Crystallography

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Structure of Y_2BaCuO_5 synthesized under strong gravity field

Akira YOSHIASA[1], Rabaya BAGUM [1], Yusuke IGUCHI[1],
Maki OKUBE[2] and Tsutomu MASHIMO[1]
[1] Graduate School of Sciences, Kumamoto Univ. Kumamoto 860-8555, Japan
[2] Tokyo Institute of Technology, Nagatsuta, Yokohama 226-8502, Japan.

Introduction

Materials research using strong gravitational field (1-10 x10^5 G, 1G =9.8 m/s^2) is still an unexploited area, even though materials science research utilizing microgravity fields is now active. To study sedimentation of atoms or crystal instability in solids under strong gravitational fields, we developed a high temperature ultracentrifuge apparatus that can generate a long duration acceleration field in excess of 10^6 G at elevated temperatures. A green phase with composition Y_2BaCuO_5 as first identified as a contaminant in the high temperature superconductor $Y_1Ba_2Cu_3O_{7-x}$. In the current research, the ultracentrifuge experiments were performed on the $Y_1Ba_2Cu_3O_{7-x}$ single crystals in the solid state to synthesize Y_2BaCuO_5 crystal by change in composition and structure and compare the structure to other previous data. The crystal structure was investigated by X-ray diffraction analysis [1].

Experimental

We used the ultracentrifuge apparatus of Kumamoto University. The gravitational field was applied along the c-axis of $Y_1Ba_2Cu_3O_{7-x}$ single crystal. The rotor could be heated by radiation from a hot carbon, hollow cylinder that is heated by a high frequency heating system. Compositions of the single crystals were determined by EPMA.

Single-crystal X-ray diffraction measurements were carried out with a four-circle diffractometer at the BL-10A beam line of the Photon Factory, Tsukuba, Japan, using monochromatized synchrotron X-ray (λ = 0.70006 Å) radiation. Structute refinements were performed using full matrix least squires program RFINE2 (Table 1). Our refinement yields full occupancies for all sites.

Results and Discussion

The lattice constants of the green Y_2BaCuO_5 single crystal are a = 7.138(5) Å, b = 12.191(1) Å and c =5.6628(3) Å. The unit cell volume, 492.8(1) Å ^{3}, is larger than that given in other previous reports.

The CuO5 pyramid in Y_2BaCuO_5 is largely distorted. The five coordinate Cu has two Cu-O1, 1.985Å and two Cu-O2, 1.988 Å bonds. The fifth Cu-O3, 2.206 Å bond lies on the mirror plane. The smallest Ba-O bond is 2.6024 Å which lies on the mirror plane. Each Y cation is surrounded by seven O atoms: six are arranged as a trigonal prism with the seventh capping one rectangular face. Details of the discussion are shown in reference [1].

Table1. Experimental data for Y_2BaCuO_5

Crystal data	Y_2BaCuO_5
Space group	*Pbnm*
a(Å)	7.1380(5)
b(Å)	12.191(1)
c(Å)	5.6628(3)
V(Å^3)	492.8(1)
Wavelength	0.70006
μ (cm^{-1})	296.9
Crystal forms	prism
Crystal size(μm^3)	20 × 20×10
Data collection	PF 10A
Data collection	ω/2θ
Scan Speed(°min^{-1})	4
No of independent reflection	645
R	0.0615
wR	0.0920

Table 2. Comparison of cation to oxygen distances (Å) and unit cell volume (Å^3) in Y_2BaCuO_5.

Average bond length	This Study	Hsu *et al.*	Barter et al.	Pei et al,
Ba-O	2.988(1)	2.983(1)	2.984(2)	2.982(3)
Cu-O	2.0298(1)	2.0376(1)	2.0380(1)	2.0404(1)
Y1-O	2.345(1)	2.336(1)	2.342(1)	2.327(1)
Y2-O	2.325(1)	2.326(1)	2.326(1)	2.335(1)
Unit cell	492.8(1)	491.6(1)	492.17(3)	491.7(1)

References

[1] Rabaya Bagum, Akira Yoshiasa, Satoru Okayasu, Yusuke Iguchi, Masao Ono, Maki Okube, Tsutomu Mashimo, JOURNAL OF APPLIED PHYSICS (2010) 108 053517 7pp

* yoshiasa@sci.kumamoto-u.ac.jp