

Thermal Expansion of Forsterite, Mg_2SiO_4 :

1. Measurements

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Thermal expansion of forsterite, Mg_2SiO_4 , is measured up to 1,600 K by the dilatometric method. The present results of volume thermal expansion γ_v is 3.20 percent from 300 to 1,200 K and expansion coefficient α_v is $40.5 \times 10^{-6} K^{-1}$ at 1,200 K. They are close to those of a natural olivine (Suzuki, 1976), but are 4.4 and 11 percent smaller as compared with those reported in the former paper (Suzuki et al., 1984). The γ_v and α_v of forsterite are 5.00 percent and $46.7 \times 10^{-6} K^{-1}$ respectively, at 1,600 K.

keywords: forsterite, olivine, thermal expansion, high temperature

1 Introduction

Olivine is one of the most important minerals in the Earth's mantle and taken great interests in by geophysicists and mineralogists. On its major end member forsterite, Mg_2SiO_4 , elasticity, thermal expansion and other thermal properties including their pressure and temperature dependencies have been measured (cf. Soga and Anderson, 1967). For discussion about constitution and equation of state in the Earth's upper mantle, such measurements up to higher temperature are much desired. We tried to measure thermal expansion of forsterite above 1,200 K ($\sim 900^\circ C$), with dilatometric method. In this report, we show results of the measurements up to 1,600 K.

2 Measurements of Thermal Expansion

In the present measurements, we detected differential linear expansion between an objective specimen and a reference one (Kajiyoshi, 1986). The reference specimen is desired to have smaller expansion coefficients and stable in measuring circumstances. Below about 1,300 K, silica glass or fused quartz is one of the best materials for such purposes (cf. Suzuki, 1975). Under higher temperatures, silica glass may crystallize during many hours of measurements and not be suitable for the reference. It is known that expansion coefficient α of many regular materials above the Debye temperature is almost linear against temperature. In the present measurements, we carefully examined linear expansion coefficient of rods made of polycrystalline aluminum

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oxide with silica glass as the reference and found that it is linear in the temperature range between 500 and 1,200 K as shown in Figure 1. The linear equation $\alpha_L = a + bT$ has the constants of $a = 5.611 \pm 0.027$ and $b = (3.178 \pm 0.032) \times 10^{-3}$ with the units of α_L in $1/\text{MK}$ and T in K. We use this equation as the reference even to higher temperature of 1,600 K, assuming linearity of the α_L . Observed values of α_L are used in the range between 300 and 500

K.

Observed differential elongation is corrected by adding the elongation of the reference material; that is,

$\Delta\ell = \ell_r \times [\exp(\int \alpha_L dT) - 1]$, where ℓ_r is the length at the reference temperature: 300 K in this report.. Possible nonlinearity in the α_L at higher temperature may result some error in corrected values, but may be expected to be smaller than a few percent in α_L of the objective specimen.

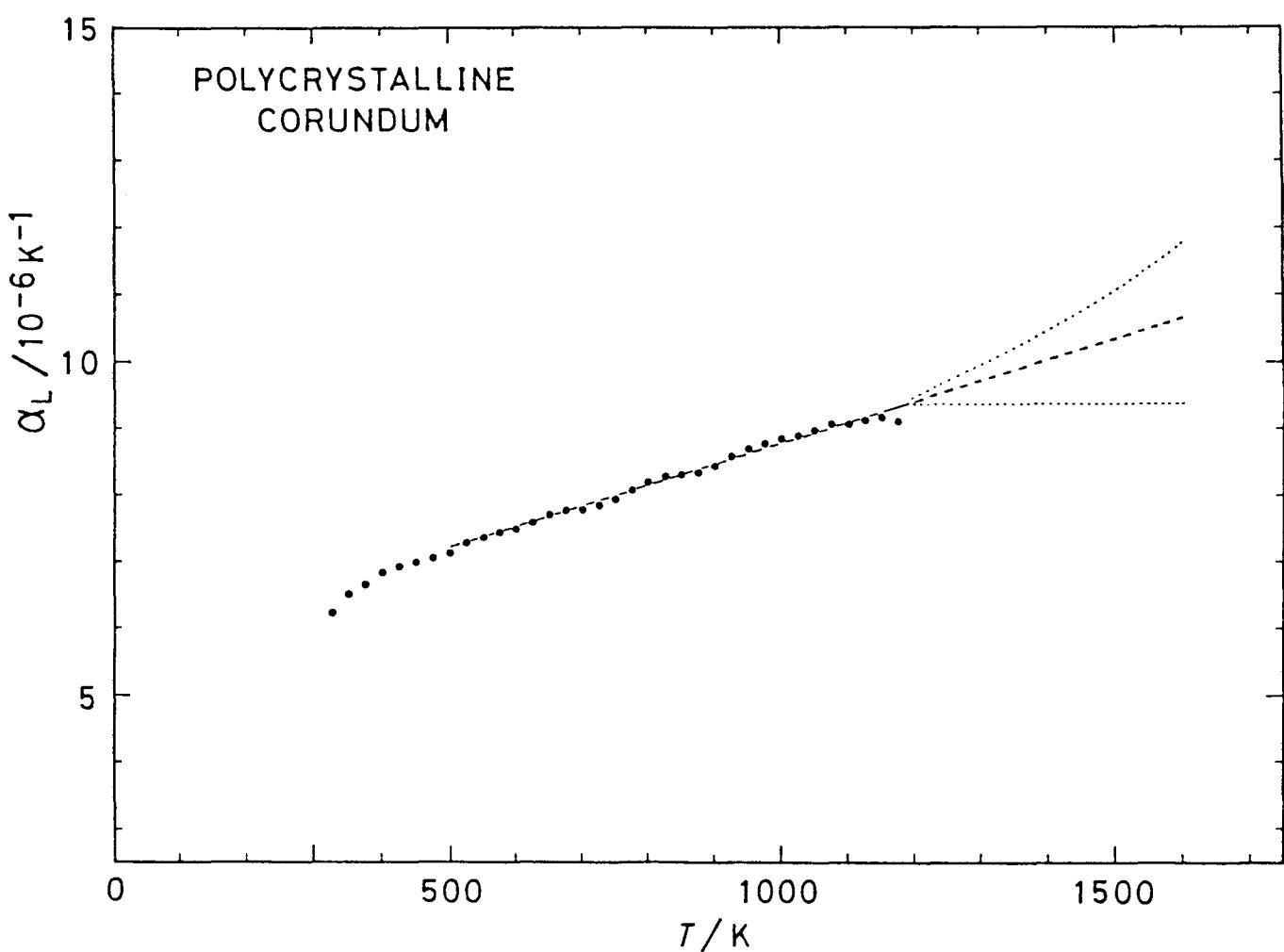


Figure 1. Observed linear expansion coefficient of polycrystalline aluminum oxide between 300 and 1,200 K. The broken line shows linear extrapolation of α_L to 1,600 K. Dotted lines show 10 percent deviations of α_L from the linear extrapolation at 1,600 K, which are given to diminish to 0 percent at 1,200 K.

Measurements were made for prismatic specimens of single-crystal forsterite. Three specimens have length of several mm along crystallographic orientations. Relative volume expansion Y_v and volume expansion coefficient α_v are calculated by the relations:

$$Y_v = (Y_a + 1)(Y_b + 1)(Y_c + 1) - 1 \quad (1)$$

$$\alpha_v = \alpha_a + \alpha_b + \alpha_c \quad (2)$$

where $Y_v = (V - V_r)/V_r$, $Y_i = (\ell_i - \ell_{ir})/\ell_{ir}$, and

$$\alpha_v = (1/V) \cdot \partial V / \partial T \quad (3)$$

$$\alpha_i = (1/\ell_i) \cdot \partial \ell_i / \partial T \quad (4)$$

The V and ℓ represent volume and linear dimension of the specimen respectively, and the subscript r is used for the reference temperature and i for three orientations of a , b or c . Theoretically, relative volume expansion may be represented by an equation as follows (Suzuki et al., 1979):

$$Y_v = (1 + 2k - \sqrt{1 - 4kE(\theta_D, T)/Q_0}) / 2ka_v - 1 \quad (5)$$

The E is internal energy evaluated by the Debye temperature θ_D , and temperature T in K. The Q_0 and k are constants, which are related to the Gruneisen parameter and pressure derivative of bulk modulus (Suzuki, 1975). The a_v is a conversion factor of theoretical reference temperature of absolute 0 K to the experimental reference temperature T_r ; that is, $a_v = V_r / V_0$.

In isotropic materials, relationship bet-

ween Y_v and Y_i is

$$Y_i = (Y_v + 1)^{1/3} - 1 \quad (6)$$

Because theoretical representation for linear thermal expansion of anisotropic materials is not well established, we use a practical relationship, simply by substituting equation (5) in equation (6) as follows:

$$Y_L = (1 + 1/2k - \sqrt{1 - 4kE(\theta_D, T)/Q_0}) / 2k^{1/3}/a_L - 1 \quad (7)$$

and $a_L = \ell_r / \ell_0$. It is found that this functional form is well applied to express linear expansion, in which each constant is not the same but has apparently orientation dependency.

Equation (5) and (7) are applied to observed data by the least squares method, and we can obtain each parameter. Thermal expansion coefficients are calculated by the definition in equations (3) and (4).

3 Results

Observed expansion data of forsterite are listed in Table 1. Smoothed values by equations (5) and (7) and their extrapolation are also listed in Table 1. Volume expansion coefficients α_v are plotted in Figure 2. The parameters in equations (5) and (7) determined by the least squares method are listed in Table 2.

Having thermal expansion data α_v , we can evaluate following anharmonic properties of forsterite, which are important in relation to equation of state and list them in Table 3.

Table 1a. Observed and calculated expansion of forsterite in a- and b-axis

a-axis	obs.			calc.			b-axis	obs.			calc.		
	T (K)	Y (%)	α (1/MK)	Y (%)	α (1/MK)	T (K)	Y (%)	α (1/MK)	Y (%)	α (1/MK)	Y (%)	α (1/MK)	
50				-0.0808	0.15	50					-0.1906	0.81	
100				-0.0781	1.08	100					-0.1785	4.26	
150				-0.0688	2.68	150					-0.1489	7.38	
200				-0.0516	4.16	200					-0.1068	9.32	
250				-0.0278	5.31	250					-0.0571	10.50	
300	0			0.0009	6.14	300	0				-0.0025	11.28	
325	0.0170	6.84		0.0167	6.47	325	0.0261	10.86			0.0260	11.57	
350	0.0342	6.98		0.0333	6.76	350	0.0543	11.47			0.0553	11.82	
375	0.0519	7.10		0.0505	7.01	375	0.0835	11.85			0.0852	12.04	
400	0.0697	7.10		0.0683	7.23	400	0.1136	12.27			0.1155	12.23	
425	0.0874	7.13		0.0866	7.42	425	0.1449	12.78			0.1464	12.41	
450	0.1054	7.29		0.1054	7.60	450	0.1776	13.06			0.1777	12.56	
475	0.1239	7.53		0.1246	7.76	475	0.2103	12.91			0.2093	12.71	
500	0.1431	7.81		0.1443	7.90	500	0.2423	12.85			0.2413	12.84	
525	0.1630	8.03		0.1642	8.03	525	0.2747	12.96			0.2736	12.96	
550	0.1833	8.15		0.1845	8.16	550	0.3073	13.06			0.3063	13.08	
575	0.2038	8.24		0.2051	8.27	575	0.3402	13.00			0.3392	13.20	
600	0.2246	8.40		0.2259	8.38	600	0.3725	12.99			0.3725	13.30	
625	0.2459	8.58		0.2471	8.49	625	0.4054	13.21			0.4060	13.41	
650	0.2676	8.66		0.2685	8.58	650	0.4388	13.48			0.4398	13.51	
675	0.2893	8.75		0.2901	8.68	675	0.4731	13.70			0.4739	13.61	
700	0.3115	8.91		0.3120	8.77	700	0.5076	13.79			0.5082	13.71	
725	0.3340	8.99		0.3341	8.86	725	0.5424	13.88			0.5428	13.81	
750	0.3566	9.07		0.3564	8.94	750	0.5774	13.90			0.5776	13.91	
775	0.3795	9.15		0.3790	9.03	775	0.6123	14.05			0.6127	14.00	
800	0.4025	9.18		0.4017	9.11	800	0.6481	14.21			0.6481	14.10	
825	0.4256	9.26		0.4247	9.19	825	0.6838	14.34			0.6837	14.20	
850	0.4490	9.34		0.4479	9.27	850	0.7203	14.50			0.7195	14.29	
875	0.4725	9.42		0.4713	9.35	875	0.7568	14.57			0.7557	14.39	
900	0.4963	9.47		0.4949	9.43	900	0.7937	14.54			0.7920	14.49	
925	0.5201	9.47		0.5187	9.51	925	0.8301	14.50			0.8287	14.59	
950	0.5439	9.53		0.5427	9.59	950	0.8668	14.59			0.8656	14.69	
975	0.5680	9.63		0.5669	9.67	975	0.9037	14.69			0.9028	14.79	
1000	0.5923	9.68		0.5913	9.76	1000	0.9409	14.68			0.9402	14.89	
1025	0.6167	9.74		0.6160	9.84	1025	0.9778	14.76			0.9779	15.00	
1050	0.6413	9.82		0.6408	9.92	1050	1.0154	14.93			1.0159	15.10	
1075	0.6661	9.89		0.6659	10.00	1075	1.0532	15.10			1.0542	15.21	
1100	0.6911	9.99		0.6912	10.08	1100	1.0917	15.23			1.0928	15.32	
1125	0.7164	10.13		0.7167	10.17	1125	1.1302	15.37			1.1316	15.43	
1150	0.7421	10.22		0.7424	10.25	1150	1.1694	15.62			1.1708	15.55	
1175	0.7679	10.30		0.7683	10.34	1175	1.2092	15.75			1.2103	15.66	
1200	0.7940	10.38		0.7945	10.43	1200	1.2491	15.84			1.2501	15.78	
1225	0.8202	10.45		0.8209	10.52	1225	1.2894	15.95			1.2902	15.90	
1250	0.8467	10.55		0.8475	10.61	1250	1.3299	16.18			1.3306	16.03	
1275	0.8734	10.65		0.8744	10.71	1275	1.3714	16.32			1.3714	16.15	
1300	0.9004	10.76		0.9015	10.80	1300	1.4126	16.39			1.4125	16.28	
1325	0.9277	10.88		0.9289	10.90	1325	1.4545	16.48			1.4539	16.42	
1350	0.9553	11.03		0.9566	11.00	1350	1.4962	16.59			1.4958	16.55	
1375	0.9834	11.27		0.9845	11.11	1375	1.5387	16.76			1.5379	16.69	
1400	1.0122	11.40		1.0126	11.21	1400	1.5813	16.81			1.5805	16.84	
1425	1.0410	11.48		1.0411	11.32	1425	1.6241	16.94			1.6235	16.99	
1450	1.0702	11.56		1.0698	11.43	1450	1.6674	17.19			1.6668	17.14	
1475	1.0994	11.59		1.0989	11.54	1475	1.7115	17.23			1.7106	17.30	
1500	1.1288	11.67		1.1282	11.66	1500	1.7550	17.30			1.7548	17.46	
1525	1.1584	11.76		1.1578	11.78	1525	1.7995	17.41			1.7994	17.63	
1550	1.1883	11.94		1.1878	11.91	1550	1.8436	17.67			1.8445	17.80	
1575	1.2188			1.2181	12.04	1575	1.8895				1.8901	17.98	
1600				1.2487	12.17	1600					1.9361	18.16	
1650				1.3110	12.45	1650					2.0297	18.55	
1700				1.3749	12.75	1700					2.1254	18.97	
1750				1.4403	13.07	1750					2.2235	19.42	
1800				1.5075	13.42	1800					2.3240	19.90	
1850				1.5766	13.80	1850					2.4272	20.43	
1900				1.6478	14.22	1900					2.5334	21.01	
1950				1.7213	14.68	1950					2.6428	21.65	
2000				1.7972	15.19	2000					2.7557	22.36	

Table 1b. Observed and calculated expansion of forsterite in c-axis and volume

c-axis	obs.	calc.	volume	obs.	calc.				
T (K)	Y (%)	α (1/MK)	Y	α	T (K)	Y (%)	α (1/MK)	Y	α (1/MK)
50		-0.1540	0.49	50		-0.4170	1.21		
100		-0.1461	2.96	100		-0.3969	7.66		
150		-0.1241	5.74	150		-0.3390	15.36		
200		-0.0902	7.68	200		-0.2475	20.96		
250		-0.0485	8.94	250		-0.1330	24.67		
300	0	-0.0015	9.79	300	0	-0.0031	27.18		
325	0.0236	9.88	0.0233	10.11	325	0.0667	27.58	0.0661	28.14
350	0.0494	10.35	0.0490	10.38	350	0.1380	28.80	0.1376	28.96
375	0.0754	10.33	0.0753	10.62	375	0.2109	29.28	0.2110	29.67
400	0.1011	10.65	0.1021	10.83	400	0.2847	30.01	0.2862	30.29
425	0.1287	11.07	0.1294	11.01	425	0.3614	30.97	0.3629	30.85
450	0.1565	11.18	0.1572	11.18	450	0.4401	31.54	0.4409	31.35
475	0.1847	11.20	0.1854	11.33	475	0.5198	31.66	0.5202	31.80
500	0.2126	11.54	0.2140	11.47	500	0.5992	32.19	0.6007	32.22
525	0.2425	11.83	0.2429	11.60	525	0.6817	32.82	0.6823	32.60
550	0.2719	11.81	0.2721	11.72	550	0.7644	33.01	0.7648	32.97
575	0.3017	11.90	0.3017	11.84	575	0.8480	33.14	0.8483	33.31
600	0.3316	11.92	0.3315	11.95	600	0.9315	33.33	0.9328	33.64
625	0.3615	11.98	0.3616	12.05	625	1.0162	33.78	1.0181	33.95
650	0.3917	12.13	0.3920	12.15	650	1.1021	34.26	1.1042	34.25
675	0.4224	12.29	0.4226	12.25	675	1.1894	34.73	1.1912	34.54
700	0.4534	12.36	0.4535	12.35	700	1.2778	35.07	1.2790	34.83
725	0.4845	12.48	0.4846	12.44	725	1.3670	35.36	1.3676	35.11
750	0.5161	12.59	0.5160	12.54	750	1.4570	35.56	1.4570	35.39
775	0.5478	12.69	0.5476	12.63	775	1.5474	35.88	1.5471	35.66
800	0.5799	12.83	0.5795	12.72	800	1.6392	36.21	1.6380	35.93
825	0.6123	12.90	0.6116	12.81	825	1.7314	36.51	1.7297	36.20
850	0.6448	12.90	0.6439	12.90	850	1.8249	36.73	1.8221	36.47
875	0.6772	12.97	0.6765	12.99	875	1.9184	36.95	1.9153	36.73
900	0.7101	13.09	0.7093	13.08	900	2.0132	37.11	2.0093	37.00
925	0.7431	13.24	0.7424	13.17	925	2.1077	37.22	2.1041	37.27
950	0.7768	13.40	0.7757	13.26	950	2.2032	37.51	2.1996	37.54
975	0.8106	13.43	0.8092	13.36	975	2.2994	37.75	2.2959	37.82
1000	0.8445	13.41	0.8430	13.45	1000	2.3963	37.77	2.3931	38.10
1025	0.8782	13.32	0.8770	13.54	1025	2.4928	37.82	2.4910	38.38
1050	0.9117	13.36	0.9113	13.64	1050	2.5901	38.09	2.5897	38.66
1075	0.9456	13.57	0.9458	13.74	1075	2.6882	38.56	2.6893	38.95
1100	0.9802	13.75	0.9806	13.83	1100	2.7881	38.97	2.7897	39.24
1125	1.0150	13.88	1.0157	13.93	1125	2.8885	39.36	2.8909	39.53
1150	1.0503	13.99	1.0510	14.04	1150	2.9906	39.85	2.9931	39.84
1175	1.0857	14.15	1.0866	14.14	1175	3.0937	40.22	3.0961	40.14
1200	1.1218	14.26	1.1225	14.24	1200	3.1979	40.47	3.2000	40.46
1225	1.1578	14.31	1.1586	14.35	1225	3.3025	40.72	3.3048	40.77
1250	1.1942	14.47	1.1951	14.46	1250	3.4082	41.22	3.4106	41.10
1275	1.2310	14.58	1.2318	14.57	1275	3.5156	41.54	3.5174	41.43
1300	1.2680	14.73	1.2688	14.69	1300	3.6232	41.88	3.6251	41.77
1325	1.3056	14.81	1.3062	14.80	1325	3.7326	42.17	3.7338	42.12
1350	1.3430	14.98	1.3438	14.92	1350	3.8419	42.60	3.8436	42.48
1375	1.3815	15.21	1.3818	15.05	1375	3.9538	43.25	3.9544	42.85
1400	1.4201	15.26	1.4201	15.17	1400	4.0667	43.47	4.0663	43.22
1425	1.4589	15.32	1.4587	15.30	1425	4.1800	43.73	4.1793	43.61
1450	1.4978	15.41	1.4977	15.43	1450	4.2945	44.16	4.2935	44.01
1475	1.5371	15.56	1.5371	15.57	1475	4.4103	44.38	4.4088	44.41
1500	1.5768	15.85	1.5768	15.71	1500	4.5262	44.81	4.5253	44.83
1525	1.6176	16.00	1.6168	15.85	1525	4.6445	45.16	4.6431	45.27
1550	1.6581	15.96	1.6573	16.00	1550	4.7625	45.57	4.7622	45.71
1575	1.6987		1.6982	16.15	1575	4.8832		4.8826	46.17
1600		1.7395	16.31	1600			5.0043	46.65	
1650		1.8233	16.64	1650			5.2521	47.65	
1700		1.9089	16.99	1700			5.5059	48.71	
1750		1.9965	17.37	1750			5.7662	49.87	
1800		2.0862	17.78	1800			6.0335	51.11	
1850		2.1781	18.22	1850			6.3084	52.46	
1900		2.2724	18.70	1900			6.5915	53.93	
1950		2.3694	19.22	1950			6.8835	55.55	
2000		2.4693	19.79	2000			7.1855	57.33	

Table 2. Expansion Parameters of Forsterite

	Tr (K)	Q ₀ (MJ/mol)	Θ _D (K)	k (-)	a - 1 (10 ⁻⁴)	σ (10 ⁻⁴)
a-axis	300	6.778 ± 0.021	829 ± 10	4.09 ± 0.03	8.1 ± 0.1	0.092
b-axis	300	4.541 ± 0.011	532 ± 10	2.61 ± 0.01	19.2 ± 0.3	0.100
c-axis	300	4.967 ± 0.009	616 ± 7	2.81 ± 0.01	15.5 ± 0.2	0.073
volume	300	5.277 ± 0.009	642 ± 6	3.06 ± 0.01	42.0 ± 0.4	0.192

Tr : reference temperature

± : probable error

Θ_D : Debye temperature

σ : standard deviation

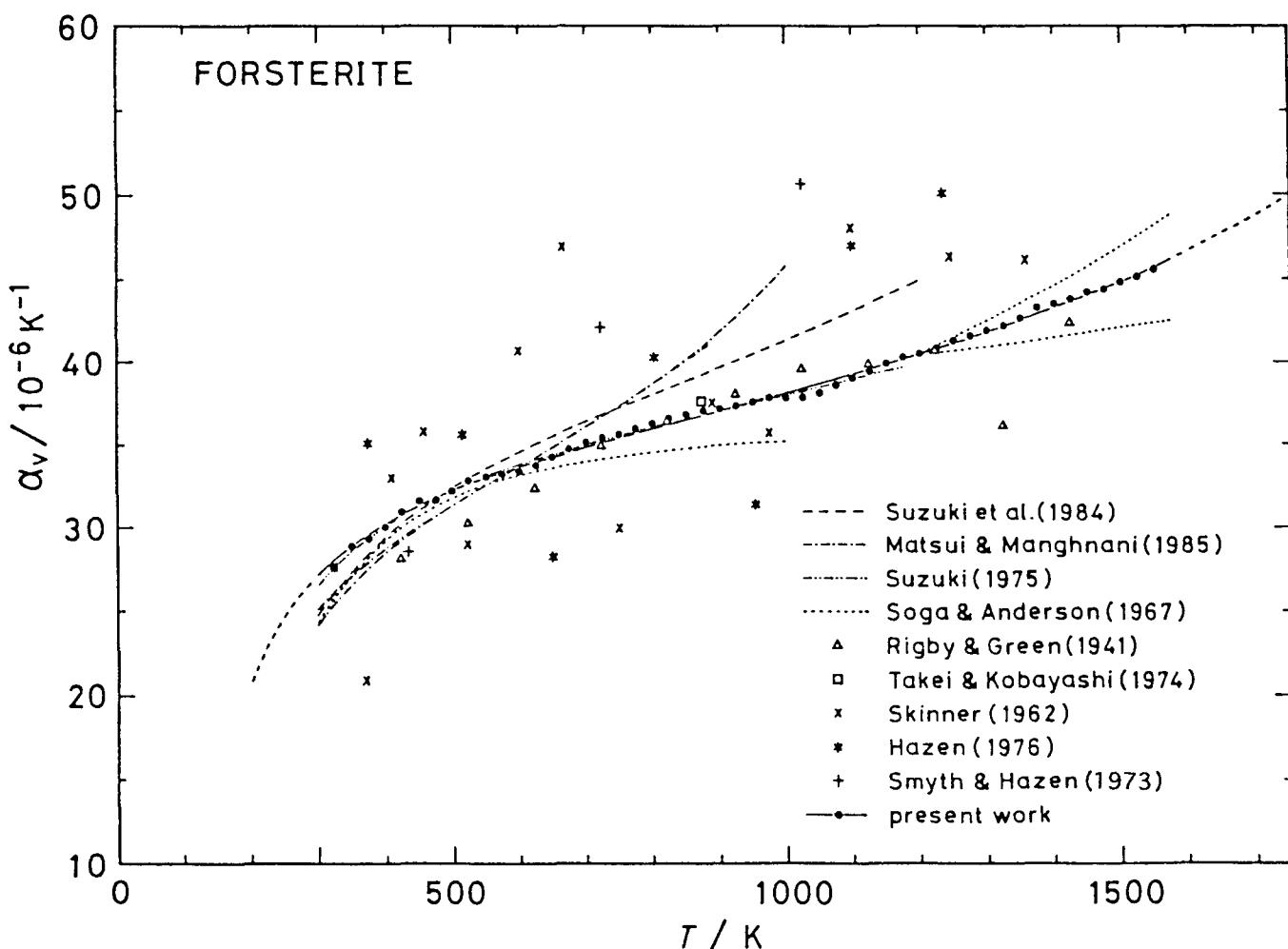
Q₀ = KoVo/γ ; k = (Ko' - 1)/2

Figure 2. Comparison of volume expansion coefficients of forsterite with previous ones.

Dotted lines attached to the present data are due to supposed variation in α_L in the reference material as shown in Figure 1.

Table 3. Anharmonic parameters of forsterite

T (K)	α (1/MK)	ρ (Mg/m ³)	C_p * (J/gK)	K_s ** (GPa)	K_T (GPa)	γ (-)	δ_s (-)	δ_T (-)	αK_T (MPa/K)	ΔP (GPa)
300	27.18	3.225	0.8412	128.8	127.5	1.290	4.54	6.21	3.464	0.0000
350	28.96	3.220	0.9142	128.0	126.4	1.259	4.29	5.83	3.660	0.1783
400	30.29	3.216	0.9704	127.2	125.3	1.235	4.15	5.58	3.796	0.3649
450	31.35	3.211	1.015	126.4	124.3	1.215	4.04	5.41	3.896	0.5573
500	32.22	3.206	1.053	125.6	123.2	1.199	3.95	5.28	3.970	0.7540
550	32.97	3.200	1.084	124.8	122.2	1.186	3.89	5.20	4.028	0.9540
600	33.64	3.195	1.111	124.0	121.1	1.175	3.84	5.13	4.075	1.157
650	34.25	3.190	1.135	123.2	120.1	1.166	3.79	5.09	4.113	1.361
700	34.83	3.184	1.156	122.4	119.0	1.158	3.75	5.05	4.146	1.568
750	35.39	3.179	1.174	121.6	118.0	1.153	3.72	5.03	4.176	1.776
800	35.93	3.173	1.191	120.8	116.9	1.148	3.69	5.01	4.202	1.985
850	36.47	3.167	1.207	120.0	115.9	1.145	3.66	5.00	4.226	2.196
900	37.00	3.161	1.221	119.2	114.8	1.142	3.63	4.99	4.249	2.408
950	37.54	3.155	1.234	118.4	113.8	1.141	3.60	5.00	4.271	2.621
1000	38.10	3.150	1.246	117.6	112.7	1.141	3.57	5.00	4.293	2.835
1050	38.66	3.143	1.257	116.8	111.6	1.142	3.54	5.01	4.315	3.050
1100	39.24	3.137	1.268	116.0	110.5	1.144	3.52	5.03	4.337	3.266
1150	39.84	3.131	1.278	115.2	109.4	1.147	3.49	5.04	4.360	3.484
1200	40.46	3.125	1.287	114.4	108.3	1.151	3.46	5.06	4.383	3.702
1250	41.10	3.119	1.296	113.6	107.2	1.155	3.43	5.08	4.407	3.922
1300	41.77	3.112	1.304	112.8	106.1	1.161	3.40	5.12	4.431	4.143
1350	42.48	3.106	1.312	112.0	104.9	1.167	3.36	5.16	4.458	4.365
1400	43.22	3.099	1.320	111.2	103.8	1.175	3.33	5.20	4.486	4.589
1450	44.01	3.092	1.327	110.4	102.6	1.184	3.29	5.24	4.516	4.814
1500	44.83	3.085	1.334	109.6	101.4	1.194	3.26	5.30	4.547	5.041
1550	45.71	3.078	1.340	108.8	100.2	1.205	3.22	5.37	4.580	5.269
1600	46.65	3.071	1.347	108.0	98.96	1.218	3.18	5.45	4.617	5.499

* : Robie et al. 1978

** : Suzuki et al. 1983

$K_T = K_S / (1 + \alpha \gamma T)$
 isothermal bulk modulus
 and adiabatic one

$\gamma = \alpha K_S / C_p$ $\rho = \alpha K_T / C_v$
 ρ
 Gruneisen parameter

$\delta_S = (-1/\alpha K_S) (\partial K_S / \partial T)$
 $\delta_T = (-1/\alpha K_T) (\partial K_T / \partial T)$
 Anderson-Gruneisen prmts

$\Delta P_{TH} = \int \alpha K_T dT$
 thermal pressure

Examination of data and discussion will be made in the following paper.

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