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Zirconia-Based Ceramics: Bridging Aesthetics and Functionality[☆]

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Abstract:
Zirconia-based materials have a wide range of applications, determined by their exceptional mechanical, chemical, electrical, and biological properties. Thus, zirconia (ZrO_2) ceramics are extensively used in dental restorations including crowns, bridges, implants, and abutments due to their high strength, fracture resistance, durability, and biocompatibility. Also, zirconia exhibits high ionic conductivity, making it suitable for solid oxide fuel cells and sensors. Moreover, due to their catalytic and reactive properties, zirconia-based nanomaterials are used as catalysts and adsorbents.

Keywords: zirconia, doping, properties, applications

1. INTRODUCTION

Zirconia (ZrO_2) is a versatile ceramic material whose properties and applications are deeply influenced by its crystalline structure, which can exist in several phases: monoclinic, tetragonal, and cubic.

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The interplay between these phases, the stabilization mechanisms, and the resulting mechanical, optical, and thermal properties make zirconia indispensable in fields ranging from dentistry to aerospace and energy [1].

Zirconia exhibits polymorphism, different crystalline structures depending on temperature and composition being evidenced. At room temperature, pure zirconia is monoclinic, but above 1170 °C it transforms to tetragonal, and above 2370 °C to cubic. The monoclinic phase is brittle and prone to cracking, while the tetragonal and cubic phases are more stable and mechanically robust [2]. Properties associated with different crystalline forms of zirconia and their applications will be presented in this study.

2. MONOCLINIC ZIRCONIA

Among zirconia polymorph, the monoclinic phase (space group $P2_1/c$) is thermodynamically stable at room temperature and ambient pressure. Upon heating at temperatures higher than ~1170 °C, it transforms into the tetragonal phase, accompanied by a volume contraction of about 4–5%, while a further heating above ~2370 °C, into the cubic phase. The reverse $t \rightarrow m$ transformation occurring upon cooling, involves a volume expansion of the same magnitude [3].

Monoclinic zirconia exhibits moderate hardness and elastic modulus compared to stabilized tetragonal or cubic zirconia. Its Vickers hardness typically lies in the range of 9–11 GPa, while the Young's modulus is around 200–210 GPa. However, its fracture toughness is relatively low (≈2–3 $\mathrm{MPa \cdot m^{1/2}}$), reflecting its brittle nature. Its low thermal conductivity (~2.0 $\mathrm{W \cdot m^{-1} \cdot K^{-1}}$) makes it suitable as a thermal barrier material or insulating additive in composite ceramics [4].

Monoclinic zirconia is chemically inert and resistant to most acids, alkalis, and molten metals, except under highly reducing conditions where Zr^{4+} may be partially reduced to Zr^{3+}. It is widely used as a protective and corrosion-resistant material in environments such as chemical reactors, crucibles, and refractory linings [5].

In terms of electrical behavior, *m*-ZrO_2 is a wide-band-gap insulator (E_g ≈ 5.0–5.5 eV), with very low electronic and ionic conductivity at room temperature. The electrical conductivity of sintered monoclinic ZrO_2, measured in the high temperature using electrical impedance spectroscopy (EIS), was 3.2×10^{-5} S/cm and 4.4×10−5 s/cm at 900 °C, for 80% and 89% TD, respectively [6]. In recent years, monoclinic zirconia has attracted attention in the field of heterogeneous catalysis and surface science [7].

Monoclinic zirconia serves as a support material for catalysts (e.g., Pt, Pd, Cu, or Ni nanoparticles), improving dispersion and thermal stability. It also participates directly in acid–base-catalyzed reactions, such as aldol condensation, Fischer–Tropsch synthesis, and transesterification [8].

Optically, monoclinic zirconia is opaque and white due to its polycrystalline nature and the strong scattering of light at grain boundaries and microcracks.

3. TETRAGONAL ZIRCONIA

In pure zirconia, at ambient pressure, the tetragonal phase (space group $P4_2/nmc$) is stable between approximately 1170 °C and 2370 °C. However, tetragonal phase is metastable, being retained at room temperature by stabilizers, the commonly used one being yttria. This phase exhibits superior mechanical properties due to transformation toughening behavior. The tetragonal phase enables zirconia to have both high strength and toughness, which is rare in ceramics [9].

In terms of electrical behavior, it is a poor electronic conductor but can act as an oxygen-ion conductor when partially stabilized. Oxygen vacancies introduced by dopants enable ionic mobility, which is exploited in oxygen sensors and fuel cell components [10].

Unlike cubic zirconia, which is fully transparent and isotropic, the tetragonal phase exhibits birefringence due to its anisotropic lattice, influencing light scattering and color perception [11].

4. CUBIC ZIRCONIA

Among the three primary polymorphs of zirconia, the cubic phase (fluorite-type, space group *Fm-3m*) is stable at temperatures above ~2370 °C. However, by substituting Zr^{4+} with lower-valent cations such as Y^{3+}, Ca^{2+}, or Ce^{4+}, oxygen vacancies are introduced to preserve charge neutrality, stabilizing the cubic phase at room temperature.

Stabilized cubic zirconia has emerged as a multifunctional material, simultaneously appreciated for its optical brilliance and technological performance (in fuel cells, oxygen sensors, and thermal barrier coatings) [12]. Cubic zirconia is notable for its low thermal conductivity (2.0–2.5 $W \cdot m^{-1} \cdot K^{-1}$). Its thermal expansion coefficient (~10.5×10^{-6} K^{-1}) and phase stability up to 2400 °C make it highly suitable for aerospace and turbine applications.

In addition, stabilized cubic zirconia demonstrates remarkable thermal shock resistance and chemical inertness even in oxidizing and corrosive atmospheres, contributing to its widespread use in refractory linings and furnace components. Cubic zirconia exhibit high oxygen-ion conductivity at elevated temperatures. Oxygen-ion conductivity is about 0.1–1.0 $S \cdot cm^{-1}$ at 1000 °C (depending on dopant type), with an activation energy for ion migration in the range 0.9–1.2 eV [13].

The combination of aesthetic and functional attributes is rooted in its unique crystal structure, which directly governs ionic mobility, thermal properties, and optical behavior.

5. CONCLUSION

Zirconia-based ceramics exhibit a unique interplay between structure, composition, and property. The monoclinic phase contributes stability and chemical durability, the tetragonal phase ensures strength and toughness, while the cubic phase provides conductivity and optical brilliance. Through judicious dopant selection and microstructural control, these phases can be stabilized or combined to meet a wide array of technological and aesthetic demands. Zirconia is thus a multifunctional material, bridging the gap between artistic design and engineering performance.

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