

YBa₂Cu₃O_{6+δ} : From Synthesis to Spectroscopy

An Interdisciplinary Approach to Research in High-Temperature Superconductivity

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Ongoing motivation for the investigation of YBCO: a material that has been discovered 30 years ago

1991: Discovery of superconductivity by *H. Kamerlingh Onnes*
1986: Discovery of high-T_c superconductivity in cuprates by *G. Bednorz and K. A. Müller* (NP 1987)

- The electronic structure of YBa₂Cu₃O_{6+δ} has been heavily debated for decades
- Much remains unclear in the understanding of its phase diagram.

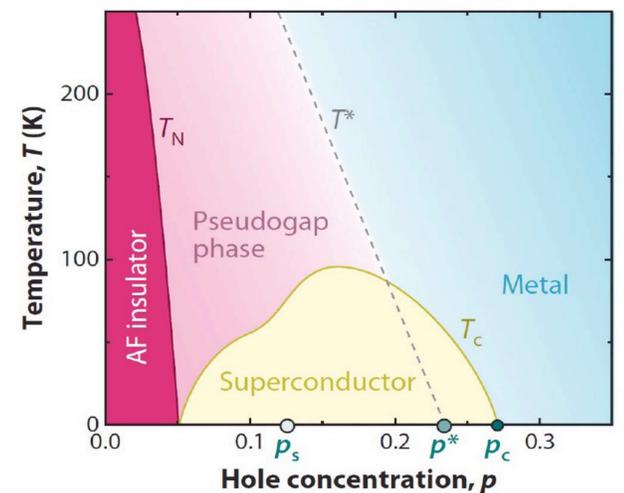
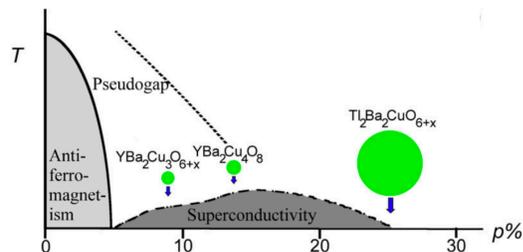
→ Pseudogap Phase

- Precursor to hidden ordered state with broken symmetry?
- Precursor to Mott insulator?

→ Fermi surface reconstruction

- Large in overdoped regime
- Small in underdoped regime

What are the causes of the reconstruction and what is its implication on high-T_c superconductivity? [1, 2]



Timeline and milestones

3 major steps:

(1) Self-flux crystal growth in crucibles

(2) Removal of twins

(3) Annealing in order to obtain specific doping

Crystal Growth

Detwinning

Annealing

- Best quality single crystals: self-flux method. SM: Y₂O₃ and a BaO–CuO melt
- Crucible material: BaZrO₃ or ZrO₂ crucibles. [3]

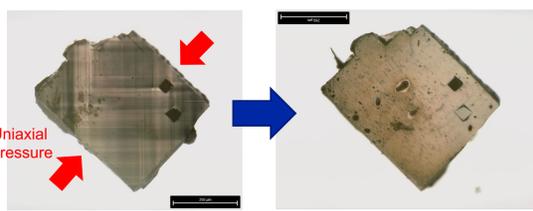
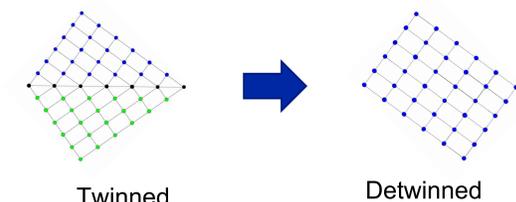


Current status

- Crystal growth of high-quality YBCO in ZrO₂ crucibles.
- Fabrication of BaZrO₃ crucibles.



- YBCO has orthorhombic structure → formation of structural domains “twinned”
- Detwinning procedure removes domain → monodomain sample “detwinned”
- Application of uniaxial pressure → 143 MPa at 250°C [4]

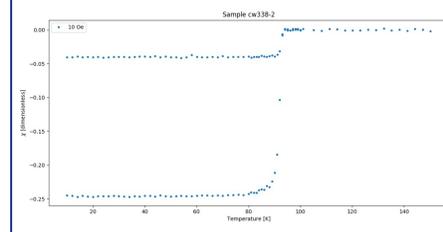


Superconductivity in YBCO emerges in the underdoped and optimally doped regimes

Oxygen annealing:

- control of the hole doping
- post crystal growth.

The exact hole doping can be verified by the T_c (SQUID) and the change of the unit cell parameter *c* (SXRD). [5]



End Product

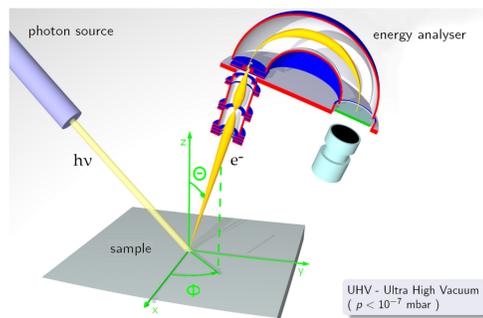
- Desired doping through annealing
- Twinned or detwinned

ARPES (Angle-resolved Photoemission Spectroscopy)

- Detailed information on band dispersion and Fermi surface
- Detection and measurement of the emitted photoelectrons at different emission angles

Research in YBCO:

Get an understanding of the Fermi surface reconstruction through the study of the three-dimensional electronic structure at different doping levels

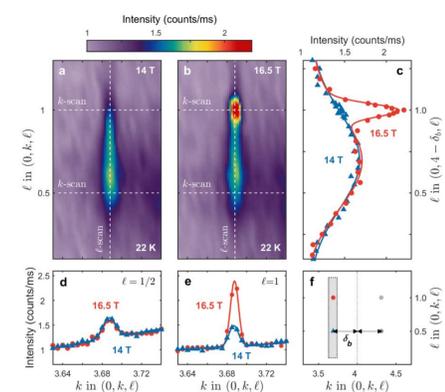
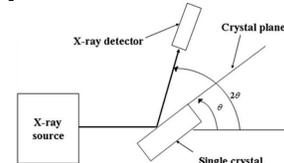


X-Ray Diffraction

- Working principle based on Bragg's law: $2d \sin \theta = n\lambda$
- Direct measurement of the structure

Research in YBCO:

Detection of charge density waves induced by field [5] and pressure [6]



Conclusion and outlook

The synthesis of high quality (pure and homogenous) single crystals is the crucial step for fundamental studies on the mechanism of superconductivity. We have successfully grown and detwinned high purity single crystals of optimally doped YBCO in ZrO₂ crucibles and will proceed with the growth in homemade BaZrO₃ crucibles. In a next step, we will tackle the annealing to obtain crystals in the underdoped regime. Meanwhile, spectroscopy experiments are in planning for 2020.

References

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- [2] M. Horio *et al.*, Phys. Rev. Lett. 2018, 121.
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