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Article

Investigation of Thermal Expansion and Compressibility of Rare-Earth Orthovanadates Using a Dielectric Chemical Bond Method

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The chemical bond properties, lattice energies, linear expansion coefficients, and mechanical properties of $ReVO_4$ (Re = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Sc, Y) are investigated systematically by the dielectric chemical bond theory. The calculated results show that the covalencies of Re−O bonds are increasing slightly from La to Lu and that the covalencies of V−O bonds in crystals are decreasing slightly from La to Lu. The linear expansion coefficients decrease progressively from $LaVO_4$ to $LuVO_4$; on the contrary, the bulk moduli increase progressively. Our calculated results are in good agreement with some experimental values for linear expansion coefficients and bulk moduli.

I. Introduction

The crystals in a zircon structure [tetragonal, $Z = 4$, space group $I4_1/amd$ (No. 141)] throughout the entire rare-earth series (plus Y, Sc) represent an ideal system for studying the relationship between the physical properties and crystal structures. In rare-earth orthovanadates, $ReVO_4$ (Re = rare-earth ions, Y, Sc), each Re ion is coordinated by eight O atoms, forming dodecahedral cages, and the V ion is coordinated by four O atoms, forming VO_4 tetrahedra. Lanthanide and related orthovanadate compounds are of interest because of their unusual magnetic characteristics and useful luminescence properties, such as YVO_4, whose most important application is in diode-pumped solid-state lasers, where it serves as a host material for Nd and other rare-earth ions. These materials have been employed as model systems for the investigation of polymorphism among the ABO_4-type compounds because the zircon-type vanadates have been found to transform reconstructively to the denser scheelite structure at pressures of a few kilobars and temperatures of less than 600 °C.[1,2] The structure refinements of zircon-type vanadates have been previously reported.[3–5] Recently, the high-precision crystal structures of $ReVO_4$ (Re = Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Sc, Y)[6,7] and $LaVO_4$[8] also have been systematically reported by employing Rietveld structure analysis of neutron powder diffraction data. The thermal expansion anisotropy, magnetoelastic effect, and compressibility of some rare-earth orthovanadates have been studied.[9–14] These results have provided accurate crystallographic data and offer the possibility of studying other properties. In this paper, the chemical bond properties, lattice energies, linear expansion coefficients, and mechanical properties of $ReVO_4$ (Re = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Sc,

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Y) are investigated systematically by the dielectric chemical bond theory. The results show that the linear expansion coefficients decrease and the bulk moduli increase progressively from $LaVO_4$ to $LuVO_4$.

II. Theoretical Method

According to the dielectric chemical bond theory of crystals,[15,16] when complex crystal structures are known, the crystal formula can be written as a linear combination of the subformula for various binary crystals. The subformula of any type of chemical bond A−B in the multibond crystal $A^1_{a1}A^2_{a2}\cdots A^i_{ai}B^1_{b1}B^2_{b2}\cdots B^j_{bj}$ can be expressed by the following formula:

$$\frac{N(B^j-A^i)ai}{N_{CAi}}A^i\frac{N(A^i-B^j)bj}{N_{CBj}}B^j = A^i_{mi}B^j_{nj} \tag{1}$$

$$mi = \frac{N(B^j-A^i)ai}{N_{CAi}}, \quad nj = \frac{N(A^i-B^j)bj}{N_{CBj}}$$

and

$$A^1_{ai}A^2_{a2}\cdots A^i_{ai}B^1_{b1}B^2_{b2}\cdots B^j_{bj} = \sum_{i,j} A^i_{mi}B^j_{nj} \tag{2}$$

A^i_{ai} and B^j_{bj} represent the different constituent elements or different sites of the same element in the crystal formula, and ai and bj represent the numbers of corresponding elements. $N(B^j-A^i)$ is the number of B^j ions in the coordination group of an A^i ion, and N^i_{CA} represents the nearest coordination number of the A^i ion. Thus, complex crystals are decomposed into the sum of different species of binary crystals such as $A^i_{mi}B^j_{nj}$. Application of this method can be used to calculate the lattice energy for simple binary crystals with the subformulas $A^i_{mi}B^j_{nj}$, but the appropriate valences must be applied. The valence Z of each ion can be obtained according to the electrostatic neutral principle of the binary crystals. For any binary crystal $(A_mB_n)^\mu$, Z_A is the normal valence of the cation A and Z_B is obtained from $Z_B = mZ_A/n$. Each chemical subformula forms a single chemical bond; for any μ kind of chemical bond, the chemical parameters such as ionicity f^μ_i, covalency f^μ_c, lattice energy $U(mn)^\mu$, and thermal expansion coefficient $\alpha_{mn}{}^\mu$ can be calculated by means of the dielectric chemical bond theory of crystals. The detailed theoretical methods can be found in refs 15–18.

The calculated method of bulk moduli is developed below.

In complex crystals, the lattice energy density $u(mn)^\mu$ of each binary crystal will be expressed as

$$u(mn)^\mu = \frac{U(mn)^\mu}{N_{AV}n^\mu v^\mu_b} \tag{3}$$

where N_{AV} is the Avogadro constant, n^μ is the number of type μ chemical bonds in one molecule, and $v_b{}^\mu$ is the chemical bond volume of the type μ chemical bonds. For simple crystals of composition A^NB^{8-N}, eq 3 becomes

$$u = \frac{U}{N_{AV}V_m} = \frac{U_m}{V_m} \tag{4}$$

V_m is the volume of one molecular unit, which is obtained from the crystal structure, and U_m is the lattice energy of one molecule. The densities of the lattice energy and bulk moduli have a good linear relationship for each type of binary crystal;[19] the slopes of the lines depend upon the properties and the crystal structures. The slopes of the fitting lines on various simple binary crystal structures, which are relating to Z_A (valence of the cation) and N_{CA} (coordination number of the cation), are different. In this situation, the valences and coordination numbers of the cation and anion are equal in the crystal. For any type μ of subformula $A^\mu_mB^\mu_n$ in a complex crystal, the valences and coordination numbers of the cation and anion are not equal. In order to apply this linear relationship between the densities of the lattice energy and bulk moduli in simple crystals of composition A^NB^{8-N}, we introduce a new parameter γ^μ for any $(A_mB_n)^\mu$ subformula:

$$\gamma(mn)^\mu = \frac{2Z^\mu_{av} + \kappa_{mn}}{4N^\mu_{av}} \tag{5}$$

where$Z^\mu_{av} = [(Z_AZ_B)(m + n)/2m]^{1/2}$ is the average valence of A and B ions in subformula A_mB_n, Z_A and Z_B are the valences of A and B ions, respectively, in A_mB_n, $N^\mu_{av} = Z_{av}N_{CA}/Z_A$ is the average coordination number of subformula A_mB_n, N_{CA} is the coordination number of the A ion in crystals, and k_{mn} is the structural correction factor.

$$\kappa_{mn} = 5 + \frac{m-n}{2m}\left(\frac{Z_{av}}{Z_B}\right)^{(m+n)/2m} \tag{6}$$

The slope is

$$\beta(mn)^\mu = -1.445 + 1.8185\exp[1.54\gamma(mn)^\mu] \tag{7}$$

The relationship between the bulk moduli $B(mn)^\mu$ and the densities of the lattice energy $u(mn)^\mu$ is

$$u(mn)^\mu = \beta(mn)^\mu[B(mn)^\mu - \delta^\mu] \tag{8}$$

$$B(mn)^\mu = \delta^\mu + \frac{u(mn)^\mu}{\beta(mn)^\mu} \tag{9}$$

Here δ^μ is a constant; we will give their empirical values as $\delta^\mu = 18/Z^\mu_{av}N^\mu_{av}$ for $N_{av} > 4$ and $\delta^\mu = 132/Z^\mu_{av}N^\mu_{av}$ for $N_{av} \le 4$.

The bulk moduli of the complex crystals are expressed as

$$B_m = \frac{1}{\kappa_m} \tag{10}$$

$$\kappa_m = \frac{\Delta V}{V_m\Delta P} = \frac{1}{V_m}\sum_\mu \frac{\Delta V_\mu}{\Delta P_\mu} = \frac{1}{V_m}\sum_\mu V^\mu\kappa_\mu = \frac{1}{V_m}\sum_\mu \frac{V^\mu}{B^\mu} \tag{11}$$

where $B(mn)^\mu$ is the bulk modulus of the kind of μth chemical bond and V^μ is the volume of the kind of μth chemical bond in one molecule.

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Table 1. Chemical Bond Parameters of $ReVO_4$ Crystals[a]

crystals	bond type	d^{μ} (Å)	f_c^{μ}	C^{μ} (eV)	E_h^{μ} (eV)	E_g^{μ} (eV)	V_m (Å^3)
$LaVO_4$[b]	La−O	2.468	0.1540	9.91	4.23	10.78	90.96
	La−O	2.550	0.1521	9.21	3.90	10.00	
	V−O	1.713	0.3569	14.04	10.46	17.51	
$CeVO_4$[c]	Ce−O	2.442	0.1542	10.17	4.34	11.06	88.96
	Ce−O	2.525	0.1522	9.43	4.00	10.24	
	V−O	1.711	0.3561	14.10	10.52	17.57	
$PrVO_4$[c]	Pr−O	2.422	0.1545	10.36	4.43	11.27	87.63
	Pr−O	2.511	0.1522	9.56	4.05	10.38	
	V−O	1.712	0.3556	14.10	10.47	17.56	
$NdVO_4$[c]	Nd−O	2.405	0.1547	10.54	4.51	11.46	86.46
	Nd−O	2.498	0.1523	9.68	4.10	10.51	
	V−O	1.711	0.3552	14.13	10.49	17.60	
$SmVO_4$[d]	Sm−O	2.368	0.1557	10.91	4.69	11.88	84.23
	Sm−O	2.483	0.1526	9.82	4.17	10.67	
	V−O	1.710	0.3551	14.16	10.51	17.63	
$EuVO_4$[d]	Eu−O	2.356	0.1558	11.04	4.75	12.02	83.27
	Eu−O	2.470	0.1527	9.94	4.22	10.80	
	V−O	1.709	0.3548	14.17	10.51	17.64	
$GdVO_4$[d]	Gd−O	2.344	0.1560	11.18	4.81	12.17	82.52
	Gd−O	2.461	0.1527	10.03	4.26	10.90	
	V−O	1.710	0.3544	14.18	10.51	17.65	
$TbVO_4$[c]	Tb−O	2.327	0.1564	11.37	4.89	12.38	81.48
	Tb−O	2.451	0.1528	10.13	4.30	11.00	
	V−O	1.709	0.3541	14.21	10.52	17.68	
$DyVO_4$[d]	Dy−O	2.308	0.1569	11.58	4.99	12.61	80.36
	Dy−O	2.442	0.1530	10.22	4.34	11.10	
	V−O	1.709	0.3540	14.21	10.52	17.68	
$HoVO_4$[c]	Ho−O	2.300	0.1570	11.67	5.04	12.71	79.77
	Ho−O	2.434	0.1530	10.30	4.38	11.19	
	V−O	1.708	0.3538	14.24	10.54	17.72	
$ErVO_4$[c]	Er−O	2.285	0.1573	11.85	5.12	12.91	78.96
	Er−O	2.426	0.1531	10.38	4.41	11.28	
	V−O	1.709	0.3534	14.23	10.52	17.70	
$TmVO_4$[c]	Tm−O	2.272	0.1578	11.99	5.19	13.07	78.18
	Tm−O	2.421	0.1532	10.43	4.44	11.34	
	V−O	1.708	0.3535	14.25	10.54	17.72	
$YbVO_4$[c]	Yb−O	2.259	0.1583	12.15	5.27	13.24	77.46
	Yb−O	2.418	0.1534	10.46	4.45	11.37	
	V−O	1.708	0.3536	14.25	10.54	17.72	
$LuVO_4$[c]	Lu−O	2.252	0.1584	12.23	5.31	13.33	76.93
	Lu−O	2.410	0.1535	10.54	4.49	11.46	
	V−O	1.706	0.3536	14.29	10.57	17.77	
YVO_4[c]	Y−O	2.298	0.1571	11.69	5.05	12.73	79.67
	Y−O	2.433	0.1530	10.31	4.38	11.20	
	V−O	1.709	0.3537	14.22	10.52	17.69	
$ScVO_4$[c]	Sc−O	2.129	0.1632	13.81	6.10	15.10	70.51
	Sc−O	2.367	0.1547	10.96	4.69	11.92	
	V−O	1.704	0.3537	14.32	10.60	17.82	

[a] d^{μ} is the chemical bond length, and f_c^{μ} is the covalency. C^{μ} and E_h^{μ} are the heteropolar and homopolar energies, respectively. E_g^{μ} is the average energy gap. V_m is the volume of one molecular unit. [b] Structural data from ref 8. [c] Structural data from ref 6. [d] Structural data from ref 7.

III. Results and Discussion

With the detailed crystallographic data, we know that the structures of $ReVO_4$ crystals have space group symmetry $I4_1/amd$ and $Z = 4$. Re has eight nearest oxygen atoms, and V has four nearest oxygen atoms. According to the above method, $ReVO_4$ can be expressed as the following sum of binary crystals:

$$ReVO_4 = Re_{1/2}O_{4/3} + Re_{1/2}O'_{4/3} + VO_{4/3} = \frac{1}{2}(ReO_{8/3} + ReO'_{8/3}) + VO_{4/3}$$

In the above formula, the single prime (′) indicates that the site of O is the same but the chemical bond length is different. According to structural data from refs 6–8, we can use the method of the chemical bond theory of the dielectric description to calculate the chemical bond parameters. The results are shown in Table 1. In the lattice energy calculation of subformulas $A^i_{mi}B^j_{nj}$, the presented valences of each ion must be applied. The formal valence Z of each ion can be obtained according to the electrostatic neutral principle of the binary crystals. For any binary crystal A_mB_n, Z_A is the normal valence of the cation A and Z_B is obtained from $Z_B = mZ_A/n$, which indicates the valence contribution of the anion in the binary crystal A_mB_n. For subformula $ReO_{8/3}$, let $Z_{Re} = 3.0$; then $Z_O = (3/8) \times 3 = 1.125$. Similarly, for $VO_{4/3}$, let $Z_V = 5.0$; then $Z_O = (3/4) \times 5 = 3.75$. From that, we can find that the presented valences of the O ion in different chemical bonds are different.

According to the chemical bond parameters in Table 1, the lattice energies, linear expansion coefficients, and bulk moduli

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Table 2. Lattice Energies, Linear Expansion Coefficients, and Bulk Moduli of $\mathrm{ReVO_4}$ Crystals[a]

crystals	bond type	v_b^μ (Å^3)	U^μ (kJ/mol)	α^μ (10^{-6} K^{-1})	α_{calcd} (10^{-6} K^{-1})	u^μ (GPa)	B^μ (GPa)	B_m^{calcd} (GPa)
$\mathrm{LaVO_4}$	La−O	9.3296	2754.7	8.8	6.1	122.5	103.8	109.1
	La−O	10.2908	2682.6	9.1		108.2	91.8	
	V−O	3.1196	22999.0	0.5		3059.6	489.8	
$\mathrm{CeVO_4}$	Ce−O	9.0793	2778.1	8.7	6.1	127.0	107.6	113.2
	Ce−O	10.0369	2703.9	9.1		111.8	94.9	
	V−O	3.1229	23022.3	0.5		3059.4	489.8	
$\mathrm{PrVO_4}$	Pr−O	8.8779	2796.5	8.6	6.0	130.7	110.7	115.9
	Pr−O	9.8930	2716.0	9.0		113.9	96.6	
	V−O	3.1354	23015.4	0.5		3046.3	487.7	
$\mathrm{NdVO_4}$	Nd−O	8.7130	2812.2	8.6	6.0 (6.0)[b]	133.9	113.4	118.4
	Nd−O	9.7634	2727.3	9.0		115.9	98.3	
	V−O	3.1374	23027.0	0.5		3045.9	487.6	
$\mathrm{SmVO_4}$	Sm−O	8.3250	2847.5	8.4	5.9	141.9	120.1	123.0
	Sm−O	9.5977	2740.7	8.9		118.5	100.5	
	V−O	3.1349	23037.1	0.5		3049.7	488.2	
$\mathrm{EuVO_4}$	Eu−O	8.2135	2858.9	8.4	5.9	144.5	122.3	125.3
	Eu−O	9.4644	2752.2	8.8		120.7	102.3	
	V−O	3.1404	23048.3	0.5		3045.8	487.6	
$\mathrm{GdVO_4}$	Gd−O	8.1045	2870.6	8.3	5.9 (4.4)[c]	147.0	124.1	127.0
	Gd−O	9.3795	2760.2	8.8		122.1	103.5	
	V−O	3.1466	23040.8	0.5		3038.8	486.5	
$\mathrm{TbVO_4}$	Tb−O	7.9422	2887.3	8.2	5.8	150.9	127.7	129.6
	Tb−O	9.2807	2769.2	8.7		123.8	104.9	
	V−O	3.1461	23052.0	0.5		3040.8	486.8	
$\mathrm{DyVO_4}$	Dy−O	7.7551	2906.2	8.2	5.8	155.5	131.5	132.3
	Dy−O	9.1858	2777.4	8.7		125.5	106.3	
	V−O	3.1485	23052.5	0.5		3038.5	486.5	
$\mathrm{HoVO_4}$	Ho−O	7.6855	2914.1	8.1	5.7	157.4	133.1	133.9
	Ho−O	9.1086	2784.7	8.7		126.9	107.5	
	V−O	3.1474	23063.1	0.4		3041.0	486.9	
$\mathrm{ErVO_4}$	Er−O	7.5482	2929.2	8.1	5.7	161.0	136.1	136.1 (136)[e]
	Er−O	9.0335	2792.0	8.6		128.3	108.7	
	V−O	3.1580	23055.6	0.5		3029.8	485.1	
$\mathrm{TmVO_4}$	Tm−O	7.4179	2942.6	8.1	5.7	164.6	139.1	137.9
	Tm−O	8.9751	2796.7	8.6		129.3	109.5	
	V−O	3.1515	23064.7	0.4		3037.2	486.4	
$\mathrm{YbVO_4}$	Yb−O	7.2847	2956.5	8.0	5.7	168.4	142.3	139.6
	Yb−O	8.9329	2800.0	8.6		130.1	110.2	
	V−O	3.1487	23067.0	0.4		3040.2	486.7	
$\mathrm{LuVO_4}$	Lu−O	7.2294	2963.3	8.0	5.7	170.1	143.8	141.2
	Lu−O	8.8603	2806.9	8.6		131.5	111.4	
	V−O	3.1429	23083.9	0.4		3048.1	488.0	
$\mathrm{YVO_4}$	Y−O	7.6661	2914.4	9.5	6.7 (6.7)[d]	157.8	133.4	134.1 (130)[f]
	Y−O	9.0982	2785.0	10.1		127.0	107.6	
	V−O	3.1532	23037.0	0.6		3032.0	485.4	
$\mathrm{ScVO_4}$	Sc−O	6.1056	3097.5	9.6	6.9	210.5	177.6	158.7
	Sc−O	8.3906	2847.8	10.7		140.9	119.3	
	V−O	3.1305	23102.1	0.4		3062.6	490.3	

[a] v_b^μ, U^μ, α^μ, u^μ, and B^μ are the chemical bond volume, the lattice energy, the linear expansion coefficient, the lattice energy density, and the bulk modulus of the μ-type chemical bond, respectively. α_{calcd} and B_m^{calcd} are the calculated values of the crystal linear expansion coefficient and the bulk modulus. [b] Experimental value from ref 9. [c] Experimental value from ref 10. [d] Experimental value from ref 11. [e] Experimental value from ref 13. [f] Experimental value from ref 14.

of various crystals were calculated; the results are shown in Table 2. From these results, we can find that the covalencies of Re−O bonds are about 15%, but they are increasing slightly from $\mathrm{LaVO_4}$ to $\mathrm{LuVO_4}$, and the covalencies of V−O bonds are about 35%, but they are decreasing slightly from $\mathrm{LaVO_4}$ to $\mathrm{LuVO_4}$. The linear expansion coefficients are decreasing progressively from $\mathrm{LaVO_4}$ to $\mathrm{LuVO_4}$; on the contrary, the bulk moduli of various crystals are increasing progressively. At the same time, in zircon-type vanadates of rare earths, we find that the bulk moduli have a linear relationship with the lattice energy densities of the crystals (see Figure 1). To date, some properties of zircon-type vanadates of rare earths have been studied; for example, the linear expansion coefficient of $\mathrm{YVO_4}$ has been measured as 6.7 (10^{-6} K^{-1})[11] and the average linear expansion coefficient of $\mathrm{NdVO_4}$ has been measured as 6.0 (10^{-6} K^{-1}),[9] which are in good agreement with our calculated values. The

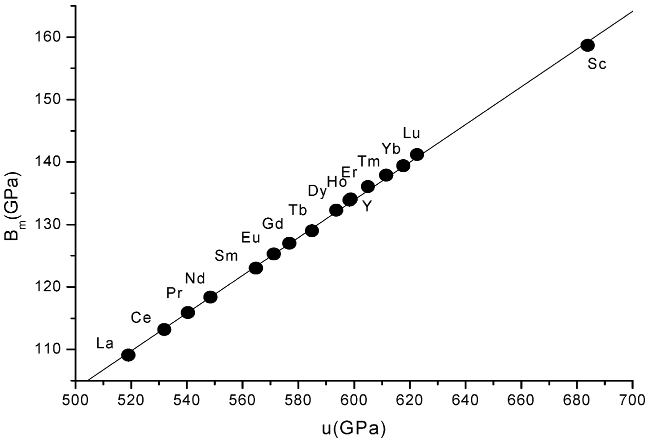

Figure 1. Relationship between the bulk moduli and lattice energy densities of rare-earth orthovanadates.

average linear expansion coefficient of $GdVO_4$ has been measured as 4.4 (10^{-6} K^{-1}),[10] which is less than our calculated result. The bulk modulus of YVO_4 had been measured by a Birch equation of state as 130 GPa;[13] according to their structural data, our calculating result is 134.6 GPa; according to the structural data reported by Chakoumakos et al., the calculated result is 134.1 GPa, and this shows that the calculated result and experimental value are in agreement. The bulk modulus of $ErVO_4$ has been given experimentally as 136 GPa[14] and is in agreement with our result 136.1 GPa.

IV. Conclusion

The chemical bond properties, lattice energies, linear expansion coefficients, and mechanical properties of $ReVO_4$ (Re = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Sc, Y) are investigated systematically by the chemical bond theory of dielectric description. We find that the various properties not only show the similarities of rare-earth ions in chemical properties but also show the difference between rare-earth ions; each property has regularities observable from La to Lu. From the expansion coefficient and bulk modulus, the VO_4 tetrahedra will behave as rigid units; the differences between different crystals come mainly from the ReO_8 group. Our calculated results are in good agreement with experimental values, which indicate that the methods are reasonable.

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