

## ***In-situ* X-ray Powder Diffraction of Electrodeposited *n*- type Cu<sub>2</sub>O and *p*-type Cu<sub>2</sub>O to Identify Phase Transformations and Thermal Expansion**

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*n*-type and *p*-type Cu<sub>2</sub>O films were electrochemically deposited on a Ti substrate in an acetate bath and lactate bath respectively. In-situ x-ray powder diffraction of electrodeposited *n*- type Cu<sub>2</sub>O and *p*-type Cu<sub>2</sub>O clearly shows same crystal orientation at room temperature and similar behaviour up to 400 °C. At 450 °C *n*-Cu<sub>2</sub>O completely converted to the CuO and *p*-Cu<sub>2</sub>O partially converted to the CuO.

**Keywords:** Cuprous Oxide, Electrodeposition, In-situ x-ray powder diffraction

### **Introduction**

The increasing global demand for energy, limited fossil fuel supplies on the planet and global climate changes due to greenhouse gas emissions from fossil fuel burning have made it necessary to use renewable, clean energy sources as energy alternatives. Among the various technologies available, photovoltaics is considered one of the cleanest ways to achieve this objective. However, the difficult task of solar cell manufacturers is to reduce production costs in relation to the resulting output power of the solar modules with a view to enhance their marketability and use. In order to solve this problem, a number of materials are being studied for their use in applications based on solar energy. Among them, recent studies show that cuprous oxide (Cu<sub>2</sub>O) has become a key candidate as it has the potential to meet global demand for electricity and reduce photovoltaic costs compared to other materials [1].

One of the main challenges for the production of Cu<sub>2</sub>O-based solar cell devices is to fabricate Cu<sub>2</sub>O *p-n* homojunctions. Since the homojunction should not present any interfacial deformation resulting from the lattice mismatch between *p*-type and *n*-type materials, the separation of photoinduced charges in the Cu<sub>2</sub>O homojunction can be considerably improved, hence improving the photoelectric conversion performance [2]. However, research on the fabrication of Cu<sub>2</sub>O homojunctions is insufficient to date due to the lack of studies on the production of *n*-type Cu<sub>2</sub>O films. Since the demonstration of the growth of *n*-type Cu<sub>2</sub>O films using the electrodeposition method by our laboratory [3] several other methods have been reported on preparation of *n*-type Cu<sub>2</sub>O films on various substrates. One way to enhance the efficiency is to improve the quality of the *n*-type and *p*-type surface and interface of the *p-n* junction. In this experiment thermal behavior of structural properties of individual films were examined.

### **Experiment**

*n*-type Cu<sub>2</sub>O films were electrochemically deposited on a Ti substrate in an aqueous solution containing 0.01 M copper acetate and 0.1 M sodium acetate at solution pH of 6.2, a deposition potential of -200 mV vs. Saturated Calomel Electrode (SCE) and at a temperature of 60 °C. *p*-Cu<sub>2</sub>O films were deposited on Ti substrates in an aqueous solution containing 0.4 M copper sulfate and 3 M sodium lactate at a solution pH of 11, the deposition potential of -450 mV vs. SCE and at a temperature of 60 °C. In order to perform powder XRD, electrodeposited sulfur treated Cu<sub>2</sub>O thin films were peeled off from Ti substrates and filled in to Lindemann glass capillary tubes of 0.3 mm internal diameter. Diffraction data of powdered samples were obtained using 25 keV photon energy

X rays of wavelength around 0.49592 Å. An XRD peak that was absent in previously reported laboratory XRD patterns could be observed using the powder XRD experiments. Thermal stability of Cu<sub>2</sub>O samples were investigated using *in-situ* X-ray powder diffraction with low signal to noise ratio and low background in the scattering angle range from 2 to 85 degree using MYTHEN detectors installed in the two-axis diffractometer at BL19B2.

## Results

Figure 1 shows the *in-situ* powder XRD patterns of electrodeposited (a) *n*-Cu<sub>2</sub>O thin films prepared at pH 6.2 in the acetate bath (b) electrodeposited *p*-Cu<sub>2</sub>O thin films prepared at pH 11 in the lactate bath.

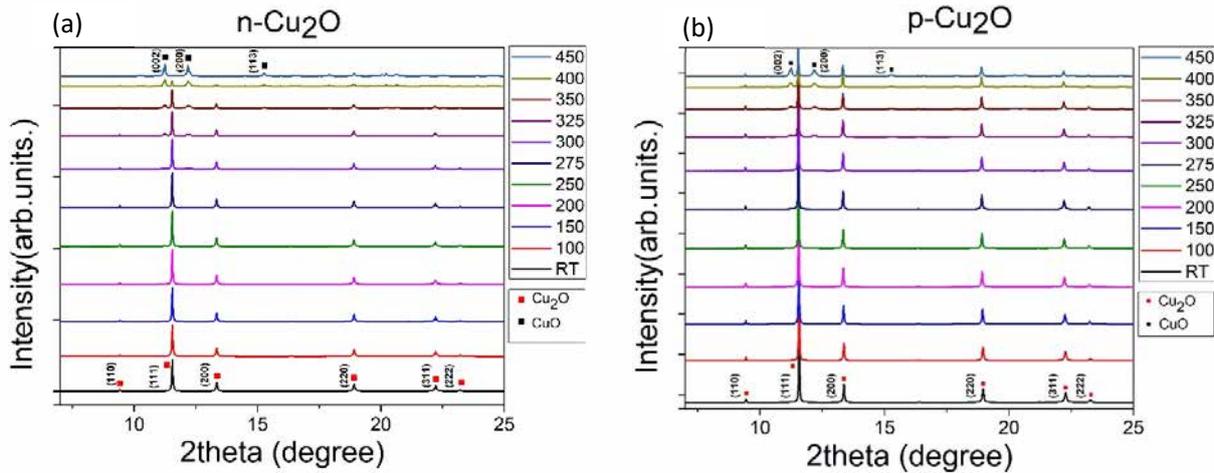


Figure 1 *In-situ* powder XRD patterns of electrodeposited (a) *n*-Cu<sub>2</sub>O thin films prepared at pH 6.2 in the acetate bath (b) electrodeposited *p*-Cu<sub>2</sub>O thin films prepared at pH 11 in the lactate bath.

Laboratory XRD was not sensitive enough to detect possible formation of phases such as Cu<sub>x</sub>O and small variation of crystallinity due to annealing. On the other hand, as shown in figure 1 the use of synchrotron powder XRD can divulge more accurate structural information due to high-energy beam with high flux as well as high counting statistics from little amount of powder sample.

In figure 1, *in-situ* powder XRD of electrodeposited *n*-type Cu<sub>2</sub>O and *p*-type Cu<sub>2</sub>O clearly shows same crystal orientation at room temperature and show that several CuO peaks have evolved after annealing at 300 °C due to the oxidation of Cu<sub>2</sub>O into CuO phase with similar behavior up to 400 °C. At 450 °C *n*-Cu<sub>2</sub>O completely converted to the CuO and *p*-Cu<sub>2</sub>O partially converted to the CuO.

## Next Step

We will obtain crystal structure information such lattice parameters and unit cell volume of *n*-Cu<sub>2</sub>O and *p*-Cu<sub>2</sub>O using FullProf suit under the Rietveld refinement method for a Pseudo-Voigt function.

## References

- [1] C. Wadiya, A. P. Alivisatos, D. M. Kammen, *Environ. Sci. Technol.* **43**, 2072-2077 (2009).
- [2] A. Baltakesmez, S. Tekmen, S. Tüzemen, *J. Appl. Phys.* **110**, 054502 (2011).
- [3] W. Siripala, J. R. P. Jayakody, *Sol. Energy Mater.* **14**, 23-27 (1986).