

 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2009B0049 実験課題名 Title of experiment Disordered crystal structure and intrinsic temperature factors of an electride by TOF neutron diffraction 実験責任者名 Name of principal investigator Kiyooki Tanaka 所属 Affiliation Nagoya institute of Technology (present address : Nagoya Industrial Science research institute)	装置責任者 Name of responsible person Ichiro Tanaka 装置名 Name of Instrument/(BL No.) iBIX at BL-03 実施日 Date of Experiment 2010/1/20 - 1/26

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. Inorganic Electrides a. $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32.529(14)}$ (C12A7:e, electric conductivity a room temperature 700S/cmm) b. $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32}$ (C12A7:2e, electric conductivity at room temperature 1500S/cmm) Both crystals were shaped into cubes with an edge of 2mm and were used for the experiment with the neutron TOF diffraction experiment.

2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons. TOF neutron diffraction experiment was done and the intensity data measured on two dimensional detector were indexed and were converged to structure factors successfully. The analysis of the data will soon start after the publication of the results on C12A7. The experiment was done as a part of our project of investigating the electron density distribution of the electrons left inside of the cages of $\text{Ca}_{12}\text{Al}_{14}\text{O}_{32+x}$ (C12A7:e), which is called as 'free' electrons here. Since the crystal structure of C12A7:e is closely related to that of C12A7 and tiny distortion of the crystal structure due to O ions included perfectly randomly in two cages among the 12 cages in the unit cell, more accurate and higher resolution single crystal diffraction experiments are necessary. Therefore, the following three kinds of experiments using the facilities of neutron diffraction at J-PARC and LANCE, and of X-ray diffraction at PF have been done in our investigation on the inorganic electride:. 1. The X-ray diffraction experiment at PF on C12A7, C12A7:e and C12A7:2e was already finished. 2. The TOF neutron diffraction experiment at LANCE on C12A7 was finished. 3. The TOF neutron experiment at J-PARC on C12A7:e and C12A7:2e is reported here.
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2. 実験方法及び結果(つづき) Experimental method and results (continued)

The results on the X-ray crystal structure of C12A7 are now being prepared for publication. The X-ray study of C12A7 revealed the detailed local deformed structure due to the O ions included in a cage and will be a firm base for further investigation on the inorganic electride. The neutron experiment at LANCE with higher resolution than the X-ray experiment will reveal more detailed splitting of atomic positions due to the included O ion. Based on these studies the diffraction data measured at J-PARC will be analysed and the detailed splitting of atoms of a cage including 'free' electrons left after the removal of O ion will be made clear. The electron density distribution measured by X-ray diffraction is the sum of those of the electrons in the cage and those around the electronic orbitals of ions. Therefore, the electron density of the 'free' electrons, which is expected to be very small, can be made clear only after analysing perfectly the splitting of ions.