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A transitional structural state and anomalous Fe-Mg order-disorder in Mg-rich orthopyroxene, $(\text{Mg}_{0.75}\text{Fe}_{0.25})_2\text{Si}_2\text{O}_6$

Hexiong Yang, Subrata Ghose

For deposit: Table 7

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Table 7. Amplitudes (\AA) and orientations of major axes of thermal ellipsoids in the $\text{En}_{75}\text{Fs}_{25}$ orthopyroxene at various temperatures

Atom	Ellipsoid	296K	1000K	1100K	1200K	1300K	
	axis (r_i)						
M1	RMS*	0.074	0.121	0.130	0.142	0.147	
	a**	70.8	69.4	62.2	69.2	65.7	
	r_1	b	92.1	91.4	94.1	94.3	99.3
		c	19.4	20.6	28.1	21.3	26.2
	RMS	0.075	0.138	0.149	0.165	0.174	
	r_2	a	101.2	88.5	98.0	92.0	97.3
		b	168.6	177.4	172.0	175.6	170.
		c	88.6	92.1	90.4	93.9	96.8
	RMS	0.087	0.151	0.165	0.173	0.178	
	r_3	a	157.5	159.3	150.9	159.1	154.5
		b	78.8	92.1	83.2	89.5	86.2
		c	70.7	67.5	61.9	69.1	64.8

Table 7. (continued)

M2		RMS	0.075	0.133	0.146	0.158	0.166
	r ₁	a	57.9	59.6	62.5	58.0	59.6
		b	81.6	87.6	90.3	86.6	83.4
		c	33.5	30.5	27.5	32.2	31.2
		RMS	0.086	0.160	0.171	0.186	0.206
	r ₂	a	80.2	75.5	74.5	75.2	74.9
		b	18.8	18.5	17.4	19.9	22.4
		c	105.9	101.2	97.7	103.0	106.1
		RMS	0.105	0.196	0.206	0.224	0.228
r ₃	a	146.0	145.6	147.7	144.0	145.3	
	b	73.3	71.7	72.6	70.4	68.7	
	c	61.4	62.0	63.8	61.1	64.0	
SiA		RMS	0.072	0.114	0.116	0.127	0.134
	r ₁	a	40.0	62.0	48.6	65.3	33.6
		b	50.4	51.1	57.9	62.6	61.0
		c	85.3	51.7	58.0	38.4	74.6
		RMS	0.074	0.117	0.120	0.129	0.137
	r ₂	a	92.4	52.5	65.8	42.1	73.2
		b	79.8	73.8	70.3	71.0	88.7
		c	169.5	138.0	148.0	125.9	163.1
		RMS	0.081	0.132	0.139	0.148	0.159
r ₃	a	129.9	50.2	51.0	58.4	62.0	
	b	41.5	136.6	141.0	145.7	150.9	
	c	80.6	75.4	90.3	78.2	83.0	

Table 7. (continued)

SiB	RMS	0.071	0.107	0.115	0.129	0.136		
	r ₁	a	55.1	46.4	44.9	40.6	55.1	
		b	116.3	111.9	93.1	100.4	110.2	
		c	46.4	51.6	45.2	51.3	41.9	
	r ₂	RMS	0.074	0.121	0.133	0.141	0.150	
		a	108.7	62.7	72.9	78.9	65.0	
		b	153.5	116.1	21.7	148.8	25.6	
		c	108.1	140.1	103.0	118.7	84.6	
		r ₃	RMS	0.081	0.131	0.133	0.146	0.159
			a	139.0	124.2	130.0	128.4	65.0
	b		87.5	144.8	68.7	119.1	25.6	
	OIA	r ₁	c	49.1	82.4	47.6	52.1	84.6
RMS			0.066	0.116	0.131	0.124	0.148	
a			151.0	156.4	173.8	167.3	165.2	
r ₂		b	109.2	105.1	95.3	92.5	82.8	
		c	69.1	72.2	86.7	77.6	77.1	
		RMS	0.085	0.138	0.148	0.153	0.167	
r ₃		a	82.1	108.5	89.9	102.3	97.5	
		b	150.9	89.9	123.2	91.1	59.3	
		c	117.8	161.5	146.8	167.6	148.2	
r ₁		RMS	0.098	0.160	0.160	0.179	0.185	
		a	62.3	104.2	83.8	87.3	77.3	
		b	111.0	15.1	146.3	177.3	31.7	
r ₂	c	36.0	85.2	57.0	89.5	61.5		

Table 7. (continued)

OIB	RMS	0.078	0.113	0.123	0.138	0.142	
	r ₁	a	17.3	22.9	19.7	30.1	18.7
		b	101.8	79.1	85.8	66.5	87.8
		c	77.5	70.1	70.8	72.3	72.0
	r ₂	RMS	0.085	0.145	0.153	0.165	0.179
		a	75.2	78.5	74.1	74.8	79.8
		b	20.6	58.9	66.2	80.9	49.1
		c	104.0	146.4	150.8	162.2	137.3
		RMS	0.092	0.165	0.174	0.176	0.204
		a	98.7	109.5	101.3	115.3	105.6
	r ₃	b	73.3	33.4	24.2	25.4	41.4
		c	19.0	64.0	68.9	88.1	52.9
O2A	RMS	0.082	0.130	0.131	0.135	0.139	
	r ₁	a	59.7	59.4	122.6	55.3	57.2
		b	30.3	31.1	147.3	35.0	33.3
		c	90.4	85.1	88.5	85.9	84.7
	r ₂	RMS	0.091	0.152	0.161	0.169	0.190
		a	117.6	105.4	104.2	103.2	99.5
		b	74.7	75.6	82.7	76.1	77.7
		c	147.7	158.7	163.9	160.6	164.4
		RMS	0.111	0.178	0.202	0.218	0.229
		a	136.7	145.0	143.7	142.2	145.5
	r ₃	b	64.5	63.1	58.4	58.6	59.6
		c	57.7	69.3	74.0	71.1	75.4

Table 7. (continued)

O2B	RMS	0.076	0.110	0.116	0.132	0.154	
	r ₁	a	60.2	61.0	60.0	56.3	125.6
		b	146.7	139.9	146.1	139.6	35.7
		c	76.1	64.9	75.7	70.5	88.0
	RMS	0.094	0.146	0.168	0.182	0.180	
	r ₂	a	108.9	84.1	75.1	71.3	89.3
		b	115.8	115.6	97.5	100.0	87.0
		c	147.1	153.6	163.2	158.6	177.0
	RMS	0.107	0.188	0.190	0.211	0.231	
r ₃	a	143.6	150.3	34.2	39.9	35.6	
	b	109.9	118.5	57.2	51.4	54.5	
	c	60.9	82.5	81.5	81.5	87.7	
O3A	RMS	0.076	0.113	0.119	0.118	0.129	
	r ₁	a	89.9	83.8	86.8	86.9	83.9
		b	64.5	65.5	65.2	67.7	63.7
		c	25.5	25.4	25.1	22.6	27.1
	RMS	0.097	0.138	0.165	0.172	0.187	
	r ₂	a	169.1	10.7	6.3	169.9	6.9
		b	80.2	100.6	86.4	79.9	90.0
		c	94.6	91.9	95.2	90.8	96.9
	RMS	0.114	0.193	0.209	0.234	0.258	
r ₃	a	100.8	98.8	84.6	99.6	86.9	
	b	152.4	153.0	154.9	155.3	153.7	
	c	65.0	64.7	65.5	67.4	63.9	

Table 7. (continued)

O3B	RMS	0.072	0.120	0.131	0.144	0.143
	a	69.8	95.0	92.3	43.2	90.6
r ₁	b	63.5	57.6	55.2	61.4	55.6
	c	34.4	32.9	34.9	60.6	34.3
	RMS	0.089	0.152	0.161	0.154	0.179
	a	70.9	24.4	14.5	48.1	8.7
r ₂	b	39.9	67.4	77.0	109.7	82.5
	c	123.5	98.6	96.3	131.7	94.4
	RMS	0.103	0.190	0.205	0.249	0.315
	a	151.6	66.2	75.6	81.3	81.3
r ₃	b	62.6	138.7	142.2	144.2	144.6
	c	83.2	58.6	55.9	55.6	55.9

* RMS--root mean square amplitude (Å).

** a,b,c---angles (°) of r_i with unit cell edges *a*, *b* and *c*, respectively.