4Q05 EPRI Project Report

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

EPRI Contract Agreement No. EP-P18263/C9013
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Activities & Results

I.   Experimental

II.   Theory & Modeling

III.   Abstract Submitted to the:

2006 Spring MRS Meeting – San Francisco

I.   Experimental

- Experiments this quarter were directed to understanding better the nature of the quasi-cubic CuO film five or so lattice constants thick that can be grown heteroepitaxially on strontium titanate (STO) substrates.

- X-ray topography measurements (described below) were performed to better ascertain that indeed cubic CuO was present.

- Inasmuch as films of materials as thin as five atomic cells often display bulk properties, we are considering including in the immediate experimental program, measurements of magnetic and conducting properties of these CuO films using nanoprobe tools unique to Stanford.

X-ray Diffraction Topography of CuO Films Grown on STO
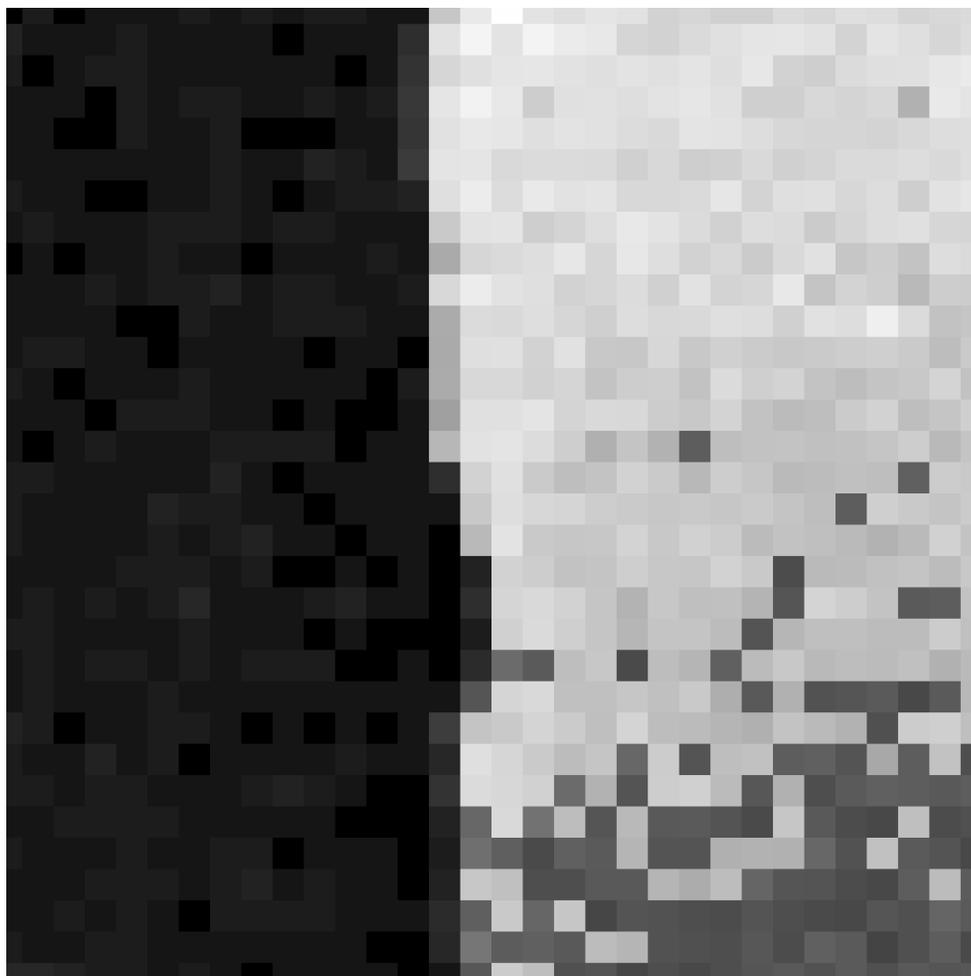
- The black area on the LHS represents the color assigned to one of the characteristic x-ray diffraction peaks of cubic STO (the CuO film has been etched away.

- The white and gray pixels (~ 1 μ^2) on the RHS represent the relative intensity of diffraction lines indicative of cubic CuO.

- Note that some pixels on the RHS are black, suggesting either the CuO film is not present in this area, or not of cubic symmetry.

II Theory & Modeling

- Modeling efforts this quarter continued to focus on testing whether the CASTEP density functional tool could optimize the values of the internal atomic coordinates in highly correlated electronic structures such as tenorite (CuO), NiO and the undoped layered cuprates

- It is known that the physical properties of such systems are reasonably well described by a variety Hubbard model extensions to DFT. We investigated how these extensions may related to determining the equilibrium crystal structures of such compounds.

- Additional and more robust numerical testing was performed with CASTEP than was reported in 3Q05. We calculated the relative ground state energies of NiO and CuO crystals where the lattice constants were varied +/- 5% from known experimental values.

- It was found that only the experimentally known lattice constant values resulted in the lowest ground state energies, again indicating that DFT can give unexpectedly reliable structural results even for quantum systems where it gives an incomplete description of most other physical properties.

Extended Hubbard Hamiltonian

Qualitative Description of the Physical Properties of Antiferromagnetic Insulators

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\downarrow} n_{i\uparrow} + \frac{V}{2} \sum_{\langle ij \rangle, \sigma, s} n_{i\sigma} n_{js}$$

This is the energy calculated in DFT which describes the physical properties of uncorrelated systems such as semiconductors and metals. This energy depends strongly on the interatomic bond length. "t" is the energy to transfer an electron from atom to atom, and the "c's" create and annihilate electrons as they move from site to site.

This term represents the repulsive force between two electrons on the same ionic site. It tends to separate spins of opposite sign on nearest neighbor ions, thus producing an antiferromagnetic state. "U" is the repelling energy, and "n" is the occupation number (either) or 1) for each spin direction on ion "i". It is independent of bond length, and thus is a simple constant for all crystallographic configurations involving the same elements.

This term is the repulsive energy between two electrons on separate ionic sites and thus dependent on bond length, but not included in the DFT formalism, and thus may play a role in setting the absolute value of the Ground State Energy for a given crystallographic configuration.

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Relative DFT GSE for NiO & CuO

Relative GSE of Mott Insulators wrt Deviations from X-Ray Lattice Parameters
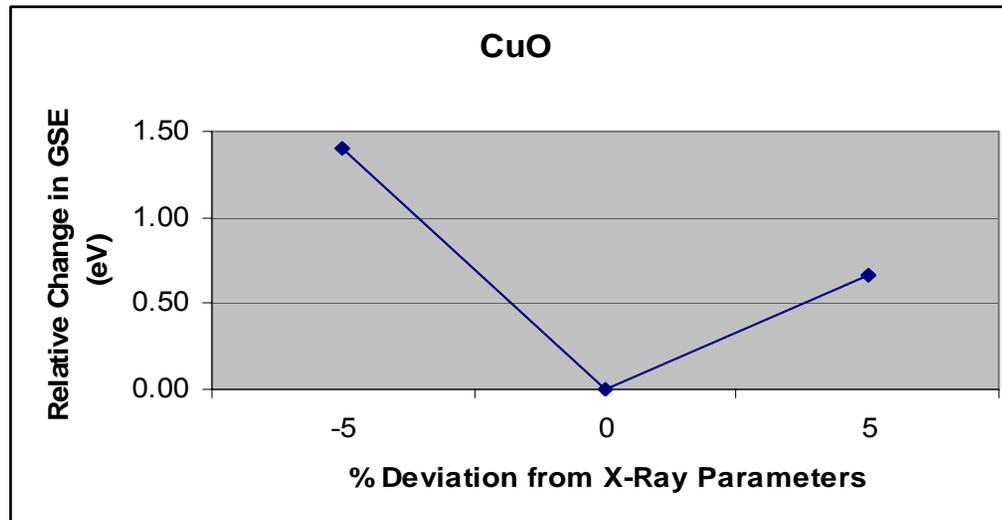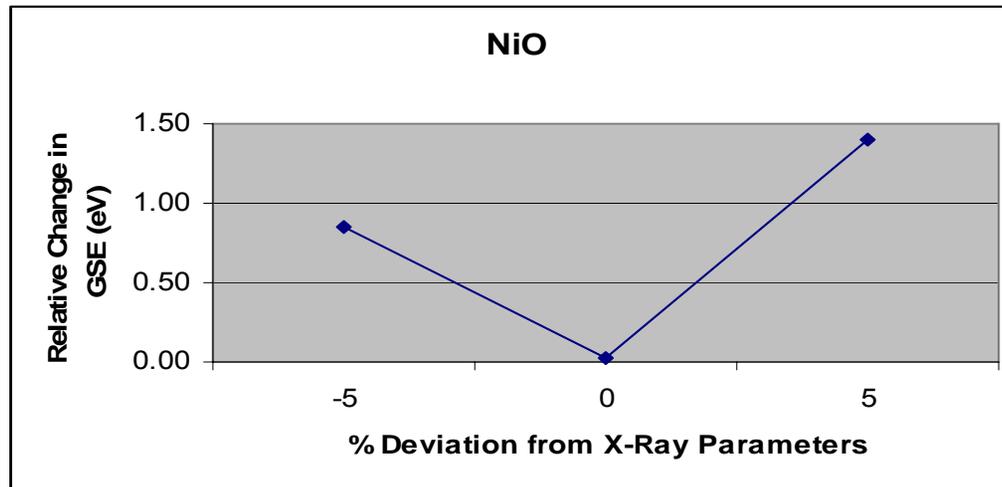
III. Abstract Submitted to the:
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Nano scale epitaxial films of Cu2O2-x; a model system
Gertjan Koster, W. Siemons, H. Yamamoto, R.H. Hammond, P.M. Grant, T.H. Geballe and M.R. Beasley

Here we present a detailed study on the growth of epitaxial CuOx thin films on single crystal substrates by MBE. *In situ* photo electron spectroscopy (XPS and UPS) is used to establish the degree of oxidation of Cu while *in situ* electron diffraction (X-ray Photo electron diffraction and RHEED) monitor the crystal structure and morphology of the growing thin film. We particularly pay attention to the valence state of Cu and the crystal symmetry as influenced by a combination of activated oxygen (O*) and/or a flux of low energy Ar+ ions. We observe a rich variety of epitaxial relationships as a function of the flux ratios of three species on the substrate surface (ie, Cu, O* and Ar+) which will be used to explore the possibility of the highest crystal symmetry possible in CuOx system.

In recent experiments we observe a new CuO phase (di-valent copper) for the first deposited unit cell layers which is found to be 45 degrees rotated with respect to the SrTiO3 substrate lattice. Both RHEED as well as preliminary X-ray Photoelectron Diffraction confirm a four fault symmetric structure. In parallel we try to establish the relationship between (electronic) properties and crystal structure at different length scales. Although the copper system is the focus of this paper, we will also address whether such an approach is feasible for other oxide materials, for example dielectric materials.

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