# Research Title Integrated approach of skills and machine learning in the measurement

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## Brief overview

Compressive sensing is introduced for observation of gold atomic nanoclusters by HAADF-STEM electron microscope. The reconstruction of three-dimensional structure from multiple imaging by electron microscope is studied in recent years, however, the present electron microscope is not made for CT usage. it is difficult to acquire a large number of observation data because of the degradation of sample due to high-energy electron beam. We introduce an algorithm capable of high precision reconstruction from rather small number of images to alleviate the effect of the above degradation and reconstructed the clusters of about 20,000 atoms.

In the course of examining the reconstruction results, it is necessary to develop a method to evaluate the reliability of the results. Since the result of compressive sensing is point estimation, it does not involve error bars. Therefore we adopt a method to generate a large number of reconstruction results by resampling from observation data and to determine the correctness of reconstruction from the statistical properties (mainly dispersion) and found a behavior that serves as a clue .

## Achievement

Three-dimensional atomic arrangement shown in Fig. 1 was obtained from three images using compressive sensing and connected-component analysis. The total number of variables is 125073, the total number of observation data is 14672, and the total number of atoms of the obtained arrangement is 24571. At the same time as obtaining the image of all atom arrangement, we extracted the atoms which are considered to have high catalytic activity from the analysis of the atomic arrangement at the adjacent lattice points (see Fig. 2).

In addition, we started to develop a method to evaluate the error with respect to compressive sensing of the structured data, and to judge correctness of reconstruction. For the reconstruction of artificial data with 2929 elements, of which the occupied number of atoms is 599, the variance obtained by resampling was calculated. As a result, a qualitative difference as shown in Fig. 3 was found in the behavior of variance for each variable of the reconstructed signal depending on the total observation data amount.

Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

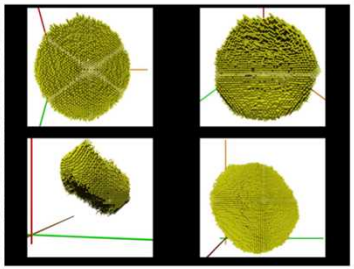

Figure 1

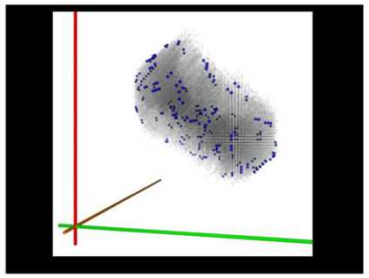

Figure 2

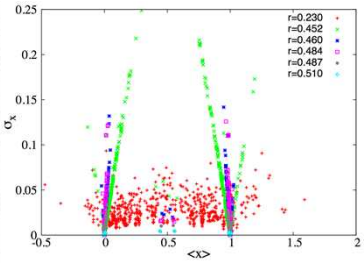


Figure 3

## Reference/Link

As for related strategic objectives related to this research area, see http://www.senryaku.jst.go.jp/teian/en/koubo/h29youkou_7_en.pdf