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Soft x-ray absorption spectroscopy of Na ions distributed in zeolite crystals

Takehito NAKANO*[1], Haruyuki HATANO[1], Daisuke KINIWA[1], Yuka IKEMOTO[2],
Tetsuya KODAIRA[3], Takuji IKEDA[4], Yoshihisa HARADA[5], Akiko FUKUSHIMA[6],
Keisuke KOBAYASHI[2], Shik SHIN[5, 6] and Yasuo NOZUE[1]
[1] Department of Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan
[2] JASRI/SPring-8, 1-1-1, Kouto, Mikazuki-cho, Sayo, Hyogo 679-5198, Japan
[3] AIST, Tsukuba, Ibaraki 305-8565, Japan, [4] AIST Tohoku, Sendai, Miyagi 983-8551, Japan
[5] RIKEN/SPring-8, 1-1-1, Kouto, Mikazuki-cho, Sayo, Hyogo 679-5148, Japan
[6]Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan

Introduction

Aluminosilicate zeolite crystals have periodically arrayed nano-size regular cages. The framework consisted of $Al_xSi_{2-x}O_4$ is negatively charged and many exchangeable cations, such as Na ions, are distributed in the space of the framework as giving an example in Fig. 1. The cations are thought to sit on a peculiar environment with strong electric filed of the framework. In the present work, we carried out Na 1s absorption spectroscopy for several different types of zeolite in order to investigate the local environment around Na cations and its effect on the optical transition process of core electrons.

Experimental procedure

We used five different types of zeolite; A, ZK-4 with Si/Al = 1.9, low silica X (LSX), Y with Si/Al = 2.8 and sodalite (SOD). Fully dehydrated powder samples were pressed and shaped into a disc in a glove box with a pure He-gas atmosphere. The disk-shaped sample was tightly fixed on a holder by a cover with a light guide hole to obtain enough electric contact. Samples were transferred into the pre-chamber of spectrometer in a N_2-gas atmosphere by using a glove bag to avoid the adsorption of water molecules. Samples were degassed again just before the measurement by irradiating the concentrated infrared light through a view port of vacuum chamber. Absorption spectra were obtained by using total electron yield method at room temperature.

Results and discussion

Figure 2 shows Na 1s absorption spectra of several different types of zeolite. There shows three prominent structures as denoted by a-c. The peak a can be attributed to the 1s-3s transition, which is also reported in NaF molecule[1]. Although this transition is originally forbidden, the absorption peaks appear quite clearly. The peaks b and c can be attributed to the 1s-3p transitions. The doublet structure is due to the splitting of the 3p orbital. According to the crystal structural data, a strong asymmetric ligand field is expected due to oxygen atoms of framework around Na ions. The strong ligand field is thought to result in the appearance of 1s-3s transition as well as the large splitting of 3p state. The difference in the peak intensities and fine structures depending on the types of zeolite is found to be consistently understood by considering the local arrangement of oxygen atoms as well as aluminum ones around Na ions.

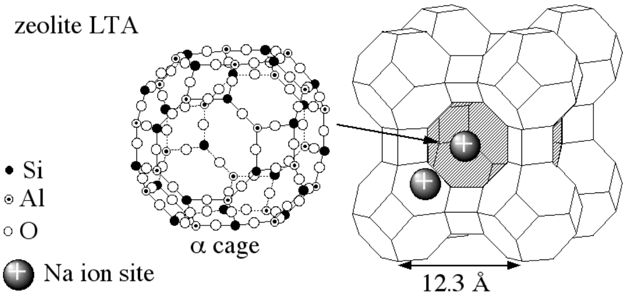

Fig. 1. Schematic illustration of framework structure of zeolite A. Typical sites of Na ions are also shown.

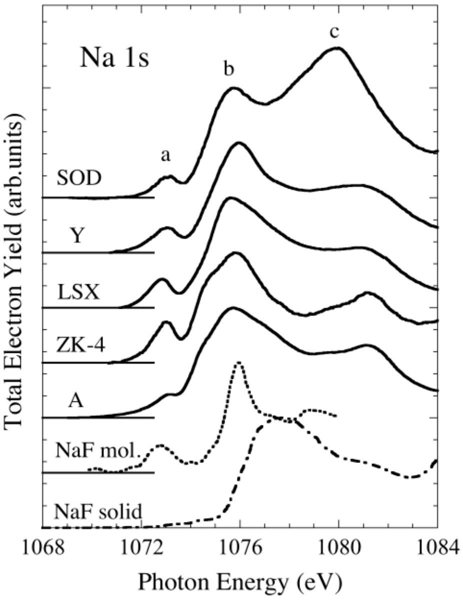

Fig. 2. Na 1s absorption spectra of zeolites and NaF, the latter of which is from Ref. [1].

References

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* nakano@nano.phys.sci.osaka-u.ac.jp