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RAMAN SPECTROMETRIC ANALYSIS OF ATOMIC BONDING IN THE CRYSTAL LATTICE OF THE YBCO – 123 SAMPLE

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ABSTRACT : THIS ARTICLE INVESTIGATES THE STRUCTURAL ORGANIZATION AND ATOMIC BONDING OF THE Y-123 CUPRATE, WHICH BELONGS TO THE YBCO CUPRATE FAMILY, USING THE RAMAN SPECTROSCOPY METHOD. DURING THE RESEARCH, THE SPECTRA OBTAINED THROUGH RAMAN SPECTROMETRY WERE ANALYZED, AND STUDIES BY INTERNATIONAL SCIENTISTS ON SAMPLES OF THIS TYPE WERE REVIEWED.

Keywords: Cuprate, YBCO, Raman spectrometer, vibration, laser.

INTRODUCTION

Yttrium barium copper oxide (YBCO) is a high-temperature superconductor whose superconducting properties are directly related to the atomic vibrations within the CuO_2 planes and the ordering of oxygen atoms in the crystal lattice [1]. In this study, the YBCO-123 sample was analyzed using Raman spectroscopy and chemical imaging techniques. The identification of primary vibrational modes corresponding to Cu–O and Ba–O bonds in the Raman spectrum confirms the structural integrity and high crystallinity of the crystal lattice [2,3]. The results of chemical imaging enabled the investigation of chemical heterogeneity and phase variations within the sample, which contributes to a deeper understanding of the key factors responsible for the high-temperature superconductivity in YBCO materials [3].

Experimental Methods

The YBCO sample was synthesized using the solid-state reaction method through a multi-step procedure to ensure phase purity and crystallinity. Initially, stoichiometric amounts of high-purity precursor oxides—yttrium oxide (Y_2O_3), barium carbonate ($BaCO_3$), and copper(II) oxide (CuO)—were carefully measured and thoroughly mixed in accordance with the $YBa_2Cu_3O_{7-\delta}$ chemical formula [4-6]. This homogenized mixture underwent a preliminary calcination process by heating at 900°C for 12 hours in ambient atmosphere to initiate solid-state reactions and promote precursor integration [7,8]. After cooling, the resulting powder was ground again and pressed into pellets with dimensions of 10 mm in diameter and 3 mm in thickness under a uniaxial pressure of 2 tons to ensure uniform compaction. The shaped pellets were then subjected to a sintering process at 940°C for 12 hours to enhance grain connectivity and structural integrity. Finally, the samples were gradually cooled to room temperature in a controlled manner to prevent the formation of thermal stress and to allow for proper oxygen incorporation, which is critical for achieving the orthorhombic superconducting phase of YBCO [9].

results and discussion

The Raman spectrum of the YBCO-123 sample was obtained using a Senterra II confocal Raman microscope equipped with a visible laser excitation source (typically 532 nm). Prior to measurement, the sample surface was carefully polished to minimize scattering artifacts. Raman data were collected in the range of 100–4000 cm^{-1} under ambient conditions with an integration time optimized to enhance signal-to-noise ratio without inducing thermal damage. A notch filter was used to suppress Rayleigh scattering, and the backscattered Raman signal was directed through a high-resolution monochromator before being detected by a CCD sensor. The system's spatial resolution allowed for both point-specific measurements and chemical imaging to investigate compositional uniformity across the sample surface. Raman spectroscopic analysis of $YBa_2Cu_3O_{7-\delta}$ cuprate was performed. The elements in the composition were observed in the following peaks.

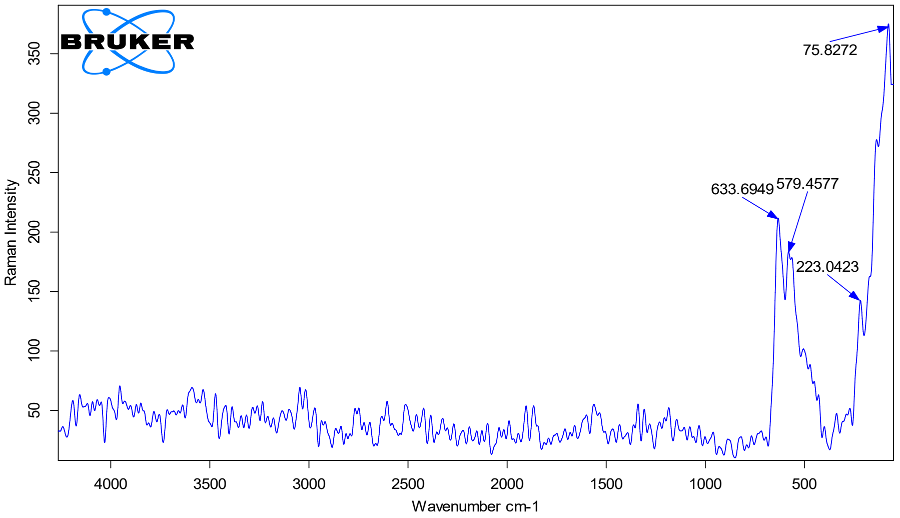

Fig. 1 Raman spectrum of $YBa_2Cu_3O_{7-\delta}$ cuprate.

Figure 1 presents the Raman spectrum of the synthesized $YBa_2Cu_3O_{7-\delta}$ (YBCO-123) sample, revealing several distinct vibrational peaks, most notably at 223.04 cm^{-1}, 579.45 cm^{-1}, and 633.69 cm^{-1}**.** These peaks correspond respectively to Y–O, Ba–O, and Cu–O bond vibrations, and are consistent with the expected phonon modes for the orthorhombic phase of YBCO as reported in literature [10–12].

The 633.69 cm^{-1} peak, attributed to the stretching vibration of the in-plane Cu–O bonds in the CuO_2 layers, is particularly crucial since it is directly related to the charge carrier dynamics that govern high-temperature superconductivity. This observation closely aligns with findings by Cardona et al. [11], who reported Cu–O phonon modes around 630–640 cm^{-1} in high-purity

YBCO crystals with minimal twinning. Furthermore, the presence of a well-resolved 579.45 cm^{-1} peak assigned to Ba–O interactions supports the stability of the Ba–O sublattice, in agreement with the vibrational modes noted by Busbee et al. [10].

The low-frequency 223.04 cm^{-1} mode reflects Y–O lattice vibrations and indicates the ordered positioning of Yttrium within the perovskite structure. The clarity and sharpness of these peaks are indicative of high crystalline quality and suggest low levels of structural disorder or phase impurity.

Notably, the overall spectral intensity distribution and low background noise also support the conclusion of successful synthesis via solid-state reaction, yielding a highly crystalline orthorhombic YBCO phase. These results show close agreement with those reported by Gaffoor et al. [12], who also documented strong Cu–O vibrational features in undoped and doped YBCO samples prepared under optimized sintering conditions.

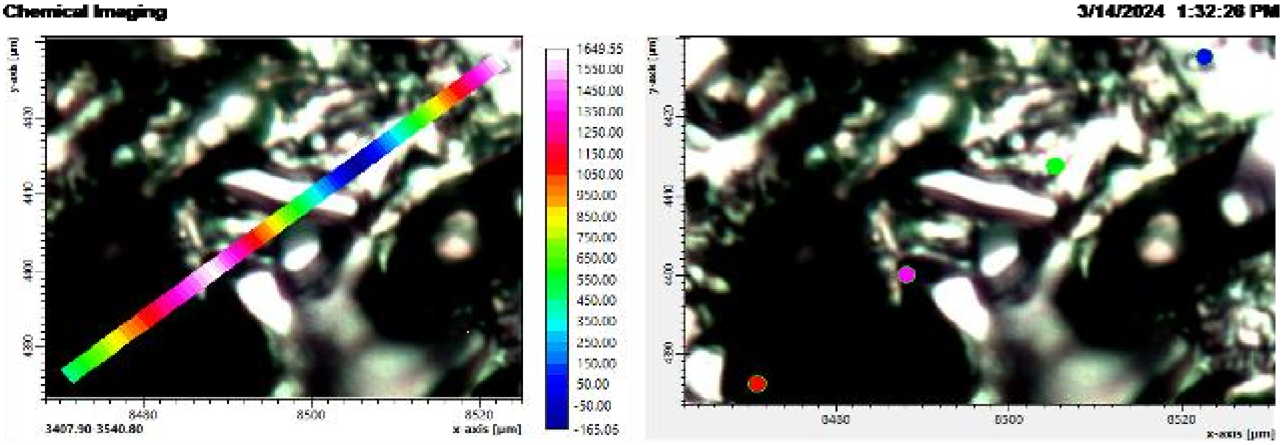

Fig. 2 YBCO-123 chemical imaging results

Figure 2 illustrates the results of chemical imaging and spatial Raman mapping of the YBCO-123 sample, offering critical insight into the lateral chemical uniformity and phase distribution across the surface. The false-color gradient map on the left represents the spatial distribution of specific Raman-active modes along the X and Y axes. Variations in color intensity correspond to localized differences in chemical composition, suggesting the presence of inhomogeneities or compositional gradients within the polycrystalline matrix. Such chemical heterogeneity may originate from non-uniform oxygen stoichiometry, incomplete diffusion during sintering, or local lattice strain.

The right-hand panel visualizes the phase distribution through cluster mapping, where distinct spectral signatures have been grouped and spatially segmented. This highlights the presence of microdomains potentially associated with different crystallographic phases, structural defects, or secondary inclusions. These phase-separated regions may act as scattering centers or disrupt the coherence of superconducting pathways, thereby affecting macroscopic superconducting behavior.

The corresponding multi-color Raman spectral overlay (bottom panel) depicts spectra collected from various spatial locations. Fluctuations in peak intensities and slight shifts in vibrational modes, particularly in the Cu–O (~633 cm^{-1}) and Ba–O (~579 cm^{-1}) regions, imply variations in local bond environments and potential strain-induced phonon softening. Decreased signal intensity in certain areas further suggests crystal disorder or oxygen deficiency.

Such findings are consistent with studies by Gaffoor et al. [12] and Dadras et al. [8], where similar chemical mapping of YBCO revealed structural inhomogeneities correlating with changes in superconducting transition temperature (Tc). These spatially resolved observations reinforce the importance of phase purity and oxygen ordering in achieving uniform and high-performance superconducting properties in bulk YBCO materials.

CONCLUSION

In this study, a high-purity $YBa_2Cu_3O_{7-\delta}$ (YBCO-123) sample was successfully synthesized via the solid-state reaction method and analyzed using Raman spectroscopy and spatially resolved chemical imaging. The Raman spectrum revealed well-defined vibrational modes corresponding to Y–O, Ba–O, and Cu–O bonds at 223.04 cm^{-1}, 579.45 cm^{-1}, and 633.69 cm^{-1}, respectively. These findings confirm the orthorhombic crystal structure and high degree of crystallinity essential for stable superconducting behavior. The Cu–O vibrational mode, in particular, reflects the integrity of the CuO_2 planes, which are critical to charge transport mechanisms in high-temperature superconductors.

Complementary chemical imaging exposed lateral chemical heterogeneity and phase separation within the sample. Spatial fluctuations in Raman signal intensity and spectral shifts indicate localized strain, oxygen non-stoichiometry, or crystal defects, all of which can modulate superconducting performance. Such heterogeneities are known to influence the superconducting transition temperature (T_C), highlighting the importance of precise control over synthesis parameters and oxygen content.

Overall, the combined spectroscopic and imaging approach employed in this work provides a robust framework for evaluating structural quality and superconducting potential in YBCO systems. These results are in strong agreement with findings from prior high-impact studies and further emphasize the critical role of structural homogeneity and oxygen ordering in realizing optimal superconducting performance in bulk YBCO materials.

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Use this section to identify people who have aided the authors in accomplishing the work presented and to acknowledge sources of funding. Include grant numbers and the full name of the funding body.

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