, of this spherical structure was indicated in Fig. 1b. If cubes orient in the statistically random direction in the solvent, their electron density distribution can be regarded approximately as that of a core-shell electron density distribution model. The electron density of the core with a radius of L is defined as $\rho 1$. Here, $\rho 1$ denotes the electron density of PbS crystal. Also, L means half the side length of a cubic particle. Fig. 1c show SAXS profiles of PbS NCs measured for their hexane solution, and simulated scattering profiles on the basis of electron density models of randomly-rotating spherical and cubic structures. L of a reasonable cubic structure was determined as 4.6 nm in average so as to minimize a difference in the peak position around q equal to 1.0 nm⁻¹ and 2.2 nm⁻¹ between measured and simulated profiles.



Fig. 1 A TEM image of PbS NCs. The shape of PbS NCs was a quasi-cube with a side length of 9.7 nm with a narrow size distribution (a). An electron density profile of a randomly-rotating cubic model in a solvent (b), scattering profiles measured for the PbS NCs (open circle) and simulated ones using spherical and cubic structures (lines) (c).