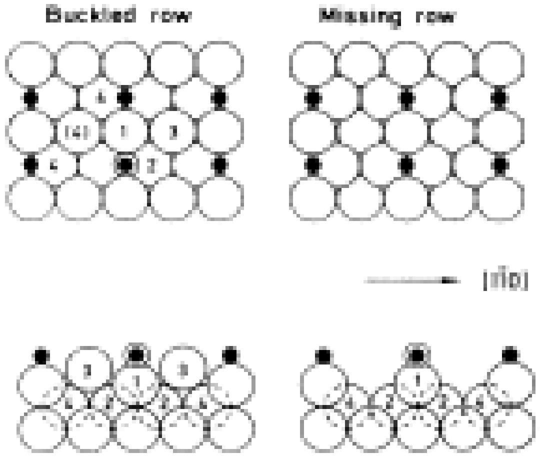
(2x1)O on Cu(110): an EXAFS study

M. Bader *et al.*, Phys.Rev. Lett. **57**, 3273 (1986)

The adsorption of O on Cu(110) at 100 K has been studied by EXAFS. The study wanted to elucidate two points:



1) Which one between the buckled row model and the missing row model describe the surface geometry after oxidation
2) Which is the exact position of an O atom respect to the surface crystalline structure. (Copper has an fcc structure with a = 3.62 Å)

1) The EXAFS spectra shown below clearly exclude the buckled row model. Why? (help: a) calculate the R position at which the peaks are expected in the EXAFS spectra following the two models and assuming the O atom placed in the top Cu plane. b) Assuming the experimental peak height due to the atom *i* equal to *Ni/Ri^2*, calculate the expected peak heights and compare with the experiment))
2) The EXAFS spectra also support an O position *d* above the Cu surface. Which is the value of *d*? (help: a) calculate the *Ni/Ri^2* for *i* = 1,2 with the new O position and compare with the experimental ratio A1/A2)

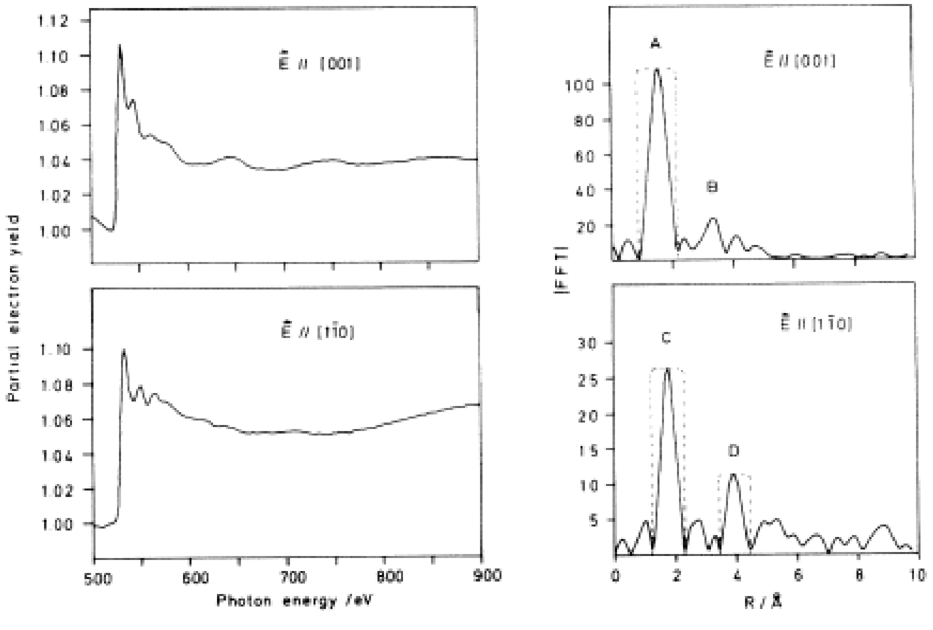
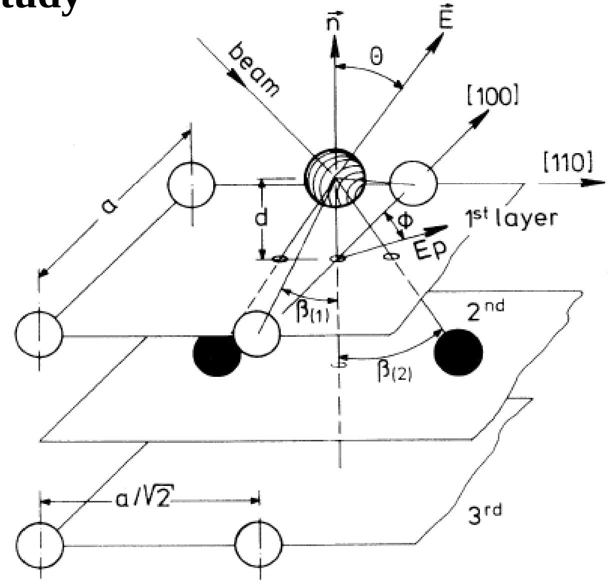


FIG. 1. Oxygen-*K*-edge SEXAFS spectra for O(2×1)/Cu(110) recorded at 100 K with E∥[001] and E∥[0$\bar{0}$1] (left), and their Fourier transforms (right). For peak notation see text.

Solution: (2x1)O on Cu(110): an EXAFS study

1)



R1= a/2 = 1.82 Å

$$R_2 = \sqrt{[(a\sqrt{2}/4)^2 + (a\sqrt{2}/4)^2} = a/2 \quad = 1.82\ \text{Å}$$

$$R_3 = \sqrt{[(a/2)^2 + (a\sqrt{2}/2)^2} = a\sqrt{3}/2 \quad = 3.13\ \text{Å}$$

$$R_4 = \sqrt{[(a\sqrt{2}/4)^2 + (3a\sqrt{2}/4)^2} = a\sqrt{5}/4 \quad = 4.05\ \text{Å}$$

The EXAFS amplitude ratio are listed in the following table: the huge difference between the two model is represented by the amplitude A3 which is expected to be close to the half of A1 in absence of reconstruction and close to 0 in case of reconstruction, as seen in the experiment

							Theory $\frac{N_i^*/R_i^2}{N_1^*/R_1^2}$
		Cu	Experiment			No	
Azimuth	θ/degrees	neighbor	R_i (Å)	A_i/A_1 ($k = 4$ Å^{-1})	R_i (Å)	reconstruction	Missing row
[001]	90	1	1.82 ± 0.02	1	1.83	1	1
[1$\bar{1}$0]	90	2	1.99 ± 0.02	0.28 ± 0.01	1.99	0.355	0.355
		3	· · ·	· · ·	3.14	0.458	· · ·
		4	4.15 ± 0.03	0.12 ± 0.01	4.16	0.354	0.354

Experimental and theoretical bond lengths and amplitude ratios.

2) Cos(θ1) = (a/2)/sqrt[(a/2)^2+d^2]
Cos(θ2) = (a sqrt(2)/4)/sqrt[(a sqrt(2)/4)^2+(a sqrt(2)/4 +d)^2]
R1^2 = (a/2)^2+d^2
R2^2 =(a sqrt(2)/4)^2+(a sqrt(2)/4 +d)^2

Substituting the right values one obtains *d* = 0.46 Å which is close to the value calculated taking into account the exact formula (*d* = 0.30 Å)

Magnetic recording technology

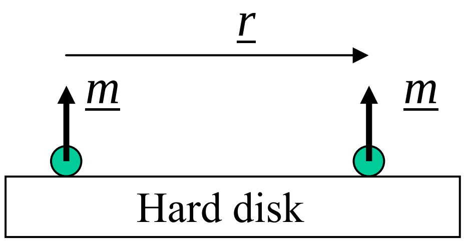
One of the limiting factor to the increase of the memory density is the bit coupling via the dipolar interaction. One way to solve the problem is to move from the nowadays longitudinal recording technique (making use of in-plane magnetized bits) to the perpendicular recording technique (making use of out-of-plane magnetized bits). Why?

Remember. Consider a magnetic particle with a magnetic moment $\underline{m}$. The dipolar field $\underline{h}$ generated by this particle at a distance $\underline{r}$ is given by:

$\underline{h} = 3(\underline{r}\ \underline{m})\ \underline{r}/r^5 - \underline{m}/r^3$.

Which is the interaction field perceived by a second particle in the following situations:

1)



2)

3)

Solution: Magnetic recording technology

The interaction field is:

1) m/r^3
2) $2m/r^3$
3) $4m/r^3$

The lowest field generated by one particle to the location of the second particle is observed in the case 1). This implies a reduced bit coupling when the bits are perpendicularly magnetized