EXAFS-study of perovskite related doped copper-tantalates

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In recent years tantalates with perovskite related structures ABO_3 have shown to be high performance dielectric materials [1, 2]. Particularly B-site doping was investigated lately by several groups to study its influence on dielectric properities [3-7].

Pure copper tantalate $Cu_{0.5}TaO_3$ is an A-site deficient perovskite with 50 % vacancies on the copper sites. The valence of copper and tantalum therein is +II and +V, respectively. In our recent studies copper tantalate is doped with Ti^{+IV}, W^{+VI} and Mo^{+VI} to examine the effect on phase formation and physical properties. All samples have been sythesized by solid state reactions of binary oxides. EXAFS measurements were performed to get a closer look at the sourroundings of the different cations used.

Xray diffraction revealed that titanium doping up to a content of 50 % causes no change in crystal structure but a small shift in lattice parameters to smaller values with increasing titanium content (to achieve charge neutrality the amount of vacancies in the A-site is subsequently reduced to 25%). XRD results were confirmed by small peak shifts in EXAFS scans at the Cu-K and Ta-L edges as shown in figure 1a and b. Parenthized values indicate the distance from the scattering atom. The attempt to obtain higher doping levels than 50% resulted in remaining titanium oxide powder.

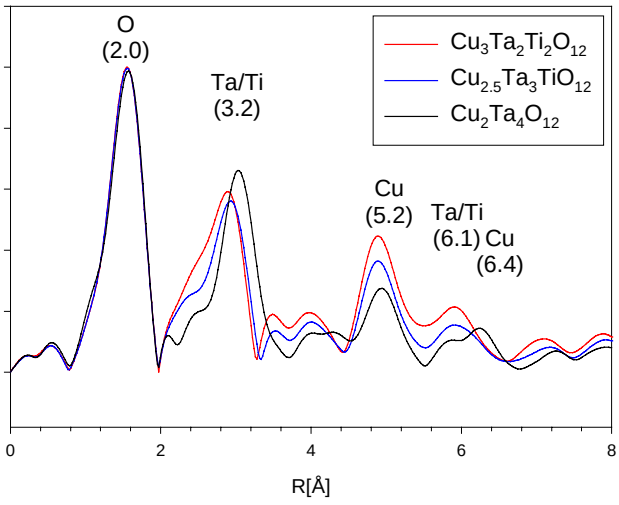

Figure 1a: FT(χ(k)*k^3) Cu-K EXAFS of Ti doped samples.

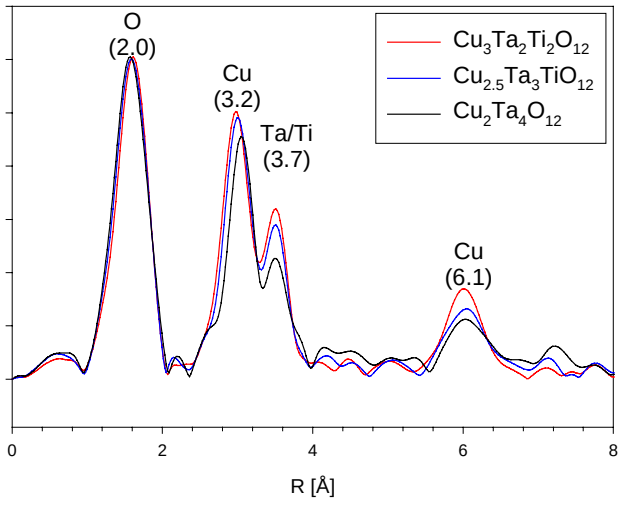

Figure 1b: FT(χ(k)·k^3) of the corresponding Ta-L EXAFS.

Doping copper tantalate with hexavalent ions did not alter lattice parameters observably. It was possible to incorporate up to 25% tungsten and even 50% molybdenum. EXAFS scans did not show shifts in the peak positions just a decrease in peak height of B-site peaks. As an example figure 2 shows the fourier transformed of $\chi(k)\cdot k^3$ of pure copper tantalate and W/Mo doped samples with 1/4 of the tantalum ions replaced by molybdenum and tungsten, respectively.

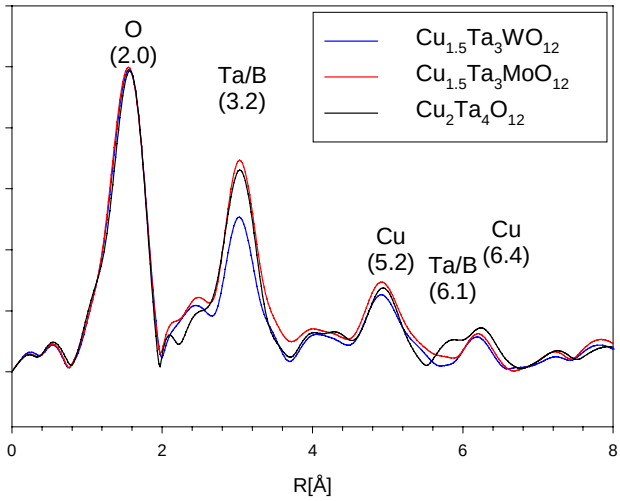

Fig. 2: FT($\chi(k)\cdot k^3$) Cu-K EXAFS of $Cu_{2-x}Ta_{4-2x}(Mo/W)_{2x}O_{12}$ (x = 0, 0.5).

Our EXAFS results reveal that the structure remains unchanged in a large region of B-site doping. Currently we are measuring the physical properties of these samples to study the influence of cations with different valences and radii. Rietveld refinements are made to determine crystal structure data and maximum doping levels will be quantified [8].

References

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