実験番号：201902042（2 シフト）

BL6N1

Sulfur-encapsulation in graphene nanospace

Shuwen　WANG，Hedeki　TANAKA

信州大学工学部先鋭材料研究所（RISM）

キーワード：Radial distribution function，Fourier transform，Structural information

1. 背景と研究目的

It is well known that XAFS contains the structural information of average distances to near-neighboring atoms and the types of neighbors about a specific atom type. We have prepared two dimensional confined nanosapce (PG-box) and encapsulate sulfur in such nanosapce. It is of significant importance to understand the structure of confined sulfur for its further application.

2. 実験内容

The EXAFS spectra of sulfur-contained PG-box was obtained in Aichi SR. The radial distribution function (RDF) of sulfur atoms can be obtianed from the EXAFS spectra by using software Athena. The RDF of interest is the spatial distribution of neighboring atoms relative to the specific type of center atom; that is, it is the partial pair correlation function about that type of atom. It is usual to display the Fourier transform (and/or its magnitude) of y(k), which is the normalized XAFS in k space.

3. 結果および考察

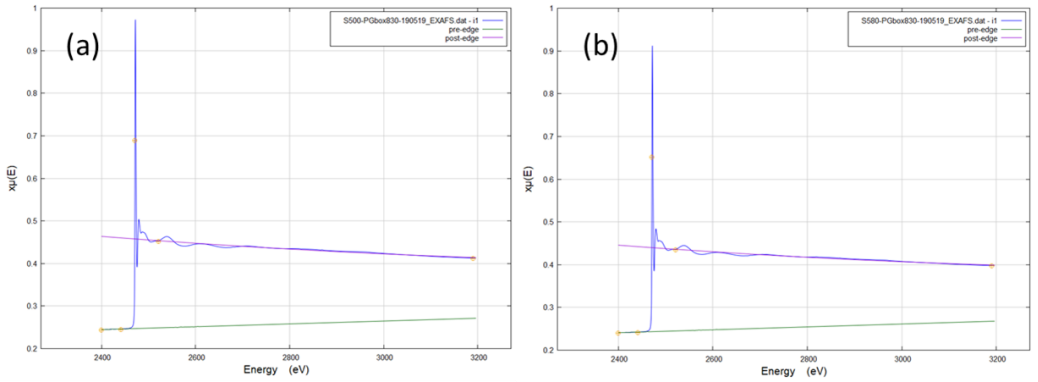

Fig 1. The EXAFS data of S@PG-box prepared at (a) 500 ºC and (b) 580 ºC.

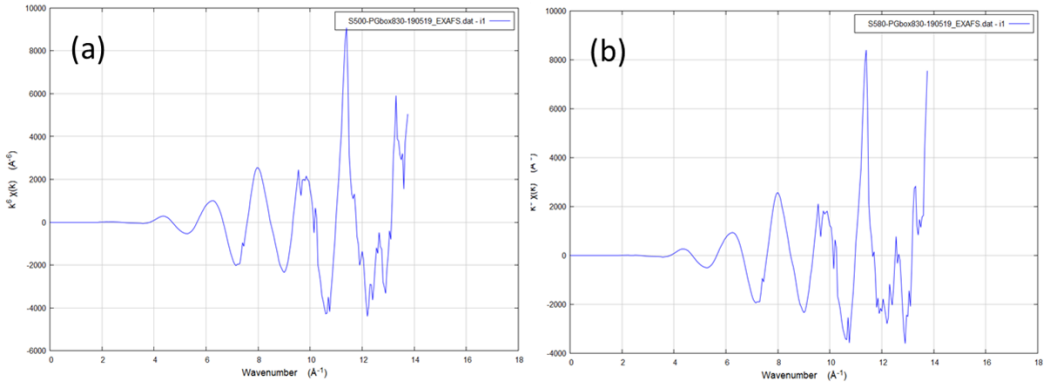

Fig 2. The EXAFS data in k space of S@PG-box prepared at (a) 500 ºC and (b) 580 ºC.

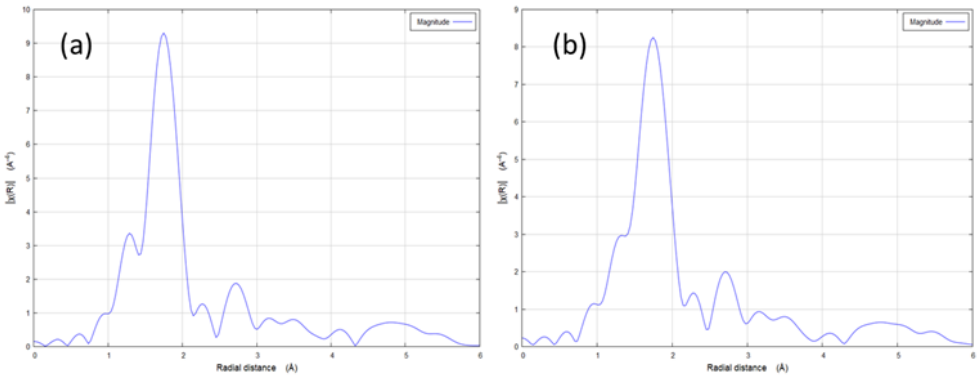

Fig 3. The radial distribution function of sulfur atoms in PG-box prepared at (a) 500 ºC and (b) 580 ºC.

The EXAFS data of S@PG-box prepared at different temperatures are shown in Figure 1. After background subtraction followed by k space transforamtion, we can obtain Figure 2. The radial distribution function of sulfur atoms can be further obtained by Fourier transformation of EXAFS data in k space, as shown in Figure 3. However, the average near-neighboring distances of surfur atoms are almost same regardless of the preparation condtions. In the following study, we will investigate the structural information of surfur confiend in different pore sizes.