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Sulfur-encapsulation in activated carbon fiber

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キーワード：**Sulfur encapsulation, Cordination number, Fourier transformaiton**

1. 背景と研究目的

We have studied the coordination number and bond length of sulfur confined in different slit-shaped pores in 201904075. We found that sulfur encapsulated in smaller pores (ACF-A5) have smaller coordination number. In current study we investigated the structure of sulfur encapsulated in ACF-A5 prepared under different temperatures.

2. 実験内容

Sulfur was encapsulated in ACF-A5 under different temperatures. 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

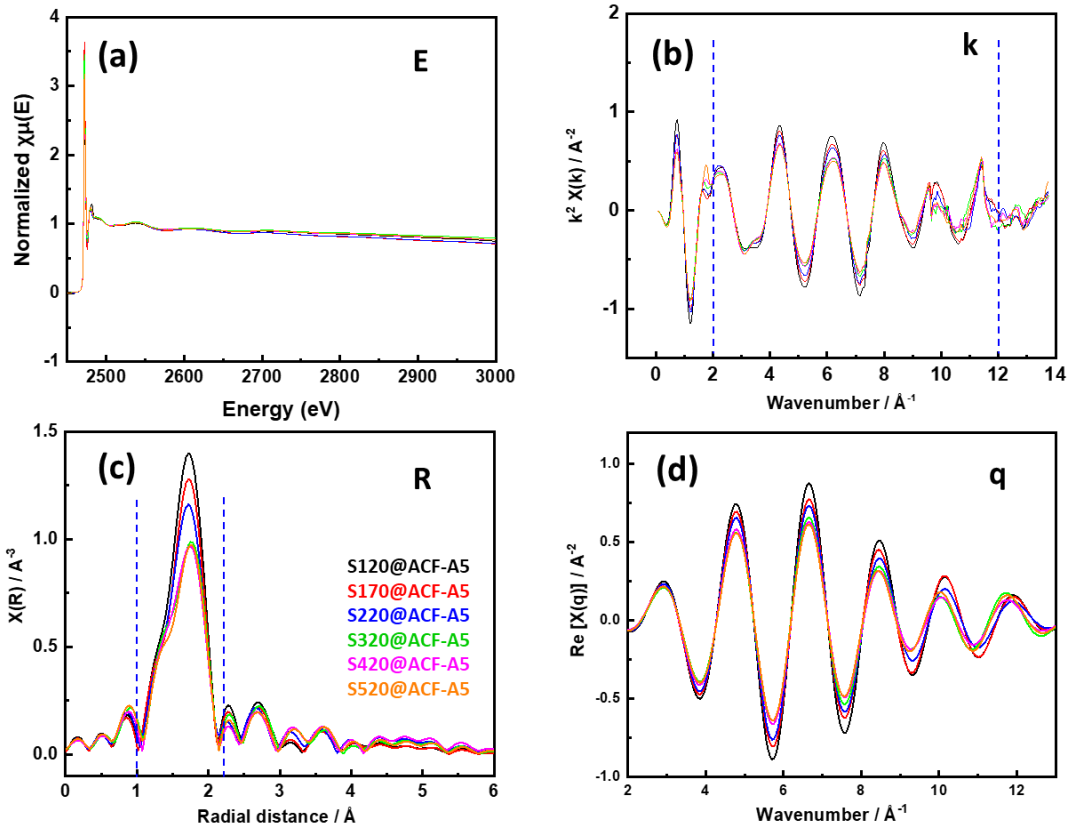

Fig 1. The EXAFS data of (a) Energy, (b) k space, (c) R space, (d) q space for sulfur encapsulated in ACF-A5 prepared under different temperatures. Some data is taken from our previous measurement.

Sulfur encapsulated in ACF-A5 under temperature of *T* is nominated as S*T*@ACF-A5.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 of S120@ ACF-A5 is close to that of bulk sulfur. The coordination number of sulfur decreases with the increase of encapsulation temperature, and becomes almost constant when encapsulation temperature is above 320 ^{o}C.