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Research Article

Thermoanalytical Evaluation of YBCO Superconductors via Energy-Reaction Index (ERI)

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Abstract – The thermochemical efficiency and phase evolution of $YBa_2Cu_3O_{7-\delta}$ (Y123) and $Y_3Ba_5Cu_8O_{18}$ (Y358) superconductors were investigated using differential thermal analysis (DTA). To provide a complementary metric to conventional conversion-factor (CF) methods, an Energy–Reaction Index (ERI) was introduced and applied to quantify the balance between exothermic and endothermic contributions during synthesis. The DTA profiles exhibited a single sharp exothermic peak for Y123 near 940 °C and multiple broader peaks for Y358 between 850 °C and 970 °C, indicating distinct formation kinetics. The calculated ERI values (1.84 for Y123 and 1.29 for Y358) revealed that Y123 undergoes a more complete and thermochemically efficient reaction process, while Y358 experiences distributed energy release associated with multi-step crystallization. Segmental ERI analysis across temperature intervals confirmed the kinetic limitation of Y358 and the progressive energy coherence of Y123. The findings demonstrate that ERI is a reliable and straightforward tool for evaluating reaction completeness and energy utilization in complex oxide superconductors. This approach can assist in optimizing heat-treatment schedules, oxygen partial pressure control, and precursor ratios for future YBCO-based materials.

Keywords: YBCO, Y123, Y358, Differential Thermal Analysis (DTA), Energy–Reaction Index (ERI), Thermochemical Efficiency.

I. INTRODUCTION

The discovery of $YBa_2Cu_3O_{7-\delta}$ (Y123) by Chu et al. in 1987 marked a significant milestone in the development of (Type-II) high-temperature superconductivity, with a critical temperature (Tc) approaching 93 K [1]. Following this breakthrough, numerous members of the Y–Ba–Cu–O (YBCO) system were explored to achieve improved superconducting performance and structural stability.

The most recently added superconducting member of this family, $Y_3Ba_5Cu_8O_{18}$ (Y358), exhibits a Tc higher than 100 K and possesses a more complex crystal structure with five CuO_2 planes and three Cu–O chains [2].

These two phases, Y123 and Y358, share similar perovskite-based frameworks but differ significantly in their lattice parameters, oxygen ordering, and phase formation dynamics. The Y123 phase contains two CuO_2 planes and one Cu–O chain, while Y358 has five and three, respectively, leading to an extended c-

axis and modified thermochemical properties [3,4]. This structural anisotropy strongly affects the oxygen diffusion kinetics, hole concentration, and ultimately the superconducting transition temperature, as discussed by Tallon and Loram [4].
Murakami [5] demonstrated that such structural variations also influence the energy flow and phase stability during sintering and peritectic transformation. Building on this, Düzgün [3] investigated the lattice strains and crystallite size distributions of Y123 and Y358, reporting that Y358 tends to form larger crystallites with higher strain energy. In another recent work, the same author critically analysed the limitations of the *conversion factor (CF)* approach used in the stoichiometric design of oxide superconductors, emphasizing that CF-based calculations may fail when oxygen nonstoichiometric and volatilization dominate [6].
To address these shortcomings, the present study introduces a novel thermochemical parameter the Energy–Reaction Index (ERI) derived from Differential Thermal Analysis (DTA) data of Y123 and Y358 samples. This semi-empirical index quantifies the relationship between exothermic and endothermic enthalpy changes to assess the energetic efficiency and reaction completeness of YBCO synthesis. By integrating experimental DTA profiles and previous structural findings, the proposed ERI provides a new perspective that links phase evolution with energy utilization, complementing conventional CF-based evaluations [1-6].

II. MATERIALS AND METHOD

Bulk samples of $YBa_2Cu_3O_{7-\delta}$ (Y123) and $Y_3Ba_5Cu_8O_{18}$ (Y358) superconductors were synthesized via the conventional solid-state reaction method. High-purity Y_2O_3 (99.99%), $BaCO_3$ (99.99%), and CuO (99.99%) powders were used as starting materials. Stoichiometric proportions were carefully calculated for each composition and thoroughly mixed in an agate mortar with ethanol as a dispersing medium. The resulting mixtures were calcined at 900 °C for 24 hours with two intermediate grindings to ensure homogeneity, followed by final sintering between 940 °C and 950 °C under ambient conditions. The synthesis procedure was designed according to standard YBCO preparation protocols described by Kuppusami and Raghunathan [7] and Murakami [8], while the stoichiometric ratios followed the author's previous methodology [3,6].
Differential Thermal Analysis (DTA) was performed using a heating rate of 10 °C/min from room temperature up to approximately 1000 °C under atmospheric air. The DTA curves of Y123 and Y358 were baseline-corrected to eliminate instrumental drift. The exothermic and endothermic regions were numerically integrated using commercial software to determine the relative enthalpy changes (in arbitrary units). Each thermogram revealed characteristic transitions: Y123 exhibited a single sharp exothermic event corresponding to its peritectic transformation, whereas Y358 showed multiple broadened exothermic peaks, indicative of sequential oxygen incorporation and complex phase evolution.
To evaluate the thermochemical reaction efficiency, a new semi-empirical parameter the Energy–Reaction Index (ERI) was proposed. It was defined as:

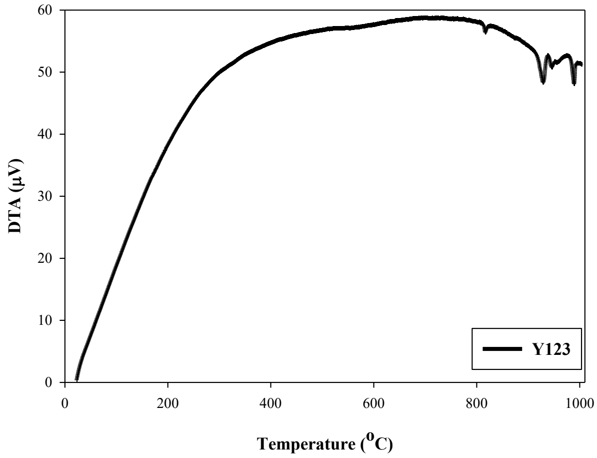
$$ERI = \frac{A_{exo}}{A_{endo}+\epsilon} \qquad (1)$$

where A_{exo} and A_{endo} represent the integrated exothermic and endothermic areas, respectively, and ϵ is a small correction factor accounting for instrumental noise and baseline uncertainty. The parameter reflects the ratio of released to absorbed energy during solid-state reaction and serves as a direct indicator of reaction completeness. High ERI values imply more efficient phase formation and oxygen diffusion, whereas low values correspond to incomplete reaction and poor structural ordering.
For detailed comparison, each DTA profile was segmented into three distinct temperature intervals:
(a) 25–400 °C – dehydration and carbonate decomposition,
(b) 400–900 °C – solid-state reactions and phase nucleation,
(c) 900–1000 °C – peritectic reaction and possible melting.
This classification follows the approach proposed by Kuppusami [7], correlating thermal events with oxygen diffusion and grain growth. The total integrated energy of each region was normalized with

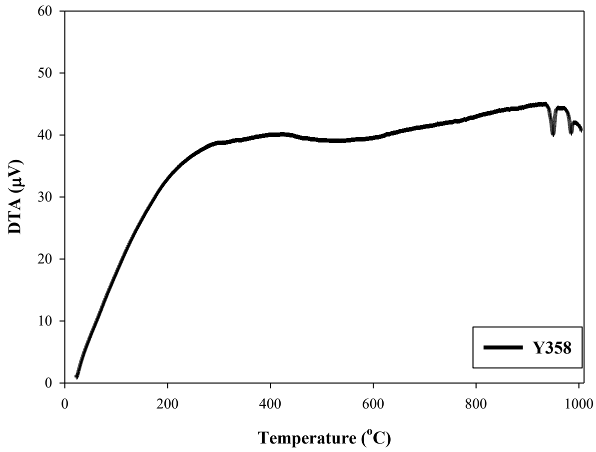
respect to the full curve area, enabling a relative comparison between the two YBCO compositions. All calculations and curve fittings were carried out using commercial software.

III. RESULTS AND DISCUSSION

Fig. 1 shows the DTA profiles of $YBa_2Cu_3O_{7-\delta}$ (Y123) and $Y_3Ba_5Cu_8O_{18}$ (Y358) superconductors. Both samples exhibit distinct thermal features reflecting their structural and compositional differences. For the Y123 compound, a single sharp exothermic peak appears around 940 °C, corresponding to its peritectic reaction and phase formation. In contrast, the Y358 curve displays multiple, broader exothermic regions between 850 °C and 970 °C, indicating a multi-step formation process involving partial melting and oxygen incorporation.



(a)



(b)

Fig. 1. DTA graphs : (a) Y123 sample (b) Y358 sample

These observations are consistent with the findings of Düzgün [3], who reported that Y358 exhibits larger crystallite size and higher lattice strain due to its extended c-axis and multi-planar structure. The broader exothermic peaks of Y358 suggest slower phase stabilization and distributed enthalpy release, typical for complex layered cuprates. Murakami [5] similarly highlighted that such broadened DTA peaks often result from incomplete diffusion driven reactions in bulk superconductors.

To quantify the relative energy efficiency of these thermal processes, the Energy–Reaction Index (ERI) was calculated using the integrated exothermic and endothermic areas from each DTA curve. Table 1 presents the normalized results. The Y123 sample yielded an ERI value of 1.84, while the Y358 sample exhibited a lower value of 1.29. This indicates that the Y123 reaction pathway is thermochemically more efficient, releasing a higher proportion of exothermic energy relative to endothermic absorption.

Table 1. Comparative ERI values derived from DTA data of Y123 and Y358 superconductors

Sample	A_{exo} (arb. units)	A_{endo} (arb. units)	ERI
Y123	3.69	2.00	1.84
Y358	3.10	2.40	1.29

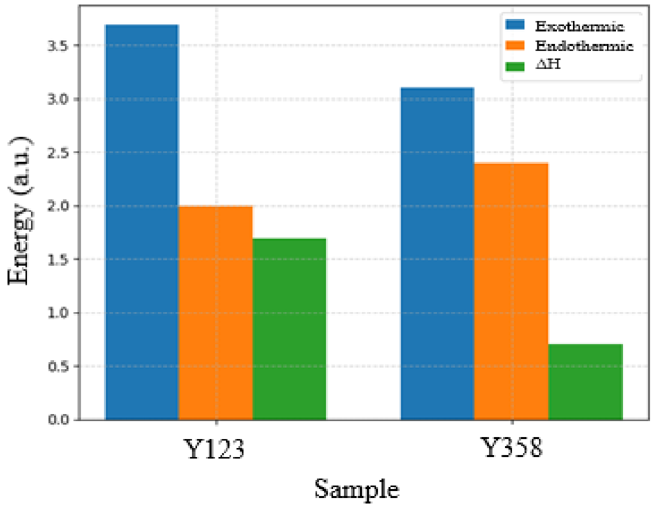


Fig. 2. Enthalpy Difference (ΔH) Comparison

To visualize the overall thermochemical energy behaviour, the total exothermic and endothermic areas of each compound were compared as shown in Figure 2. The calculated enthalpy difference ($\Delta H = A_{exo} - A_{endo}$) represents the net released energy during the synthesis reaction. Y123 exhibited a higher ΔH value of 1.69 a.u., whereas Y358 showed a smaller difference of 0.70 a.u. The higher ΔH for Y123 confirms its more exothermic and energetically favourable formation route, consistent with its sharper DTA peak and higher ERI value.

The higher ERI for Y123 suggests a more complete reaction and better phase homogeneity, consistent with its well-defined peritectic transition. In Y358, the lower ERI indicates partial reaction completion, possibly due to oxygen vacancies or incomplete rearrangement of Cu–O chains. The presence of multiple exothermic peaks reflects overlapping sub-reactions related to the formation of intermediate oxygen-deficient phases.

This behaviour supports the idea that the Y358 phase requires finer control of stoichiometry and oxygen partial pressure to achieve full crystallization.

To further analyse the temperature-dependent reaction dynamics, the DTA curves were segmented into three characteristic regions. The integrated exothermic and endothermic areas within each range were used to compute a partial Energy–Reaction Index (ERI) for both samples, as summarized in Table 2.

Table 2. Segmental ERI across Temperature Intervals

Temperature Interval (°C)	Y123	Y358
25-400	0.94	0.78
400-900	1.20	1.02
900-1000	1.84	1.29

These results demonstrate that the Y123 sample exhibits a steady increase in ERI with temperature, suggesting progressive enhancement of thermochemical efficiency toward its peritectic reaction near 940 °C. In contrast, Y358 shows smaller incremental gains, reflecting incomplete energy release and phase overlap during its multi-step crystallization. This comparison confirms that Y123 follows a more thermodynamically efficient reaction pathway than Y358.

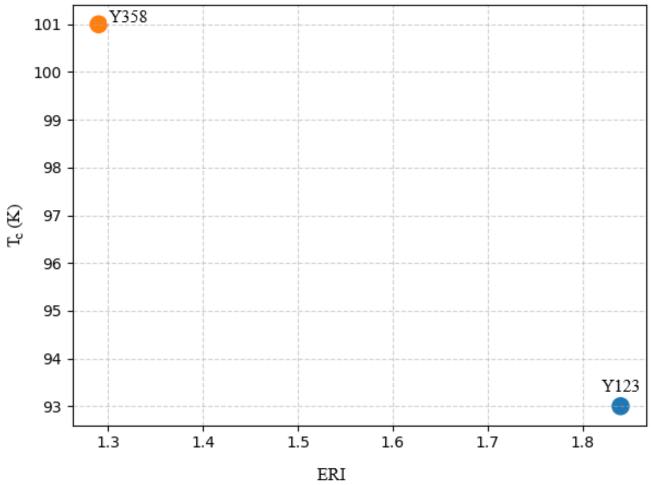


Fig. 3. Correlation between ERI and T_c

Figure 3 shows the relationship between the Energy–Reaction Index (ERI) and the superconducting transition temperature (T_c). A general positive correlation can be observed; however, the slightly higher Tc of Y358 despite its lower ERI suggests that kinetic factors and oxygen stoichiometry may dominate over thermochemical efficiency in determining superconducting performance.

In summary, the Energy–Reaction Index provides a simple yet powerful tool to evaluate thermochemical efficiency in complex oxide superconductors. By integrating energetic and structural information, ERI complements the traditional conversion-factor (CF) method [6] and offers a new approach for assessing reaction completeness in multi-phase YBCO systems. These findings may guide optimization of heat-treatment protocols and precursor ratios for advanced superconducting materials.

Fig. 4. Schematic representation of the energy flow and phase evolution in YBCO superconductors.

Y123 follows a single-step peritectic formation path with high thermochemical efficiency, whereas Y358 undergoes multiple intermediate reactions with distributed energy release, reflecting its more complex phase structure. The schematic in Figure 4 highlights the fundamental difference in energy utilization during synthesis. Y123 achieves complete structural conversion through a dominant exothermic process, while Y358 exhibits sequential sub-reactions associated with partial oxygen incorporation and local energy losses. This conceptual model provides a visual framework for interpreting DTA-derived energetic parameters and their link to phase stability in complex YBCO systems.

IV. CONCLUSION

In this study, the thermochemical characteristics of $YBa_2Cu_3O_{7-\delta}$ (Y123) and $Y_3Ba_5Cu_8O_{18}$ (Y358) superconductors were comparatively evaluated using differential thermal analysis (DTA). The Energy–Reaction Index (ERI) was introduced as a complementary parameter to traditional conversion factor methods for assessing energy efficiency and reaction completeness during synthesis.

The DTA and ERI results consistently revealed that Y123 undergoes a single-step peritectic reaction around 940 °C, corresponding to a sharp exothermic peak and higher thermochemical efficiency (ERI = 1.84). In contrast, Y358 exhibits a multi-step reaction sequence with distributed exothermic behaviour and a lower ERI (1.29), indicating incomplete phase formation and partial oxygen incorporation.

Segmental ERI analysis across temperature intervals confirmed that Y123 maintains a steady increase in energy efficiency with temperature, while Y358 remains kinetically limited due to its complex layered structure. The schematic energy flow model further visualized this distinction, demonstrating that Y123 achieves efficient, single-step crystallization, whereas Y358 follows a multi-step diffusion-limited mechanism.

Overall, the proposed ERI framework provides a simple yet effective thermodynamic indicator for evaluating phase formation pathways in complex oxide superconductors. This approach may serve as a useful guideline for optimizing synthesis routes, oxygen control, and heat-treatment parameters in future high-temperature superconducting materials.

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