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Structural and Mössbauer studies in $REBaCuFeO_{5+x}$ compounds.

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We have studied the non superconducting phase $REBaCuFeO_{5+x}$ (where RE=rare earth). with neutron, x-ray powder diffraction and Mössbauer spectroscopy.

1. Introduction

The oxygen deficient perovskite $YBaCuFeO_{5+x}$ was isolated for the first time by L.Er-Rakho et al[1]. Recently, Meyer et al[2] presented Mössbauer spectra which revealed the existence of a single Fe^{3+} site and concluded that only the ($1b_1$) site is occupied with iron whereas ($1b_2$) is occupied with copper. Detailed analysis with Mössbauer spectroscopy in the same series for RE=Y,Nd,Sm,Cd,Dy,Lu and Tm has been presented by M.Pissas et al[3].

2.Results and discussion

We have performed Rietveld refinements for all our x-ray diffraction profiles in space group P4mm using the site $1b_1$ (z=0.27) for the iron and site $1b_2$ (z=0.74) for copper, with excellent results. R_B-factors, for example, for Sm and Nd compounds are 3.43% and 6.51%, correspondingly. Figure 1 shows the dependence of the lattice constants and the extra oxygen in relation with rare earth.

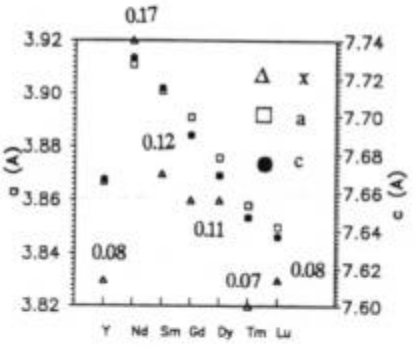

Figure 1.
Lattice constants and additional oxygen content vs lanthanide supporting cation in $ReBaCuFeO_{5+x}$.

Figure 2 shows part of Neutron diffraction profiles of $YBaFeCuO_{5+x}$ from 320-500K. The mag-

netic reflections indexed as (h/2,k/2,l/2) h,k,l=odd and the magnetic unit cell involves a doubling of the nuclear one along all three directions.

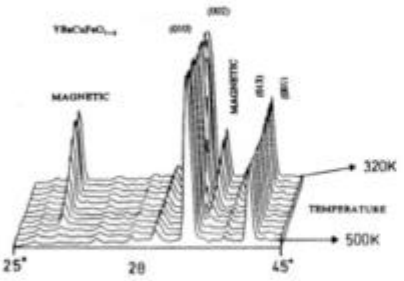

Figure 2
Part of Neutron diffraction profiles (320-500K).

The Mössbauer spectra do not substantially differ for the whole $REBaCuFeO_{5+x}$ series. They consist of a site which corresponds to ferric iron in the high spin state with a saturated hyperfine magnetic field of approximately 510KG. The quadrupole splitting of the paramagnetic region ($\Delta E_Q = e^2qQ/2$) was 0.22mm/s. In addition the Mössbauer spectra present a temperature dependent inhomogeneous broadening of the absorption lines. Under the Neel point the spectra are composed from a broadened Zeeman-split component and a paramagnetic one. This behavior could be attributed to a distribution of T_N's due to the inhomogeneity of the crystallites with respect to their content in oxygen. We also found that the Mössbuaer spectra are influenced from the percentage of the additional oxygen[3]. Figure 3 shows representative Mössbuaer spectra for the $SmBaCuFeO_{5+x}$ compound at 393K, RT and 85K.

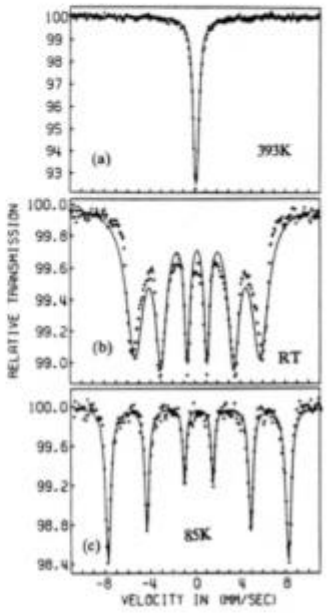

Figure 3
Mössbauer spectra for the $SmBaCuFeO_{5+x}$ compound at (a) 393K, (b) RT, (c) 85K.

REFERENCES

1. L.Er-Rakho et al, J.Solid State Chem. 73 (1988) 531.
2. C.Mayer et al, Solid State Commun. 76,(1990) 163.
3 M.Pissas et al, Submitted for publication in Physica C (May). 1991