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Crystal Structural Behavior of CoCu$_2$O$_3$ at High Temperatures

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Abstract:
High temperature structure of CoCu$_2$O$_3$
The spin ladder compounds have received much attention recently due to their relation to the high transition temperature superconductivity. Also the study of spin ladder compounds is of great interest to explore the specific characteristics that result in their behavior. The CoCu$_2$O$_3$ spin ladder crystal structure is similar to SrCu$_2$O$_3$, which is apparent composition for many high temperature superconductors. The effects of temperature on structural change are investigated for this system. High temperature x-ray diffraction patterns were collected up to 1000°C and the variation of lattice parameters as a function of temperature up to decomposition is studied.

The thermal stability of CoCu$_2$O$_3$ has been studied at elevated oxygen pressures beyond a high temperature of 1000°C [1]. Temperatures at which CoCu$_2$O$_3$ undergoes decomposition reactions were studied along with the products of the reactions. The study introduced here provides structural details and the linear coefficient of thermal expansion (CTE) before progressive decomposition.

Experimental Details:
Sample Preparation:
Powder samples of (Ca$_{1-x}$Co$_x$)Cu$_2$O$_3$ (x=0.05) were prepared by the solid state reaction method as described elsewhere [2]. The phase purity of the sample was verified by powder XRD measurements on polycrystalline samples and found to be in single phase. The chemical compositions of the synthesized samples were determined [2].

High Temperature X-Ray Diffraction:

A circular corundum sample stage was loaded with fine powdered CoCu$_2$O$_3$ and loaded into the vacuumed high temperature stage in the Bruker D8 Advance X-Ray Diffractometer (Figure 1). Sample was heated at a rate of 0.5°C/sec from 30°C to 400°C. XRD data was collected at temperatures of 30 °C, 100 °C, 200 °C, 300 °C, and 400 °C then cooled at a rate of 1°C/sec back to 30 °C for a final collection of data. Another run from 30 °C to 1000 °C was conducted to track the decomposition of the sample. XRD data was collected starting at 30 °C, and every 200 °C up to 1000 °C, and back to 30 °C. TOPAS was used to analyze the x-ray diffraction patterns and the track percent compositions of the sample at various temperatures. Origin8 was used to analyze the data and obtain the linear coefficient of thermal expansion.

Results:
- TOPAS was used to display the intensity peaks which are characteristic of the material (Figure 2 and Figure 3) from 30°C to 400°C. As the temperature increases the shift of the peaks to the lower 2θ shows an expansion of the cell.
- Length of lattice parameter vs. temperature data is linear only to 300°C, so linear CTE was determined using data from 30°C to 300°C using Origin8 (Figure 4-a).
- Linear CTE for each lattice parameter can be seen in Table 1.

Conclusions:
- Lattice parameters do not have the same coefficient of thermal expansion, therefore the volume expansion is not isotropic.
- Products of the reaction between 400°C and 600°C are in good agreement with previous TGA/DTA study [1].
- CoCu$_2$O$_3$ decomposes at 537°C [1]. There are no temperature induced phase changes observed before decomposition.

References:

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