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Study on water vapor corrosion resistance of rare earth monosilicates RE_2SiO_5 (RE = Lu, Yb, Tm, Er, Ho, Dy, Y, and Sc) from first-principles calculations

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Abstract

Corrosion resistance of rare earth monosilicates (RE_2SiO_5 , RE = Lu, Yb, Tm, Er, Ho, Dy, Y, and Sc) in water vapor has been studied using the first-principles calculations. The results show that the water vapor corrosion resistance of RE_2SiO_5 demonstrates the following order: $Sc_2SiO_5 > Dy_2SiO_5 > Y_2SiO_5 > Ho_2SiO_5 > Er_2SiO_5 > Yb_2SiO_5 > Tm_2SiO_5 > Lu_2SiO_5$. To further improve their water vapor resistance, a doping strategy has been employed for the first time. Two scenarios have been investigated: one is a half mole proportion of substitution of various rare earth elements for Yb in the Yb_2SiO_5 lattice; the other is a half mole fraction substitution of rare earth elements in RE_2SiO_5 (RE = Lu, Yb, Er and Y) by scandium. It is unveiled that the water vapor resistance of $YbScSiO_5$ and $YScSiO_5$ has been greatly improved in contrast to other rare

earth monosilicates. The current study provides guidelines for the selection of environmental barrier coatings with a better water vapor corrosion resistance.

Keywords: Materials chemistry, Inorganic chemistry, Structural engineering

1. Introduction

The silicon-based non-oxide ceramic materials, as hot section components of aero-engines, suffer from rapid recession at a high temperature combustion environment owing to water vapor corrosion [1, 2, 3]. As a result, environmental barrier coatings (EBCs) are usually mandatory to be applied on those substrates to prevent them from reacting with water vapor, thereby alleviating such rapid recession problems [4, 5, 6, 7]. Recently rare earth monosilicates (RE_2SiO_5) are proposed as one of the most promising EBC topcoat materials due to their excellent properties for EBC applications [8, 9, 10].

For an EBC topcoat, good water vapor corrosion resistance is a prerequisite. However, regarding the water vapor resistance property of different rare earth monosilicates, there are contradictions in different literature. For instance, K.N. Lee et al. [8] shows that the water vapor resistance of RE_2SiO_5 has the following order: $Yb_2SiO_5 > Er_2SiO_5 > Y_2SiO_5 > Lu_2SiO_5$. While, Ref. [11] unveils a slightly different trend, with Yb_2SiO_5 and Lu_2SiO_5 possessing best and poorest water vapor resistance but indicating that Y_2SiO_5 has better water vapor resistance than Er_2SiO_5 . In addition, as these experimental results were tested in an alumina tube, it is reported that the alumina contamination can probably change water vapor corrosion resistance of RE_2SiO_5 [12]. However, as the working conditions of EBCs are alumina free, the above testing results cannot probably represent the genuine water vapor corrosion resistance of rare earth monosilicates in combustion environment of gas turbines that is normally free of alumina species. Therefore, these data on water vapor corrosion resistance are required to test in an atmosphere that is similar to combustion environments and free of alumina species. Unfortunately, experimentally it is difficult to conduct water vapor corrosion resistance tests without introducing alumina at such a high temperature, as there are rare water vapor inert media that is suitable to conduct such experiments.

Alternatively, these water vapor corrosion resistance data can be obtained by theoretical calculations. The first-principle calculations have been proven to be a powerful tool to predict the properties of compounds with identical crystalline structure but various elements. For instance, the water vapor corrosion resistance of $RE_2Si_2O_7$ with the same crystal structure could be reflected by the strength of Si-O bonds [13]. It is worth pointing out that, a stronger Si-O bond is usually reflected by a higher Mulliken population, given Si-O bonds in an identical crystallographic environment. In addition, the water vapor resistance of $0.75BaO \cdot 0.25SrO \cdot Al_2O_3 \cdot 2SiO_2$ (BSAS) with

a hexagonal crystal structure had also been predicted by the strength of Si-O bonds and the calculated results were in good agreement with the experimental data [14]. These all studies suggest the feasibility of a computational method for comparing water vapor corrosion resistance of different materials with the same crystal structure.

Therefore, in the current work, in order to unveil RE_2SiO_5 with best water vapor corrosion resistance, the strength of Si-O bonds (or Mulliken population) in RE_2SiO_5 is calculated by first-principles. Apparently, RE_2SiO_5 have the identical crystalline structure, and thus the Si-O bond strength can be a reflection of their water vapor corrosion resistance. Further, motivated by a possible improvement of water vapor corrosion resistance by doping strategy, we employ different rare earth elements (Lu, Er, Y and Sc) to substitute a half proportion of Yb in Yb_2SiO_5 . In addition, as YbScSiO_5 exhibits a larger value of Mulliken population, i.e. better water vapor corrosion resistance, the Sc element is then used to substitute 50% of rare earth elements in A_2SiO_5 ($\text{A} = \text{Lu}, \text{Er}$ and Y). Finally, we rank all RE_2SiO_5 currently investigated on water vapor corrosion resistance, which might provide some beneficial guidelines for the selection of EBC topcoats with a better water vapor corrosion resistance.

2. Methods

The first principles calculations were carried out by using CASTEP code [15]. The plane wave basis was employed under periodic boundary conditions. The kinetic energy cutoff was set to 450 eV for expanding Bloch waves in the reciprocal space. For the energy integrations, a discretized $2 \times 3 \times 4$ \mathbf{k} sampling grid was applied in the first irreducible Brillouin zone based on Monkhorst-Pack method [16]. For the exchange correlation energy, polarized local density approximation (LDA) was used [17]. The crystal structures were fully optimized by independently modifying lattice parameters and internal atomic coordinates. The Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization scheme [18] was employed to minimize the total energy and interatomic forces. For the pseudo-atoms, the ultra-soft type pseudopotentials were applied for RE, Si, and O atoms to account the electrostatic interactions between valence electrons and the ionic core. The criteria for convergence in geometry optimization were selected as follows: the difference in total energy within 1×10^{-6} eV/atom, the ionic Hellmann-Feynman forces within $0.002 \text{ eV}/\text{\AA}$, the maximum stress within 0.01 GPa and the maximum ionic displacement within 1×10^{-4} \AA . After geometric optimization, the Mulliken bond populations were analyzed. The distance cut-off for bond populations was 3.0 \AA .

3. Result and discussion

Table 1 illustrates experimental and calculated lattice parameters of the optimized RE_2SiO_5 ($\text{RE} = \text{Lu}, \text{Yb}, \text{Tm}, \text{Er}, \text{Ho}, \text{Dy}, \text{Y}$, and Sc). The calculated lattice

Table 1. Experimental and calculated lattice parameters of RE₂SiO₅, YbBSiO₅ (B = Lu, Er, Y, Sc) and AScSiO₅ (A = Lu, Er, Y).

	Method	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
Lu ₂ SiO ₅	Expt. [19]	14.254 (9)	10.241 (8)	6.641 (7)	122.20 (8)	819.3 (10)
	Calc.	14.3509	10.2609	6.6322	122.511	823.566
Yb ₂ SiO ₅	Expt. [19]	14.28 (1)	10.28 (1)	6.653 (5)	122.2 (1)	824.0 (7)
	Calc.	14.1935	10.0753	6.5739	122.134	796.028
Tm ₂ SiO ₅	Expt. [19]	14.302 (9)	10.313 (9)	6.662 (6)	122.21 (9)	828.5 (9)
	Calc.	14.1607	10.1037	6.5541	122.113	806.709
Er ₂ SiO ₅	Expt. [19]	14.32 (2)	10.35 (2)	6.69 (1)	122.3 (3)	836.7 (41)
	Calc.	14.1717	10.1761	6.5822	122.189	803.295
Ho ₂ SiO ₅	Expt. [19]	14.35 (2)	10.37 (2)	6.71 (1)	122.2 (3)	843.0 (38)
	Calc.	14.1961	10.14563	6.5792	122.101	802.632
Dy ₂ SiO ₅	Expt. [19]	14.382 (2)	10.42 (2)	6.74 (1)	122.0 (3)	856.5 (72)
	Calc.	14.2331	10.1645	6.5833	122.113	806.709
Y ₂ SiO ₅	Expt. [20]	14.371 (3)	10.388 (3)	6.710 (4)	122.17 (4)	848 (1)
	Calc.	14.2556	10.2188	6.5854	122.309	810.801
Sc ₂ SiO ₅	Expt. [21]	13.679 (1)	9.967 (1)	6.4257 (6)	121.12 (1)	750.0
	Calc.	13.6452	9.6243	6.3202	121.848	705.042
YbLuSiO ₅	Calc.	14.2672	10.1342	6.6640	122.142	815.844
YbErSiO ₅	Calc.	14.3747	10.2637	6.6607	122.143	832.071
YbYSiO ₅	Calc.	14.1806	10.1410	6.6063	122.143	832.071
YbScSiO ₅	Calc.	13.6904	10.2753	6.6009	120.635	798.964
LuScSiO ₅	Calc.	13.6993	10.1693	6.5320	120.729	782.221
ErScSiO ₅	Calc.	13.9797	10.0158	6.6000	121.812	785.308
YScSiO ₅	Calc.	13.6695	10.3210	6.6145	120.510	803.976

parameters deviate from the experimental data by around 1.05% for a, 1.43% for b, and 1.34% for c, respectively, suggesting that the current optimized structures are reasonable. The crystal structures of RE₂SiO₅ are shown in Fig. 1. The unit cell of RE₂SiO₅ contains 32 atoms, which occupy 8 different crystallographic sites including two different RE³⁺ sites (labeled as RE1 and RE2), one Si site and five O sites (labeled as O1–O5). Four oxygen (O1–O4) atoms form a Si-centered distorted tetrahedron SiO₄, whilst O5, without any Si atom as its nearest neighbor, is loosely bonded to four rare earth cations, forming a distorted polyhedron REO₆ and REO₇. Hence, the RE₂SiO₅ consists of SiO₄ tetrahedra, REO₆ and REO₇ polyhedra [19]. When exposed to water vapor environment at high temperature, SiO₄ is subjected to water vapor attacking. As for the Si-O bond in the same environment, the higher Mulliken population represents stronger Si-O bond. Given a compound possessing a higher Mulliken population of Si-O bonds, it tends to give a better water vapor corrosion resistance, owing to the fact that those SiO₄ polyhedra with a higher Mulliken population of Si-O bonds are more difficult to be completely corroded. According to Fig. 4 or Table 2, Sc₂SiO₅ has the highest value of Mulliken population

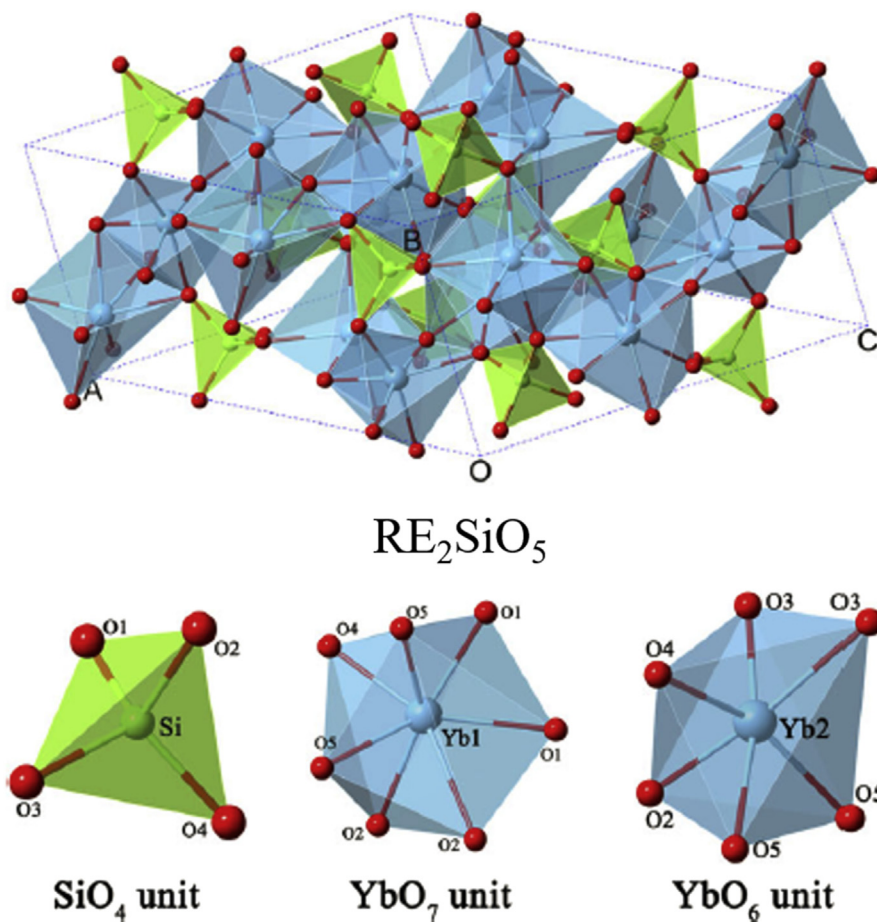


Fig. 1. The crystal structures of RE_2SiO_5 and SiO_4 polyhedron.

than other rare earth monosilicates, indicating that Sc_2SiO_5 possesses the best water vapor corrosion resistance. Moreover, the water vapor resistance of RE_2SiO_5 has the following order: $\text{Sc}_2\text{SiO}_5 > \text{Dy}_2\text{SiO}_5 > \text{Y}_2\text{SiO}_5 > \text{Ho}_2\text{SiO}_5 > \text{Er}_2\text{SiO}_5 > \text{Yb}_2\text{SiO}_5 > \text{Tm}_2\text{SiO}_5 > \text{Lu}_2\text{SiO}_5$. Except for Lu_2SiO_5 , other rare earth monosilicates have rather close Mulliken population, suggesting that they have close water vapor resistance. Lu_2SiO_5 exhibits the lowest value of Mulliken population, even much lower than the average value of Mulliken population, suggesting that the water vapor corrosion resistance of Lu_2SiO_5 is much weaker than that of other rare earth monosilicates. As the Lu_2SiO_5 has a smaller ionic radius than silicon-based non-oxide ceramic materials, the Lu-O bond will be shorter. On the other hand, the volume of Lu_2SiO_5 is the same as other rare earth monosilicates (as shown in Table 1). Thus, the Si-O bond needs to become longer to remain the volume and consequently mulliken population of Si-O bond in Lu_2SiO_5 becomes the lowest.

As our primary concern is the bonding strength of Si-O bonds in RE_2SiO_5 , which directly relates to the water vapor corrosion resistance of a rare earth monosilicate,

Table 2. Mulliken bond populations, bond length and density of Mulliken Population (Mulliken bond populations/bond-length) of Si–O bonds in RE₂SiO₅, YbBSiO₅ (B = Lu, Er, Y, Sc) and AScSiO₅ (A = Lu, Er, Y).

	Si–O bond population	Si–O bond length (Å)	Density of Si–O bond Population (Å ³)
Lu ₂ SiO ₅	0.5233	1.6246	0.3221
Yb ₂ SiO ₅	0.5609	1.6237	0.3454
Tm ₂ SiO ₅	0.562	1.6233	0.3462
Er ₂ SiO ₅	0.564	1.6216	0.3478
Ho ₂ SiO ₅	0.5633	1.6219	0.3473
Dy ₂ SiO ₅	0.5664	1.6216	0.3493
Y ₂ SiO ₅	0.5652	1.6216	0.3485
Sc ₂ SiO ₅	0.5696	1.6187	0.3519
YbLuSiO ₅	0.5413	1.6211	0.3339
YbErSiO ₅	0.5206	1.6311	0.3192
YbYSiO ₅	0.5522	1.6295	0.3389
YbScSiO ₅	0.5719	1.6172	0.3536
LuScSiO ₅	0.5626	1.6185	0.3476
ErScSiO ₅	0.5487	1.6279	0.3371
YScSiO ₅	0.5801	1.6177	0.3586

it appears that there exists another strategy to tailor the Si–O bonding length (or strength) in a fixed RE₂SiO₅. As already mentioned, the RE₂SiO₅ consists of SiO₄ tetrahedra, REO₆ and REO₇ polyhedra. Due to the chemical property similarity of the lanthanide elements, it is easy to introduce a second lanthanide element in the RE₂SiO₅ lattice. The introduction of a second rare earth element, i.e. doping, can potentially alter the size of REO₆ and REO₇ polyhedra, which can result in an opposite change of SiO₄ tetrahedra, thereby causing the corresponding Si–O bond length (or bond strength) change. In the current study, Yb₂SiO₅ is selected as the ‘matrix’ compound and a half proportion of Yb in Yb₂SiO₅ is substituted by a second rare earth element, such as Lu, Er, Y and Sc. Fig. 2 shows the optimized structure of YbBSiO₅ (B = Lu, Er, Y and Sc). As discussed, RE³⁺ has two crystallographic sites, RE1 and RE2, in the RE₂SiO₅ lattice. It is found that Yb in the RE2 sites has been replaced by a second rare earth element B (B = Lu, Er, Y and Sc). The results suggest that the substitution of Sc for Yb in Yb₂SiO₅ can dramatically improve the water vapor corrosion resistance and the Mulliken population value of YbScSiO₅ exceeds the highest value of all undoped rare earth monosilicates. However, the substitution of the other three rare earth elements, i.e. Lu, Er and Y, for Yb in Yb₂SiO₅ reduces the water vapor resistance.

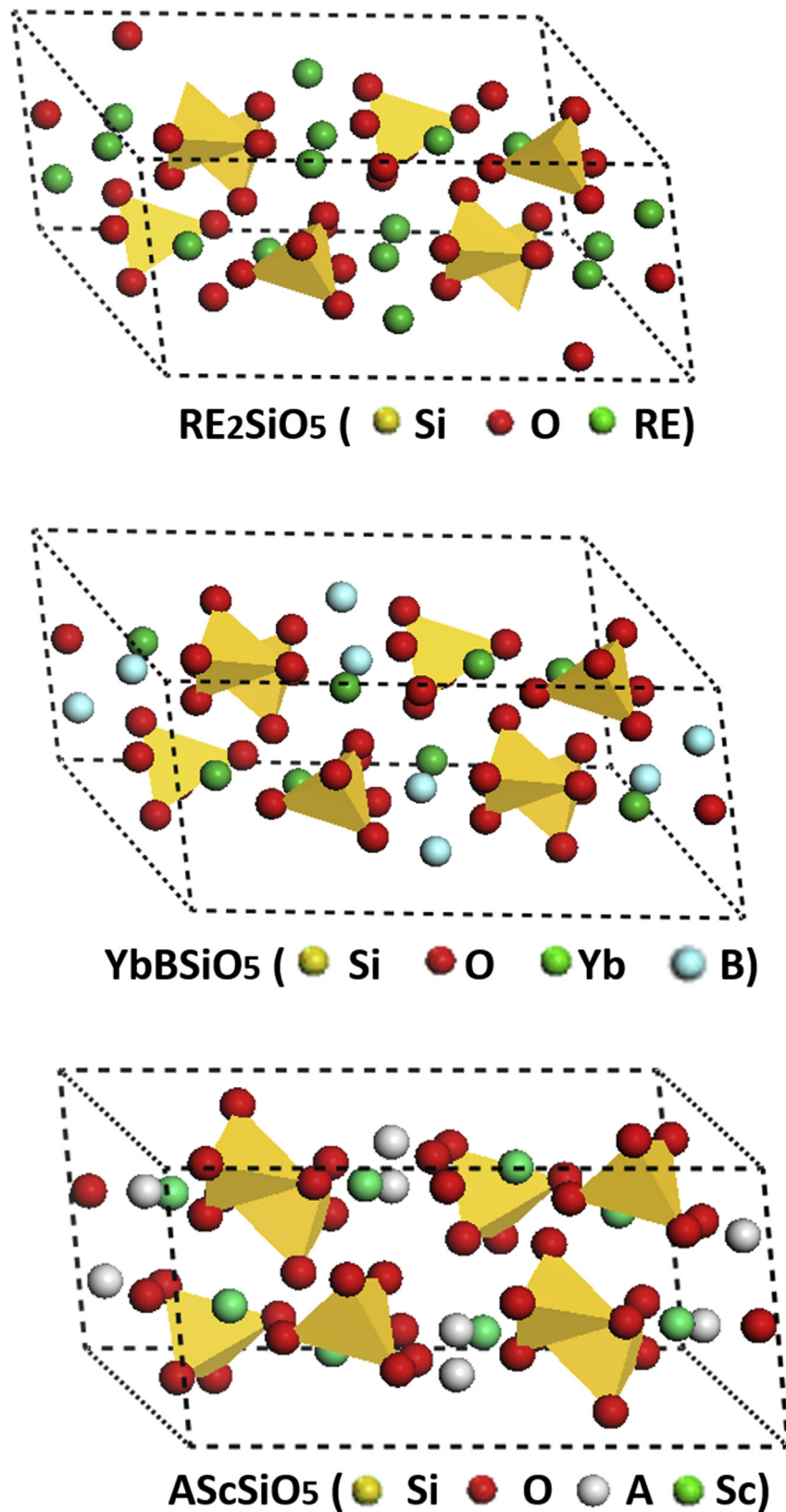


Fig. 2. The optimized crystal structures of RE_2SiO_5 , YbBSiO_5 (B = Lu, Er, Y and Sc) and AScSiO_5 (A = Lu, Er and Y).

Further, regarding the dramatic improvement of the Mulliken population by the substitution of Sc for Yb in Yb_2SiO_5 , a half mole fraction substitution of Sc for various 'matrix' rare earth monosilicate compounds, A_2SiO_5 ($\text{A} = \text{Lu}, \text{Er}$ and Y), has been investigated. As shown in Fig. 2, the RE2 sites in A_2SiO_5 ($\text{A} = \text{Lu}, \text{Er}$ and Y) are occupied by Sc. As illustrated in Fig. 3, the values of Mulliken population of RScSiO_5 ($\text{R} = \text{Lu}, \text{Yb}$ and Y) have been improved by at least 10%. In particular, the Mulliken population of YScSiO_5 has been dramatically improved, which perhaps has the best water vapor resistance in all rare earth silicates currently investigated.

The half mole fraction substitution of Sc for R in R_2SiO_5 ($\text{R} = \text{Lu}, \text{Yb}$ and Y) improves water vapor resistance, whereas the half mole fraction substitution of Sc for Er in Er_2SiO_5 reduces water vapor resistance. This can be accounted for in the context of the crystal lattice energy. Due to a smaller radius of Sc^{3+} , when a half proportion of rare earth elements in R_2SiO_5 ($\text{R} = \text{Lu}, \text{Yb}$ and Y) are substituted by Sc, the doped rare earth monosilicate crystals will contract in order to reduce the system energy. As a result, Si-O bonds in RScSiO_5 ($\text{R} = \text{Lu}, \text{Yb}$ and Y) will become shorter than R_2SiO_5 ($\text{R} = \text{Lu}, \text{Yb}$ and Y) as shown in Fig. 3, leading to an increase of Mulliken population. According to Table 1, the volume of ErScSiO_5 crystal structure is smaller than that of Er_2SiO_5 . However, as the volume contraction of ErScSiO_5 can probably be realized by shortening Er-O or Sc-O bonds, the Si-O bonds can even become longer so as to reduce the system energy of ErScSiO_5 . Thus, as shown in Figs. 3 and 4, Si-O bonds in ErScSiO_5 become longer than these

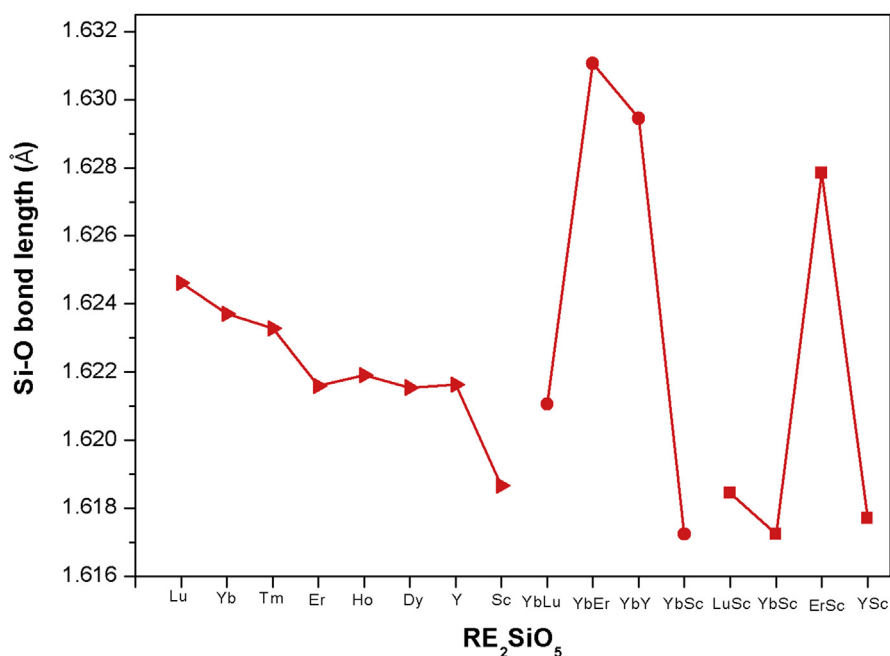


Fig. 3. Bond length of Si–O bonds in RE_2SiO_5 , YbBSiO_5 ($\text{B} = \text{Lu}, \text{Er}, \text{Y}$ and Sc) and AScSiO_5 ($\text{A} = \text{Lu}, \text{Er}$ and Y).

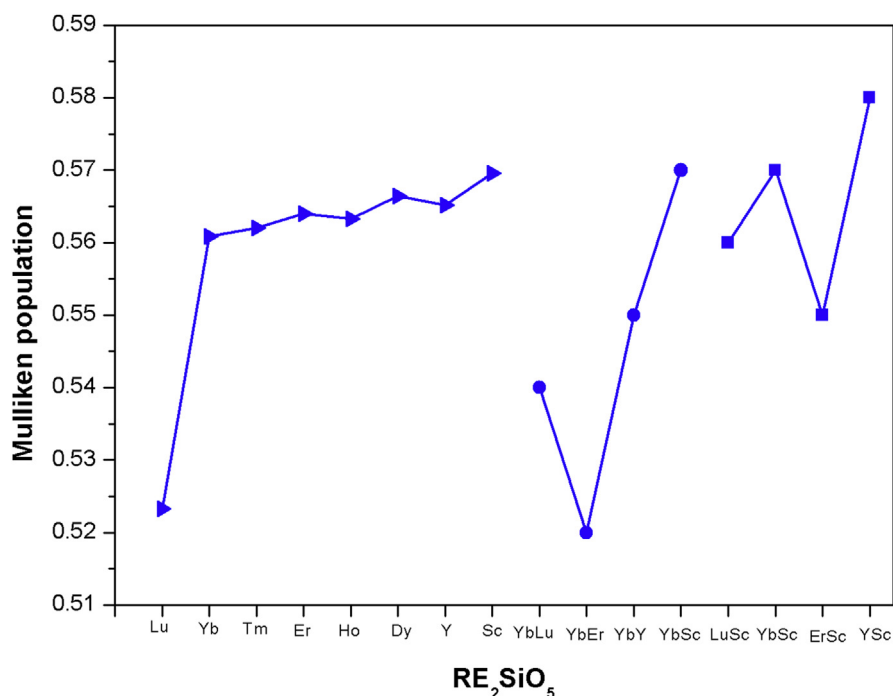


Fig. 4. Mulliken bond populations of Si–O bonds in RE₂SiO₅, YbBSiO₅ (B = Lu, Er, Y and Sc) and AScSiO₅ (A = Lu, Er and Y).

in Er₂SiO₅ and Mulliken population of Si–O bonds in ErScSiO₅ correspondingly decreased, suggesting that water vapor resistance of ErScSiO₅ decreases. In brief, when the substitution of Sc for Er in ErScSiO₅ occurred, water vapor resistance of ErScSiO₅ became weaker to reduce crystal lattice energy. By contrast, water vapor resistance of RScSiO₅ (R = Lu, Yb and Y) became stronger to reduce crystal lattice energy.

Density of Mulliken bond populations of Si–O bonds has also been performed to compare water vapor resistance of rare earth monosilicates. Density of Mulliken bond populations represents Mulliken bond population/bond-length. The calculated data are displayed in Table 2 and Fig. 5. Obviously, the trend of water vapor resistance is essentially the same as results from Mulliken bond populations in Fig. 4. However, there are two differences in water vapor resistance. The new order is: Sc₂SiO₅ > Dy₂SiO₅ > Y₂SiO₅ > Er₂SiO₅ > Ho₂SiO₅ > Tm₂SiO₅ > Yb₂SiO₅ > Lu₂SiO₅. In the previous order, water vapor resistance of Er₂SiO₅ and Ho₂SiO₅ is similar and Er₂SiO₅ is closely following Ho₂SiO₅. Whereas, the current results reveal that water vapor resistance of Er₂SiO₅ and Ho₂SiO₅ is still similar but Ho₂SiO₅ is closely following Er₂SiO₅. Likewise, water vapor resistance of Tm₂SiO₅ and Yb₂SiO₅ has changed and Yb₂SiO₅ is currently following closely Tm₂SiO₅ according to density of Mulliken bond populations of Si–O bonds in RE₂SiO₅. The trend of water vapor resistance of other rare earth silicates is in good agreement with that from Mulliken bond populations.

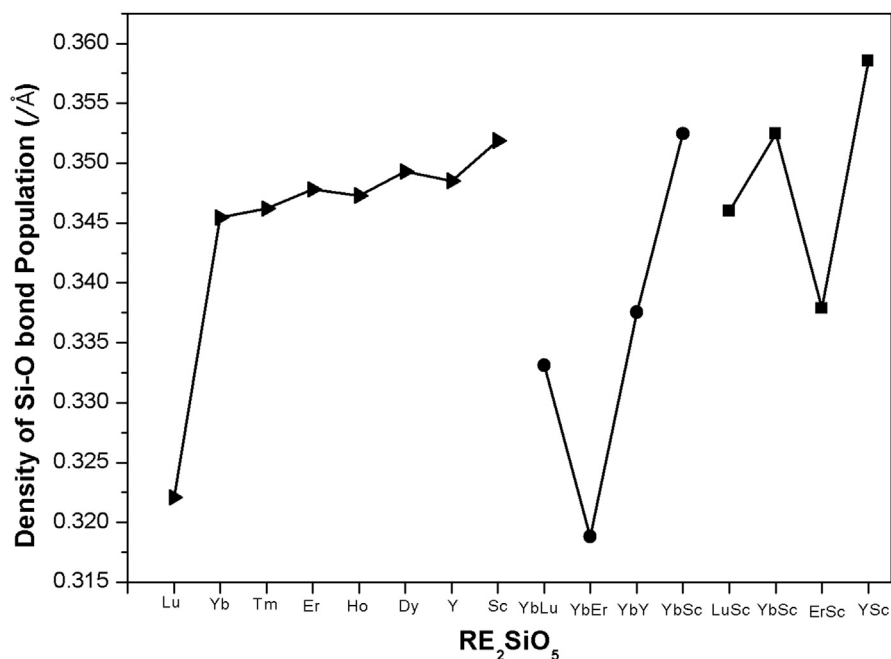


Fig. 5. Density of Mulliken bond populations of Si–O bonds in RE₂SiO₅, YbBSiO₅ (B = Lu, Er, Y, Sc) and ASiO₅ (A = Lu, Er, Y).

4. Conclusion

The water vapor resistance of RE₂SiO₅ (RE = Lu, Yb, Tm, Er, Ho, Dy, Y, and Sc) has been studied using first-principles calculations. By comparing the Mulliken population of Si–O bonds, it is found that the currently investigated rare earth monosilicates except Lu₂SiO₅ have similar water vapor corrosion resistance. Lu₂SiO₅ shows much lower water vapor resistance. In addition, a doping strategy of RE₂SiO₅ by a second rare earth element on the RE site has been employed for the first time to seek a compound with better water vapor corrosion resistance. Two series of calculations have been carried out: the first is using different rare earth element dopants, i.e. Lu, Er, Y and Sc, to substitute a half mole proportion of Yb in the Yb₂SiO₅ lattice; the second is using Sc as a dopant to substitute a half mole proportion of rare earth elements in different rare earth monosilicates, i.e. Lu₂SiO₅, Er₂SiO₅ and Y₂SiO₅. The results show that the Sc substitution of Yb₂SiO₅ can greatly improve its water vapor resistance, whereas the substitution of Lu, Er and Y for Yb in Yb₂SiO₅ is not beneficial to the water vapor resistance. Further, the Sc substitution for Y in Y₂SiO₅ can noticeably improve its water vapor corrosion resistance. Indeed, the solid solution of ScYSiO₅ exhibits the best water vapor resistance of all rare earth monosilicates currently investigated. The current study ranks water vapor resistance of common rare earth monosilicates and suggests the doping on the RE site could possibly further improve its water vapor resistance, which provides guidelines for the selection of environmental barrier coating topcoat materials with water vapor corrosion resistance.

Declarations

Author contribution statement

Jing Han: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Yanfei Wang: Conceived and designed the experiments; Wrote the paper.

Rongjun Liu: Conceived and designed the experiments.

Di Jiang: Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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