11B/2002G260

Spatial distribution of metal induced gap state at alkali halide/metal interface

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Introduction

At the insulator (or semiconductor)/metal interface, a free-electron-like metal wave function penetrates into an insulating side and new electronic states metal induced gap states (MIGS) are formed in the insulator (or semiconductor) band gap. MIGS is considered to determine the Schottky barrier height at the semiconductor/metal interface, and they have attracted wide attention especially for semiconductor/metal interfaces. However, there is little experiments to observe MIGS, because well-defined interfaces are hard to prepare, and the signal from the interface is obscured by that from the substrate in conventional experimental methods. Recently, we succeeded in observing MIGS by preparing well defined LiCl/Cu(001) and LiCl/Ag(001) interfaces, and using NEXAFS. In the present study, we investigated more detailed character of MIGS, focusing on the spatial distribution of MIGS in surface parallel direction.

Experiment

Mechanically and electrochemically polished Cu(001) and Ag(001) were cleaned by repeated cycles of Ar^+ sputtering and annealing. Alkali halides were evaporated from a Knudsen cell in a custom-designed ultrahigh-vacuum system with a base pressure of 4×10^{-8} Pa and the growth rate was on the order of 0.1 nm/min. Cl K-edge NEXAFS was carried out at the station BL-11B of the Photon Factory in the Institute of Materials Structure Science.

Results and Discussion

The Cl-*K* and K-*K* edges NEXAFS provide information on the unoccupied Cl-p and K-p electronic densities of states. In case of alkali halide (001) film, each layer consists of the same number of cations and anions, and cations and anions align alternately. Therefore, we can discuss the spatial distribution of MIGS in the surface parallel direction by comparing the intensity of the MIGS peak in Cl edge and K edge NEXAFS for KCl film grown on metal substrate. Figure 1 shows both Cl-*K* and K-*K* edges NEXAFS for KCl/Cu(001). The pre-peak originated from MIGS is clearly observed for Cl edge, while the pre-peak is not observed for K-edge. These NEXAFS results reveals that MIGS are localized at only the anion site. Figure 2 shows the systematic view of the spatial distribution of MIGS for alkali halide/metal interface determined by the present NEXAFS results.

The localization of MIGS at anion site can be discussed by considering recent theoretical calculation results. With the help of *ab initio* calculation performed by Arita *et al.*, charge transfer from the insulator to the metal commonly occurs for alkali halide/metal systems, indicating that MIGS has a valence band (anion) character. On the other hand, the localization of MIGS at anion sites determined by the present study provides another possibility of superconductivity proposed by Kuroki and Aoki

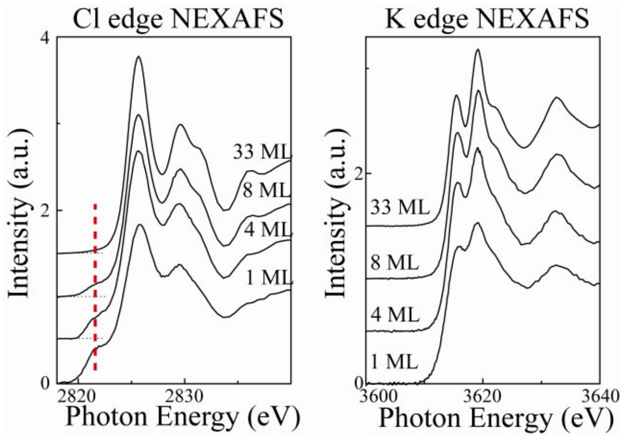

Figure 1: The Cl-*K* and K-*K* edge NEXAFS spectra in KCl films grown on Cu(001) for various thicknesses of the KCl layer taken at the X-ray incidence angle of 15°, except the bottom one (normal incidence). All the spectra are normalized by their edge-jump.

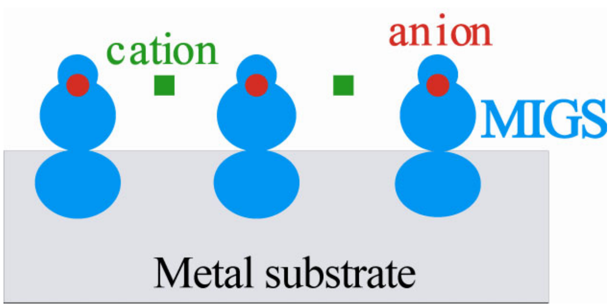

Figure 2: Systematic view of the spatial distribution of MIGS for alkali halide/metal interface. The position of cation (box) and anion (circle) is shown in the figure.

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