

## High-Pressure Induced Structural Phase Transition in $\text{Li}_2\text{CuO}_2$

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### Abstract

In situ high-pressure energy dispersive X-ray diffraction measurements on polycrystalline powder  $\text{Li}_2\text{CuO}_2$  has been performed by using diamond anvil cell instrument with synchrotron radiation. The results showed that  $\text{Li}_2\text{CuO}_2$  undergoes a structural transition at 8.1GPa. The structural transition is reversible.

### Introduction

Since the discovery of superconductivity in heavily Ca doped  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  at 12k under pressure of 3GPa in 1996[1], cuprates with edge-sharing  $\text{CuO}_2$  chains have been considered as another family of transition metal oxides in connection with high  $T_c$  superconductors. As a typical one dimensional cuprate,  $\text{Li}_2\text{CuO}_2$  was in favored for both experimental and computational studies. Recently we performed a series of in situ high pressure XRD measurements up to 36.9GPa and a structural phase transition was observed at 8.1GPa in this compound.

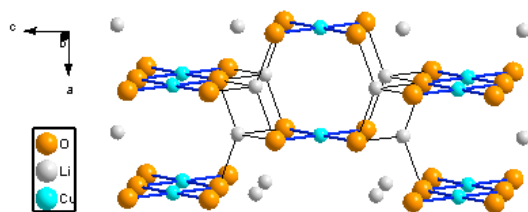


Fig 1 structure of  $\text{Li}_2\text{CuO}_2$

### Methods and Materials

The *in situ* high pressure X-ray energy dispersive diffraction experiment on  $\text{Li}_2\text{CuO}_2$  was carried out at room temperature in a diamond anvil cell (DAC) using the white-radiation from the synchrotron radiation source at the Beijing Synchrotron Radiation Laboratory (BSRL). The size of the X-ray spot was  $30\mu\text{m} \times 20\mu\text{m}$ . The culet of the DAC was  $500\mu\text{m}$ . The powder of the sample was loaded into a  $300\mu\text{m}$  hole in a T301 stainless steel gasket. The applied pressure of the DAC was monitored by the position of the luminescence line  $R_2$  from a small piece of ruby placed in the gasket hole. In our experiments, the relation of energy and channel was  $E=0.5444+0.0885*\text{chn}$ . According to the formula  $\sin\theta=0.619925/[d(\text{nm})*E(\text{KeV})]$ , we got the exact value of  $\theta=7.465^\circ$ .

### Results

The spectra of energy dispersive X-ray diffraction(EDXD) of the  $\text{Li}_2\text{CuO}_2$  sample under various pressures at room temperature are shown in Figure 2. The maximum pressure applied in our experiment is 36.9 GPa. From the spectra we can find that, when the pressure is lower than 6.5GPa, all diffraction peaks shift toward higher energy as the pressure increases.

However, two new peaks(signed with \* ) emerge when the pressure loaded from 8.1GPa to 10.4GPa. As pressure increases, the intensity of the new peaks gets stronger with that of all the initial diffraction peaks of  $\text{Li}_2\text{CuO}_2$  weakening and finally indistinguishable at 36.9GPa. The new diffraction peaks shift

toward lower energy as the pressure released, and most of the initial diffraction peaks of  $\text{Li}_2\text{CuO}_2$  come back to original sites when the pressure returns to ambient

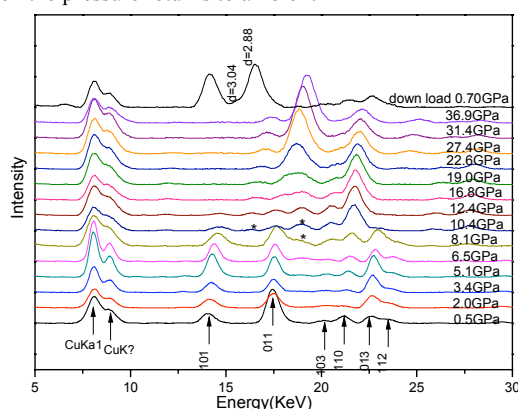


Fig 2 The spectra of EDXD of the  $\text{Li}_2\text{CuO}_2$  sample under various pressures at room temperature

### Discussion

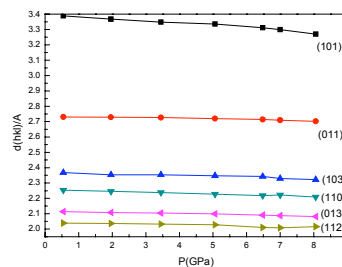


Fig 3 Pressure dependence of the d values ( $d_{hkl}$ ) in  $\text{Li}_2\text{CuO}_2$

According to the high pressure experiment and the results described above, we suggest that  $\text{Li}_2\text{CuO}_2$  sample undergoes a structural phase transition from 8.1GPa. Fig. 3 presents the results of the lattice evolution with pressure. Due to the relatively low resolution of the instrument, it is difficult to determine the exact structure of the new phase at the moment.

### Acknowledgement:

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### Reference

- [1] M. Uehara, T. Nagata, et al, J. Phys. Soc. Jpn. 65(9), 2764 (1996).
- [2] P. Novak, J. Power Source 15(1985)101