Crystal Structure of High Temperature Superconductors

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Introduction

History of Superconductors

Superconductors are material which exhibit no resistance below a certain temperature. Superconductors were discovered in 1911 by Scientist Kamerlingh Onnes. superconductivity was first observed in mercury with a critical temperature of 4.2 Kelvin.

Applications of Superconductors

Some of the applications of superconductors that are currently being used includes: magnetic shielding devices, medical imaging systems, superconducting quantum interference devices (SQUIDS), infrared sensors, analog signal processing devices, microwave devices, power transmission, superconducting magnets in generators, energy storage devices, particle accelerators, levitated vehicle transportation, rotating machinery, magnetic separators, Josephson devices, MRI imagers, Electric motors, fault-current devices.

Motivation

The purpose of our experiment was to prepare YBCO and to determine is properties by a careful analysis of its x-ray diffraction pattern.

Motivation

Preparation of HTS

High temperature superconductors are prepared using the Solid State reaction method. Using this method you follow these four steps: step1- mixing the chemicals, step 2- Calcinations, step 3- the intermediate firings, step 4- the final oxygen annealing. This reaction takes place at high temperature. After the reaction has taken place, the YBCO should be reground to a powder and then pressed into a pellet.

Superconducting Systems

Simple Metals and Alloys

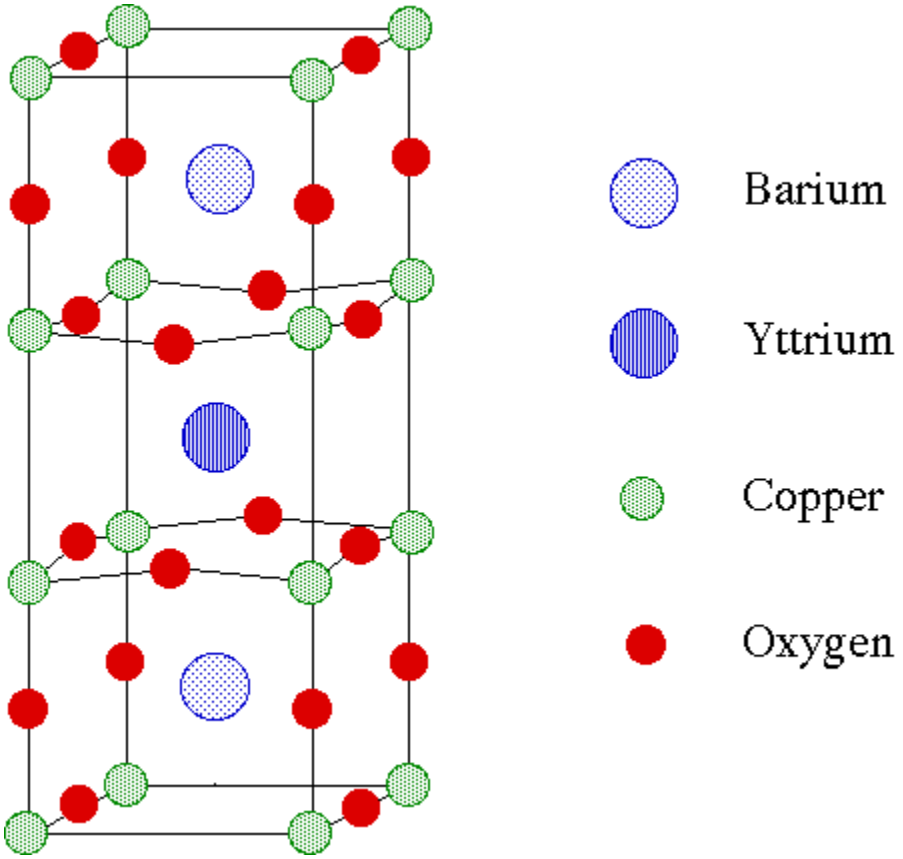
Material	Critical Temperature (K)
Titanium (Ti)	0.4 K
Zinc (Zn)	0.85
Aluminum (Al)	1.175
Tantalum (Ta)	4.47
Lead (Pb)	7.2
NbN	16.0
La_3In	18.05
Nb_3Ge	16.0

High Temperature Superconductors

Material	Critical Temperature (K)
$La_{1.85}Ba_{0.15}CuO_4$	36
$YBa_2Cu_3O_7$	92
$Tl_2Ba_2Ca_2Cu_3O_{10}$	120
$Tl_{1.8}Ba_2Ca_{2.6}Cu_3O_{10}$ (at high pressure)	255

Crystal Structure of $YBa_2Cu_3O_{6+x}$

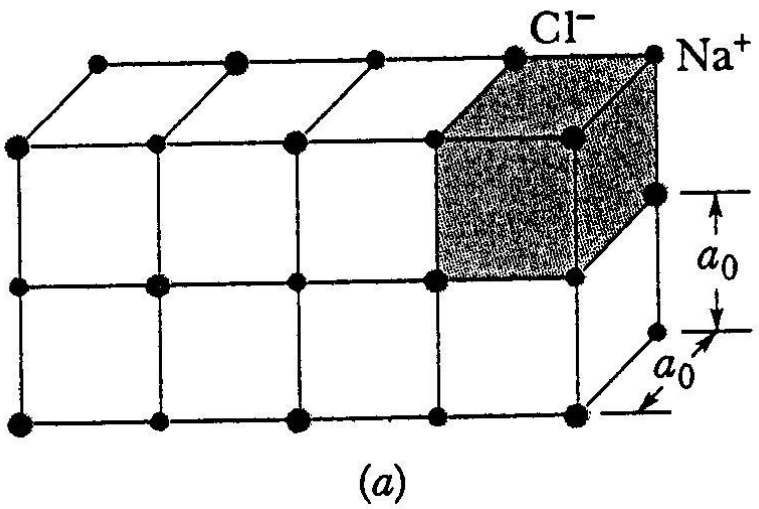
Unlike the original simple metals and alloys high temperatures superconductors such as YBCO have very complicated crystal structures. We prepared YBCO and determined the purity of the sample by x-ray diffraction methods. The complicated structure produced a intricate diffraction pattern.



Taken from http://imr.chem.binghamton.edu/labs/super/superc.html

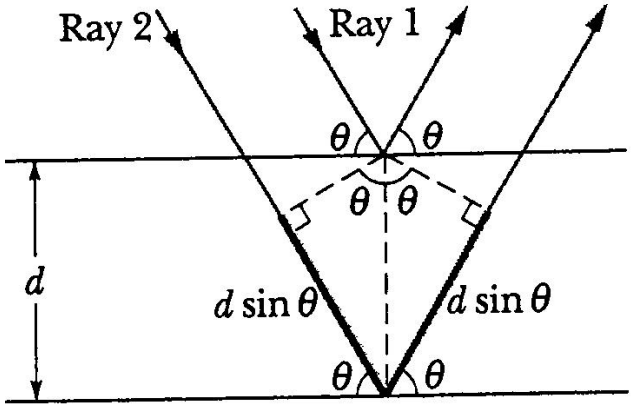
X-Ray Diffraction for Structure Determination: Lattice Planes

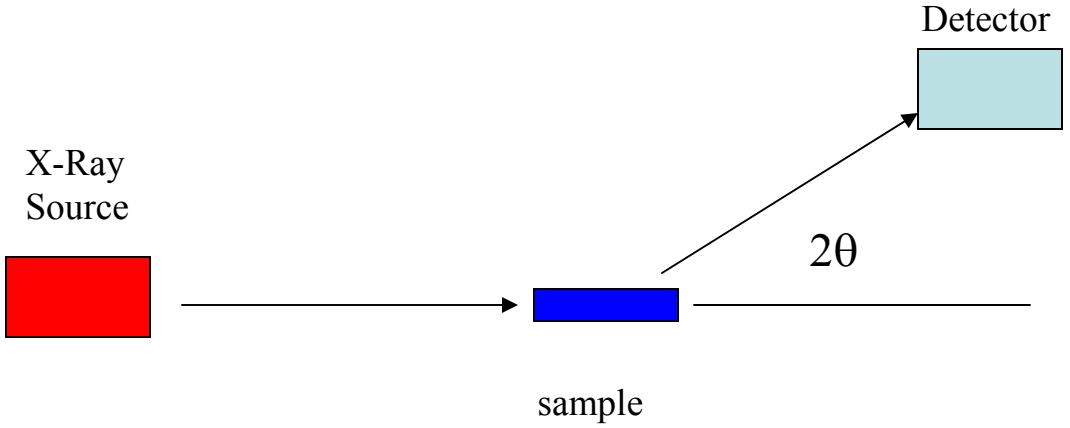
Crystalline solids are composed of planes of atoms. If radiation with wavelength close to that of the spacing between the planes scatters off of the material waves from different planes interfere and create an interference patter called a diffraction pattern. Since a unique structure produces a distinct diffraction pattern. X-ray diffraction can be used to identify the a material. We show the case for NaCl (table salt) on the left.



X-Ray Diffraction for Structure Determination: Diagrams of Experiment

X-rays generated by electrons colliding with a Cu target are scattered off of the sample. The diffraction pattern is obtained by scanning the detector over a continuous range of angles. Our objective was to determine if our synthesized sample was YBCO. The d-spacing can be determined from the diffraction pattern if the angle of a peak and wavelength of the radiation are known.



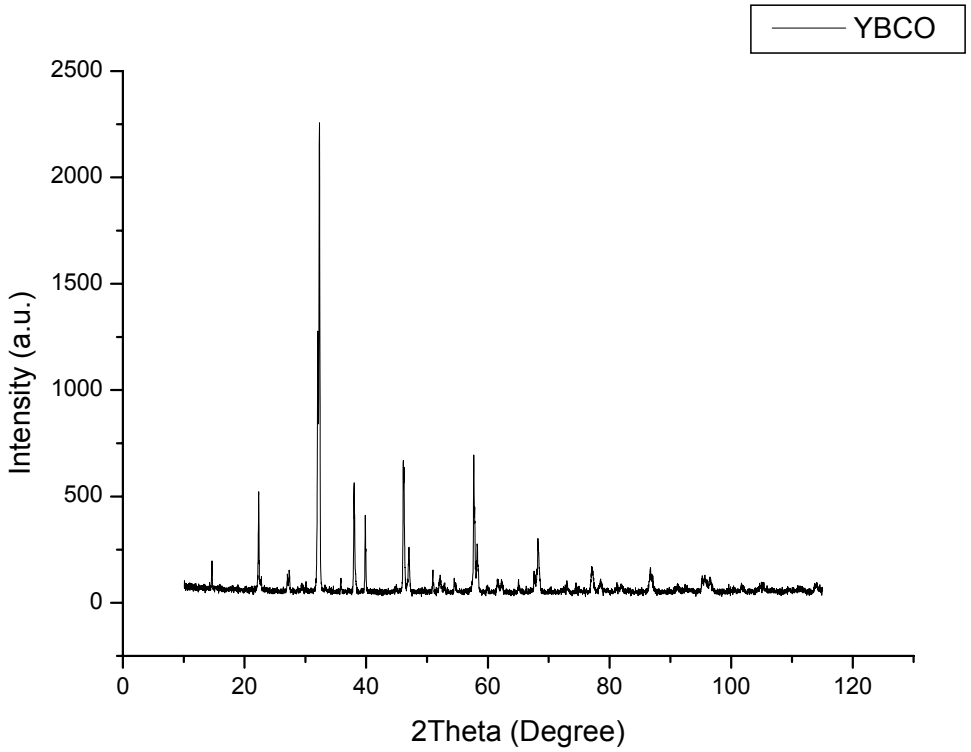


X-Ray Diffraction for Structure Determination: Diffractometer

The upper right shows the x-ray diffractometer used to measure the diffraction pattern for your YBCO sample. Note the large water cooled Cu x-ray source on the left (bottom figure), the sample and the detector. The measured x-ray diffraction pattern follows.

YBCO X-Ray Diffraction Pattern

The intensity vs. angle is shown. In order to identify the compound we found all of the peak positions and made a table of peak position and intensity as a function of angel. Using Braggs Law we can obtain the plane separation (d).



Braggs Law

$2 d \sin(\theta) = n \lambda$

For Cu $\lambda = 1.54060$ Å (1 A=10^{-10} m)

Peak Positions from XRD

2 Theta	d (A)	Intensity
15.07	5.875	5
22.73	3.909	18
27.45	3.246	3
27.77	3.210	4
32.43	2.759	54
32.72	2.735	100
36.23	2.477	4
38.41	2.342	26
40.26	2.238	19
46.53	1.950	31
47.43	1.915	9
51.38	1.777	5
52.50	1.742	4
54.89	1.671	4
58.10	1.586	34
58.68	1.572	12
62.02	1.495	3
62.62	1.482	4
65.42	1.425	4
68.01	1.377	5
68.68	1.366	11
73.42	1.289	3
77.51	1.231	5
78.89	1.212	4
87.11	1.118	5
87.57	1.113	3
91.59	1.075	3
95.69	1.039	4
96.16	1.035	3
96.93	1.029	4
102.10	0.990	2
105.69	0.96649	3

TABLE I. Powder x-ray diffraction pattern for $Ba_2YCu_3O_{6.9}$. Orthorhombic unit cell, $a = 3.8218(7)$ Å, $b = 3.8913(7)$ Å, $c = 11.677(2)$ Å.

h	k	l	d_{OBS} (Å)	I/Io (%)
0	0	2	5.844	2
0	0	3	3.893	11
1	0	0	3.822	3
0	1	2	3.235	3
1	0	2	3.198	5
0	1	3	2.750	60
1	0	3	2.726	100
1	1	0		
1	1	1	2.653	2
1	1	2	2.469	3
0	0	5	2.336	11
1	0	4	2.321	3
1	1	3	2.232	13
0	2	0	1.946	23
0	0	6		
2	0	0	1.911	10
1	1	5	1.775	3
0	1	6	1.741	2
0	2	3		
1	0	6	1.734	2
1	2	0		
2	0	3		
2	1	0	1.716	2
1	2	1		
1	2	2	1.662	1
1	2	3	1.584	24
1	1	6		
2	1	3	1.569	11

Taken from Phys. Rev. Lett. 58, 1676 (1987).

Lattice Parameters Extracted from XRD Pattern

For orthorhomic unit cells such as that for YBCO
$d(h,k,l, a, b, c) = 1/\mathrm{sqrt}[(h/a)^2+(k/b)^2+(l/c)^2]$
By using this formula you can find a, b, c if the diffraction peaks have been indexed. On the right is an example of the determination of peak positions from the d-spacings. A more accurate set of values can be obtained by fitting the full pattern.

h=0, k=0, l=2
$d(h,k,l) = 1/[(h/a)^2+(k/b)^2+(l/c)^2]^{1/2}$

$d(0\ 0\ 2) = 1/[(2/c)^2]^{1/2} = c/2$
$c = 2\ d(0\ 0\ 2) = 2(5.875) = 11.75$
$c = 11.75$ Å

$d(h\ k\ l) = d(0\ 1\ 3) = [(1/b)^2+(3/c)^2]^{1/2}$
$1/d(0\ 1\ 3)^2 = (1/b)^2+(3/c)^2$
$1/d(0\ 1\ 3)^2-(9/c)^2=1/b^2$
$b = 1/[1/d(1\ 0\ 3)^2-(3/c)^2]^{1/2}$
$= 1/[1/2.759^2 - 9/11.75^2]^{1/2}$
$b = 3.887$ Å

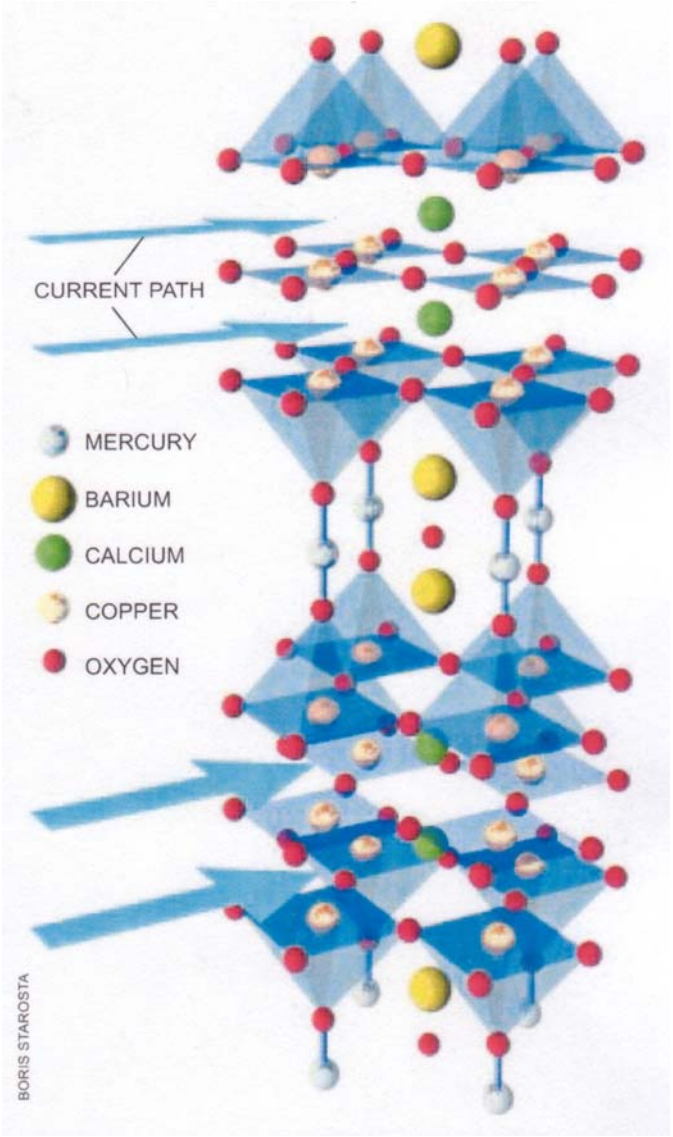
$d(h\ k\ l) = d(2\ 0\ 0) = 1.915$
$d(2\ 0\ 0) = 1/[(2/a)^2]^{1/2} = a/2$
$a = d(2\ 0\ 0)*2$
$a = 3.830$ Å

Discussion

delta	0.07	0.27	0.4	0.45	0.52	0.55	0.59	0.62
x	0.93	0.73	0.6	0.55	0.48	0.45	0.41	0.38
a	3.8227	3.8275	3.8349	3.8362	3.8415	3.8433	3.8468	3.8510
b	3.8872	3.8875	3.8851	3.8808	3.8778	3.8764	3.8736	3.8700
c	11.6802	11.7063	11.7279	11.7286	11.747	11.7512	11.7601	11.7711
Tc	93K	93K	60K	60K	55K	40K	30K	10K

Based on the d(200) peak which is the strongest we estimate the x value for the sample was between 0.73 and 0.55. The sample is possibly mixed phase with some parts of the sample having x near 0.55 (Tc ~60k) and some with x near 0.27 (Tc ~93). In fact the resistivity measurements show evidence of percolation or the motion of electrons through a mixed phase system.

We show here a graphic of the conduction of electrons electron through the crystal structure. Note that the transport or current is highly anisotropic.



Taken from Scientific American, Sept. 1995.

Summary

The main purpose of the project was to synthesize YBCO and ascertain is properties such as the oxygen content by analysis of the x-ray diffraction pattern. YBCO has a very complicated structure. Analysis of the XRD pattern revealed that oxygen content must be carefully controlled to obtain a single phase material. Precise control of the oxygen pressure is required. We propose to prepare samples under high oxygen pressure next time.

Acknowledgments

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