Research Article

Low thermal conductivity and anisotropic thermal expansion of ferroelastic $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ ceramics

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Abstract: In this paper, $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ ceramics have been fabricated by solid-phase synthesis reaction. Each sample was found to crystallize in a monoclinic phase by X-ray diffraction (XRD). The properties of $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ were optimized by adjusting the ratio of Gd/Y. $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ had a low high-temperature thermal conductivity (1.37–2.05 W·m$^{-1}$·K$^{-1}$), which was regulated by lattice imperfections. The phase transition temperature of the $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ ceramics was higher than 1500 °C. Moreover, the linear thermal expansion coefficients (TECs) were 10.5×10$^{-6}$ K$^{-1}$ (1200 °C), which was not inferior to yttria-stabilized zirconia (YSZ) (11×10$^{-6}$ K$^{-1}$, 1200 °C). $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ had anisotropic thermal expansion. Therefore, controlling preferred orientation could minimize the TEC mismatch when $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ coatings were deposited on different substrates as thermal barrier coatings (TBCs). Based on their excellent properties, it is believed that the $(\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4$ ceramics will become the next generation of high-temperature thermal protective coatings.

Keywords: thermal barrier coatings (TBCs); thermal conductivity; high-temperature phase stability; high-temperature X-ray diffraction (XRD); anisotropic thermal expansion

1 Introduction

Thermal barrier coatings (TBCs) are regarded as components of diesel generators, aero-engines, and high-speed aircraft for improved efficiency and power [1,2]. At present, the most widely used TBC material is 6–8 wt% yttria-stabilized zirconia (YSZ). High thermal expansion coefficients (TECs) (11×10$^{-6}$ K$^{-1}$, 1200 °C) and ferroelastic toughening effect of YSZ are the main reasons for its wide application [3–5].

Nevertheless, if the use temperature is higher than 1200 °C, YSZ will undergo a phase transition. The t’ (metal-stable tetragonal)-phase YSZ will become the tetragonal (t) phase and the monoclinic (m) phase, such that the phase transition can be accompanied by a small bulk expansion and lead to material failure [3]. Therefore, much effort has been devoted to exploring novel TBCs, such as rare-earth (RE) zirconates, cerium oxides, phosphates, and silicates [6–11]. The above materials have lower fracture toughness compared to YSZ, which is important for TBCs operating in high-temperature environments. Consequently, we need to look for a new material similar to YSZ with ferroelastic...
toughening mechanism and high fracture toughness.

Our previous research [12–16] found that tantalate ceramics had good properties and can be further optimized and used as TBCs. The investigation of thermal conductivity of YSZ found that the difference of valence between doping ions Y\(^{3+}\) and Zr\(^{4+}\) would produce high concentrations of lattice defects, resulting in enhanced phonon scattering and reduced thermal conductivity [17–20]. Feng et al. [21] and Shian et al. [22] reported that the ferroelastic toughening mechanism of yttrium tantalate was similar to that of YSZ. Wang et al. [23] reported that the thermal conductivity of YTaO\(_4\) ceramics was 1.4 W·m\(^{-1}\)·K\(^{-1}\) (800 °C). Yang and Ye [24] reported that the TECs of GdTaO\(_4\) exceed 14×10\(^{-6}\) K\(^{-1}\) (1350 °C). Wu et al. [25] obtained the lowest thermal conductivity (1.7 W·m\(^{-1}\)·K\(^{-1}\) at 900 °C) of (Y\(_{1-x}\)Dy\(_x\))TaO\(_4\) by doping. The YTaO\(_4\) and GdTaO\(_4\) ceramics with the m phase possess ferroelastic transformation and excellent performance. The structure of the materials determines their properties, and various defects have a leading role in the thermal conductivity. Y and Gd have large misfits in atomic mass and ionic size, which will contribute to large strain field fluctuations and effective phonon scattering [26]. Gd\(^{3+}\) can partially replace Y\(^{3+}\) to enhance phonon scattering and slightly increase TECs [27].

From the above statement, RETaO\(_4\) (RE = rare-earth elements) are candidates for TBCs, based on their excellent thermal insulation, high TECs, relatively low modulus, and high toughness. Further, Lu et al. [28] studied the linear expansion coefficient and anisotropic thermal expansion of Yb\(_2\)SiO\(_5\) ceramics by high-temperature X-ray diffraction (XRD). The average linear TECs are 6.3×10\(^{-6}\) K\(^{-1}\) (473–1673 K), and the anisotropic TECs are \(\alpha_a = (2.98 \pm 0.16) \times 10^{-6} \text{ K}^{-1}\), \(\alpha_b = (6.51 \pm 0.19) \times 10^{-6} \text{ K}^{-1}\), and \(\alpha_c = (9.08 \pm 0.16) \times 10^{-6} \text{ K}^{-1}\). Ridley et al. [29] found five silicate RE\(_2\)SiO\(_5\) (RE = Sc, Y, Dy, Er, and Yb) with the average linear TECs of (6–9)×10\(^{-6}\) K\(^{-1}\) through the in-situ XRD studies, of which Sc\(_2\)SiO\(_5\) has the lowest TECs and anisotropic TECs. The anisotropic TECs are vital for the applications of RETaO\(_4\) as TBCs. Herein, we investigate the anisotropic TECs of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) solid solution via the powder high-temperature XRD. The changes of the lattice parameters, unit cell volumes, TECs of different axis, and linear TECs are key points of this work. It is found that, the phase transition temperature of the prepared (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) solid solution is higher than 1450 °C, which is similar to that of YTaO\(_4\). Moreover, (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) has low thermal conductivity, suitable modulus, and high hardness. This work further advances the research and application of ferroelastic RETaO\(_4\) as high-temperature protecting coatings.

2 Experimental and calculated details

2.1 Specimen preparation

The (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics were obtained via sintering at 1700 °C for 10 h by the solid-phase reaction method. The raw materials used in this work were Y\(_2\)O\(_3\), Gd\(_2\)O\(_3\), Ta\(_2\)O\(_5\), and absolute ethanol. All the raw materials were sourced from Aladdin, China, the powder purity is 99.99%, and the particle sizes were less than 10 μm. First, we weighed the raw materials in the required molar ratio, put them into the cleaned ball mill tank, and added absolute ethanol to two-thirds of the volume of the ball mill tank. Then we used a planetary ball mill (Nanjing NanDa Instrument Co. Ltd., QM-3SP2, China) to mix for 24 h, and then put it into an oven at 70 °C to obtain a dry mixed powder. We sieved the dried powder until its particle size was less than 48 μm, and then put it into a tablet machine to obtain a block of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\). Finally, the columns were placed at 1700 °C for 10 h to synthesize circular specimens.

2.2 Characterization of high-temperature phase stability

The crystal structures of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) were identified by the X-ray diffractometer (Rigaku, MiniFlex600, Japan). To gather more information about the unit cell parameters, the XRD refinement was performed by GSAS software.

The microscopic morphologies of the specimen were observed by the scanning electron microscope (SEM; ZEISS, SIGMA-300, Germany). The measurements of the grain size of the samples were conducted within ImageJ software.

To analyze the high-temperature phase stability of the materials, the thermogravimetric (TG) and differential scanning calorimetry (DSC) analyses were performed on (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) by a simultaneous thermal analyzer (NETZSCH, STA 449 F3, Germany). The sample had a mass of 10 mg, which was ultrasonically cleaned before measuring, and then kept in a bake-out furnace at 70 °C for 1440 min.

The high-temperature phase transition of the sample
was measured by the powder high-temperature X-ray diffractometer (Panalytical, Empyrean, the Netherlands), whose measurement accuracy was ±0.0001°, and the measurement range was 10–70 °C. During the measurement, the scanning speed was 6 (°)/min, the measurement temperature was from 25 to 1500 °C, and the sample was held at each temperature for 30 min before the measurement.

2.3 Thermal property measurement

The thermal diffusivity (\(d\)) of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) was measured by a laser scintillation apparatus (NETZSCH, LFA 457, Germany). The sample needed to be made into a cylinder with a diameter of 6 mm and a height of 1 mm. A layer of carbon was sprayed on both sides of the sample, and then the thermal conductivity (\(k\)) was obtained by Eq. (1):

\[
k = d \times c_p \times \rho
\]

where \(c_p\) is the heat capacity, and \(\rho\) is the actual density of the sample.

The (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramic bulk is difficult to achieve complete densification, considering that voids will have a certain impact on the thermal conductivity results, so the theoretical thermal conductivity \(k_0\) can be obtained by Eq. (2):

\[
\frac{k}{k_0} = 1 - \frac{4}{3\phi}
\]

where \(\phi\) is the porosity.

The thermal expansion characteristics of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) samples were measured by a thermal mechanical analyzer (NETZSCH, TMA 402 F3, Germany). The TECs were calculated by Eq. (3):

\[
\text{TEC} = \frac{\Delta L}{L} \times \frac{1}{\Delta T}
\]

where \(L\), \(\Delta L\), and \(\Delta T\) represent the room-temperature length of the sample, the change in length, and the change in temperature, respectively. To obtain the TECs of the high-temperature XRD data, the refinement of XRD was conducted by UnitCell. UnitCell was a least-square refinement software that can obtain the lattice parameters from the XRD results.

2.4 Modulus and hardness

The Young’s modulus (\(E\)) of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) was measured within an ultrasound reflection equipment (Teclab, UMS-100, France). The NanoBlitz 3D (Nanomechanisc, Inc iMicro, USA) was further used to measure the moduli and hardness of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics. During the test, with a load of 50 mN and no holding time, there are 30 × 30 = 900 points evenly distributed in a square area of 300 μm × 300 μm.

3 Results and discussion

3.1 Structure characterizations

Figure 1(a) reveals the XRD patterns of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics, compared with the ICDD PDF No. 24-0441 of m-GdTaO\(_4\) and ICDD PDF No. 24-1415 of m-YTaO\(_4\). The prepared (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) have identical crystal structures, and there is no second phase, suggesting that the phase structure of each sample is the m phase. As shown in Fig. 1(b), the main XRD peak of (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) shifts to higher angles with \(x\) increasing. The ionic radius of Gd\(^{3+}\) (1.053 Å) is larger than...
that of $Y^{3+}$ (1.019 Å) [30], and the reduced unit cell volume causes the XRD peaks to shift to higher angles.

The Rietveld refinement results are plotted in Figs. 2(a)–2(g). The accuracy of the Rietveld refinement can be assessed by the weighted graph variance factor ($R_{wp}$) and graph variance factor ($R_p$). $R_{wp}$ is less than 9%, and $R_p$ is less than 7% for each sample, indicating the refinement results with high confidence. The unit cell volumes and lattice parameters are listed in Table 1. The lattice parameters and theoretical densities are found to shrink by the increase in the $x$ value. The lattice constant decreases with the decrease in RE $^{3+}$ ionic radii. The unit cell volume varies with $x$ of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics, as shown in Fig. 2(h). Figure 2(i) demonstrates the crystal structure of (Gd$_{1-x}$Y$_x$)TaO$_4$; the unit cell of YTaO$_4$ is composed of tetrahedra [TaO$_4$] and dodecahedron [YO$_8$], and the coordination number of Y atom can be obtained [31].

Figures 3(a)–3(g) display the in-situ XRD results. The XRD patterns of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics correspond to that of the m-phase PDF cards at temperatures up to 1450 °C. As the temperature increases to 1500 °C, the m phase peaks disappear, while the t phase peaks become more expressed and sharper. We can see that each (Gd$_{1-x}$Y$_x$)TaO$_4$ sample crystallizes in the m phase when the temperature is reduced to 25 °C. This proves that the high-temperature phase transition of (Gd$_{1-x}$Y$_x$)TaO$_4$ is reversible. The XRD peaks of the t phase are derived from the gradual merging of the m phase without sudden changes, and the XRD peaks reflect the changes of the unit cell parameters. It is believed that the transformation of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics from the m phase to the t phase does not produce large volume differences, and the phase change has seldom intention on the TECs of the materials [32]. Interestingly, when $x = 4/6$, the sample does not undergo a phase transition at 1500 °C and maintains the m phase, which may be caused by the

![Figure 2 XRD Rietveld refinement results of (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, and 6/6$): (a) $x = 0/6$; (b) $x = 1/6$; (c) $x = 2/6$; (d) $x = 3/6$; (e) $x = 4/6$; (f) $x = 5/6$; and (g) $x = 6/6$. (h) Unit cell volume is plotted as a function of $x$. (i) Characteristic crystal structure of YTaO$_4$ ceramics with $I2(5)$ space group.](www.springer.com/journal/40145)
Table 1  Lattice parameters (a, b, and c), unit cell volumes (V), and theoretical densities (ρ) of (Gd$_{1-x}$Y$_x$)TaO$_4$ (x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, and 6/6) ceramics

| x    | a (Å) | b (Å) | c (Å) | V (Å$^3$) | ρ (g·cm$^{-3}$) |
|------|-------|-------|-------|-----------|-----------------|
| 0/6  | 5.407 | 11.073| 5.082 | 302.877   | 8.82            |
| 1/6  | 5.391 | 11.047| 5.077 | 301.042   | 8.63            |
| 2/6  | 5.381 | 11.028| 5.074 | 299.704   | 8.41            |
| 3/6  | 5.356 | 10.987| 5.065 | 296.733   | 8.24            |
| 4/6  | 5.354 | 10.980| 5.056 | 295.908   | 8.01            |
| 5/6  | 5.339 | 10.956| 5.059 | 294.556   | 7.79            |
| 6/6  | 5.328 | 10.936| 5.055 | 293.241   | 7.56            |

measurement error. (Gd$_{2/6}$Y$_{4/6}$)TaO$_4$ and the other components are similar and should have similar high-temperature phase change points, so the phenomenon is considered to be a measurement error. For the high-temperature XRD measurement, the powder to be measured is placed on the platinum carrier table, and the thermocouple measures the temperature of the carrier table instead of the temperature of the powder directly tested; so the measurement error is generated, and the size of the error is mainly determined by the thickness of the powder.

Fig. 3  Original and three-dimensional (3D) in-situ XRD patterns for (Gd$_{1-x}$Y$_x$)TaO$_4$ (x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, and 6/6) ceramics: (a) x = 0/6; (b) x = 1/6; (c) x = 2/6; (d) x = 3/6; (e) x = 4/6; (f) x = 5/6; and (g) x = 6/6.
To further understand the thermal stability of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics from 50 to 1450 °C, the DSC and TG curves are plotted in Figs. 4(a)–4(g). The mass loss and heat flow of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) samples are revealed by the blue and red curves, respectively. The mass loss of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics is less than 1%. No endothermic or exothermic peak (50–1450 °C) is observed in the DSC and the first derivative of the DSC (DDSC) curves of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics, which show that (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) has admirable thermal stability [33]. Therefore, the m–t phase transition of the (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) ceramics occur between 1450 and 1500 °C as discussed in conjunction with the high-temperature XRD results.

Fig. 4 DDSC, DSC, and TG curves as a function of temperature for (Gd\(_{1-x}\)Y\(_x\))TaO\(_4\) (\(x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, \) and \(6/6\)) ceramics: (a) \(x = 0/6\); (b) \(x = 1/6\); (c) \(x = 2/6\); (d) \(x = 3/6\); (e) \(x = 4/6\); (f) \(x = 5/6\); and (g) \(x = 6/6\).
3.2 Microstructure

The microstructures of the \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) ceramics are shown in Fig. 5. Each grain of the sample is uniform in size, separated by clear grain boundaries. The average grain size and area of \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) are 12–15 μm and 117–167 μm², respectively. In \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\), a little quantity of pore and crack is observed. Figure 5(d) shows the local magnification of the \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) ceramic grains. There are some stripe-like structures pointing in different directions. Combined with Refs. [25,34] on tantalate, it can be concluded that the structure is a ferroelastic structure. The ferroelastic structure is derived from the phase transition process and can enhance fracture toughness by absorbing stress.

3.3 Thermal conductivity

Based on the Neumann–Kopp law, Fig. 6(a) displays that the specific heat capacity of \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) increases slightly with the increasing temperatures.

![Figure 5](image1.jpg)

Fig. 5 Microstructures of \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) \((x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, \text{and} 6/6)\) ceramics: (a) \(x = 0/6\); (b) \(x = 1/6\); (c) \(x = 2/6\); (e) \(x = 3/6\); (f) \(x = 4/6\); (g) \(x = 5/6\); and (h) \(x = 6/6\). (d) Local magnification of the \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) ceramic grains.

![Figure 6](image2.jpg)

Fig. 6 Temperature-dependent thermal properties of \((\text{Gd}_{1-x}\text{Y}_x)\text{TaO}_4\) \((x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, \text{and} 6/6)\) ceramics: (a) specific heat capacity; (b) thermal diffusivity; (c) thermal conductivity; and (d) thermal conductivity as a function of composition parameter \((x)\) at different temperatures.
As expressed in Fig. 6(b), the thermal diffusivities of high-temperature (Gd₁₋ₓYₓ)TaO₄ are significantly lower than those of low-temperature (Gd₁₋ₓYₓ)TaO₄, tending to an extreme value at 900 °C. As depicted in Fig. 6(c), with the temperature increasing, the thermal conductivity gradually decreases. Obviously, the thermal properties of the material are significantly changed after Y and Gd doping. When x = 3/6, the thermal conductivity of the prepared sample was significantly reduced (1.37 W·m⁻¹·K⁻¹, 900 °C) compared with 8YSZ (2.5 W·m⁻¹·K⁻¹, 1000 °C) [31]. (Gd₁₋ₓYₓ)TaO₄ dropped by nearly half [35]. The composition-dependent thermal conductivity of (Gd₁₋ₓYₓ)TaO₄ is plotted in Fig. 6(d). Since the phonon scattering coefficients of (Gd₁₋ₓYₓ)TaO₄ with different compositions are different, the variation of conductivity with x at different temperatures exhibits a concave parabolic law. Y and Gd have a large gap in volume and mass, which will generate mass and volume fluctuations and produce phonon scattering [36]. The main phonon scattering is controlled mainly by Umklapp scattering and point defect scattering processes in (Gd₁₋ₓYₓ)TaO₄. For an ideal crystal, most of the thermal resistance is created by Umklapp scattering. Slack [40] calculated the theoretical thermal conductivity (k_{Stack}) by Eq. (11):

\[ k_{Stack} = \frac{A \bar{M} \theta_0^3 \Omega}{\gamma^2 n^3 T} \]

where \( A = 3.04 \times 10^7 \text{W} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \cdot \text{m}^{-2} \cdot \text{K}^{-3} \), \( \bar{M} \), \( \theta_0 \), \( \Omega \), \( n \), and \( T \) are the average atomic mass, the Debye temperature, the average atomic volume, the number of atoms in the original unit cell, and the absolute temperature, respectively. \( \theta_0 \) and \( \gamma \) can be obtained by Eqs. (12) and (13), respectively [41]:

| Table 2 Phonon scattering coefficients (Γ), average masses of (Gd, Y) sites (\( M_{(Gd,Y)} \)), average radii of (Gd, Y) sites (\( \bar{\Delta}_{(Gd,Y)} \)), average masses of (Gd₁₋ₓYₓ)TaO₄ ceramics (\( \bar{M} \)), and strain fields factors (ε) of (Gd₁₋ₓYₓ)TaO₄ (x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, and 6/6) ceramics |
|---|---|---|---|---|
| x | \( M_{(Gd,Y)} \) | \( \bar{M} \) | \( \Delta_{(Gd,Y)} \) | ε | Γ |
| 0/6 | 157.3 | 67.03 | 105.3 | 175.27 | 0.000 |
| 1/6 | 145.9 | 67.03 | 104.7 | 165.13 | 0.048 |
| 2/6 | 134.5 | 67.03 | 104.2 | 161.33 | 0.070 |
| 3/6 | 123.1 | 67.03 | 103.6 | 184.87 | 0.078 |
| 4/6 | 111.7 | 67.03 | 103.0 | 164.27 | 0.061 |
| 5/6 | 100.3 | 67.03 | 102.5 | 181.27 | 0.037 |
| 6/6 | 88.9 | 67.03 | 101.9 | 160.62 | 0.000 |

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Fig. 7 Experimental, theoretical, and ultimate thermal conductivities of (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, \text{and} 6/6$) ceramics: (a) $x = 0/6$; (b) $x = 1/6$; (c) $x = 2/6$; (d) $x = 3/6$; (e) $x = 4/6$; (f) $x = 5/6$; and (g) $x = 6/6$. (h) Phonon scattering coefficient and thermal conductivity as a function of $x$.

$$\theta_D = \frac{h}{k_B} \left( \frac{3N}{4\pi V} \right)^{1/3} \times v_m$$  

(12)

$$\gamma = \frac{3}{2} \left(1 + \sigma\right) \left(2 - 3\sigma\right)$$  

(13)

where $h$, $k_B$, $N$, and $V$ are the Plank’s constant, the Boltzmann constant, the number of atoms in a unit cell, and the volume of a unit cell, respectively [41]. The $k_{\text{Slack}}$ of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics are compared with the experimental thermal conductivities, as plotted in Figs. 7(a)–7(g). Obviously, the experimental and theoretical thermal conductivities have an identical trend with the increasing temperatures. However, there are still some differences between the experimental and theoretical values. One is that the theoretical data of (Gd$_{1-x}$Y$_x$)TaO$_4$ in the high-temperature stage are smaller than the experimental thermal conductivity. The reasons are as follows: Firstly, the Slack model ignores the contribution of thermal radiation at high temperatures, and secondly, the Slack model ignores the energy of the optical branch phonons [42]. The relaxation time of the optical branch phonon is much shorter than that of the acoustic branch phonon. However, it carries relatively large energy, which can also increase the thermal conductivity of the material to a certain extent [40,43].

Another difference is that the experimental thermal conductivity at a low temperature is lower than the theoretical thermal conductivity. The large difference in mass number and volume of impurity atoms and matrix atoms in this study causes structural disorder and reduced lattice energy, resulting in increased non-resonant parameters and increased phonon scattering. Thus, the experimental thermal conductivity is lower than the calculated thermal conductivity at low temperatures [44].

The dominant role is played by the strong scattering among phonons due to the increase in temperature. With the further increase in temperature, the average free range of phonons reaches the minimum value, which is close to the atomic spacing, and the thermal conductivity reaches the limit value. The main models for describing the limited thermal conductivity of solids are the Clarke model [45] and Cahill model [44]. The expressions for the Clark model ($k_{\text{min1}}$) and Cahill model ($k_{\text{min2}}$) are

\begin{table}
\centering
\begin{tabular}{ccccc}
\hline
\textbf{$x$} & \textbf{$\sigma$} & \textbf{$v_t$ (m s$^{-1}$)} & \textbf{$v_l$ (m s$^{-1}$)} & \textbf{$\rho_0$ (g cm$^{-3}$)} \\
\hline
0/6 & 0.34 & 2500 & 5185 & 2810 & 8.57 \\
1/6 & 0.34 & 2470 & 5062 & 2775 & 8.51 \\
2/6 & 0.35 & 2521 & 5205 & 2833 & 8.31 \\
3/6 & 0.35 & 2517 & 5280 & 2831 & 8.17 \\
4/6 & 0.34 & 2574 & 5270 & 2892 & 7.83 \\
5/6 & 0.35 & 2715 & 5670 & 3053 & 7.65 \\
6/6 & 0.34 & 2782 & 5670 & 3124 & 7.48 \\
\hline
\end{tabular}
\caption{Poisson’s ratios ($\sigma$), transverse acoustic velocities ($v_t$), longitudinal acoustic velocities ($v_l$), average acoustic velocities ($v_\text{m}$), and measured densities ($\rho_0$) of (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, \text{and} 6/6$) ceramics at room temperature}
\end{table}
\[ k_{\text{min}1} = 0.87k_BN_A^{2/3}m^{2/3} \rho^{1/6}E^{3/2}/M^{2/3} \]  
\[ k_{\text{min}2} = k_B \cdot \frac{2.48}{\pi} \rho^{2/3} \left(2v_1 + v_1\right) \]

where \(N_A\) and \(m\) are the Avogadro’s number and the number of atoms in a single cell, respectively. Figures 7(a)–7(g) show \(k_{\text{min}1}\) and \(k_{\text{min}2}\) of \((\text{Gd}_{1-x} \cdot \text{Y}_x)\text{TaO}_4\). The \((\text{Gd}_{3/6} \cdot \text{Y}_{3/6})\text{TaO}_4\) ceramics have a thermal conductivity similar to the limited thermal conductivity.

### 3.4 Thermal expansion

The TECs are one of the key influencing factors for TBC service. TBCs consist of a ceramic layer, an adhesive layer, and a metal substrate. It is well known that metals have larger TECs than ceramics, and the bonding layer is the thermal expansion moderating layer of the two materials. The TBCs operate under the condition of cooling and heating cycles. To avoid thermal stress caused by different TECs, it is necessary to find ceramic layers with high TECs.

It is widely accepted that micro-cracks are induced in the ceramics owing to the large anisotropy of TECs [46]. The cell parameters for each sample are calculated from the X-ray data for the corresponding temperature of the sample. The error between the measured values of the room-temperature unit cell parameters and the values of the ICDD database is less than 0.3%, and the specific values are listed in Table 4. More detailed cell parameters for each sample calculated by the high-temperature XRD data are shown in Tables 5–11. The normalized lattice parameters of \((\text{Gd}_{1-x} \cdot \text{Y}_x)\text{TaO}_4\) are shown in Figs. 8(a)–8(g). The lattice constants \((b\) and \(c)\) and unit cell volumes \((V)\) are positively related to temperature, while the lattice constant \((a)\) increases slightly, and then decreases slowly when the temperature is higher than 1000 K. The angle between the \(a\)-axis and the \(c\)-axis \((\beta)\) gradually decreases with the increasing temperature until it is 90° after the \(m\)-\(t\) phase transition. The crystal transformation process of \(\text{GdTaO}_4\) is shown in Fig. 8(h), where the transformation process of the \(\beta\) angle is consistent with the data obtained via the high-temperature XRD.

The anisotropic TECs of \((\text{Gd}_{1-x} \cdot \text{Y}_x)\text{TaO}_4\) are calculated via the lattice constants at different temperatures. When the temperature is higher than 600 K, the volumetric TECs are defined by Eq. (16) [47]:

\[ \ln(V/V_0) = \alpha_V(T - T_0) \]

where \(V_0\) is the volume at 25 °C, \(T_0\) is the room temperature, and \(\alpha_V\) is the temperature-dependent volumetric TECs.

### Table 4 Difference between measured values of room-temperature unit cell parameters and ICDD database values of \(\text{YTaO}_4\)

| Method   | \(a\) (Å) | \(b\) (Å) | \(c\) (Å) | \(V\) (Å³) |
|----------|-----------|-----------|-----------|-----------|
| ICDD     | 5.326     | 10.931    | 5.050     | 292.600   |
| Unit cell| 5.320     | 10.922    | 5.047     | 291.903   |
| Error (%)| 0.11      | 0.08      | 0.06      | 0.24      |

### Table 5 Unit cell parameters of \(\text{GdTaO}_4\) ceramics at various temperatures

| Temperature (°C) | \(a\) (Å) | \(b\) (Å) | \(c\) (Å) | \(V\) (Å³) |
|------------------|-----------|-----------|-----------|-----------|
| 25               | 5.396     | 11.051    | 5.075     | 95.614    | 301.119   |
| 200              | 5.400     | 11.070    | 5.082     | 95.414    | 302.434   |
| 400              | 5.403     | 11.094    | 5.092     | 95.136    | 303.996   |
| 600              | 5.404     | 11.121    | 5.105     | 94.889    | 305.677   |
| 800              | 5.402     | 11.150    | 5.119     | 94.479    | 307.397   |
| 1000             | 5.397     | 11.179    | 5.139     | 93.914    | 309.318   |
| 1200             | 5.381     | 11.215    | 5.168     | 93.111    | 311.390   |
| 1300             | 5.366     | 11.233    | 5.192     | 92.521    | 312.648   |
| 1400             | 5.342     | 11.255    | 5.228     | 91.482    | 314.236   |
| 1500             | 5.288     | 11.291    | 5.288     | 90.000    | 315.742   |

### Table 6 Unit cell parameters of \((\text{Gd}_{3/6} \cdot \text{Y}_{3/6})\text{TaO}_4\) ceramics at various temperatures

| Temperature (°C) | \(a\) (Å) | \(b\) (Å) | \(c\) (Å) | \(V\) (Å³) |
|------------------|-----------|-----------|-----------|-----------|
| 25               | 5.382     | 11.035    | 5.072     | 95.550    | 299.853   |
| 200              | 5.388     | 11.053    | 5.079     | 95.405    | 301.137   |
| 400              | 5.393     | 11.077    | 5.088     | 95.135    | 302.757   |
| 600              | 5.395     | 11.103    | 5.102     | 94.848    | 304.506   |
| 800              | 5.394     | 11.129    | 5.119     | 94.488    | 306.334   |
| 1000             | 5.389     | 11.160    | 5.141     | 94.039    | 308.424   |
| 1200             | 5.380     | 11.197    | 5.169     | 93.252    | 310.893   |
| 1300             | 5.370     | 11.218    | 5.188     | 92.680    | 312.225   |
| 1400             | 5.355     | 11.243    | 5.217     | 92.003    | 313.886   |
| 1500             | 5.286     | 11.288    | 5.286     | 90.000    | 315.446   |

### Table 7 Unit cell parameters of \((\text{Gd}_{4/6} \cdot \text{Y}_{2/6})\text{TaO}_4\) ceramics at various temperatures

| Temperature (°C) | \(a\) (Å) | \(b\) (Å) | \(c\) (Å) | \(V\) (Å³) |
|------------------|-----------|-----------|-----------|-----------|
| 25               | 5.381     | 11.023    | 5.076     | 95.615    | 299.674   |
| 200              | 5.386     | 11.042    | 5.084     | 95.409    | 300.992   |
| 400              | 5.390     | 11.066    | 5.094     | 95.193    | 302.559   |
| 600              | 5.392     | 11.091    | 5.106     | 94.855    | 304.286   |
| 800              | 5.392     | 11.118    | 5.124     | 94.489    | 306.205   |
| 1000             | 5.389     | 11.151    | 5.141     | 93.978    | 308.169   |
| 1200             | 5.375     | 11.186    | 5.170     | 93.120    | 310.397   |
| 1300             | 5.362     | 11.211    | 5.191     | 92.595    | 311.716   |
| 1400             | 5.344     | 11.235    | 5.223     | 91.784    | 313.439   |
| 1500             | 5.280     | 11.302    | 5.277     | 90.000    | 314.905   |

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The volumetric TECs of (27.9–33.3)×10^{-6} K^{-1} (1400 °C) of the (Gd_{1/6}Y_{5/6})TaO_{4} ceramics are obtained by Eq. (16), and the results are shown in Fig. 9(d). The calculated TECs of three axes at 1400 °C are \(a_{\alpha} = (-7.3–(-2.1)) \times 10^{-6} \text{ K}^{-1} \), \(a_{\beta} = (11.1–13.9) \times 10^{-6} \text{ K}^{-1} \), and \(a_{\gamma} = (16.2–21.6) \times 10^{-6} \text{ K}^{-1} \), and the results are plotted in Figs. 9(a)–9(c). Due to this high anisotropic thermal expansion, the thermal mismatch can be minimized by controlling the preferred orientation, making (Gd_{1/6}Y_{5/6})TaO_{4} more widely used in the technical field of TBCs. The axial TECs of (Gd_{1/6}Y_{5/6})TaO_{4} ceramics gradually increase along the \(a\)-axis at first, and then gradually decrease when the temperature exceeds 600 °C, and the prepared samples finally show a negative TECs. The TECs along the \(b\)-axis and \(c\)-axis gradually increase with the increasing temperatures, while their values are quite different. The anisotropic TECs may generate internal stress during thermal cycling, and lead to micro-cracks in the coatings. The TECs of the (Gd_{1/6}Y_{5/6})TaO_{4} ceramics increase linearly before 600 °C, but the TECs increase slowly above 600 °C, which may be related to the negative value of the \(a\)-axis TECs after 600 °C.

Figures 10(a) and 10(b) show the thermal expansion rates (\(dL/L_{0}\)) and TECs of (Gd_{1/6}Y_{5/6})TaO_{4} measured via the TMA analyzer, respectively. Apparently, \(dL/L_{0}\) is linearly related to temperature, indicating that (Gd_{1/6}Y_{5/6})TaO_{4} has excellent phase stability. When \(x = 1/6\), the TECs of (Gd_{1/6}Y_{5/6})TaO_{4} reach 10.5×10^{-6} \text{ K}^{-1} (1200 °C), which is comparable with YSZ (11×10^{-6} \text{ K}^{-1}). Dopant creates point defects that further induce lattice distortion, which results in the enhanced lattice stress fields and increased off-resonance of lattice vibrations, and it ultimately leads to high TECs. The linear TECs were calculated by dividing the volumetric TECs by 3, as shown in Fig. 10(c) [29,48]. When \(x = 1/6\), the TECs are up to 10.3×10^{-6} \text{ K}^{-1} (1200 °C), which is similar to the TECs measured via the TMA analyzer. When the temperature rises to 1500 °C, the TECs increase slightly compared with those before the phase transition, and the value is 11.5×10^{-6} \text{ K}^{-1}.

![Image](www.springer.com/journal/40145)
Fig. 8  Normalized unit cell parameters of (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6,$ and $6/6$) as a function of temperature: (a) $x = 0/6$; (b) $x = 1/6$; (c) $x = 2/6$; (d) $x = 3/6$; (e) $x = 4/6$; (f) $x = 5/6$; and (g) $x = 6/6$. (h) Schematic diagram of the crystal transformation process of GdTaO$_4$ from the m phase to the t phase, where the purple ball is the Gd atom, the yellow ball is the Y atom, and the red ball is the O atom.

Fig. 9  Axial TECs for (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6,$ and $6/6$): (a) $a$-axis; (b) $b$-axis; and (c) $c$-axis. (d) Volumetric TECs of (Gd$_{1-x}$Y$_x$)TaO$_4$. 

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3.5 Mechanical properties

$E$ is a physical quantity related to the resistance of the material to deformation, and can also characterize the bonding strength of the material [49,50]. During the operation of the turbine engine, it will be hit by some foreign objects, which will cause cracks in the coating and eventually damage [51]. Consequently, as a TBC material, $E$ needs to be considered. The nanoscale $E$ of (Gd$_{1-x}$Y$_x$)TaO$_4$ were measured by the nanoindentation method, and the results are plotted in Figs. 11(a)–11(g).

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**Fig. 10** Temperature dependence of thermal expansion properties of (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6,$ and $6/6$) ceramics via the TMA analyzer: (a) $dL/L_0$; (b) TECs. (c) Linear TECs of (Gd$_{1-x}$Y$_x$)TaO$_4$ from 200 to 1500 °C by the high-temperature XRD.

**Fig. 11** 3D distributions of $E$ for (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6,$ and $6/6$) ceramics: (a) $x = 0/6$; (b) $x = 1/6$; (c) $x = 2/6$; (d) $x = 3/6$; (e) $x = 4/6$; (f) $x = 5/6$; and (g) $x = 6/6$. (h) $E$ as a function of $x$. 
The 3D topography shows a small wave motion with the change of position. We speculate that this might be because the sample contains some microscopic voids and cracks, which will affect the accuracy of the measurement, but this error can be eliminated to a certain extent through multiple measurements [52]. Figure 11(h) shows the mean values of $E$ obtained by nanoindentation. To verify the accuracy of the data measured by the nanoindentation method, we use the ultrasonic pulse method to further measure $E$, and the results are shown in Table 12. The mean $E$ of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics are 137.5–150.9 GPa measured by the NanoBlitz 3D method, which is almost the same as the ultrasonic pulse method and far below that of YSZ (240 GPa) [53]. Figures 12(a)–12(g) show the mean values of hardness obtained by the nanoindentation, and the hardness and $E$ have a linear relationship. Figure 12(h) shows the mean values of the hardness,

| x     | Method       | $E$  | $B$  | $G$  | $H$  |
|-------|--------------|------|------|------|------|
| 0/6   | Ultrasonic pulse | 144.4| 158.9| 53.5 | —    |
| 0/6   | NanoBlitz 3D   | 146.4| —    | —    | 9.54 |
| 1/6   | Ultrasonic pulse| 139.6| 148.8| 51.9 | —    |
| 1/6   | NanoBlitz 3D   | 150.8| —    | —    | 9.51 |
| 2/6   | Ultrasonic pulse| 142.2| 154.7| 52.8 | —    |
| 2/6   | NanoBlitz 3D   | 148.2| —    | —    | 9.64 |
| 3/6   | Ultrasonic pulse| 140.1| 158.7| 51.8 | —    |
| 3/6   | NanoBlitz 3D   | 150.9| —    | —    | 9.61 |
| 4/6   | Ultrasonic pulse| 139.4| 148.2| 51.9 | —    |
| 4/6   | NanoBlitz 3D   | 139.9| —    | —    | 9.36 |
| 5/6   | Ultrasonic pulse| 152.5| 170.9| 56.4 | —    |
| 5/6   | NanoBlitz 3D   | 137.5| —    | —    | 9.42 |
| 6/6   | Ultrasonic pulse| 155.4| 163.4| 40.5 | —    |
| 6/6   | NanoBlitz 3D   | 137.5| —    | —    | 9.39 |

Fig. 12 3D distributions of $H$ for (Gd$_{1-x}$Y$_x$)TaO$_4$ ($x = 0/6, 1/6, 2/6, 3/6, 4/6, 5/6, and 6/6$) ceramics: (a) $x = 0/6$; (b) $x = 1/6$; (c) $x = 2/6$; (d) $x = 3/6$; (e) $x = 4/6$; (f) $x = 5/6$; and (g) $x = 6/6$. (h) $H$ as a function of $x$. 

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and the mean hardness of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics is 9.4–9.6 GPa, which is close to that of YSZ (10 GPa). The high $H$ and relatively low $E$ help the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics to resist thermal shock during service and improve their service life [54].

4 Conclusions

In this work, structural characterization, high-temperature phase stability, thermal conductivity, and anisotropic TECs of (Gd$_{1-x}$Y$_x$)TaO$_4$ are investigated as potential TBCs. The results of the research are as follows:

1) The SEM results show that the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics have ferroelastic domains similar to YSZ. The (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics have excellent high-temperature phase stability, and the $m$–$t$ phase transition temperature is higher than 1450 °C.

2) (Gd$_{1-x}$Y$_x$)TaO$_4$ has extremely low thermal conductivity (1.37–2.05 W·m$^{-1}$·K$^{-1}$, 900 °C) compared with 8YSZ (2.5 W·m$^{-1}$·K$^{-1}$, 1000 °C), which dropped by nearly half. The linear TECs reach $11.5\times10^{-6}$ K$^{-1}$ (1500 °C), and the anisotropic TECs are $a_o = (-7.3$–$(-2.1))\times10^{-6}$ K$^{-1}$, $a_l = (11.1$–$13.9)\times10^{-6}$ K$^{-1}$, and $a_c = (16.2$–$21.6)\times10^{-6}$ K$^{-1}$.

3) The mean $E$ of (Gd$_{1-x}$Y$_x$)TaO$_4$ ranges from 137.5 to 150.9 GPa, and they are far less than that of YSZ (240 GPa), when the mean hardness of the (Gd$_{1-x}$Y$_x$)TaO$_4$ ceramics is 9.4–9.6 GPa.

4) Considering that the TBC materials should possess low thermal conductivity and suitable TECs, (Gd$_{3/6}$Y$_{3/6}$)TaO$_4$ is the best TBC material among all the components.

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