Investigation on the Thermal–Mechanical Properties of YbRESiO$_5$ (RE = Yb, Eu, Gd, Ho, Tm, Lu, Y, Sc): First-Principles Calculations and Thermal Performance Experiments

Shilong Yang $^{1,†}$, Tianying Wang $^{2,†}$, Kaibin Li $^{1,*}$, Weize Wang $^{1,3,*}$, Yangguang Liu $^1$ and Ting Yang $^1$

**Abstract:** Environmental barrier coatings are critically needed in the future to safeguard SiC-based ceramic matrix composites (SiC CMCs) used in gas turbines. Element doping of rare earth monosilicates could further improve the properties of the coating. The crystal structure, elastic properties, and resistance to water vapor corrosion of Yb$_2$SiO$_5$ and YbRESiO$_5$ (where RE = Sc, Y, Eu, Gd, Ho, Tm, Lu) were examined in this study using first-principles calculations. When RE is Yb, the material is Yb$_2$SiO$_5$. Based on the outcomes of the calculation, we prepared YbRESiO$_5$ (RE = Sc, Yb, Eu) and studied the thermodynamic properties. The findings show that YbRESiO$_5$’s resistance to water vapor corrosion is as follows: YbLuSiO$_5$ < YbEuSiO$_5$ < YbGdSiO$_5$ < YbYSiO$_5$ < YbTmSiO$_5$ < YbHoSiO$_5$ < YbScSiO$_5$. YbScSiO$_5$ has a lower unit cell volume, average Re-O bond length, and thermal expansion coefficient than Yb$_2$SiO$_5$, while YbEuSiO$_5$ has the reverse pattern. Moreover, of the eight materials, YbScSiO$_5$ has the greatest elastic modulus and lattice distortion. After doping with Eu, YbEuSiO$_5$ exhibits a decrease in thermal conductivity by nearly thirty percent compared to Yb$_2$SiO$_5$, due to the formation of oxygen vacancies. The development of environmental barrier coating materials may benefit from these discoveries.

**Keywords:** rare earth monosilicate; environment barrier coating; first-principles calculation; water vapor corrosion resistance; thermal properties

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1. **Introduction**

As the aviation sector develops, thrust–weight ratios increase in new generations, and internal gas temperatures exceed the bearing limits of nickel-based superalloys [1,2]. According to the needs of the current development, the surface temperature of the hot end components of the new generation of aero-engines can reach 1400 °C, while the maximum working temperature of single-crystal nickel-based superalloys is 1100 °C and Ni3Al single-crystals have a high-temperature limit of 1200 °C, so there is an urgent need to develop a new type of material matrix [3]. The most promising high-temperature structural materials to replace nickel-based superalloys in the hot sections of aircraft engines are SiC-based ceramic matrix composites (SiC CMCs) [1,4,5]. SiC CMCs have a high temperature resistance, low density, high strength, high elastic modulus, oxidation resistance, erosion resistance, and crack insensitivity [6]. But in real high-temperature service conditions, SiC CMCs face substantial hurdles, especially with regard to considerable water vapor corrosion issues [4]. Poor environmental durability still prevents them from being used in combustion environments due to the presence of two chemical degradation mechanisms,
recession and thermal corrosion. (i) Recession is the loss of silicon-based ceramics due to repeated oxidation and volatilization when exposed to high-velocity water vapor in a turbine. (ii) Thermal corrosion is caused by alkaline salts in the combustion environment, which form liquid silicates and cause craters in silicon-based ceramics [7–9]. Alkaline salts are salts formed by the reaction of an alkaline metal (e.g., sodium, potassium) or an alkaline earth metal (e.g., calcium, magnesium) with an acid. Experimental results from NASA et al. show that the loss rate of the ceramic surface is about 270 µm/kh in a combustion environment (1200 °C; pressure 1013.25 KPa; airflow velocity 90 m/s). For the protection of the substrate, environmental barrier coatings (EBCs) must be used. Due to their resistance to water vapor corrosion, high temperature phase stability, and matching thermal expansion coefficient with SiC CMCs substrates, rare earth silicate materials in EBC systems are currently receiving a lot of attention [1,10,11].

EBCs have evolved through three generations since the 1990s [12]. The initial generation of EBC systems, YSZ/Mullite, could not meet the practical application requirements under continuous thermal cycling because of crack propagation, which limited its ability to resist a few hundred hours in a water vapor atmosphere at 1300 °C [13,14]. Later, BSAS (1-xBaO·xSrO-Al2O3·2SiO2, 0 ≤ x ≤ 1) materials with low thermal expansion coefficients (4 × 10⁻⁶ K⁻¹–5.15 × 10⁻⁶ K⁻¹, and thus a close match with SiC, 4.02 × 10⁻⁶ K⁻¹) and a low elastic modulus (60–70 Gpa) were used to develop the second generation of EBCs [15]. These materials replaced YSZ as the surface coating, or they enhanced Mullite with BSAS or Mullite to form the BSAS/Mullite/Si system. Unfortunately, at 1584 K, the BSAS material system experiences a glass phase shift that shortens the coating’s lifespan by causing cracking [13,14,16]. BASA’s volatilization loss for 1000 h at 1400 °C, 6 atm total pressure and 24 m/s gas flow rate is as high as 70 µm. The third-generation rare earth silicate system has a high melting point (1950 °C), a low thermal conductivity (2.3 W·m⁻¹·K⁻¹–1.5 W·m⁻¹·K⁻¹), and a coefficient of thermal expansion (6–8 × 10⁻⁶ K⁻¹) similar to that of silicon-based ceramic materials (5 × 10⁻⁶ K⁻¹). And according to research, it can serve thousands of hours in a water vapor environment at 1482 °C, with excellent water vapor corrosion resistance. Therefore, rare earth silicate materials are drawing more and more attention [13,14,17–19].

Two distinct crystal phases can be distinguished in RE₂SiO₅ based on variations in rare earth elements (RE). All RE₂SiO₅ are monoclinic and stable as either space group P2₁/c or C2/c, which are generally termed the X1 and X2 structure. RE₂SiO₅ forms the X1 phase when the radius of the rare earth elements (RE = La, Ce, Pr, Nd, Sm, Eu, Tb, and Gd) is bigger, i.e., in the atomic numbers from 57 to 64. RE₂SiO₅ forms the X2 phase when the radius of the rare earth elements (RE = Dy, Ho, Er, Tm, Yb, and Lu) is lower [20], i.e., in the atomic numbers from 66 to 71. According to Mackenzie Ridley’s research, RE₂SiO₅ is in the X2 phase when the average radius of rare earth elements is less than 0.95 Å [21]. Two crystal structures are present in rare earth monosilicates; the X1 phase is stable at low temperatures (800–1200 °C) and the X2 phase emerges and is stable at high temperatures (1450–1950 °C) [22]. Volume differences brought forth by changes in the crystal shape affect stress fields and raise the possibility of cracking. Consequently, X2-phase monosilicates at high temperatures (1450–1550 °C) are frequently utilized in Environmental Barrier Coatings (EBCs). RE₂SiO₅, in X2 phase compounds, includes one silicon atom (Si), five oxygen atoms (O₁–O₅), and two distinct locations for rare earth elements (RE₁ and RE₂). While the other oxygen atom forms a loose link with the rare earth elements, the four separate oxygen atoms (O₁–O₄) combine to create a [SiO₄] tetrahedron with Si. The two distinct rare earth atoms have coordination numbers of 7 and 6, respectively, resulting in the compounds [REO₇] and [REO₆]. Whereas [REO₇] and [REO₆] are comparatively softer, the [SiO₄] tetrahedral structure is strong and has stiff characteristics. The mechanical and thermal properties of the material are greatly impacted by these features. The rigidity of the [SiO₄] tetrahedra endows the material with a higher modulus of elasticity and lower coefficient of thermal expansion, and thus the material typically exhibits better structural stability. In contrast, the weaker bonding of the [REO₇] and [REO₆] units allows for increased flexibility.
of the material, but may result in higher coefficients of thermal expansion and lower moduli of elasticity [20,21,23].

For multi-component rare earth monosilicates, the introduction of rare earth elements needs to be carefully selected, and different rare earth elements will have an impact on the Si-O bond strength and mechanical properties. It has been shown that the strength of the Si-O bond is proportional to the water vapor corrosion resistance of multi-component rare earth monosilicates, and the higher the strength of the Si-O bond, the stronger the water vapor corrosion resistance. For example, K. N. Lee [17] experimentally showed that the water vapor corrosion resistance of Yb$_2$SiO$_5$ is greater than that of Lu$_2$SiO$_5$. And Han et al. [24] calculated the Si-O bond length of Yb$_2$SiO$_5$ to be 1.6137 Å by the first nature principle, which is smaller than the Si-O bond length of Lu$_2$SiO$_5$ of 1.6246 Å [24]. The flexural strength, elastic modulus, and thermal shock resistance of monoclinic Re$_2$SiO$_5$ for orthosilicates are dependent on the mass and radius of the rare earth cations, as demonstrated by both experimental and Density Functional Theory (DFT) calculations. For example, according to the experiments, RE$_2$SiO$_5$ increases the elastic modulus from Tb$_2$SiO$_5$ (143.72 GPa) to Lu$_2$SiO$_5$ (171.3 GPa) and the shear modulus from Tb$_2$SiO$_5$ (61 GPa) to Lu$_2$SiO$_5$ (71 GPa) as the radius of the rare earth elements decreases [7].

In order to study the lattice distortions as well as the mechanical properties of Yb$_2$SiO$_5$ and YbRESiO$_5$ (where RE = Sc, Y, Eu, Gd, Ho, Tm, Lu), we calculated the crystal structures and the elastic properties of the materials using first-principles calculation. Furthermore, the Si-O bond lengths of eight different rare earth monosilicates were simulated to assess the materials’ resistance to water vapor corrosion. Additionally, Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$ bulk materials were produced utilizing solid-phase reaction techniques based on the outcomes of first-principles calculations in order to precisely investigate the impact of various rare earth cations on the mechanical and thermodynamic properties of the materials. Microstructural analysis and thermodynamic property evaluations of the composite materials were conducted. Last but not least, by investigating the effects of the crystal structure, coefficient of thermal expansion, thermal conductivity, and elastic constants of different rare earth monosilicates, this study may provide a theoretical framework for the creation of novel EBC materials.

2. Computational Models and Experimental Procedures

2.1. Computational Models

One silicon atom (Si), five oxygen atom sites (O1–O5), and two distinct rare earth atom sites (Yb1 and Yb2) make up the Yb$_2$SiO$_5$ unit cell. While the remaining oxygen atom loosely connects with the rare earth atoms, four of the oxygen atoms (O1–O4) form a [SiO$_4$] tetrahedron with the silicon atom. The two distinct rare earth atoms have coordination numbers of 7 and 6, respectively, resulting in the formation of [YbO$_7$] and [YbO$_6$] polyhedra [25]. Therefore, in the actual process, because larger atomic radius elements tend to occupy sites with larger coordination numbers, in the model of Yb$_2$SiO$_5$, to better approximate real conditions, rare earth elements (RE = Eu, Gd, Ho, Tm, Lu) with atomic radii larger than Yb were added into the Re1 site, while rare earth elements (RE = Sc, Y, Lu) with atomic radii smaller than Yb were added into the Re2 site [26]. The conventional and primitive cells of Yb$_2$SiO$_5$ are shown in Figure 1 a and b, respectively.

CASTEP was used to do computations from first principles. The most stable crystal structure at zero temperature was obtained by geometric optimization of the crystal structure of each rare earth silicate, which was then analyzed before the material’s resistance to water vapor corrosion and its thermodynamic properties were assessed. The crystal structure optimization method was carried out by expanding Bloch waves in reciprocal space with a cutoff energy of 450 eV using a plane wave basis set under periodic boundary conditions [27]. The first irreducible Brillouin zone was used as the discrete $2 \times 3 \times 4k$ sample grid for the Monkhorst-Pack technique of energy integration. The first irreducible Brillouin zone is the smallest, uniquely defined region in reciprocal space that contains all the distinct momentum states of a crystal, crucial for simplifying electronic band structure
calculations. Regarding exchange-correlation energies, the local density approximation (LDA) was employed [28]. To maximize the crystal structure, separate modifications were performed to the lattice constants and the relative locations of interior atoms. We used the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization approach to minimize both the interatomic forces and the overall energy [29]. We computed the electrostatic interactions between valence electrons and ionic cores using ultra-soft pseudopotentials. Atomic forces within 0.03 eV/Å, energy differences within $1 \times 10^{-5}$ eV/atom, maximum stress within 0.05 GPa, and maximum ion displacement within $1 \times 10^{-3}$ Å were the convergence conditions for geometric optimization. A distance of 3 Å was chosen as the Mulliken population cutoff distance (which is the threshold distance used to determine which atomic contributions to electronic charge density are considered significant in the Mulliken population analysis) [24].

Figure 1. (a) Conventional cell and (b) primitive cell of Yb$_2$SiO$_5$.

By linearly fitting stress against applied homogeneous elastic strains, the elastic constants were found. The strain–stress relationship approach developed by Milman and Warren was used to derive second-order elastic constants [30]. Four sets of uniform strain configurations (which refer to four different strain states applied in various directions and magnitudes to study changes in a material’s structure and properties) were used to calculate the 13 independent elastic constants ($c_{11}$, $c_{22}$, $c_{33}$, $c_{44}$, $c_{55}$, $c_{66}$, $c_{12}$, $c_{13}$, $c_{23}$, $c_{15}$, $c_{25}$, $c_{35}$, and $c_{45}$) of Yb$_2$SiO$_5$. Internal atomic degrees of freedom were optimized to yield the stresses. The linear fitting of computed stresses as a function of strain allowed for the determination of elastic stiffness. Maximum ion displacement differences were defined at $2 \times 10^{-4}$ Å, total energy differences within $2 \times 10^{-6}$ eV/atom, and Hellmann–Feynman force (which is the force on an atom or particle derived directly from the gradient of the potential energy with respect to atomic positions) differences within $0.006$ eV/Å as the convergence criterion for optimizing internal atomic degrees of freedom. The average sound velocity ($v_m$), Debye temperature ($\theta_D$), bulk modulus ($B$), shear modulus ($G$), Young’s modulus ($E$), and Poisson’s ratio ($\nu$) were then calculated using the elastic stiffness constants ($c_{ij}$) [31].

2.2. Material Preparation and Microstructure Characterization

The Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$ bulk materials were prepared using the solid-state reaction method. The raw materials included Sc$_2$O$_3$, Ho$_2$O$_3$, Yb$_2$O$_3$ (≥99.9 wt.% from Shanghai Maclin Biochemical Technology Co., Ltd., Shanghai, China), and SiO$_2$ (≥99.99 wt.% from Shanghai Maclin Biochemical Technology Co., Ltd.). The powdered raw materials were first placed in crucibles and dried in an oven for two hours at 393 K. After that, they were weighed using a molar ratio of 2:1 for silicon to rare earth elements. After that, a clean stainless-steel tank was filled with the materials, milling balls, and anhydrous ethanol in a mass ratio of 1:2:1. The tank was then subjected to a 10 h ball milling process at 270 revolutions per minute. The slurry that had been ground was dried in ovens for 12 h at 353 K and 393 K. Subsequently, the coarse oxides were crushed into powders using an agate grinding disc and sieved through an 80-mesh screen to achieve fine powders. After that, these fine powders were put into molds measuring φ15 mm, and they were uniaxially
pressed for five minutes at 15 MPa before oil pressure was applied. For thirty minutes, an oil pressure of 300 MPa was applied. To obtain the final products, the samples were sintered for 10 h at 1823 K.

Phase analysis of the sintered samples was carried out with an X-ray diffractometer (XRD, D/Max, 2550VB/PC, Rigaku, Tokyo, Japan) filtered with Cu Kα radiation at 18 KV accelerating voltage and 450 mA current. Using a step size of 10°/min, the diffraction angles were scanned from 10° to 80°. A scanning electron microscope (SEM, HITACHI S-3400 N, Japan) fitted with an energy-dispersive spectrometer (EDS, AMETEK APOLLO X, Berwyn, PA, USA) was used for microstructural examination.

2.3. Thermal Properties

Using standard metallographic techniques, all samples used in the thermal treatment experiments were cut from sintered bulk silicate.

Using a laser flash analyzer (NETZSCH, LFA 427, Germany), the bulk silicate’s thermal diffusivity was determined throughout a temperature range of 300 K to 1473 K. Sample dimensions were 12.7 mm × 2 mm. To reduce heat radiation, a thin layer of graphite was applied to the samples’ two sides prior to testing.

The thermal conductivity (k) of the material was calculated using the following formula, derived from thermal diffusivity (Dth), density (ρ), and specific heat capacity (c_p) [32]:

\[ k = D_{th} \cdot \rho \cdot c_p \]  

(1)

Additionally, the density (ρ) was determined using Archimedes’ method (which is using the principle of buoyancy to determine the volume of an irregularly shaped object) [33], while the specific heat capacity (c_p) was calculated using the Neumann–Kopp law (which states that the heat capacity of a substance is proportional to the number of atoms or molecules in a compound) [34]. Furthermore, the thermal conductivity of fully dense samples (k_0) was computed [35].

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

(2)

k is the theoretical thermal conductivity, ψ is the porosity. Additionally, thermal expansion coefficient-related parameters of bulk silicates were measured using a vertical high-temperature dilatometer (NETZSCH, DIL 402C, Germany) in the range of 303 K to 1473 K. The formula for calculating the thermal expansion coefficient (a) is as follows [31]:

\[ a = \frac{\Delta L}{L \cdot \Delta T} \]  

(3)

Here, L represents the original length of the sample, and ΔL denotes the length change of the sample under the temperature difference ΔT. The samples used were rectangular rods measuring 2 mm × 6 mm × 11 mm in the three dimensions.

3. Result and Discussion

3.1. First-Principles Calculations

After geometric optimization, the computed and theoretical lattice parameters of Yb₂SiO₅ are shown in Table 1. Deviation in this section is defined as the gap between the geometrically optimized lattice parameters of the material and the theoretical lattice parameters. Less than 3% separates the lattice constants from their theoretical values, indicating that the computations are reliable.

The crystal structures of YbRESiO₅ (RE = Sc, Y, Ho, Eu, Tm, Lu, Gd) following geometric optimization are displayed in Figure 2. Due of variations in rare earth element types, the locations of Si and O atoms vary during geometric optimization, leading to changes in lattice constants and subsequently affecting the unit cell volumes. The crystal
forms with various rare earth element dopants following geometric optimization are shown in Figure 2.

Table 1. The lattice parameters of Yb$_2$SiO$_5$ after lattice optimization and the theoretical lattice parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Yb$_2$SiO$_5$ Theory [20]</th>
<th>Yb$_2$SiO$_5$ Calculation</th>
<th>Deviation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$ (Å)</td>
<td>14.2800</td>
<td>14.1961</td>
<td>0.5021</td>
</tr>
<tr>
<td>$b$ (Å)</td>
<td>10.2800</td>
<td>10.0852</td>
<td>1.9052</td>
</tr>
<tr>
<td>$c$ (Å)</td>
<td>6.6530</td>
<td>6.5614</td>
<td>1.3013</td>
</tr>
<tr>
<td>$\gamma$ (°)</td>
<td>122.200</td>
<td>122.2250</td>
<td>0.0220</td>
</tr>
</tbody>
</table>

Figure 2. Geometrically optimized crystal structure of YbRESiO$_5$ (RE = Sc, Y, Lu, Tm, Ho, Gd, Eu). (a) YbScSiO$_5$, (b) YbYSiO$_5$, (c) YbLuSiO$_5$, (d) YbTmSiO$_5$, (e) YbHoSiO$_5$, (f) YbGdSiO$_5$, and (g) YbEuSiO$_5$. 
After geometric optimization with addition of different rare earth elements, Table 2 shows the lattice parameters and unit cell volumes of YbRESiO$_5$. According to computational analysis, the largest unit cell volume is produced by doping with the largest atomic radius element, Eu, and the smallest unit cell volume is produced by adding the element Sc. The overall trend is YbScSiO$_5$ (750.4240 Å$^3$) < YbHoSiO$_5$ (794.8210 Å$^3$) < Yb$_2$SiO$_5$ (794.7620 Å$^3$) < YbTmSiO$_5$ (800.1510 Å$^3$) < YbGdSiO$_5$ (806.6770 Å$^3$) < YbYSiO$_5$ (809.2980 Å$^3$) < YbLuSiO$_5$ (812.4510 Å$^3$) < YbEuSiO$_5$ (813.6240 Å$^3$).

Table 2. Geometrically optimized lattice parameters of YbRESiO$_5$ (RE = Sc, Y, Lu, Eu, Gd, Ho, Yb).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>a(Å)</th>
<th>b(Å)</th>
<th>c(Å)</th>
<th>γ(°)</th>
<th>V(Å$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>YbYSiO$_5$</td>
<td>14.2749</td>
<td>10.1817</td>
<td>6.5710</td>
<td>122.0710</td>
<td>809.2980</td>
</tr>
<tr>
<td>YbLuSiO$_5$</td>
<td>14.3203</td>
<td>10.1851</td>
<td>6.5834</td>
<td>122.2090</td>
<td>812.4510</td>
</tr>
<tr>
<td>YbHoSiO$_5$</td>
<td>14.1741</td>
<td>10.1046</td>
<td>6.5834</td>
<td>122.3620</td>
<td>794.8210</td>
</tr>
<tr>
<td>YbGdSiO$_5$</td>
<td>14.2360</td>
<td>10.1655</td>
<td>6.5936</td>
<td>122.2250</td>
<td>806.6770</td>
</tr>
<tr>
<td>YbScSiO$_5$</td>
<td>13.9188</td>
<td>9.94632</td>
<td>6.4012</td>
<td>122.1350</td>
<td>750.4240</td>
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<tr>
<td>YbTmSiO$_5$</td>
<td>14.1493</td>
<td>10.1100</td>
<td>6.6152</td>
<td>122.2340</td>
<td>800.1510</td>
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<tr>
<td>YbYSiO$_5$</td>
<td>14.1916</td>
<td>10.0858</td>
<td>6.5616</td>
<td>122.2250</td>
<td>794.7620</td>
</tr>
<tr>
<td>YbEuSiO$_5$</td>
<td>14.2760</td>
<td>10.1632</td>
<td>6.6205</td>
<td>122.2340</td>
<td>813.6240</td>
</tr>
</tbody>
</table>

3.1.1. Crystal Lattice Distortion Calculation

To quantitatively describe the distortion of polyhedra, the following equation is used to calculate the lattice distortion within the material [25]:

$$\Delta d = \frac{1}{n} \sum_n \left( \frac{d(\text{MO})_n - [d(\text{MO})_{\text{RE}}]}{d(\text{MO})_{\text{RE}}} \right)^2$$

(4)

Here, $d(\text{MO})_{\text{RE}}$ represents the average bond length of Re-O and Si-O in YbReSiO$_5$ (Re = Sc, Y, Lu, Eu, Gd, Ho). The average bond lengths between the rare earth element (Re) or silicon (Si) and the nth oxygen atom.

Table 3 gives the bond lengths, average bond lengths, and lattice distortions of [SiO$_4$], [REO$_6$], and [REO$_7$] in YbRESiO$_5$ (RE = Sc, Y, Lu, Eu, Gd, Ho, Yb). We discovered that adding Sc, the element with the smallest atomic radius in our investigation, drastically alters the bond lengths and lattice distortions of the material when compared to Yb$_2$SiO$_5$. In comparison to Yb$_2$SiO$_5$, YbScSiO$_5$ has the highest lattice distortions in [REO$_6$] and [REO$_7$], rising by approximately 50% and 60%, respectively. It also has the shortest average RE-O bond lengths in [REO$_6$] and [REO$_7$]. Compared to Yb$_2$SiO$_5$, its average RE-O bond lengths decrease by 0.5% and 4.4%. Conversely, among elements that increase the RE-O bond lengths, adding Eu resulted in the longest RE-O bond lengths in [REO$_6$] and [REO$_7$] for YbEuSiO$_5$, rising by roughly 1.3% and 1.5%, respectively, compared to Yb$_2$SiO$_5$.

In this study, the average RE-O bond lengths in [REO$_6$] polyhedra for the eight different rare earth monosilicates are ordered as follows: YbScSiO$_5$ (2.10674 Å) < YbHoSiO$_5$ (2.21699 Å) < YbTmSiO$_5$ (2.21344 Å) < Yb$_2$SiO$_5$ (2.21750 Å) < YbLuSiO$_5$ (2.24643 Å) < YbGdSiO$_5$ (2.23314 Å) < YbEuSiO$_5$ (2.23771 Å). In [REO$_7$] polyhedra, the average RE-O bond lengths are ordered as: YbScSiO$_5$ (2.29198 Å) < Yb$_2$SiO$_5$ (2.30098 Å) < YbTmSiO$_5$ (2.30253 Å) < YbYSiO$_5$ (2.31480 Å) < YbLuSiO$_5$ (2.31456 Å) < YbHoSiO$_5$ (2.32545 Å) < YbGdSiO$_5$ (2.32157 Å) < YbEuSiO$_5$ (2.33001 Å). The lattice distortion in [REO$_6$] is ranked as follows: YbEuSiO$_5$ (1.26024‰) < YbGdSiO$_5$ (1.27335‰) < Yb$_2$SiO$_5$ (1.63300‰) < YbTmSiO$_5$ (1.68293‰) < YbLuSiO$_5$ (1.82196‰) < YbYSiO$_5$ (2.07000‰) < YbHoSiO$_5$ (2.37837‰) < YbScSiO$_5$ (3.31675‰). The lattice distortion in [REO$_7$] polyhedra is ranked as: YbYSiO$_5$ (0.06170‰) < YbLuSiO$_5$ (0.07019‰) < YbGdSiO$_5$ (0.11984‰) < Yb$_2$SiO$_5$ (0.12334‰) < YbTmSiO$_5$ (0.20894‰) < YbHoSiO$_5$ (0.31473‰) < YbEuSiO$_5$ (0.37126‰) < YbScSiO$_5$ (0.47114‰). Among the eight rare earth monosilicates, YbScSiO$_5$ has the biggest lattice distortion and the shortest RE-O bond length. We relate this to the considerable difference in atomic radii between Yb and Sc elements. Additionally, the introduction of various
elements also affects the lattice distortion of [SiO$_4$] tetrahedra, but because of their rigid nature, the amplitude of variation is not significant in this study and thus is not discussed in detail here. YbScSiO$_5$ exhibits the largest lattice distortion and shortest RE-O bond length as a result of this heterogeneity in rare earth cation radii.

Table 3. Lattice distortion values of different rare earth monociliate.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Bond</th>
<th>Polyhedra</th>
<th>Bond Length (Å)</th>
<th>Average Bond Length (Å)</th>
<th>Degree of Distortion (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yb$_2$SiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.17365, 2.26578, 2.27687, 2.28556, 2.29827, 2.3003, 2.50635</td>
<td>2.30098</td>
<td>1.63300</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.17305, 2.20835, 2.21083, 2.22665, 2.22665, 2.24791</td>
<td>2.21750</td>
<td>0.12334</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.5915, 1.60382, 2.60696, 1.6228</td>
<td>1.60627</td>
<td>0.04824</td>
</tr>
<tr>
<td>YbTmSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.1845, 2.23035, 2.24948, 2.28916, 2.31377, 2.35425, 2.4962</td>
<td>2.30253</td>
<td>1.68259</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.15346, 2.20741, 2.21105, 2.22142, 2.2615, 2.2616</td>
<td>2.21344</td>
<td>0.20894</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59125, 1.60026, 2.60967, 1.62292</td>
<td>1.60592</td>
<td>0.05333</td>
</tr>
<tr>
<td>YbEuSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.22305, 2.26695, 2.31138, 2.35425, 2.4962</td>
<td>2.32157</td>
<td>1.27335</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.15427, 2.22478, 2.23663, 2.25526, 2.26148, 2.29384</td>
<td>2.23771</td>
<td>0.37126</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59478, 1.60692, 2.61483, 1.61983</td>
<td>1.60759</td>
<td>0.03971</td>
</tr>
<tr>
<td>YbGdSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.2152, 2.26505, 2.29988, 2.31368, 2.35175, 2.49526</td>
<td>2.32157</td>
<td>1.27335</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.19257, 2.21548, 2.23483, 2.23147, 2.25323, 2.26769</td>
<td>2.23314</td>
<td>0.11984</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59321, 1.60148, 2.6151, 1.62029</td>
<td>1.60752</td>
<td>0.04468</td>
</tr>
<tr>
<td>YbHoSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.20992, 2.25368, 2.28601, 2.30662, 2.34039, 2.58406</td>
<td>2.32545</td>
<td>2.37837</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.20766, 2.22172, 2.22778, 2.23061, 2.27294, 2.14123</td>
<td>2.21699</td>
<td>0.31473</td>
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<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59119, 1.5994, 2.61279, 1.62194</td>
<td>1.60633</td>
<td>0.05451</td>
</tr>
<tr>
<td>YbLuSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.17016, 2.28852, 2.28869, 2.30331, 2.30836, 2.31393, 2.52894</td>
<td>2.31456</td>
<td>1.82196</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.21116, 2.23925, 2.24528, 2.25512, 2.25873, 2.26928</td>
<td>2.24643</td>
<td>0.07019</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59393, 1.60716, 2.61992, 1.61873</td>
<td>1.60744</td>
<td>0.03059</td>
</tr>
<tr>
<td>YbScSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.15248, 2.21908, 2.23995, 2.2501, 2.28767, 2.29817, 2.59642</td>
<td>2.29198</td>
<td>3.31675</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.11166, 2.02535, 2.08059, 2.11853, 2.13039, 2.17394</td>
<td>2.10674</td>
<td>0.47114</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.59075, 1.5956, 2.60682, 1.61564</td>
<td>1.60243</td>
<td>0.05863</td>
</tr>
<tr>
<td>YbYSiO$_5$</td>
<td>RE1-O</td>
<td>[REO$_7$]</td>
<td>2.17206, 2.28342, 2.29012, 2.29846, 2.30223, 2.30753, 2.54975</td>
<td>2.31480</td>
<td>2.07000</td>
</tr>
<tr>
<td></td>
<td>RE2-O</td>
<td>[REO$_6$]</td>
<td>2.19854, 2.23202, 2.23482, 2.23868, 2.24511, 2.25553</td>
<td>2.23415</td>
<td>0.06170</td>
</tr>
<tr>
<td></td>
<td>Si-O</td>
<td>[SiO$_4$]</td>
<td>1.5952, 2.60773, 1.60961, 1.61904</td>
<td>1.60620</td>
<td>0.02906</td>
</tr>
</tbody>
</table>

3.1.2. Water Vapor Corrosion Resistance

Testing the water vapor corrosion resistance in environments similar to combustion but without alumina is necessary because the majority of current experiments on environmental barrier coatings for water vapor corrosion are carried out in alumina tubes, and there are reports that alumina contamination may alter the water vapor corrosion resistance of RE$_2$SiO$_5$ [9]. It is difficult, though, to carry out useful research in such hot conditions without adding alumina materials. Thus, in order to acquire theoretical information on the water vapor corrosion resistance of eight materials, this work uses first-principles calculations. It has been demonstrated that using first-principles calculations to predict the properties of compounds with various components but the same crystal structure works well [24]. For example, the strength of the Si-O linkages can reflect the water vapor corrosion resistance of RE$_2$SiO$_5$ with the same crystal structure.

The Si-O bonds in rare earth silicates are broken down by steam during high-temperature water vapor corrosion, which corrodes environmental barrier coatings by Si-O degradation.
The pace of corrosion is slower if the Si-O bonds are generally stable; on the other hand, the rate of corrosion is higher if the Si-O bonds are weak. As a result, by determining the strength of the Si-O linkages, the water vapor corrosion resistance of rare earth monosilicates may be compared [36]. Si-O bond density, which is defined as the ratio of Si-O bond energy to Si-O bond length, usually directly correlates with the strength of Si-O bonds. Determining the Si-O bond information through first-principles calculations on materials enables evaluation of the water vapor corrosion performance of various rare earth monosilicates.

Eight distinct rare earth monosilicates are shown in Figure 3 and Table 4 along with their Si-O bond densities, Milliken populations, and Si-O bond lengths. Our calculations show that, out of the eight materials, YbScSiO$_5$ has the highest resistance to water vapor corrosion because it has the shortest Si-O link length (1.60243 Å), the highest Milliken population (0.63500), and the greatest bond density (0.3963 Å$^{-1}$). Following Eu addition, YbEuSiO$_5$ has the longest Si-O bond length (0.61000 Å); nevertheless, it also has a lower Milliken population (0.61000) and bond density (0.3794 Å$^{-1}$) than Yb$_2$SiO$_5$, suggesting that it is less resistant to water vapor corrosion than Yb$_2$SiO$_5$. The water vapor corrosion resistance of Yb$_2$SiO$_5$ is generally enhanced by adding Sc, Ho, and Tm, and decreased by doping with Gd, Eu, Y, and Lu. Overall, the ranking of water vapor corrosion resistance among the eight different rare earth monosilicates is as follows: YbLuSiO$_5$ (0.3764 Å$^{-1}$) < YbEuSiO$_5$ (0.3794 Å$^{-1}$) < YbGdSiO$_5$ (0.3810 Å$^{-1}$) < YbYSiO$_5$ (0.3811 Å$^{-1}$) < Yb$_2$SiO$_5$ (0.3844 Å$^{-1}$) < YbTmSiO$_5$ (0.3851 Å$^{-1}$) < YbHoSiO$_5$ (0.3860 Å$^{-1}$) < YbScSiO$_5$ (0.3963 Å$^{-1}$).

![Graphs](image-url)

Figure 3. (a) Si-O bond lengths, (b) Milliken population, and (c) density of Si-O bonds for YbRESiO$_5$ (RE = Yb, Sc, Y, Lu, Tm, Ho, Gd, Eu).
Table 4. Si-O bond information for YbRESiO$_5$ (RE = Yb, Sc, Y, Lu, Tm, Ho, Gd, Eu).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Bond Average (Å)</th>
<th>Population of Bond</th>
<th>Density (Å$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yb$_2$SiO$_5$</td>
<td>1.60627</td>
<td>0.61750</td>
<td>0.3844</td>
</tr>
<tr>
<td>YbTmSiO$_5$</td>
<td>1.60603</td>
<td>0.61850</td>
<td>0.3851</td>
</tr>
<tr>
<td>YbEuSiO$_5$</td>
<td>1.60759</td>
<td>0.61000</td>
<td>0.3794</td>
</tr>
<tr>
<td>YbGdSiO$_5$</td>
<td>1.60752</td>
<td>0.61250</td>
<td>0.3810</td>
</tr>
<tr>
<td>YbHoSiO$_5$</td>
<td>1.60620</td>
<td>0.6200</td>
<td>0.3860</td>
</tr>
<tr>
<td>YbLuSiO$_5$</td>
<td>1.60744</td>
<td>0.6050</td>
<td>0.3764</td>
</tr>
<tr>
<td>YbScSiO$_5$</td>
<td>1.60243</td>
<td>0.63500</td>
<td>0.3963</td>
</tr>
<tr>
<td>YbYSiO$_5$</td>
<td>1.60630</td>
<td>0.61720</td>
<td>0.3811</td>
</tr>
</tbody>
</table>

3.1.3. Elastic Constants

The elastic constants of YbRESiO$_5$ (RE = Yb, Eu, Gd, Ho, Tm, Lu, Y, Sc) that were determined using first-principles techniques are shown in Table 5. The average sound velocity, Debye temperature, bulk modulus, shear modulus, and Young’s modulus of Yb$_2$SiO$_5$ are all markedly increased by the equimolar addition of Sc, while the addition of Gd has the reverse effect. Poisson’s ratio is the lowest when adding Ho. The order of magnitude for average sound velocity is as follows: YbGdSiO$_5$ (2875.6370 m/s) < YbEuSiO$_5$ (3027.7198 m/s) < YbHoSiO$_5$ (3047.4524 m/s) < YbTmSiO$_5$ (3115.4777 m/s) < Yb$_2$SiO$_5$ (3116.0476 m/s) < YbLuSiO$_5$ (3136.1570 m/s) < YbYSiO$_5$ (3282.3078) < YbScSiO$_5$ (3669.7119 m/s). The ranking of the Debye temperature is YbGdSiO$_5$ (367.7621 K) < YbEuSiO$_5$ (392.4537 K) < YbHoSiO$_5$ (394.2189 K) < YbTmSiO$_5$ (395.7621 K) < Yb$_2$SiO$_5$ (400.2373 K) < YbLuSiO$_5$ (403.6193 K) < YbYSiO$_5$ (419.4569 K) < YbScSiO$_5$ (481.4030 K). The ranking of Young’s modulus is YbGdSiO$_5$ (125.8217 Gpa) < YbEuSiO$_5$ (134.4732 Gpa) < YbHoSiO$_5$ (139.7532 Gpa) < YbYSiO$_5$ (145.4985 Gpa) < YbTmSiO$_5$ (145.6084 Gpa) < YbLuSiO$_5$ (151.7248 Gpa) < Yb$_2$SiO$_5$ (153.4019 Gpa) < YbScSiO$_5$ (162.0600 Gpa).

Table 5. Elastic constants of YbRESiO$_5$ (RE = Yb, Tm, Eu, Gd, Lu, Ho, Sc, Y).

<table>
<thead>
<tr>
<th>Compound</th>
<th>$v_{sh}$ (m/s)</th>
<th>$\Theta_D$ (K)</th>
<th>$B$ (Gpa)</th>
<th>$G$ (Gpa)</th>
<th>$E$ (Gpa)</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yb$_2$SiO$_5$</td>
<td>3116.0476</td>
<td>400.2373</td>
<td>116.9618</td>
<td>59.8568</td>
<td>153.4019</td>
<td>0.2696</td>
</tr>
<tr>
<td>YbTmSiO$_5$</td>
<td>3115.4777</td>
<td>395.7621</td>
<td>105.4786</td>
<td>57.3296</td>
<td>145.6084</td>
<td>0.2699</td>
</tr>
<tr>
<td>YbEuSiO$_5$</td>
<td>3027.7198</td>
<td>392.4537</td>
<td>102.4666</td>
<td>57.1057</td>
<td>134.4732</td>
<td>0.2677</td>
</tr>
<tr>
<td>YbGdSiO$_5$</td>
<td>2875.6370</td>
<td>367.7621</td>
<td>92.0294</td>
<td>49.4669</td>
<td>125.8217</td>
<td>0.2721</td>
</tr>
<tr>
<td>YbHoSiO$_5$</td>
<td>3136.1570</td>
<td>403.6193</td>
<td>106.2719</td>
<td>60.1105</td>
<td>151.7248</td>
<td>0.2621</td>
</tr>
<tr>
<td>YbLuSiO$_5$</td>
<td>3047.4524</td>
<td>394.2189</td>
<td>97.2663</td>
<td>55.4342</td>
<td>139.7532</td>
<td>0.2605</td>
</tr>
<tr>
<td>YbScSiO$_5$</td>
<td>3669.7119</td>
<td>481.4030</td>
<td>126.2605</td>
<td>63.0056</td>
<td>162.0600</td>
<td>0.2861</td>
</tr>
<tr>
<td>YbYSiO$_5$</td>
<td>3282.3078</td>
<td>419.4569</td>
<td>95.0679</td>
<td>53.6648</td>
<td>145.4985</td>
<td>0.2625</td>
</tr>
</tbody>
</table>

Studies have indicated that the atomic number of the rare earth element has a substantial impact on the elastic modulus and flexural strength of X$_2$-RE$_2$SiO$_5$ samples. This discovery could be explained by the rare earth element’s decreased ionic radius increasing rare earth–oxygen interactions. In X$_2$-RE$_2$SiO$_5$ samples, the bond strength can be represented by the cation field strength (CFS) [7]. The calculation formula for CFS is as follows [37]:

$$CFS = Z_c/r_c^2$$

(5)

$Z_c$ represents the cation charge, and $r_c^2$ represents the cation radius squared.

It is clear from the data in Table 6 that when the ionic radius of rare earth elements falls, so does the bonding strength between oxygen and rare earth in X$_2$-RE$_2$SiO$_5$. Consequently, the cation field strength (CFS) of cations having larger radii, including Gd$^{3+}$, Eu$^{3+}$, Ho$^{3+}$, Tm$^{3+}$, and Y$^{3+}$, is lower than that of Yb$_2$SiO$_5$. As a result, when adding cations such as Gd$^{3+}$, Eu$^{3+}$, Ho$^{3+}$, Tm$^{3+}$, and Y$^{3+}$, the Young’s modulus lowers. Of the eight rare earth monosilicates, the element Sc$^{3+}$ with the shortest cation radius has the highest CFS and,
consequently, the highest Young’s modulus. The findings of the computed elastic modulus, however, do not quite match the CFS ranking. This disparity can be explained by the fact that materials containing Yb frequently show aberrant characteristics in comparison to other lanthanide elements, such as a different melting and boiling point and density. This observation might be explained by the fact that Yb ([Xe]4f^{14}6s^2) has a closed-shell atomic configuration, meaning that there are only two 6s valence electrons accessible for chemical bonding [7].

Table 6. CFS of rare earth cations in YbRESiO₅ (RE = Yb, Sc, Y, Lu, Tm, Ho, Gd, Eu).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Average Ionic Radius</th>
<th>CFS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yb₂SiO₅</td>
<td>0.86</td>
<td>4.056</td>
</tr>
<tr>
<td>YbTmSiO₅</td>
<td>0.865</td>
<td>4.009</td>
</tr>
<tr>
<td>YbEuSiO₅</td>
<td>0.905</td>
<td>3.662</td>
</tr>
<tr>
<td>YbGdSiO₅</td>
<td>0.9</td>
<td>3.370</td>
</tr>
<tr>
<td>YbHoSiO₅</td>
<td>0.88</td>
<td>3.387</td>
</tr>
<tr>
<td>YbLuSiO₅</td>
<td>0.855</td>
<td>4.104</td>
</tr>
<tr>
<td>YbScSiO₅</td>
<td>0.835</td>
<td>4.303</td>
</tr>
<tr>
<td>YbYSiO₅</td>
<td>0.875</td>
<td>3.918</td>
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</table>

3.2. Phases and Microstructure of Sintered Bulk Materials

Three materials’ XRD patterns are displayed in Figure 4: Yb₂SiO₅, YbScSiO₅, and YbEuSiO₅. There is no second phase in the prepared silicate bulk materials, according to the measured diffraction peaks between the prepared monosilicates and the standard PDF of the Yb₂SiO₅ card (97-000-4446). Shifts in the diffraction peaks of YbScSiO₅ and YbEuSiO₅ relative to the standard Yb₂SiO₅ PDF card are detected upon doping Yb₂SiO₅ with Sc and Eu. The diffraction peaks move to larger angles when the smaller cation radius element (Sc³⁺) is incorporated into Yb₂SiO₅. This is due to a change in lattice parameters. On the other hand, adding a higher cation radius element (Eu³⁺) increases the lattice parameters and causes the peaks of diffraction to move to smaller angles. These outcomes agree with the XRD patterns in Figure 4 and the simulated computations in Table 2. The unit cell volume of Yb₂SiO₅ drops by 5.1% when equal moles of Sc are added, but increases by 2.3% when doped with the same moles of Eu. Consequently, YbScSiO₅ (750.4240 Å³) < Yb₂SiO₅ (794.7620 Å³) < YbEuSiO₅ (813.6240 Å³) is the order in which the unit cell volumes of the three materials are arranged.

Figure 4. XRD patterns of YbReSiO₅ (Re = Yb, Sc, Eu).
As seen in the XRD patterns in Figure 4, which show no further phases, the produced rare earth monosilicates often have few pores and no noticeable fissures. Furthermore, porosity levels within 5% were demonstrated by the density and porosity calculations of \( \text{Yb}_2\text{SiO}_5 \), \( \text{YbScSiO}_5 \), and \( \text{YbEuSiO}_5 \), as indicated in Table 3. The microstructures of cross-sections of the materials \( \text{Yb}_2\text{SiO}_5 \), \( \text{YbScSiO}_5 \), and \( \text{YbEuSiO}_5 \) are displayed in Figure 5. A homogeneous distribution of elements is revealed by EDS scans of the elemental distribution in the three materials (Figure 6). When paired with the XRD results shown in Figure 4, these results show that the \( \text{Yb}_2\text{SiO}_5 \), \( \text{YbScSiO}_5 \), and \( \text{YbEuSiO}_5 \) sample preparation procedures were accurate and produced materials that were reasonably pure. The results of various densities and porosities of the three materials are shown in Table 7.

![Figure 5](image-url)  
Figure 5. (a) Microstructure of \( \text{Yb}_2\text{SiO}_5 \), (b) microstructure of \( \text{YbScSiO}_5 \), and (c) microstructure of \( \text{YbEuSiO}_5 \).

![Figure 6](image-url)  
Figure 6. (a) Element distribution of \( \text{Yb}_2\text{SiO}_5 \), (b) element distribution of \( \text{YbScSiO}_5 \), and (c) element distribution of \( \text{YbEuSiO}_5 \).

<table>
<thead>
<tr>
<th>Compound</th>
<th>( \rho(\text{Re}_2\text{SiO}_3) ) (g cm(^{-3}))</th>
<th>( \omega(\text{Re}_2\text{SiO}_3) ) (wt.%)</th>
<th>( \omega(\text{SiO}_2) ) (wt.%)</th>
<th>( \rho(\text{Exp.}) ) (g cm(^{-3}))</th>
<th>( d ) (%)</th>
<th>( \psi ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Yb}_2\text{SiO}_5 )</td>
<td>7.28</td>
<td>86.77</td>
<td>13.23</td>
<td>7.12</td>
<td>97.80</td>
<td>2.20</td>
</tr>
<tr>
<td>( \text{YbEuSiO}_5 )</td>
<td>5.76</td>
<td>81.57</td>
<td>18.43</td>
<td>5.49</td>
<td>95.31</td>
<td>4.69</td>
</tr>
<tr>
<td>( \text{YbScSiO}_5 )</td>
<td>6.69</td>
<td>86.13</td>
<td>13.87</td>
<td>6.40</td>
<td>95.66</td>
<td>4.34</td>
</tr>
</tbody>
</table>
3.3. Thermal Performance Test
3.3.1. Thermal Conductivity

Figure 7 shows the thermal expansion coefficients and specific heat capacities of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$ within the temperature range of 300 K to 1473 K. For these three rare earth monosilicates, the thermal expansion coefficients often decrease with increasing temperature, which is consistent with the typical trend of phonon thermal conductivity [25,38]. Both the thermal conductivity and the thermal expansion coefficient, however, exhibit a rising trend at 800 °C, most likely as a result of radiation heat transfer effects, which have also been noted in other tests [39]. Consequently, statistics on laser thermal conductivity above 800 °C should be regarded as approximations. The thermal diffusivity of Yb$_2$SiO$_5$ ranges from 0.470 mm$^2$·s$^{-1}$ to 0.788 mm$^2$·s$^{-1}$ between 300 K and 1473 K. YbScSiO$_5$ exhibits a thermal diffusivity ranging from 0.506 mm$^2$·s$^{-1}$ to 0.751 mm$^2$·s$^{-1}$. The lowest thermal expansion coefficient is shown by YbEuSiO$_5$, which ranges from 0.352 mm$^2$·s$^{-1}$ to 0.610 mm$^2$·s$^{-1}$.

![Figure 7](image)

**Figure 7.** (a) Thermal diffusivity of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$, (b) specific heat capacity of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$.

Three distinct rare earth monosilicates’ actual and theoretical thermal conductivities are displayed in Figure 8. In this investigation, the porosity of all three samples stayed below 5%. The estimated theoretical value of 2.17 W·m$^{-1}$·K$^{-1}$ for Yb$_2$SiO$_5$ at ambient temperature closely matches the reported value of 2.2 W·m$^{-1}$·K$^{-1}$ for Yb$_2$SiO$_5$ in the literature [40]. The theoretical thermal conductivity of Yb$_2$SiO$_5$ at normal temperatures is 2.07 W·m$^{-1}$·K$^{-1}$. Microstructural variations, such as variations in grain size and the impact of infrared radiation at high temperatures, may be the cause of the poorer thermal conductivity and thermal diffusivity of Yb$_2$SiO$_5$ in this investigation. Additionally, YbScSiO$_5$ has a range of 1.85 W·m$^{-1}$·K$^{-1}$ to 1.67 W·m$^{-1}$·K$^{-1}$, YbEuSiO$_5$ exhibits the lowest thermal conductivity among the three materials, ranging from 1.44 W·m$^{-1}$·K$^{-1}$ to 1.07 W·m$^{-1}$·K$^{-1}$, and Yb$_2$SiO$_5$ varies from 2.07 W·m$^{-1}$·K$^{-1}$ to 1.52 W·m$^{-1}$·K$^{-1}$. Overall, the addition of Sc elements results in very little change in thermal conductivity and thermal diffusivity; at 650 K, YbScSiO$_5$ exhibits slightly higher values than Yb$_2$SiO$_5$, but before this temperature, the tendency is the opposite. On the other hand, YbEuSiO$_5$’s diffusivity and thermal conductivity dramatically drop with the addition of Eu. The experiment’s observation of radiation heat transfer may be the cause of the rise in thermal conductivity at 1073 K.
This study states that the thermal conductivity of Sc₂SiO₅ material is 1.67 times greater than that of Yb₂SiO₅ and varies from 2.50 W·m⁻¹·K⁻¹ to 3.50 W·m⁻¹·K⁻¹ between 400 K and 1673 K. Eu₂SiO₅ has a lower thermal conductivity than Yb₂SiO₅, ranging from 1.50 W·m⁻¹·K⁻¹ to 1.25 W·m⁻¹·K⁻¹. As a result, it drops to 1.25 W·m⁻¹·K⁻¹, which is less than Yb₂SiO₅ [26,35]. Thus, it can be deduced that there may be a positive correlation between the thermal conductivity of rare earth monosilicate materials doped with binary equimolar elements and the thermal conductivity of their parent materials. Additionally, YbScSiO₅ and YbEuSiO₅ exhibit greater specific heat capacity than Yb₂SiO₅, with the inclusion of Sc elements having a particularly notable effect. Yb₂SiO₅ with Sc may somewhat raise the material’s thermal conductivity, while doping the material with Eu may result in a minor drop in thermal conductivity. Nonetheless, the square root of thermal conductivity and phonon scattering coefficient are inversely proportional in materials with added point defects because of the large lattice distortion in YbScSiO₅ and the adherence to phonon heat transfer principles in those materials. Higher phonon scattering coefficients can result from larger lattice distortions and mismatched rare earth cation weights and radii. This could account for YbScSiO₅’s weaker thermal diffusivity and conductivity than Yb₂SiO₅ at temperatures lower than 600 K.

The outer electron structure of Eu, which is 4f⁷6s², is another factor contributing to YbEuSiO₅’s lowest thermal conductivity. Its outer electron structure becomes 4f⁷ when it loses two electrons. Based on Hund’s rule, 4f⁷ is in a stable half-filled state. Eu²⁺ ions, which encourage the creation of oxygen vacancies and drastically lower thermal conductivity, may therefore be present in YbEuSiO₅ [26]. Overall, compared to Yb₂SiO₅, the insertion of Sc components exhibits little overall change in thermal conductivity and thermal diffusivity. On the other hand, compared to Yb₂SiO₅, the addition of Eu elements leads to much decreased thermal diffusivity and thermal conductivity because of the development of oxygen vacancies. In particular, YbEuSiO₅ has a minimum thermal conductivity of 1.07 W·m⁻¹·K⁻¹ in the temperature range of 303 K to 1473 K, which is 29% less than Yb₂SiO₅’s (1.52 W·m⁻¹·K⁻¹). Moreover, YbEuSiO₅’s (1.44 W·m⁻¹·K⁻¹ to 1.07 W·m⁻¹·K⁻¹) thermal conductivity fluctuates less in this temperature range than Yb₂SiO₅’s (2.07 W·m⁻¹·K⁻¹ to 1.52 W·m⁻¹·K⁻¹). Furthermore, the stability of the temperature and stress fields is aided by the low range of thermal conductivity parameters. For materials that are monosilicate, these elements are essential.

3.3.2. CTE

Figure 9 shows the coefficient of thermal expansion (CTE) and ΔL/L curves of Yb₂SiO₅, YbScSiO₅, and YbEuSiO₅ from 303 K to 1473 K. Compared to Yb₂SiO₅, YbEuSiO₅ exhibits...
an increasing trend in $\Delta L/L$, while YbScSiO$_5$ shows a decreasing trend. Here, $\Delta L$ is the only representation of the change because $L$, the original length, is a constant. In contrast to Yb$_2$SiO$_5$, the effects of Sc and Eu doping on $\Delta L$ are opposite. In order to get precise coefficients of thermal expansion for monosilicate materials, as shown in Figure 8, it is noted that, for Yb$_2$SiO$_5$, the CTE varies between $5.86 \times 10^{-6}$ K$^{-1}$ and $8.05 \times 10^{-6}$ K$^{-1}$ over the 600 K to 1473 K temperature range. The results of this investigation closely match those of Tian et al. and mistakes lower than $0.5 \times 10^{-6}$ K$^{-1}$ can often be ignored, as they are most likely the result of experimental and sampling mistakes. The addition of Eu to YbEuSiO$_5$ raises its CTE in comparison to Yb$_2$SiO$_5$, while Sc doping lowers the CTE of YbScSiO$_5$, following the $\Delta L/L$ trends. YbScSiO$_5$ and YbEuSiO$_5$ show CTE values of $5.64 \times 10^{-6}$ K$^{-1}$ to $7.56 \times 10^{-6}$ K$^{-1}$ and $6.16 \times 10^{-6}$ K$^{-1}$ to $8.6 \times 10^{-6}$ K$^{-1}$, respectively, throughout the 600 K to 1473 K range. Compared to Yb$_2$SiO$_5$, the addition of Sc lowers the material’s overall CTE as well as the amplitude of its temperature-dependent CTE variation. On the other hand, Eu’s introduction has the opposite impact.

![Figure 9](image-url) (a) Thermal expansion coefficient (CTE) of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$. (b) $\Delta L/L$ curves of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$.

The coefficient of thermal expansion (CTE) of YbScSiO$_5$ doped with Sc is often lower than that of Yb$_2$SiO$_5$, but the CTE of YbEuSiO$_5$ doped with Eu is higher. YbScSiO$_5$ has the lowest CTE at 1473 K, $7.56 \times 10^{-6}$ K$^{-1}$, 7% less than Yb$_2$SiO$_5$, whereas YbEuSiO$_5$ has the greatest CTE at $8.6 \times 10^{-6}$ K$^{-1}$, 7.5% more than Yb$_2$SiO$_5$.

The coefficient of thermal expansion (CTE) of rare earth monosilicates should be correlated with the parent silicate, based on the experimental data presented in this work [31]. Based on Mackenzie et al.’s research, we discovered that Sc$_2$SiO$_5$ has a thermal expansion coefficient between $4 \times 10^{-6}$ K$^{-1}$ and $6 \times 10^{-6}$ K$^{-1}$ in the 200 °C to 1200 °C temperature range. This is much lower than that of Yb$_2$SiO$_5$. As reported by Chen et al., we discovered that the thermal expansion coefficient of Eu$_2$SiO$_5$ is significantly larger than that of Yb$_2$SiO$_5$ in the temperature range of 200 °C to 1200 °C, ranging from $7 \times 10^{-6}$ K$^{-1}$ to $8.5 \times 10^{-6}$ K$^{-1}$ [26,40]. This could be the reason for the difference in material CTE seen when doping Yb$_2$SiO$_5$ with Sc versus Eu. Because this phenomenon is not examined in further detail in the current work, more theoretical and experimental research is required to validate it.

4. Conclusions

The crystal structure, elastic constants, Si-O bond lengths, and bond energies of YbRESiO$_5$ (RE = Yb, Eu, Gd, Ho, Tm, Lu, Y, Sc) were investigated in this work using first-principles calculations. Using a solid-state reaction, dense polycrystalline ceramics of Yb$_2$SiO$_5$, YbScSiO$_5$, and YbEuSiO$_5$ were created. The created ceramic samples were subjected to thermal tests. The following is a summary of the primary conclusions:

1. According to first-principles calculations, the crystal structure and elastic properties of Yb$_2$SiO$_5$ are affected differently when equimolar amounts of rare earth elements
RE (RE = Eu, Gd, Ho, Tm, Lu, Y, Sc) are added. In particular, doping the material with Eu, which has the largest atomic radius, and Sc, which has the smallest, seems to have opposite effects. While YbEuSiO₅ has the opposite behavior, YbScSiO₅ has the biggest lattice distortion, average sound velocity, Debye temperature, and Young’s modulus. It also has the least average RE-O bond length and unit cell volume. The material’s Young’s modulus is increased when Yb₂SiO₅ is doped with Sc, mostly as a result of an increase in cation field strength and a decrease in average cation radius.

(2) The Si-O bond lengths and bond energies of YbRESiO₅ (RE = Yb, Eu, Gd, Ho, Tm, Lu, Y, Sc) were calculated using first-principles methods. The seven aforementioned elements can be divided into two groups based on the outcomes of the simulation: In comparison to Yb₂SiO₅, one group (Gd, Eu, Y, and Lu) decreases the bond energy and lengthens the Si-O bond when replacing Yb, which lowers the material’s resistance to oxygen and water corrosion. When doped, the other group (Sc, Ho, and Tm) shortens the Si-O bond and lengthens the bond energy, improving the material’s resistance to oxygen and water corrosion.

(3) According to thermal conductivity measurements, below 600 K, YbScSiO₅ has somewhat less thermal diffusivity and thermal conductivity than Yb₂SiO₅. They are marginally greater than Yb₂SiO₅ beyond 600 K, but the overall difference is negligible. When Eu is added, YbEuSiO₅ exhibits much reduced thermal conductivity and diffusivity in comparison to Yb₂SiO₅. In particular, for YbEuSiO₅, the minimum thermal conductivity is 1.072 W·m⁻¹·K⁻¹ between 400 °C and 1200 °C, while for Yb₂SiO₅, it is 1.52 W·m⁻¹·K⁻¹. This indicates that when YbEuSiO₅ is compared to Yb₂SiO₅, its minimum thermal conductivity decreases by 29.4%. The primary cause of YbEuSiO₅’s notable reduction in thermal conductivity is the addition of Eu, which results in the introduction of oxygen vacancies.

(4) Coefficient of thermal expansion (CTE) testing results show that YbScSiO₅ has a lower CTE than Yb₂SiO₅, but adding Eu raises the CTE of YbEuSiO₅. In particular, at 1473 K, YbScSiO₅ exhibits the lowest CTE (7.56 × 10⁻⁶·K⁻¹) compared to Yb₂SiO₅ (7% lower) at the same temperature. YbEuSiO₅, on the other hand, has the highest CTE at 8.6 × 10⁻⁶·K⁻¹, which is 7.5% more than Yb₂SiO₅. According to an analysis of the experimental data, there may be a positive correlation between the base material and the CTE of multi-component silicates.


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