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Metal induced gap states at LiCl/Cu(001) interface studied by x-ray absorption fine structure

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Introduction

There has been a growing interest in metal/insulator systems due to their importance in catalysis, device applications and fundamental science. However, the large difference in chemical bond between metals and insulators makes it difficult to form an well-ordered interface. Recently, we could reveal that some alkali halide film grow heteroepitaxially on metal surfaces in a layer-by-layer fashion. In the present study, the electronic structures of LiCl/Cu(001) and LiCl/Ag(001) have been studied using NEXAFS, as a model system of the metal/insulator (alkali halide) interface.

Experiment

A mechanically and electrochemically polished Cu(001) and Ag(001) crystals were cleaned by repeated cycles of Ar$^+$ sputtering and annealing at 900 K. LiCl was evaporated from a Knudsen cell. Cl-*K* edge NEXAFS measurements were carried out at the soft x-ray double-crystal monochromator station BL-11B of the Photon Factory in National Laboratory for High Energy Physics.

Results and Discussion

Figure 1 shows the thickness and polarization dependence of the Cl K-edge NEXAFS for LiCl film grown on Cu(001). A well-pronounced pre-peak (peak 1) was observed on the bulk edge onset for the thin LiCl film grown on Cu(001). The intensity of the pre-peak increased with a decrease in film thickness. The pre-peak extended approximately 4 eV on the low energy side. The pre-peak was also observed for LiCl/Ag(001). LiCl grows on Cu(001) with its [100] axis rotated by 45^{o} from that of the metal substrate ([100]$_{film}$//[110]$_{substrate}$), while LiCl grows on Ag(001) without azimuthal rotation ([100]$_{film}$//[100]$_{substrate}$). The pre-peak was observed irrespective of the interface structure. The energy of Cu MMM AES for LiCl/Cu(001) was the same as that for Cu(001) within 0.1 eV, indicating that Cu-Cl bond was not formed at the interface. Furthermore, the Cl 1s XPS results shows that only Li-Cl bond was formed for LiCl/Cu(001), since there is no sub-peak. These experimental results indicate that the pre-peak did not derive from the local Cu-Cl bond at the interface. The Cl-*K* edge pre-peak, and the gap state which they reflected, could be qualitatively understood as metal-induced gap state (MIGS). The MIGS were first introduced for semiconductor/metal junctions, but are also applicable to insulator/metal interfaces, such as MgO/Cu. In the present study, we could observe the MIGS for alkali halide/metal interfaces. The MIGS are the tails of the metal wave functions that decay exponentially into the insulating side of the interface. Next, we would discuss the character of MIGS formed at LiCl/Cu(001) interface. The MIGS peak was most enhanced at grazing x-ray incidence, implying that MIGS spread toward the surface normal direction. By analyzing the thickness dependence of the intensity of pre-peak, the decay length( ) of MIGS was determined to be 0.2 nm. The decay length is shorter for states that are farther in energy from the band edge, that is,   decreases with the band gap. For Si/Cu interface, the band gap of Si is 1.2 eV and   is 0.6 nm. On the other hand, the band gap of LiCl is as large as 9.4 eV, it is, thus, natural that   is 0.2 nm for LiCl/Cu.

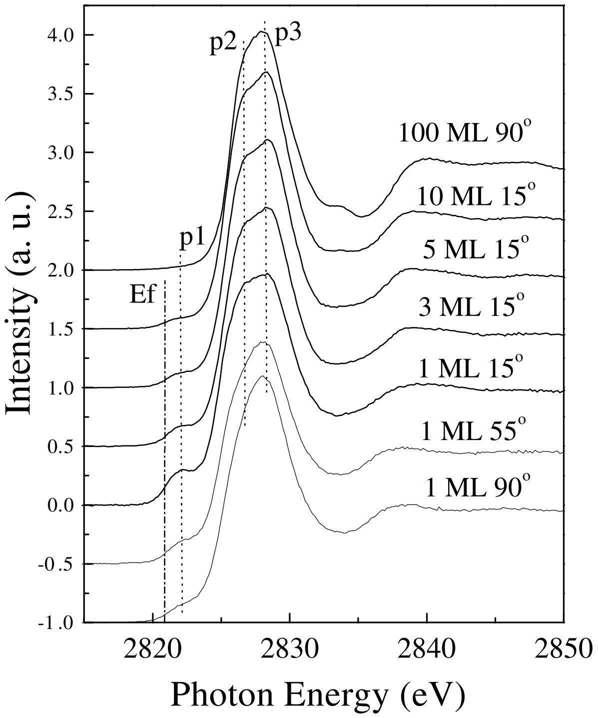

Fig. 1: Thickness and polarization dependence of the Cl K-edge NEXAFS for LiCl film grown on Cu(001).

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