

## Decay length of metal induced gap states at alkali halide/metal interface

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### Introduction

Insulator/metal interfaces attract wide attention, since they provide fascinating possibilities such as metal-insulator transition, band gap narrowing and superconductivity as well as technological ones such as catalysis, magnetic tunneling junctions, etc. Among the insulators, we concentrated on alkali halides because they can be grown epitaxially on some metal or semiconductor substrates and are expected for the ultra-thin insulating films. We have revealed the existence of metal induced gap states (MIGS) at the alkali halide/metal interfaces. In the present study, we investigated more detailed character of MIGS, focusing on the decay length in surface normal direction.

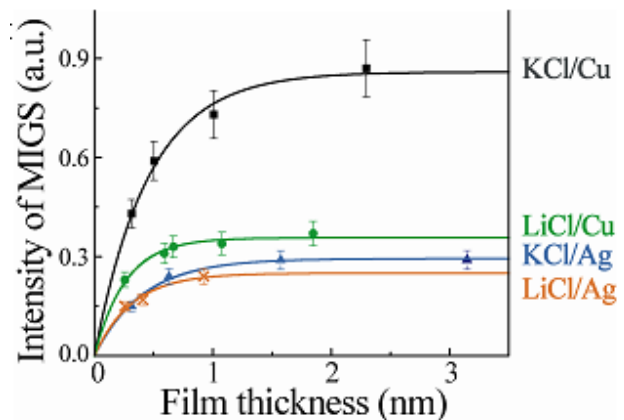
### Experiment

Mechanically and electrochemically polished Cu(001) and Ag(001) were cleaned by repeated cycles of Ar<sup>+</sup> sputtering and annealing. Alkali halides were evaporated from a Knudsen cell in a custom-designed ultrahigh-vacuum system with a base pressure of  $4 \times 10^{-8}$  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 spatial distribution of MIGS in the surface normal direction is discussed in terms of decay length of MIGS by the thickness dependent NEXAFS. Figure shows the intensity of the pre-peak (not normalized by the edge-jump) as a function of the film thickness. Here, we assume that the probing depth of NEXAFS is much greater (typically >1000 nm) than the atomic scale, and the density of MIGS ( $f(x)$ ) at the distance  $x$  can be represented as  $I_0 \exp(-x/\lambda)$ , where  $I_0$  and  $\lambda$  are the intensity of MIGS at the interface, decay length. The intensity of MIGS ( $F(X)$ ; film thickness  $X$ ) observed by NEXAFS is, thus, represented as  $I_0 \lambda (1 - \exp(-X/\lambda))$  by integrating  $f(x)$  from 0 to  $X$ . By fitting the experimental data with  $F(X)$ , the decay length is determined to be 0.26 nm for LiCl/Cu(001), 0.29 nm for LiCl/Ag(001), 0.46 nm for KCl/Cu(001), and 0.41 nm for KCl/Ag(001), which indicates that the MIGS are indeed localized within a sub-nm of the interface. The result for the fitting is included in Figure.

The decay length of MIGS depends on an alkali halide,



**Figure:** Intensity of MIGS peak (not normalized by the edge-jump) versus the film thickness for LiCl/Cu, LiCl/Ag, KCl/Cu, and KCl/Ag. The curves are the least-square fit to  $F(n)$ .

and does not depend on a metal. We then discuss these facts using the finite square-well potential problem. In the quantum mechanics, the penetration depth of the wave function of the bound state is proportional to  $V^{-1/2}$ , where  $V$  is the height of the potential well. Since MIGS originates from a penetration of the metal wave function into an insulating side, the penetration depth of the wave function corresponds to the decay length of MIGS. The height of the potential in alkali halide/metal is the energy difference between the Fermi level and the valence band maximum. Assuming that the Fermi level locates at the center of the band gap, the height of the potential is half of the band gap energy. The band gap energy is 8.5 eV for KCl and 9.4 eV for LiCl, and hence the penetration of wave function (decay length of MIGS) of KCl with smaller band gap energy is larger than that of LiCl. Since the height of the potential well does not depend on metal, the decay length of MIGS does not depend on a metal. On the other hand, the intensity of MIGS at the interface depends on the distance between an alkali halide and a metal, and it varies with the combination of a metal and an alkali halide.

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