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Sulfur-encapsulation in carbon nanotubes

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キーワード：Cordination number, bond length, Fourier transformaiton

1. 背景と研究目的

The present study is a continuous work of 201904075.

We have studied the coordination number and bond length of sulfur confined in slit-shaped pores. In the present study we investigate those structural information of sulfur confined in cylindrical-shaped pores.

2. 実験内容

Sulfur was encapsulated in a series of carbon nanotubes (EC1.5, EC2.0, SWCNH) of different diameters. The EXAFS spectra of sulfur-contained carbon nanotubes were obtained in Aichi SR. The k space of EXAFS data can be obtained by normalization of The XAFS spectra. Fourier transformation of k space gives R space of EXAFS data, and reverse Fourier transformation of R space gives q space.

3. 結果および考察

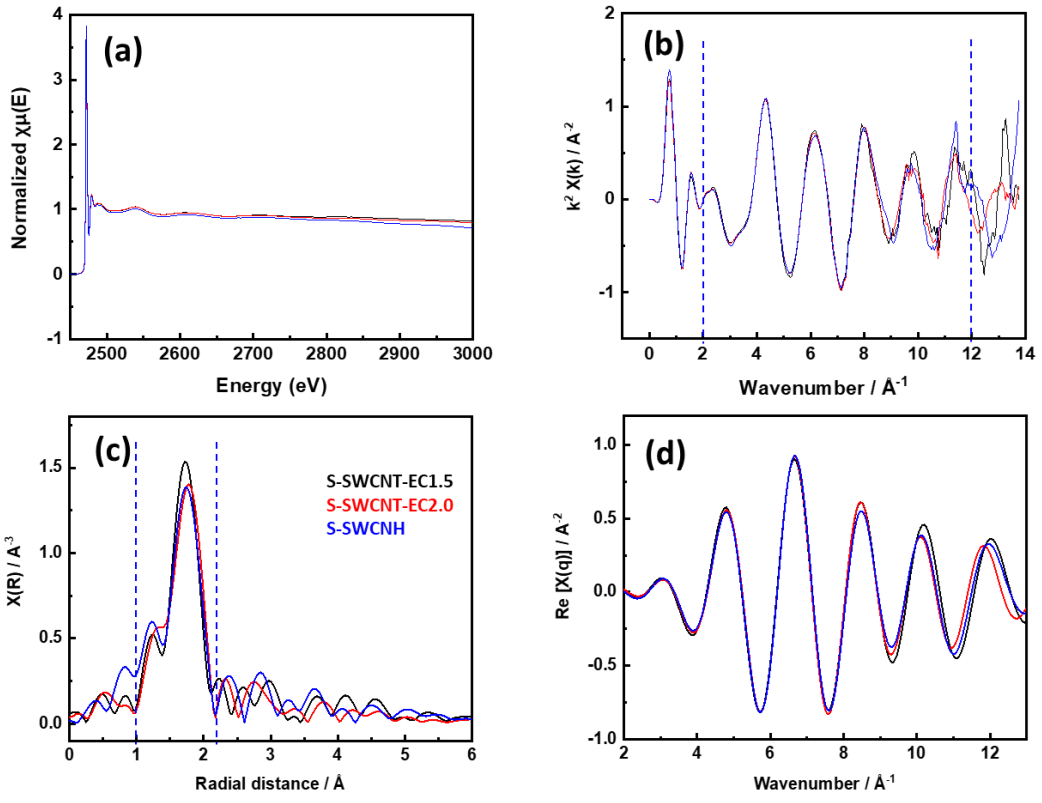

Fig 1. The EXAFS data of (a) Energy, (b) k space, (c) R space, (d) q space for sulfur encapsulated in carbon nanotubes with different diameters. Sulfur encapsulated in EC1.5: black, sulfur encapsulated in EC2.0: red, sulfur encapsulated in SWCNH: blue.

The normalized X-ray absorption spectroscopy is shown in Figure (a). The EXAFS data (k space) of sulfur encapsulated in different carbon nanotubes are shown in Figure (b). After Fourier transformation of k space, we can obtain the radial distribution function of sulfur atoms (R space), as shown in Figure (c). The reverse Fourier transformation of R space gives q space (Figure (d)), from which the coordination number and bond length can be obtained by using software Artemis. Results indicate that the coordination numbers and bond length of the confined sulfur in carbon nanotubes larger than 1.5 nm are similar to that of bulk sulfur, being around 2.0 and 0.206 nm.