# EFFECT OF THE Cu–O–Cu BUCKLING ANGLE ON THE CRITICAL CURRENT DENSITY OF Y123

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**Abstract.** The relationship between the Cu(2)–O–Cu(2) bond angle (φ) in the $CuO_2$ planes and the critical current density ($J_c$) of the $YBa_2Cu_3O_{7-\delta}$ (Y123) superconductor is analysed. An expression for φ in terms of atomic coordinates and its uncertainty are given; for orthorhombic Y123, φ ≈ 164.7° (O(2)) and 164.9° (O(3)). A shift of 0.001 in the oxygen z-coordinate is shown to change φ by ≈ 0.7°. A 2 K decrease in $T_c$ is estimated to reduce the intergranular $J_c$ at 77 K by 17–21 %.

**Keywords:** $YBa_2Cu_3O_{7-\delta}$, $CuO_2$ plane, Cu–O–Cu bond angle, buckling, critical current density, Rietveld refinement, grain boundaries.

## Introduction

The practical value of Y123 is set not by its $T_c \approx 92$ K but by its critical current density at 77 K. While epitaxial films reach $J_c(77\ K) \sim 10^6$ A/cm$^2$, bulk ceramics typically do not exceed $10^2$–$10^3$ A/cm$^2$; this gap is attributed to intergranular weak links [3, 4].

The $CuO_2$ planes in Y123 are not flat: the O(2) and O(3) atoms are displaced towards the Y layer, while the Cu(2) atoms are displaced towards the Ba–O layer. As a result, the Cu(2)–O–Cu(2) angle is smaller than 180° and the plane is buckled (dimpled) [1].

The importance of buckling for superconductivity has been established experimentally: across the cuprate family, $T_{c,max}$ increases as buckling decreases [2]. Theoretically, this is linked to the overlap of the Cu $3d_{x^2-y^2}$ and O $2p_\sigma$ orbitals and to changes in the band parameter $t'/t$ [7, 8]. In addition, buckling enables linear coupling of the out-of-phase O(2)/O(3) $B_{1g}$ vibration (≈ 340 cm$^{-1}$) to the electrons [5].

While the effect of φ on $T_c$ has been widely studied, its effect on $J_c$ has not been assessed systematically. **The aim of this work** is to quantify the mechanisms by which the Cu–O–Cu bond angle affects $J_c$ and to define the requirements for determining φ by Rietveld refinement.

## Materials and methods

The object of analysis is orthorhombic (Pmmm) Y123 ceramics. Structural parameters are obtained by Rietveld refinement of X-ray diffraction patterns using FullProf [6]; neutron diffraction data were used for comparison [1]. The Cu(2)–O–Cu(2) angle is calculated from the c-axis offset between the Cu(2) and oxygen atoms, $\Delta z = z(O) - z(Cu2)$:

$$\varphi_{O(2)} = 180° - 2\cdot\arctan(2c\cdot\Delta z / a), \quad \varphi_{O(3)} = 180° - 2\cdot\arctan(2c\cdot\Delta z / b) \qquad (1)$$

where a, b and c are the lattice parameters and $\beta = (180° - \varphi)/2$ is the tilt (buckling) angle of each Cu–O bond out of the plane. The uncertainty in φ follows from the uncertainties in the z-coordinates:

$$\sigma_\varphi = [(4c/a) / (1 + (2c\cdot\Delta z/a)^2)]\cdot[\sigma_z^2(O) + \sigma_z^2(Cu2)]^{1/2} \qquad (2)$$

The critical current density is determined at 77 K either by the four-probe transport method with a 1 μV/cm criterion or from magnetic hysteresis using the Bean model [9]:

$$J_c = 20\cdot\Delta M / [a_s\cdot(1 - a_s/3b_s)] \qquad (3)$$

where ΔM is the width of the hysteresis loop (emu/cm$^3$) and $a_s < b_s$ are the sample cross-section dimensions (cm). The temperature dependence of $J_c$ was taken in the form

$$J_c(T) = J_c(0)\cdot(1 - T/T_c)^n \qquad (4)$$



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where n = 1 corresponds to tunnel-type (SIS) and n = 2 to metallic (SNS) weak links; for ceramics, typically n = 1.5–2.

**Results and discussion**

**1. Geometry of the bond angle.** For a near-$O_7$ composition with a = 3.82 Å, b = 3.89 Å, c = 11.68 Å, z(Cu2) ≈ 0.356 and z(O2) ≈ z(O3) ≈ 0.378, $c \cdot \Delta z \approx 0.257$ Å [1]. Equation (1) then gives $\beta \approx 7.7°$ and $\varphi_{O(2)} \approx 164.7°$, and $\beta \approx 7.5°$ and $\varphi_{O(3)} \approx 164.9°$. The $CuO_2$ plane is therefore bent by ≈ 15°, and the bending differs between the a and b directions.

**2. Precision requirements.** According to Eq. (2), a change of only 0.001 in the z-coordinate changes φ by ≈ 0.7°. Because oxygen scatters X-rays weakly, $\sigma_z(O) \approx 0.001–0.002$, giving an uncertainty in φ of ≈ 1°. Reliable detection of changes in φ of order 0.5° therefore requires high-angle ($2\theta > 100°$) data or neutron diffraction.

**3. The φ → $T_c$ → $J_c$ link.** Increased buckling (smaller φ) reduces the Cu $3d_{x^2-y^2}$–O $2p_\sigma$ overlap and lowers $T_{c,max}$ [2, 8]. Since the 77 K operating temperature is close to $T_c$, $J_c$ is highly sensitive to this change. Relative values calculated from Eq. (4) are given in Table 1.

Table 1

**Relative change in $J_c$(77 K) with decreasing $T_c$ (relative to $T_c$ = 92 K)**

| $T_c$, K | $J_c$(77 K)/$J_{c,92}$, n = 1.5 | $J_c$(77 K)/$J_{c,92}$, n = 2 |
|---|---|---|
| 92 | 1.000 | 1.000 |
| 91 | 0.917 | 0.890 |
| 90 | 0.834 | 0.785 |
| 89 | 0.752 | 0.684 |
| 88 | 0.671 | 0.588 |

Thus, a $T_c$ decrease of only 2 K reduces the intergranular $J_c$ by 17–21 %, and a 4 K decrease by 33–41 %. In other words, the relative sensitivity of $J_c$ to structural parameters is roughly an order of magnitude higher than that of $T_c$.

**4. Effect of grain boundaries.** The current across a grain boundary decreases as $J_{c,gb} = J_{c,g} \cdot \exp(-\theta/\theta_0)$, with $\theta_0 \approx 4–5°$ [3]. Mechanical strain and oxygen deficiency near the boundary increase local buckling. This widens the layer of suppressed order parameter and strengthens weak-link behaviour. Conversely, nanoscale fluctuations of φ within the grains may act as $\delta T_c$-type pinning centres.

**5. Upper-limit estimate.** The depairing current density

$$J_d = \Phi_0 / (3\sqrt{3} \cdot \pi \cdot \mu_0 \cdot \lambda^2 \cdot \xi) \quad (5)$$

gives $\approx 3 \cdot 10^8$ A/cm$^2$ for λ ≈ 150 nm and ξ ≈ 1.5 nm. Since $\lambda^{-2}$ is proportional to the superfluid density, flattening of the planes (φ → 180°) is also expected to raise $J_d$. The actual $J_c$ of ceramics lies 5–6 orders of magnitude below this limit, so the main reserve lies in the intergranular connections.

**6. Rapid characterisation.** The frequency and Fano asymmetry of the $B_{1g}$ Raman mode (≈ 340 cm$^{-1}$) directly reflect the degree of buckling [5]. Raman spectroscopy combined with Rietveld refinement is therefore proposed as a non-destructive means of monitoring φ and $J_c$.

**Conclusions**

1. In Y123 the Cu(2)–O–Cu(2) angle is ≈ 164.7° (O(2)) and ≈ 164.9° (O(3)); the $CuO_2$-plane buckling angle is ≈ 7.5–7.7°.


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2. Determining φ to within 0.5° requires the oxygen z-coordinate to be refined to better than ±0.0005, which calls for high-angle X-ray or neutron diffraction data.

3. A decrease in φ lowers $T_c$, which at 77 K sharply reduces $J_c$: a 2 K drop in $T_c$ lowers $J_c$ by 17–21 %.

4. Local buckling at grain boundaries strengthens weak-link behaviour; processing factors that flatten the $CuO_2$ planes (full oxygenation, cation substitution, texturing) offer a promising route to higher $J_c$.

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