1Q06 EPRI Project Report

"Consultant to EPRI Project Management on the Fabrication of New Superconducting Materials"

EPRI Contract Agreement No. EP-P18263/C9013

Contractor: Paul M. Grant

EPRI Project Manager: Steven Eckroad

15 April 2006

Activities & Results

I. Experimental

II. Theory & Modeling

III. Siemons MRS Presentation

I. Experimental

- New XPS results substantiate growth of "cubic" CuO on STO. Uncertainty exists regarding "perpendicular" cell parameter (could be tetragonal).
- With greater thickness, the film begins to take on the tenorite structure, a tendency which is exacerbated on removing sample from vacuum to ambient (water?).
- That a new structure exists is demonstrated by "chemical shifting" of indicator XPS peaks differently from tenorite for films grown on STO.
- Future experiments will explore out-of-plane lattice constant value, doping effects, and magnetic properties.

Return

II Theory & Modeling

- Studies examining the relevance of single particle DFT calculations on determining the equilibrium lattice constants of Mott-Hubbard insulators continue. Using the "geometry optimization" features of CASTEP, we were able to obtain the cell constants of La_2CuO_4 to within two percent, thus indicating DFT methods can successfully locate the relative equilibrium structures of materials with strong coulomb correlation.
- Over the next two quarters of this year, we will explore using CASTEP in an attempt to predict the structural properties of thin CuO layers separated by NiO films to determine if a "cubic" multilayer of these two compounds is energetically stable.

Return

Wolter's MRS Talk

2006 Spring MRS, San Francisco

19 April 2006

Return

Nanoscale Epitaxial Films of Cu_2O_{2-x}

An attempt to make cubic CuO

Wolter Siemons

MRS Spring meeting

HH4.9: Novel materials

Wednesday, April 19th 2006, 4:30pm

People and funding

At Stanford University:

Wolter Siemons, Gertjan Koster, Hideki Yamamoto, Bob Hammond, Ted Geballe, Paul Grant, Malcolm Beasley

At University of Twente: Guus Rijnders and Dave Blank

This research is funded by EPRI, DoE, and NanoNed

Motivation

- Model system related to High-T_c cuprates
  - Expected to be 3D system, compared to the 2D planes
  - Increased superfluid density (raising T_c?)
  - Exploration of doping methods
  - More general: Exploration epitaxial stabilization

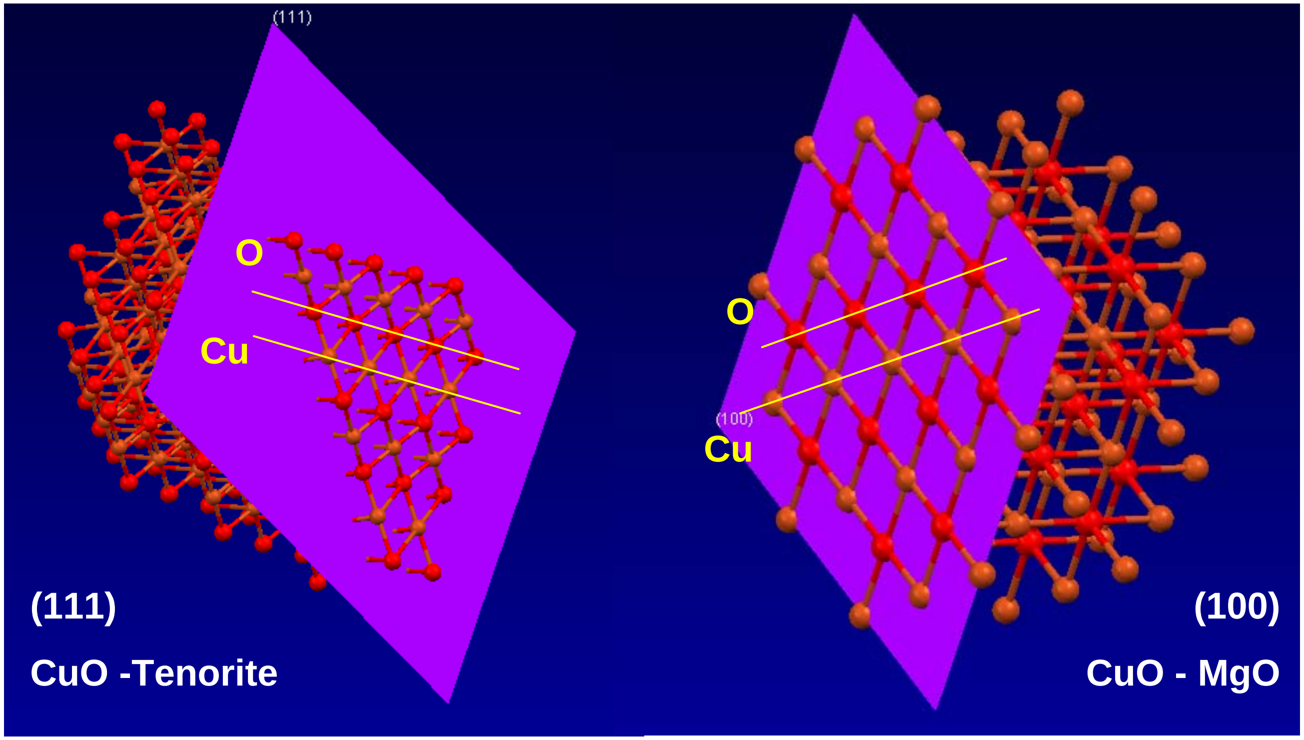
Material specifics

- CuO (tenorite) naturally has a monoclinic unit cell
- Charge transfer system (Mott-Hubbard), insulating in undoped form

Growth parameters:

- Grown in 10^{-5} Torr O_2 pressure with 600 W atomic oxygen source
- Various substrates at 500-600 ^{o}C
- Can be grown both with MBE and PLD

Proxy structure

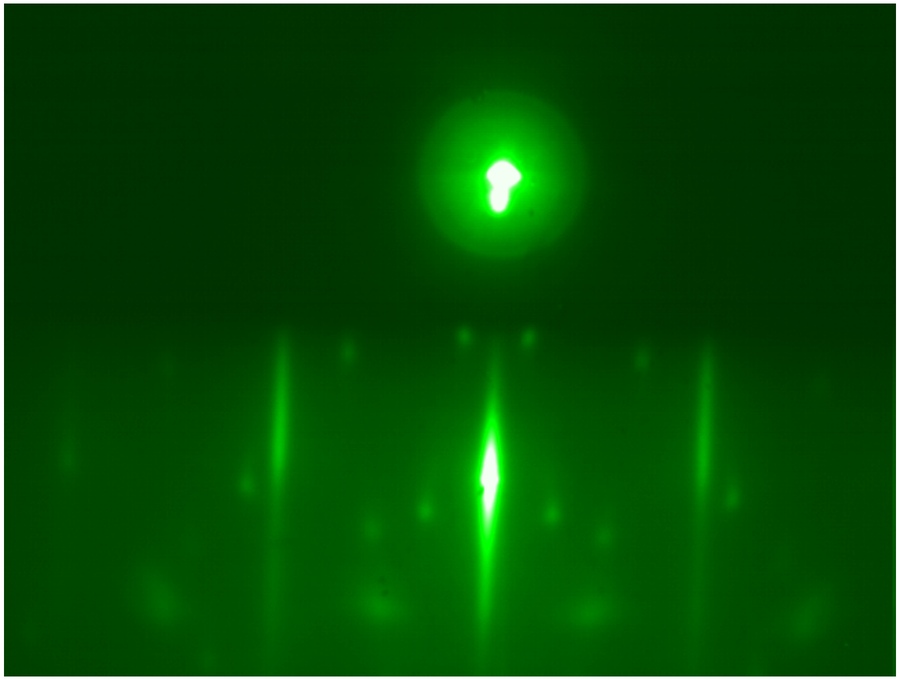


Average bond length:
1.92 A
(Shorter than cuprates)

Average bond length:
2.10 A

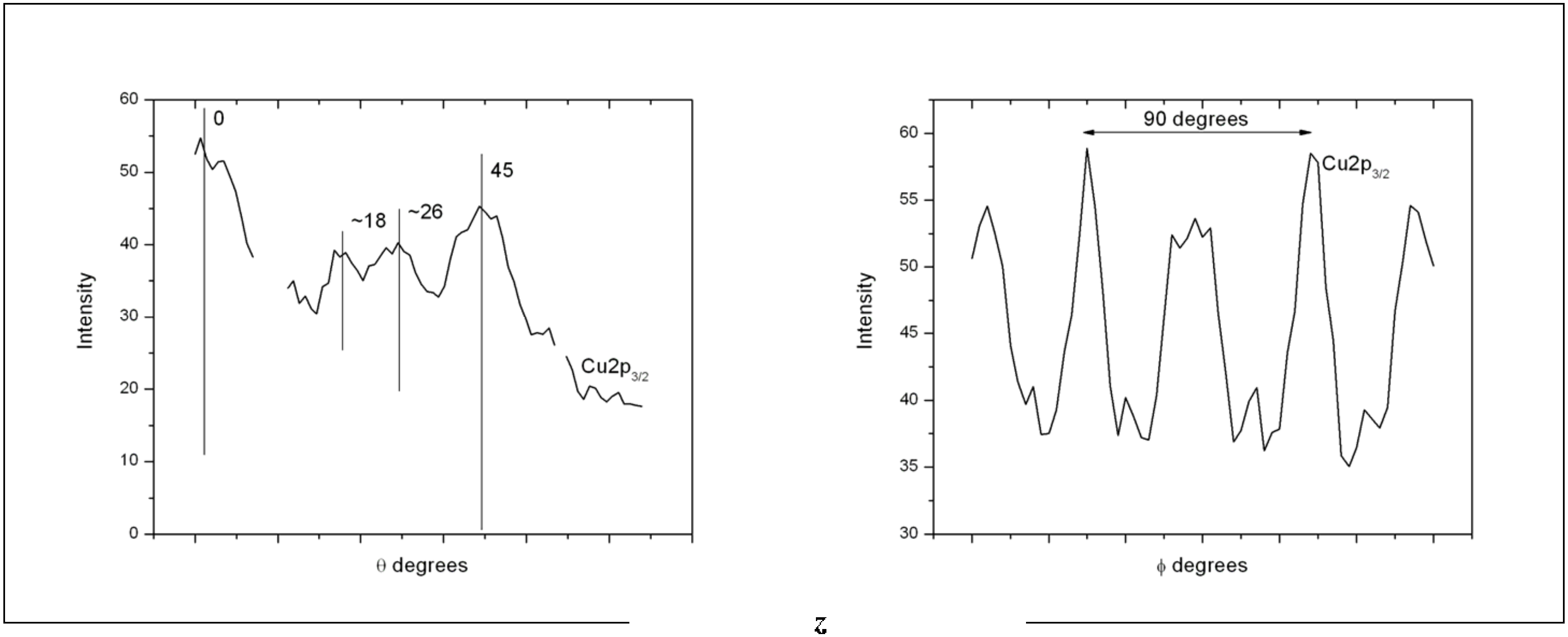
- Stabilized Cu_2O_2 by epitaxy on TiO_2 terminated $SrTiO_3$ substrates

RHEED

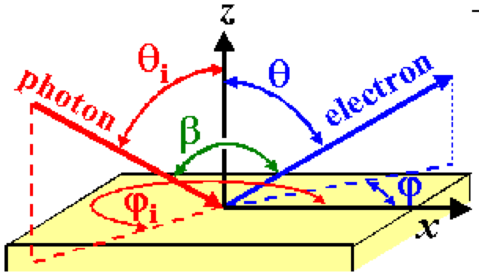


- CuO, like MgO and NiO, grows epitaxially on $SrTiO_3$
- Grows 45 degrees rotated with respect to substrate
- After critical thickness (~25-30A) structure changes to tenorite
- Critical thickness depends on temperature, substrate, and oxidation conditions

X-ray Photoelectron Diffraction



Along $SrTiO_3$ 110



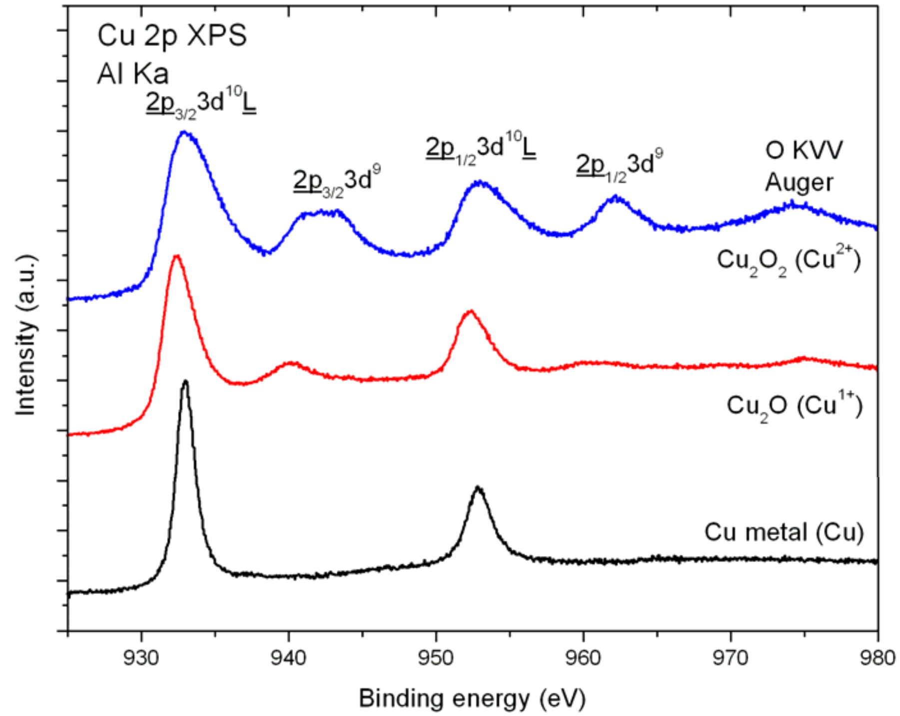
Instability

- Structure wants to change to tenorite structure
- Taking sample out of vacuum might have this effect, and certainly does this going beyond the critical thickness

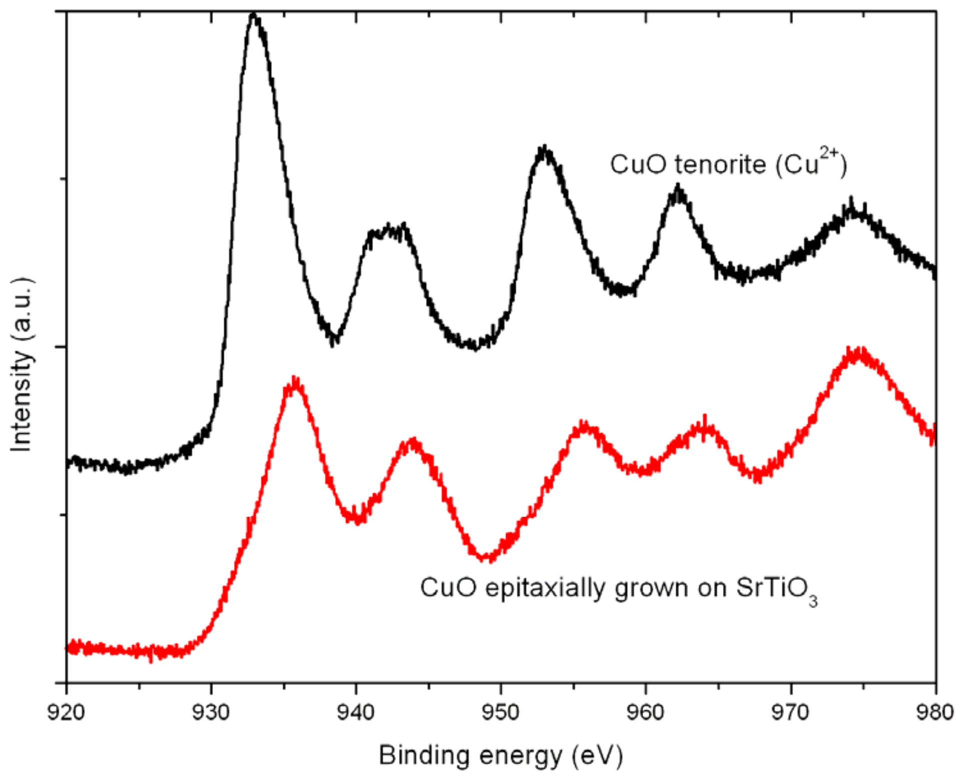
In situ XPS from Cu to CuO

In situ technique to avoid degradation of the material

Detailed studies of the XPS Cu 2p multiplet structure have been used to estimate the charge transfer energy (Δ)



XPS shifts



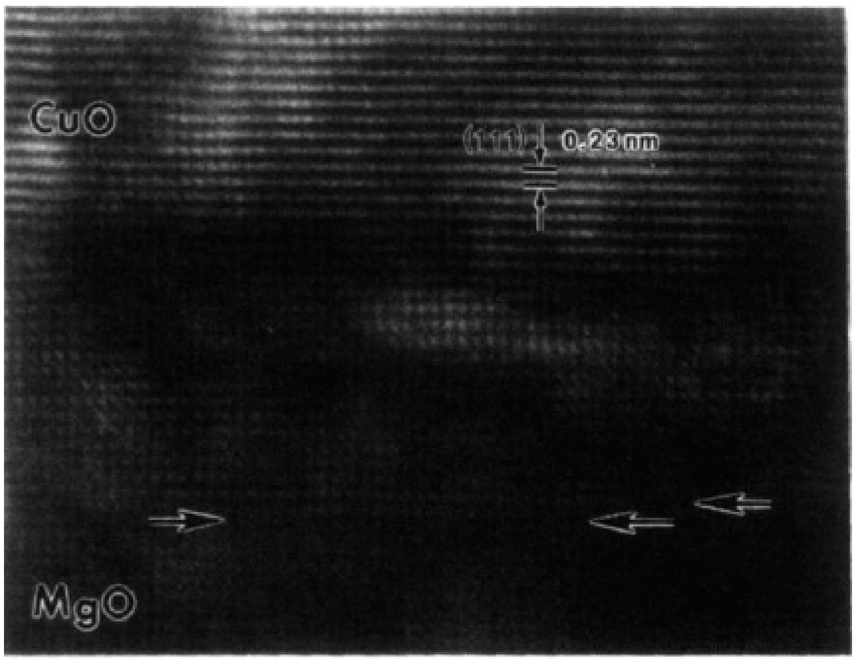
Different chemical environment

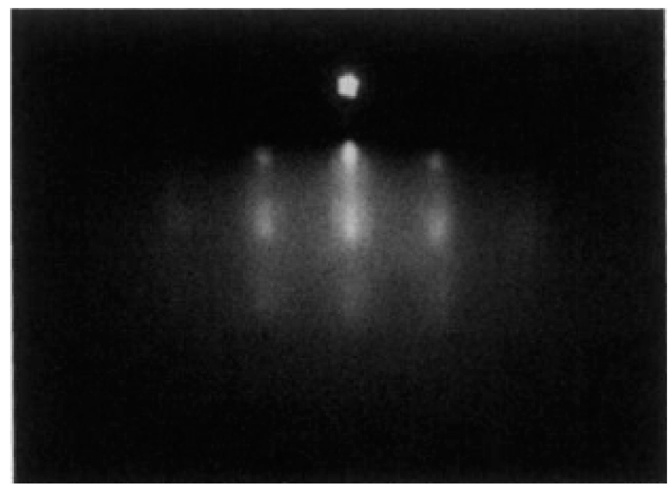
Future experiments

- Determine the out of plane lattice constant (through simulation of XPD)
- Doping of CuO: chemical, charge transfer overlayers and field effect
- Determination (with Kapitulnik and Xia) of the magnetic properties, with the help of a sagnac interferometer, by measuring Kerr rotation (could be done *in situ*)

Work by other groups

Critical thickness and instability make it very hard to analyze the material. XRD, TEM, etc. almost impossible.





Catana, Locquet, Paik, and Schuller, PRB 46, 15477 (1992)