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# XAS experiment on Cu/MoO$_3$ layered thin films

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## 1．背景と研究目的

MoO$_3$ is a transition metal oxide with high work function (α-MoO$_3$ work function is 6.5 eV). Even though it is a high-k insulator, its electronic structure and conductivity properties can be modified by means of Oxygen vacancy defects formation (n-type doping, which results in the formation of sub-oxides MoO$_{3-x}$) or the introduction of substitutional Copper atoms (p-type doping, which results in the formation of alloys Cu$_y$MoO$_{3-x}$), making it a promising material for applications which require interfaces with high work function and a relatively low surface resistivity [1]. In a recent work the shortest Mo-O bond length in multilayer Cu/MoO3 samples, subjected to different thermal treatment, has been measured by means of the Raman technique and correlated with the oxidation state of Mo, measured by linear combination fitting of XAS data [2,3]. In particular a regular trend of shortening of the first-neighbor Mo-O bond with increasing valence state of Mo has been found. This trend can be explained, at least for small deviations from the stochiometric α-MoO$_3$ structure, by the formation of oxygen vacancies with the lowest formation energy, namely concerning the inter-layer O1 oxygen site [4] and the simultaneous diffusion of Copper atoms between layers of MoO$_3$ [5]. In order to verify this hypothesis we propose to use XAS to monitor the local environment around Mo and Cu atoms. Understanding the formation of the Cu$_y$MoO$_{3-x}$ alloy is expected to open new prospective about employment of the metal/metal-oxide interface in various applications which require high work function and low resistivity materials, such as for Radio Frequency protective coating and in organic electronics.

## 2．実験内容

We measured three multilayer samples, Cu(3.0 nm)/MoO$_3$ (33.0 nm) x 3 layers, total thickness 108 nm, grown on Carbon (graphite) substrate (0.2 mm thick) as grown and annealed at different partial pressures of air at 435°C. Measurements were done at the Cu K-edge and Mo K-edge in fluorescence mode, by putting the sample at 45 degress angle with respect to the incoming beam and towards the SDD. MoO$_3$ and MoO$_2$ reference materials were also measured in quick XAFS mode.

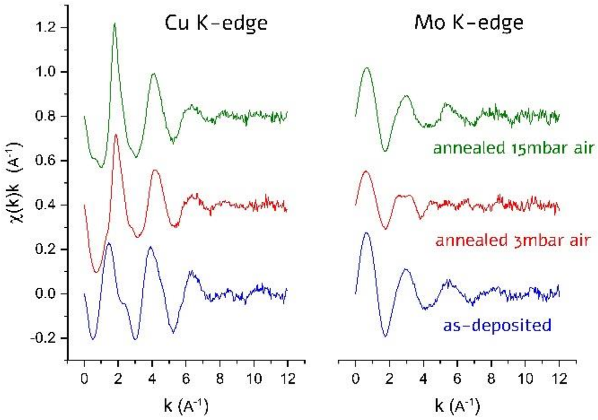


*Figure 1 Structural signal kχ(k) of the measured samples, for the Cu K-edge (left column) and Mo K-edge (right column). Spectra of 15 mbar annealed, 3 mbar annealed and as-deposited samples are shown, respectively, in the upper, middle and lower rows.*

## 3．結果および考察

The measured XAS spectra indicate a clear structural change occurring on the sample annealed at 435°C in 3mbar and 15 mbar of air, as can be deduced from both the Cu K-edge and Mo K-edge structural signals of Fig. 1. An EXAFS analysis of the measured spectra is currently in progress.

## 4．参考文献

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