2Q05 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

30 June 2005

Activities & Results

I. Experimental

II. Theory & Modeling

III. Abstracts Submitted

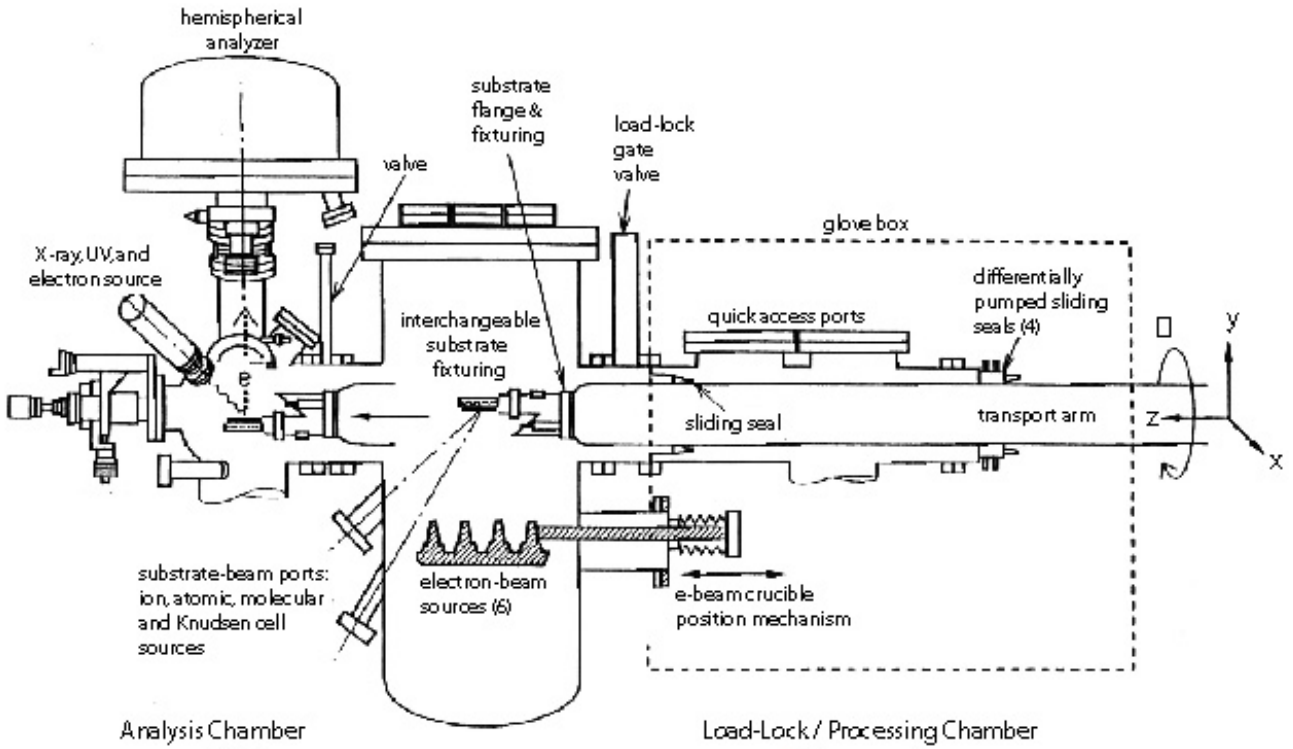
I. Experimental

- The MBS system for the last six weeks has been diverted to other research efforts at GLAM[1] pending the fabrication and installation of an IBAD gun more suitable to texturing CuO.
- The need for a new ion beam gun arises from the lower bombardment energy (25 V) of the impinging Ar^+ (or O^+) so as not to unduly damage the growing CuO film other than to remove atoms not positioned in cubic lattice positions.
- However, the requirement for lower energies also results in a decreased beam flux intensity, thus the ion gun must be placed closer to the substrate than was the case for ion etching of MgO buffer layers for YBCO[2] coated conductors.
- The result of this “close-in” placement is a higher stray magnetic field interference from the permanent magnets surrounding the ion gun with the electron beam emanating from the RHEED and essentially destroying the diffraction pattern necessary to analyze the progress of film growth.
- Bob Hammond has finished the design of a new ion gun with mu-metal[3] shields surrounding the deflection magnets which is now being fabricated with expected installation in the next week or so. Upon completion, CuO growth runs will re-commence in earnest on the MBS system.

Return

MBS Machine

MOLECULAR BEAM SYNTHESIS SYSTEM (MBS)



Analysis Chamber

- LEED
- XPS
- UPS

UHV Deposition Chamber

- Electon beam sources (6 emitters, 10 crucibles)
- Atomic Absorption rate control
- Atomic Oxygen Sources (2)
- Ion beam processing
- RHEED
- 4000 L/sec cryopump

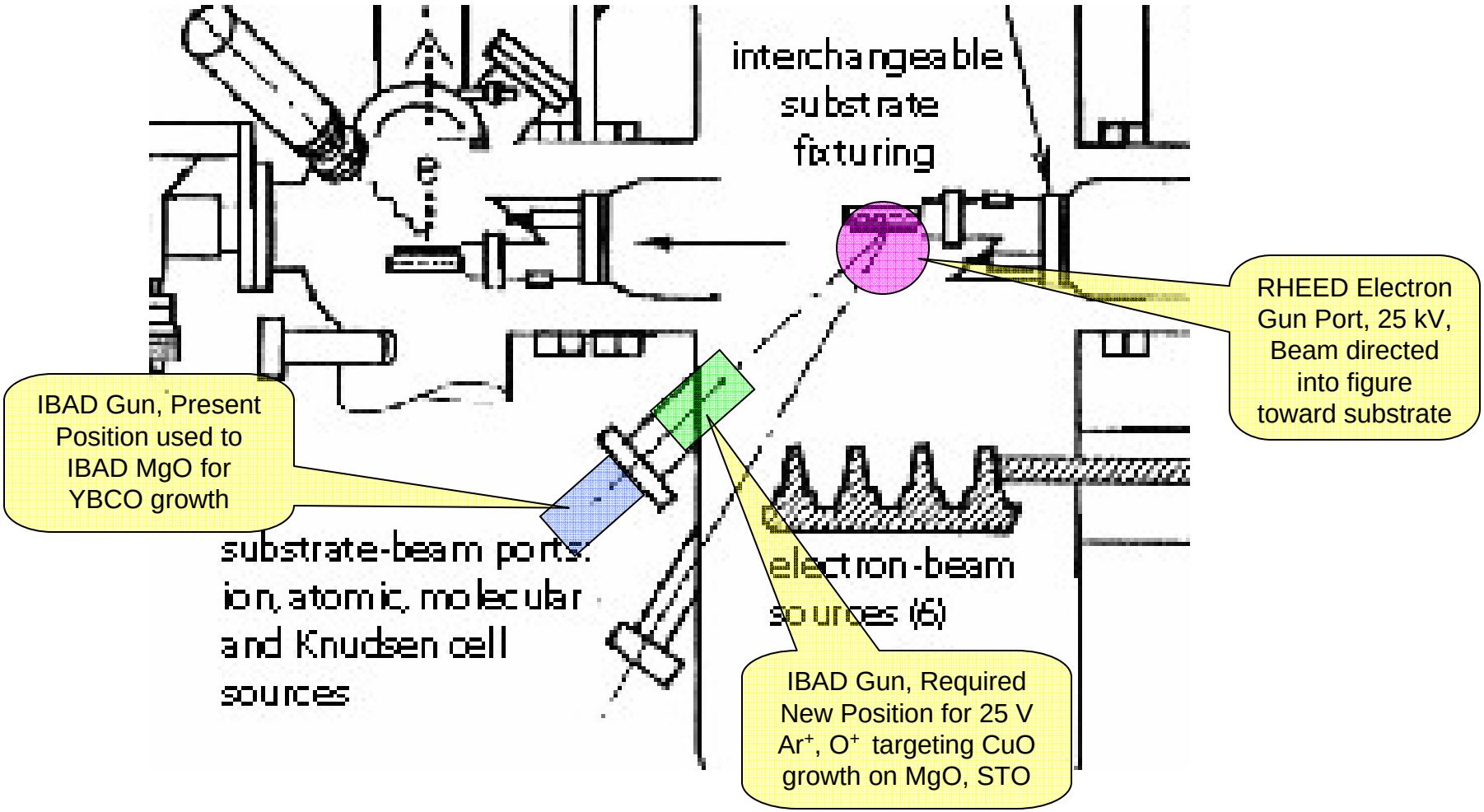
Load-Lock / Processing Chamber

- Gas annealing

Return

IBAD – RHEED Port Positions

(Stray Magnetic Field from New IBAD Gun Position Interferes with RHEED Diffraction Pattern)



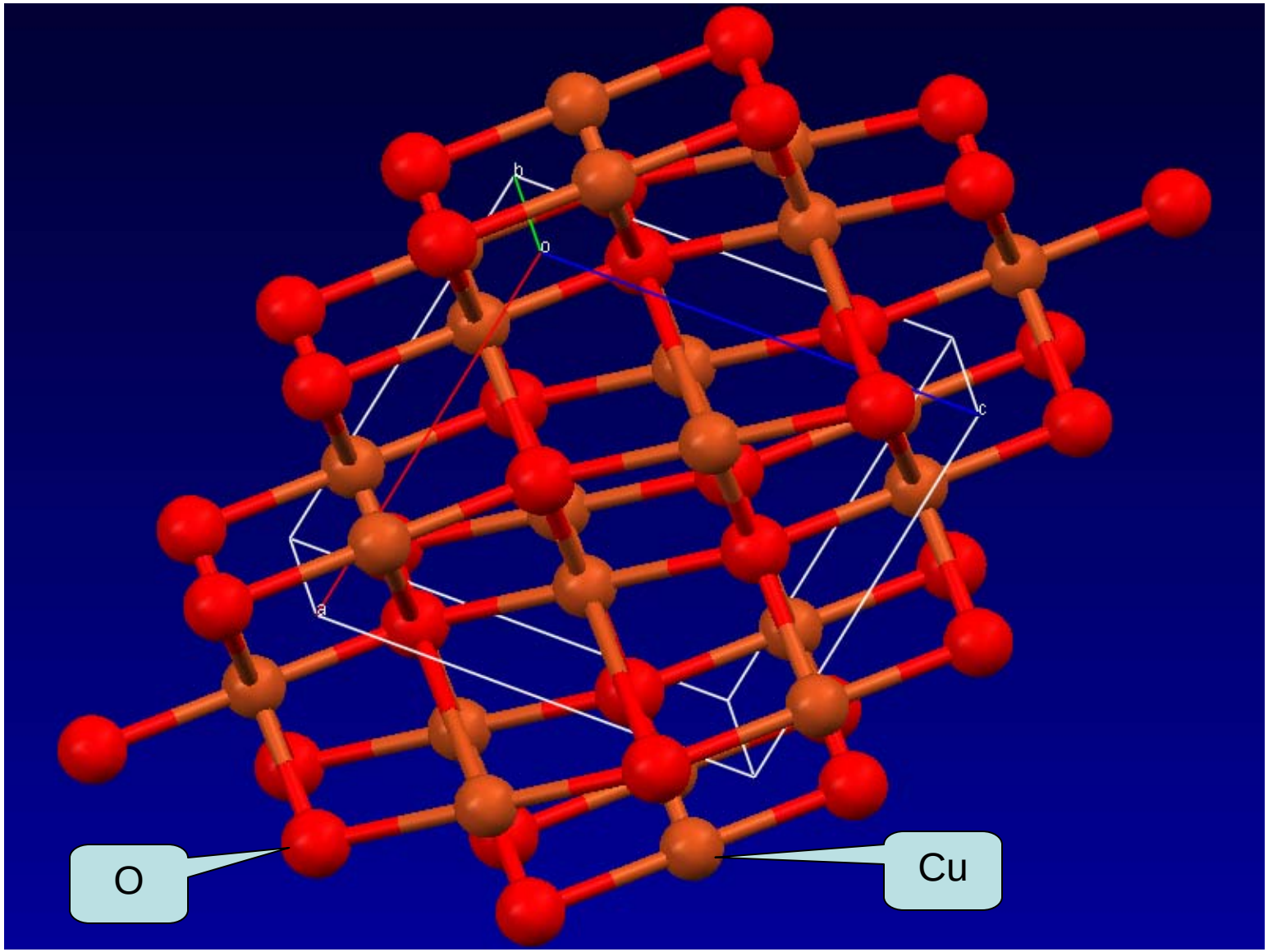
Return

II Theory & Modeling

- Agenda
  - Estimate relative “ground state” energies for native monoclinic tenorite CuO and growth as a meta-equilibrium structure[1] on cubic substrates beginning with cubic MgO as a proxy lattice for potentially cubic CuO using modern ab-initio single-particle electronic structure methodology.[2]
- Results & Observations
  - The calculations suggest a small metastable rock salt state for CuO between +/- 1% of the lattice constants[3] for pristine MgO, but not nearly as stable as the monoclinic structure.
  - The SCF convergence[4] behavior may provide a better indicator of the relative stability of these various structures than the energy/CuO unit. Observe the very rapid convergence of the tenorite structure found in nature.
- Current Conclusions
  1) It appears there is a slightly stable formation region for CuO on MgO, despite the 10% increase in Cu – O bond length vis-à-vis tenorite.
  2) Our current experimental evidence, as reported in the Trimester Report 2005 report, is that CuO does indeed epi-grow for the first few monolayers.
  3) The simulations suggest growth may most optimally occur between the tenorite (111) plane onto the (100) surface of MgO. Possible extensions of this present study would include testing the match to STO[5] and doping of the NiO rock salt structure with Cu up to and perhaps beyond the known solubility limit of 25%.

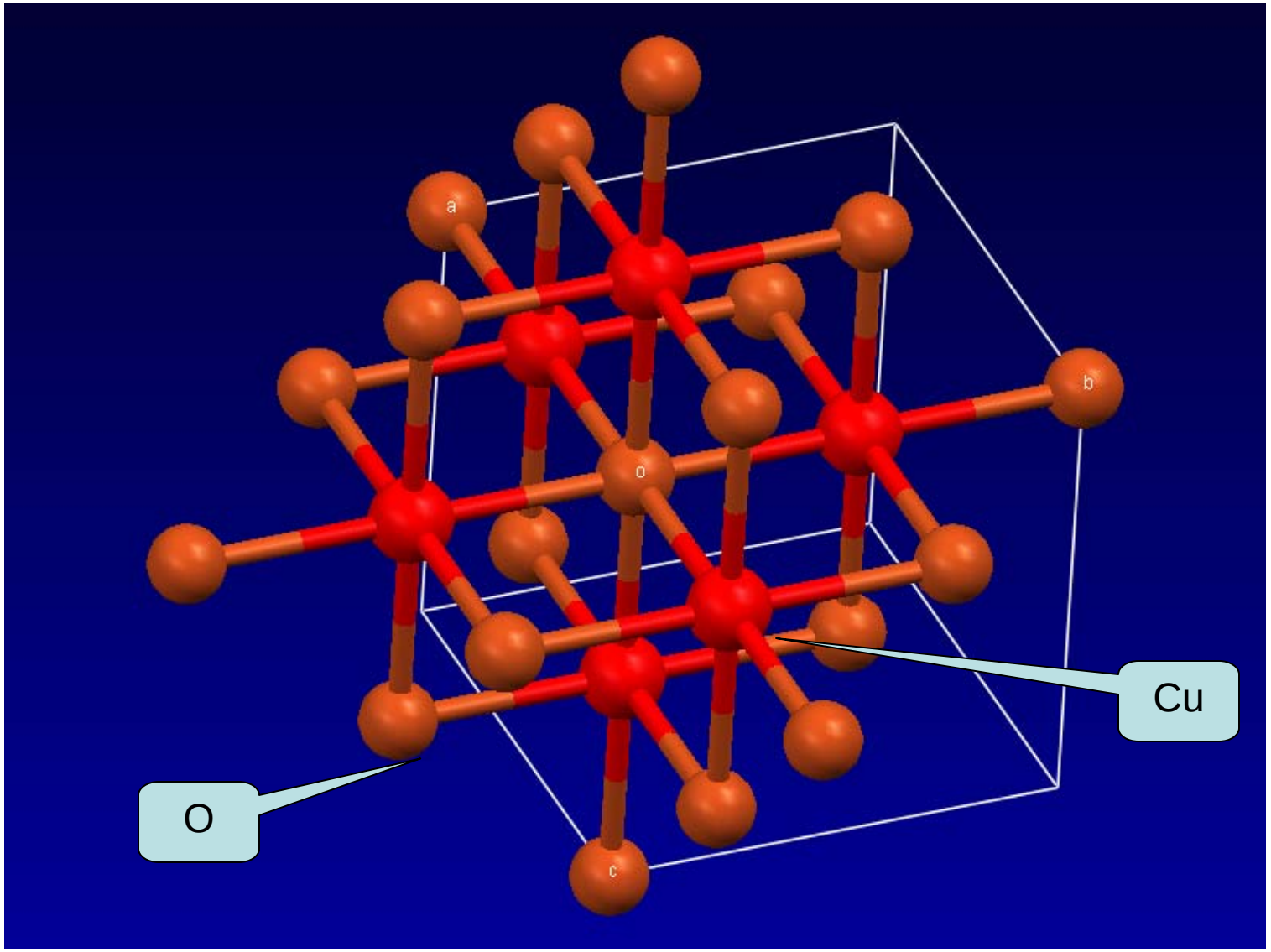
Return

Tenorite (Monoclinic CuO)



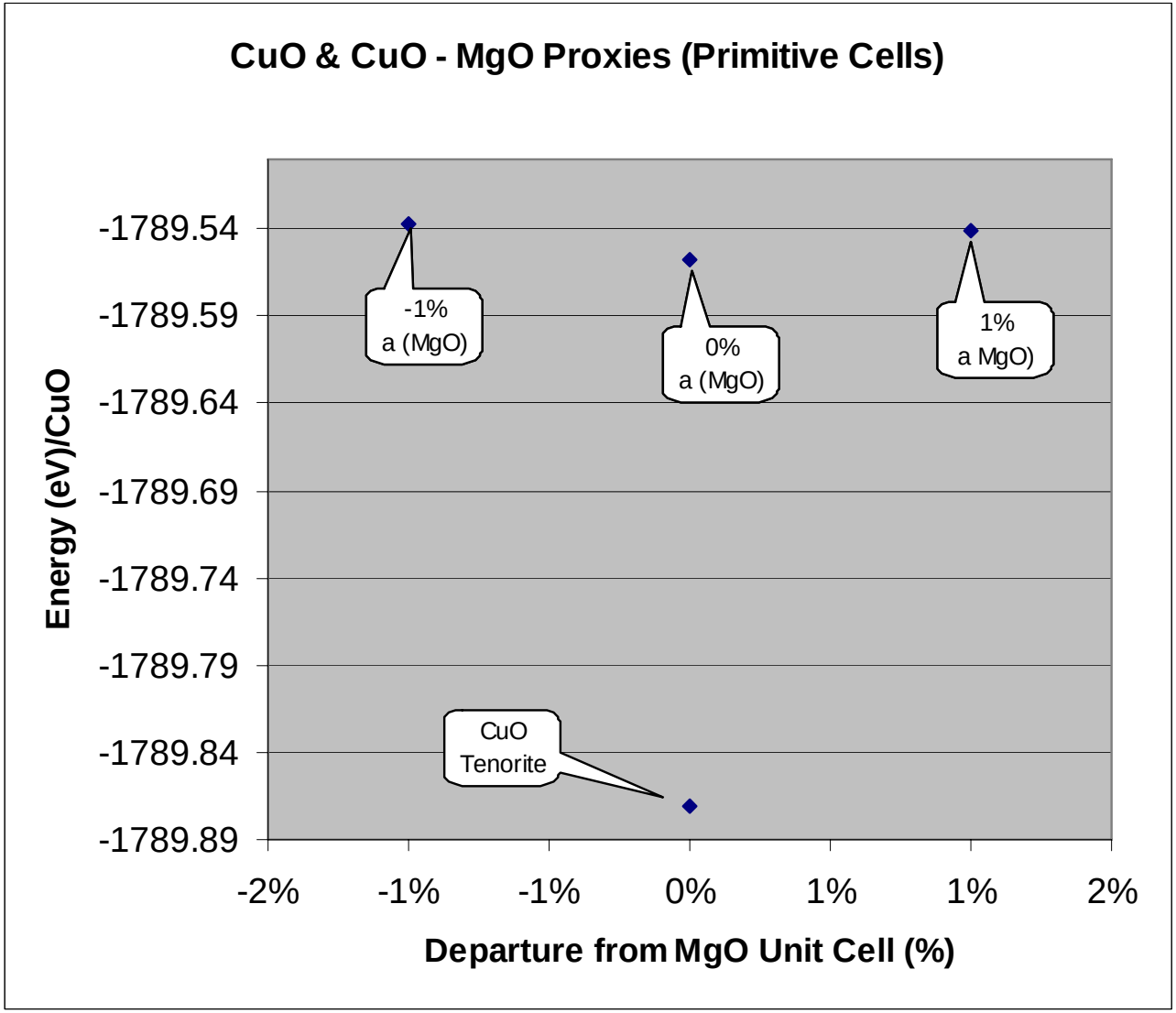
Return

CuO as Cubic MgO



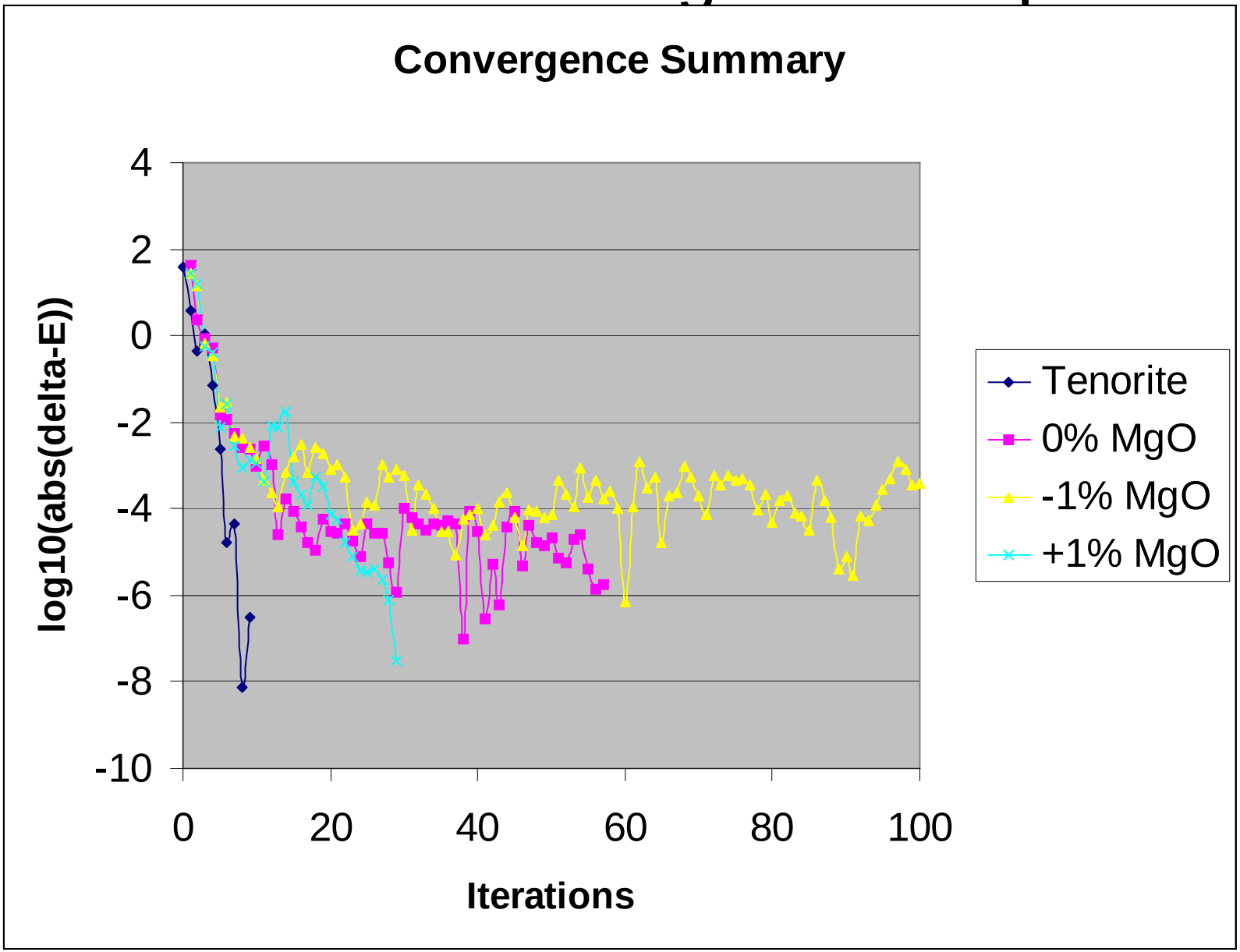
Return

“CuO – MgO Proxy” Converged Energies



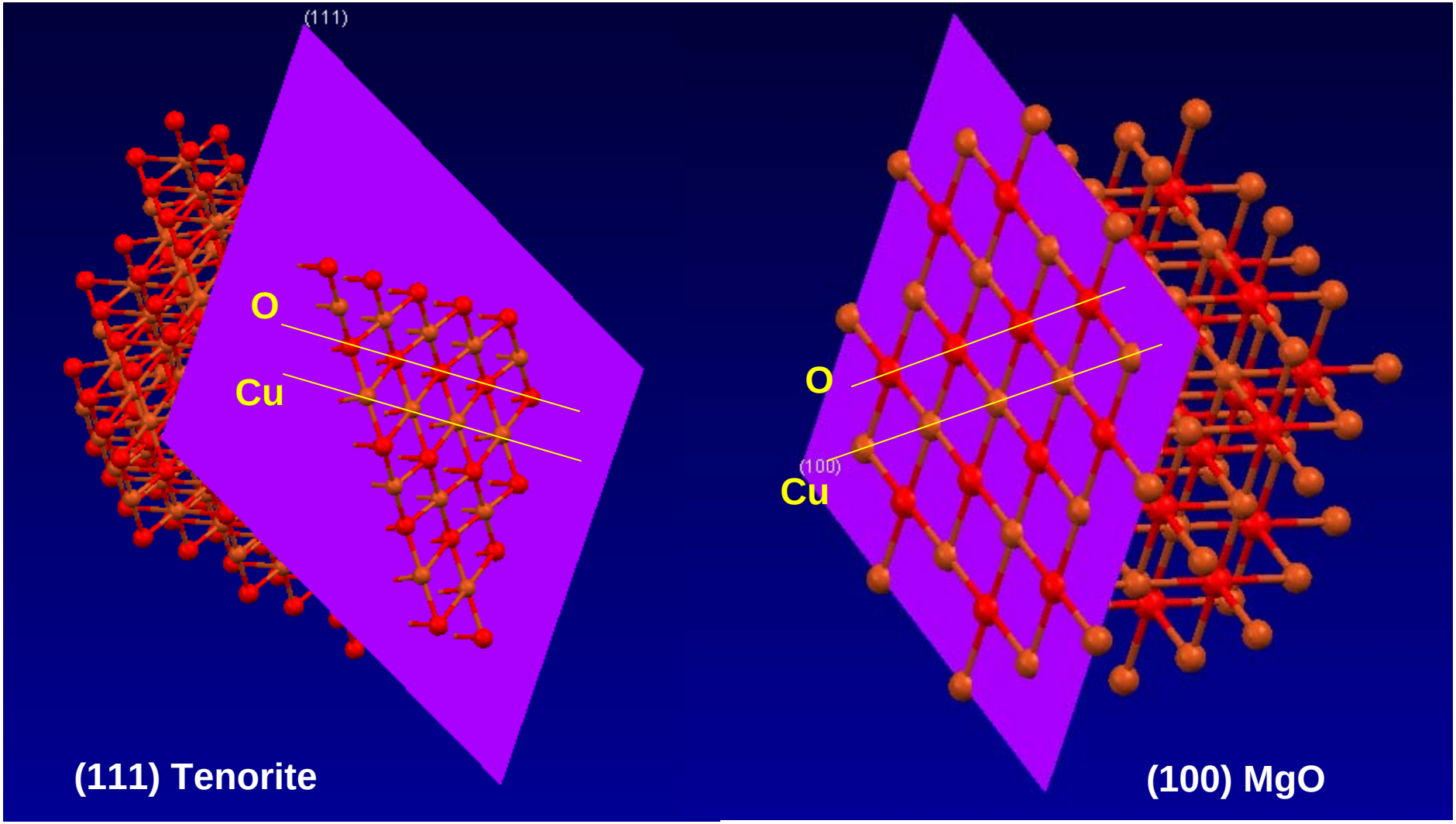
Return

Trial Runs Convergence Properties



Return

Comparison of Tenorite (111) to CuO – MgO Proxy (100)



Return

III. Paper Submitted to:

The 12th International Workshop on Oxide Electronics

Chatham, Cape Cod, Massachusetts, USA

October 2-5, 2005

The effect of low energy Ar^+ ion bombardment on epitaxy and oxidation of thin films of CuO_x

Gertjan Koster[1], Hideki Yamamoto[1,2], Wolter Siemons[1,3], Arturas Vailionis[1], R.H. Hammond[1], P.M. Grant[4], T.H. Geballe[1] and M. Beasley[1]

[1]Geballe Laboratory for Advanced Materials, Stanford University, Stanford, CA

[2]NTT Basic Research Laboratories, Kanagawa, Japan

[3]Inorganic Materials Science, Faculty of Science and Technology, Twente University, The Netherlands

[4]W2AGZ Technologies, Palo Alto, CA

Here we present a detailed study on the growth of epitaxial CuOx thin films on single crystal substrates (MgO and $SrTiO_3$) 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 (LEED and RHEED) monitor the crystal structure 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 the substrate, activated oxygen and 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 achievable in CuO_x system. The relationship between (electronic) properties and crystal structure is being investigated at different lengths using scanning probes. Although the copper system is the focus of this paper, we will also address whether such an approach is feasible for other oxide materials

.

This work is supported by DOE, EPRI and Netherlands Organization for Scientific Research (VENI).

Return