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# Insulating properties of ultrathin KF layers on Cu(100): Resonant Auger spectroscopy

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**Abstract**

Solid-state effects in the creation and decay of K 2p core excitations in thin KF films on Cu(100) surface have been studied in resonant Auger spectra, excited using synchrotron radiation. The spectra of films of various thickness starting from a single monolayer were measured.

The photoabsorption spectra reveal crystal field splitting already at film thickness of about 1 monolayer. The Auger decay spectra of the K $2p^{-1}3d$ core excitations in films of thickness up to 2 monolayers exhibit a band characteristic of the decay of core ionised states, showing that the excited electron delocalises into substrate before the core hole decays. In thicker films the coexistence of the decay of excited states in the bulk of the KF crystalline film and of ionised states at the KF–metal interface is observed, indicating that the charge transfer probability from the upper layers of the film into the metallic substrate is strongly reduced.


*Keywords:* Alkali halides; KF; Copper; Photoelectron spectroscopy; Auger electron spectroscopy; Insulating films

## 1. Introduction

Recent progress in nanosciences has stimulated the interest in ultrathin insulating films of (a few) monolayer thickness and in their production process with the prospect to use these films as insulators in microelectronic industry. Mostly oxides, but also alkali halide films have been extensively studied in recent years (for example, see Refs. [1–5]). Alkali halides are the simplest insulators, where the electronic processes can be regarded in a good approximation to involve

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only a single ion and therefore the well-established and accurate methods of atomic ab initio calculations provide a good starting point for studying electronic processes such as photoabsorption and core hole decay in ionic compounds.

We present here an experimental study of potassium fluoride as an adsorbate with thickness ranging from one to several monolayers (ML) on Cu(1 0 0) surface. Our study focusses mainly on the formation of insulating properties, characteristic of the solid. For this purpose we investigated the photoexcitation and the Auger decay of potassium 2p excitations, created by monochromatised synchrotron radiation. The resonant Auger (RA) spectra of K in solids as well as of free potassium atoms have been reported and analysed earlier [6–10]. To our knowledge, no such studies exist of KF adsorbates or free molecules. The 2p photoabsorption of the KF crystal reveals strong effects due to the lowered symmetry in comparison to the free $K^+$ ion. Namely, the atomic 3d orbital, to which the K 2p electrons are excited, is split by the cubic crystal field into two components of different energy and spatial orientation. Also the intensity distribution in the RA electron spectra of the decay of the $2p^{-1}3d$ states shows strong dependence on the symmetry of the excited state as well as on the spin–orbit coupling of the K 2p electrons [6,7].

A question that invariably arises in connection with resonant excitations in adsorbates concerns the probability and extent of the delocalisation of the excited electron. In weakly bound physisorbed systems the delocalisation has been shown to have a comparable time-scale with the RA decay that fills the core hole [11,12], whereas in some chemisorbed systems the delocalisation is much faster [13–15]. Given the prominent role of the excited 3d electron in our case of KF, its delocalisation should have a major impact on the observed Auger electron spectra. Its behavior serves as a probe of charge dynamics (for example, see recent review [16]) and thus carries information about the build-up of insulating properties. Studying the crystal–adsorbate sequence gives an excellent opportunity to elaborate on these aspects.

## 2. Experimental set-up

The experiments were performed at beamline D1011 of MAX-II storage ring (Lund, Sweden). The beamline was equipped with a modified SX-700 plane grating monochromator and a Scienta SES-200 electron energy analyser. In our experiments the photon energy resolution was set to 0.3 eV and the electron energy resolution was about 0.15 eV. The energy calibration of the SX700 monochromator was performed using the photoelectron spectra of Au, excited with the first and second order radiation. The photoabsorption spectra were obtained by measuring the total yield of the emitted electrons with a microchannel plate detector. For the preparation of the films a separate growth chamber was connected to the UHV preparation chamber of the beamline. The base pressure in the growth chamber was $8 \times 10^{-10}$ Torr. The mechanically and electrochemically polished Cu(1 0 0) (Metal Crystals Ltd.) single crystal surface was used as the substrate onto which the films of KF were evaporated from a tantalum crucible. Resistive heating of the Ta support wires allowed the sample to be rapidly heated to a temperature of up to 800 K at a rate of 2.5 K $s^{-1}$. The Cu(1 0 0) sample was initially cleaned in situ by standard procedures consisting of argon ion bombardment while annealing at 700 K over a period of several days and was deemed clean when no contaminants could be observed above noise level of electron spectra. Between the growth of films with different thicknesses the Cu(1 0 0) single crystal was routinely cleaned by $Ar^+$-ion sputtering followed by annealing at 650 K for 20 min. After cleaning and annealing, no contamination was observed in the photoelectron spectra.

The thickness and morphology of each overlayer were determined by using the inelastic electron background analysis of the Cu 3s photoelectron peak (the binding energy of 123 eV) according to the QUASES software package [17]. The QUASES method provides quantitative information regarding both the overlayer coverage and its morphology. It relies on the phenomenon that the energy loss structure that accompanies photoelectron or Auger electron peaks carries information on the depth of origin of the detected