

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2017A0119 実験課題名 Title of experiment Understanding microscopic structural transformations of coals on heat-treatment 実験責任者名 Name of principal investigator Hideki Tanaka 所属 Affiliation Department of Chemical Engineering, Kyoto University	装置責任者 Name of responsible person Toshiya Otomo 装置名 Name of Instrument/(BL No.) NOVA / (BL-21) 実施日 Date of Experiment October 26-29, 2017

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.
Low-grade and high-grade coals heat-treated at 600, 700, 800, and 900 °C

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.
<p>The low-grade and high-grade coals heat-treated at different four temperatures (600, 700, 800, and 900 °C) in powder form (ca. 1 cc) were put into glass cells and evacuated at 110 °C using a turbo molecular pump for 2 hours to remove adsorbed water. Then, the samples were transferred to V-Ni cells in a helium-filled glove box and sealed by PTFE. Neutron diffraction measurements were measured by NOVA at room temperature. The structure factors for the low-grade and high-grade coals obtained by the detector at angle of 45° are shown in Figures 1 and 2. It is clear that the peak at a wave vector of $Q = 1.8 \text{ \AA}^{-1}$ for the low-grade coals becomes pronounced with increasing temperature of heat treatment (Figure 1), which suggests that the number of stacking of a nano-graphene is increased. On the other hand, in the case of the high-grade coal treated at 600 °C, the peak at $Q = 1.8 \text{ \AA}^{-1}$ has already been pronounced compared with that of low-grade coal heat-treated at 900 °C (Figure 2). The peak at $Q = 1.8 \text{ \AA}^{-1}$ is also increased with increasing temperature of heat treatment, which is again attributed to the development of the layer structure of stacked nano-graphenes. These facts demonstrate that the structural transformations of the low-grade coals and high-grade coals on the heat-treatment are different, which would be related to the shrinkage behavior of the low-grade coal.</p>

2. 実験方法及び結果(つづき) Experimental method and results (continued)

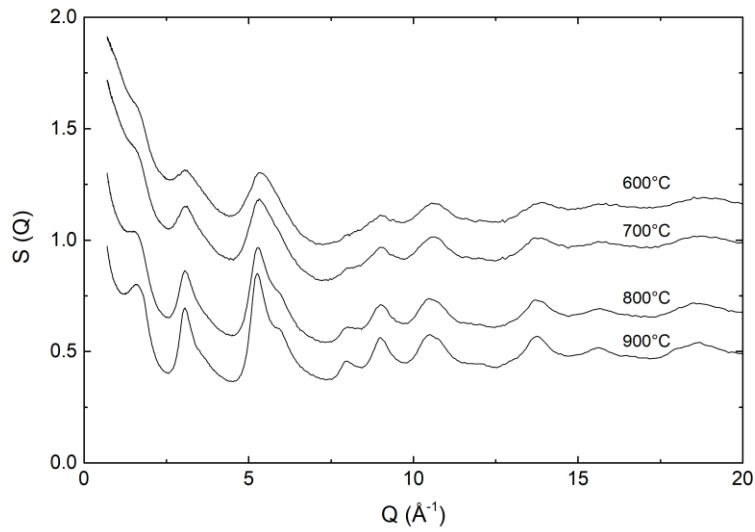


Figure 1 Wave vector dependence of the structure factor of the low-grade coals heat-treated at four temperatures.

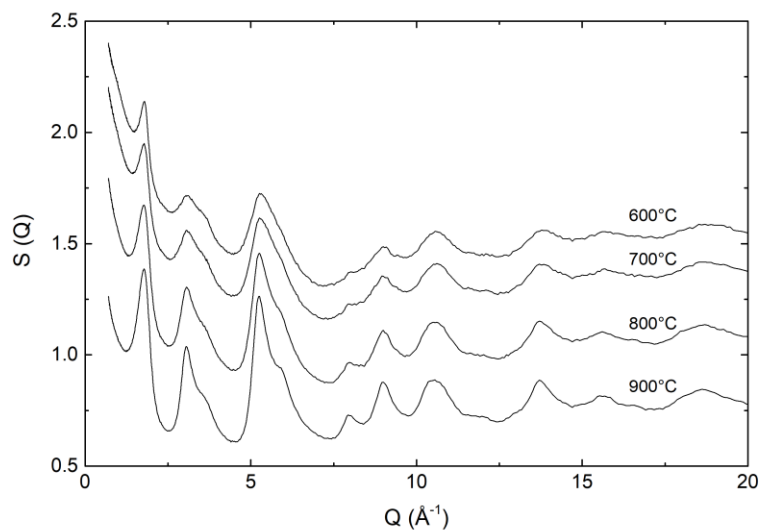


Figure 2 Wave vector dependence of the structure factor of the high-grade coals heat-treated at four temperatures.

We have already determined the density of coals with exception of macropores by using a mercury porosimeter and the composition of hydrogen atoms in coals by the elementary analysis. These data will be used to obtain the pair distribution function of the coals in collaboration with Dr. Suzuya and Dr. Otomo.