The compressibility and high pressure structure of diopside from first principles simulation: supplementary material

A. M. Walker[1,*], R. P. Tyer[2], R. P. Bruin[1] and M. T. Dove[1]

[1] Department of Earth Sciences,
University of Cambridge,
Downing Street,
Cambridge, CB2 3EQ, UK

[2] STFC Daresbury Laboratory,
Warrington, Cheshire, WA4 4AD, UK

[*] amw75@cam.ac.uk

Results of convergence tests for k-point (Figures 1–3) sampling and plane-wave cutoff (Figures 4–6) are presented. In each of the cases we compare the total energy (Figures 1 and 4) along with energy derivatives with respect to changes in cell parameters (Figures 3 and 6) and internal co-ordinates (Figures 2 and 5). These are calculated from one particular geometry, without geometry optimization. Only the energy derivatives strictly need to be converged and these converge much more rapidly then the total energy. By 600 eV and a 2x2x2 grid all three measures are converged.

Table 1 shows the variation of the size and orientation of the unit strain ellipsoid with pressure. Tables 2–4 shows the variation in polyhedral bond lengths and bond lengths for Si, Mg and Ca, respectively.

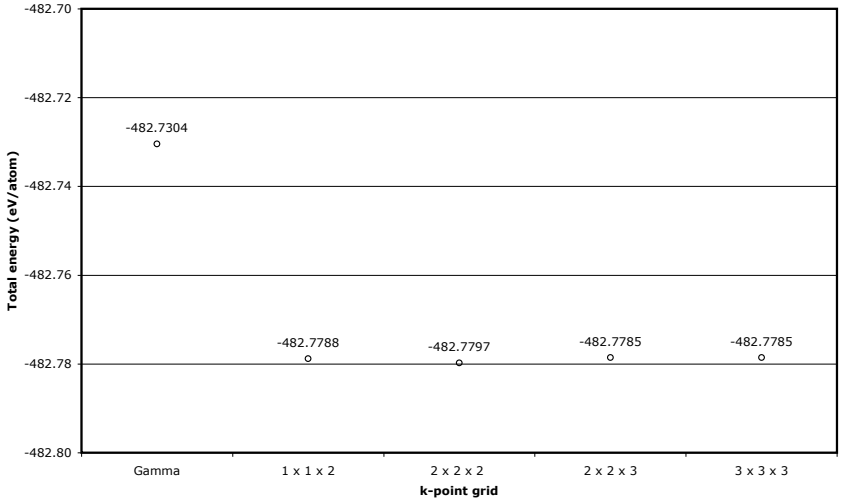

Figure 1: Convergence of total energy with increasing k-point sampling

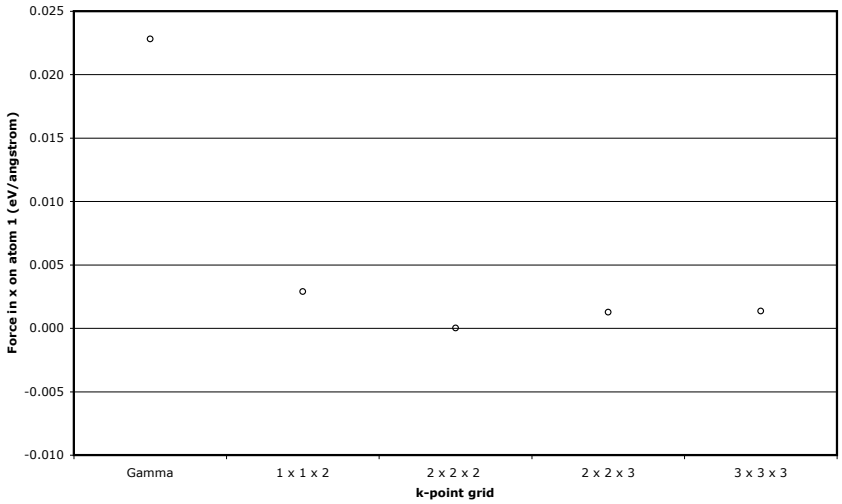

Figure 2: Convergence of atomic forces with increasing k-point sampling

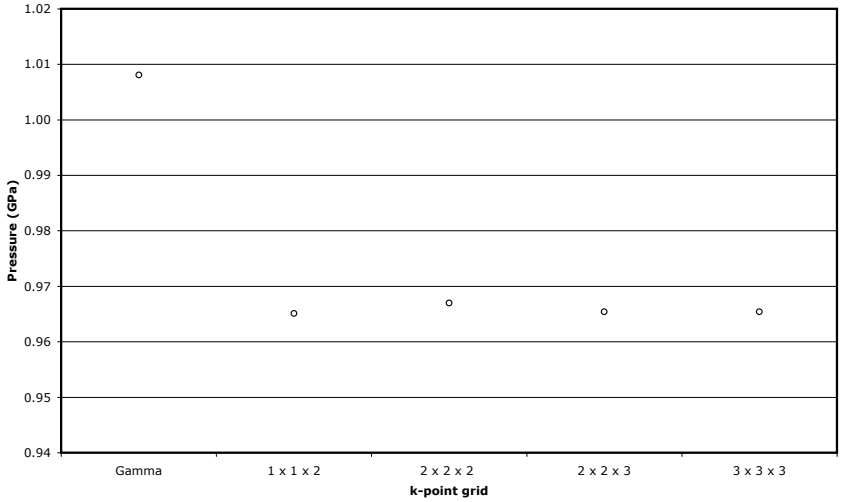

Figure 3: Convergence of total pressure with increasing k-point sampling

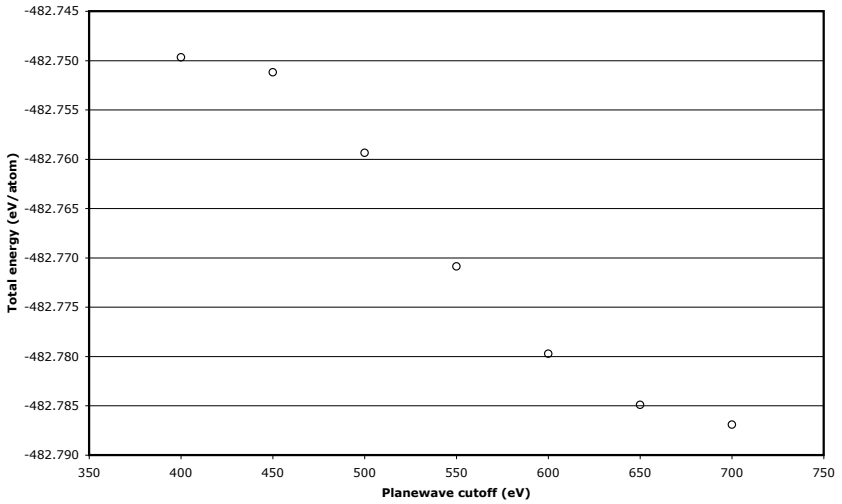

Figure 4: Convergence of total energy with increasing basis size

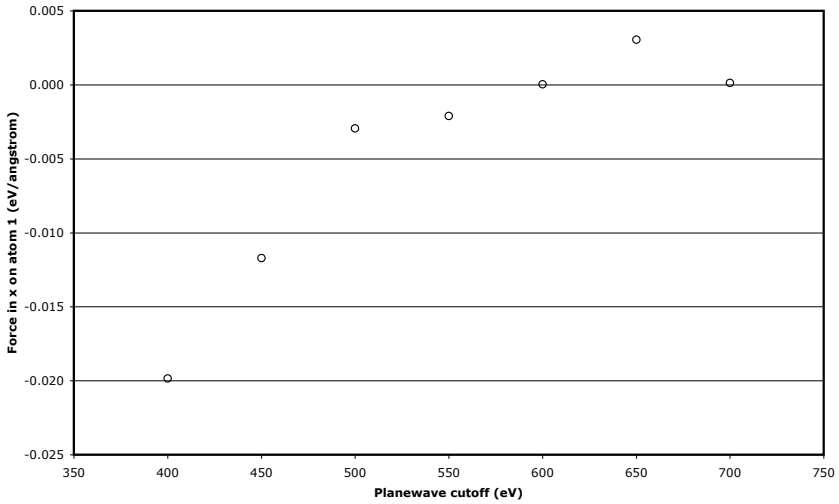

Figure 5: Convergence of atomic forces with increasing basis size

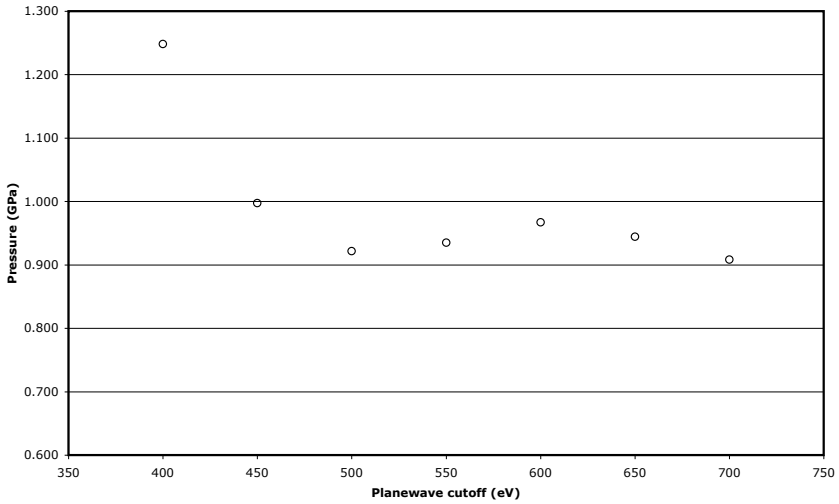

Figure 6: Convergence of total pressure with increasing basis size

P GPa	Axial lengths (x100)			Ellipsoid orientation (°)			
	$-\varepsilon_1$	$-\varepsilon_2 \parallel b$	$-\varepsilon_3$	$\varepsilon_1 \wedge a$	$\varepsilon_1 \wedge c$	$\varepsilon_3 \wedge a$	$\varepsilon_3 \wedge c$
1.0	0.079	0.431	0.544	49.5	57.0	139.6	33.0
2.0	0.076	0.397	0.517	51.8	54.8	141.8	35.2
3.0	0.088	0.381	0.491	52.2	54.3	142.2	35.7
4.0	0.132	0.369	0.449	52.0	54.6	142.0	35.4
5.0	0.128	0.358	0.435	51.9	54.7	141.9	35.3
6.0	0.127	0.348	0.421	51.8	54.8	141.8	35.2
7.0	0.136	0.341	0.402	51.7	54.9	141.7	35.1
8.0	0.123	0.333	0.396	51.8	54.8	141.8	35.2
9.0	0.127	0.327	0.381	51.7	54.8	141.7	35.2
10.0	0.136	0.322	0.364	51.5	55.0	141.5	35.0
11.0	0.132	0.316	0.355	51.5	55.0	141.5	35.0
12.0	0.132	0.312	0.345	51.5	55.1	141.5	34.9
13.0	0.128	0.307	0.338	51.5	55.1	141.4	34.9
14.0	0.127	0.303	0.329	51.4	55.2	141.4	34.8
15.0	0.127	0.299	0.320	51.3	55.3	141.3	34.7
16.0	0.133	0.296	0.309	51.0	55.6	141.0	34.4
17.0	0.134	0.292	0.301	50.8	55.7	140.8	34.3
18.0	0.127	0.289	0.298	50.9	55.6	140.9	34.4
19.0	0.130	0.286	0.289	50.6	55.9	140.6	34.1
20.0	0.124	0.282	0.286	50.7	55.8	140.7	34.2
21.0	0.131	0.282	0.276	50.4	56.2	140.4	33.8
22.0	0.131	0.279	0.271	50.2	56.4	140.2	33.6
23.0	0.130	0.277	0.266	50.1	56.5	140.1	33.5
24.0	0.127	0.274	0.262	50.0	56.5	140.1	33.5
25.0	0.123	0.271	0.260	50.1	56.5	140.1	33.5

Table 1: Unit strain ellipsoid as a function of pressure.

P GPa	Si–O1	Si–O2	Si–O3a	Si–O3b	$\overline{\mathrm{Si-O}}$	r_{Si}	V_{Si}
0.0	1.611	1.594	1.692	1.678	1.644	1.642	2.261
1.0	1.608	1.592	1.693	1.677	1.643	1.640	2.255
2.0	1.606	1.591	1.692	1.676	1.641	1.639	2.248
3.0	1.604	1.589	1.691	1.674	1.639	1.637	2.242
4.0	1.602	1.588	1.690	1.673	1.638	1.635	2.235
5.0	1.600	1.586	1.689	1.671	1.636	1.634	2.229
6.0	1.598	1.585	1.688	1.670	1.635	1.632	2.223
7.0	1.596	1.584	1.686	1.668	1.634	1.631	2.217
8.0	1.594	1.582	1.685	1.667	1.632	1.629	2.212
9.0	1.593	1.581	1.684	1.665	1.631	1.628	2.206
10.0	1.591	1.580	1.683	1.664	1.629	1.627	2.200
11.0	1.589	1.579	1.682	1.662	1.628	1.625	2.195
12.0	1.588	1.578	1.681	1.661	1.627	1.624	2.189
13.0	1.586	1.576	1.679	1.660	1.625	1.623	2.184
14.0	1.584	1.575	1.678	1.658	1.624	1.621	2.179
15.0	1.583	1.574	1.677	1.657	1.623	1.620	2.174
16.0	1.581	1.573	1.676	1.656	1.622	1.619	2.169
17.0	1.580	1.572	1.675	1.654	1.620	1.617	2.164
18.0	1.578	1.571	1.674	1.653	1.619	1.616	2.159
19.0	1.577	1.570	1.673	1.652	1.618	1.615	2.154
20.0	1.576	1.569	1.672	1.651	1.617	1.614	2.149
21.0	1.574	1.568	1.671	1.649	1.616	1.613	2.144
22.0	1.573	1.567	1.670	1.648	1.615	1.612	2.140
23.0	1.571	1.566	1.669	1.647	1.614	1.611	2.135
24.0	1.570	1.566	1.668	1.646	1.612	1.609	2.131
25.0	1.569	1.565	1.667	1.645	1.611	1.608	2.127

Table 2: Variation in bond lengths in the Si tetrahedera with pressure

P GPa	Mg–O1a	Mg–O1b	Mg–O2	$\overline{\mathrm{Mg-O}}$	r_{Mg}	V_{Mg}
0.0	2.098	2.172	2.088	2.119	2.120	12.630
1.0	2.094	2.164	2.082	2.113	2.112	12.491
2.0	2.089	2.153	2.075	2.106	2.105	12.358
3.0	2.085	2.142	2.068	2.098	2.097	12.232
4.0	2.080	2.133	2.061	2.091	2.090	12.112
5.0	2.075	2.124	2.055	2.085	2.084	11.999
6.0	2.070	2.116	2.050	2.079	2.078	11.892
7.0	2.066	2.108	2.044	2.073	2.072	11.790
8.0	2.061	2.101	2.039	2.067	2.066	11.693
9.0	2.057	2.094	2.034	2.062	2.061	11.600
10.0	2.053	2.088	2.029	2.056	2.055	11.510
11.0	2.049	2.081	2.024	2.051	2.050	11.425
12.0	2.045	2.075	2.019	2.046	2.045	11.342
13.0	2.041	2.069	2.015	2.042	2.041	11.262
14.0	2.037	2.064	2.010	2.037	2.036	11.184
15.0	2.033	2.058	2.006	2.032	2.032	11.110
16.0	2.029	2.053	2.002	2.028	2.027	11.037
17.0	2.026	2.048	1.998	2.024	2.023	10.966
18.0	2.022	2.043	1.994	2.020	2.019	10.897
19.0	2.018	2.039	1.990	2.016	2.015	10.830
20.0	2.015	2.034	1.987	2.012	2.011	10.765
21.0	2.011	2.030	1.983	2.008	2.007	10.702
22.0	2.008	2.025	1.980	2.004	2.003	10.640
23.0	2.004	2.021	1.976	2.001	2.000	10.580
24.0	2.001	2.017	1.973	1.997	1.996	10.521
25.0	1.998	2.013	1.970	1.994	1.993	10.464

Table 3: Variation in bond lengths in the M1 octahedron with pressure

P GPa	Ca–O1	Ca–O2	Ca–O3a	Ca–O3b	$\overline{\mathrm{Ca-O}}$	r_{Ca}	V_{Ca}
0.0	2.381	2.345	2.838	2.557	2.530	2.521	27.168
1.0	2.371	2.341	2.819	2.562	2.523	2.509	26.781
2.0	2.366	2.338	2.785	2.561	2.512	2.499	26.455
3.0	2.360	2.335	2.754	2.560	2.502	2.490	26.152
4.0	2.355	2.332	2.725	2.559	2.493	2.481	25.863
5.0	2.350	2.329	2.699	2.558	2.484	2.472	25.595
6.0	2.345	2.326	2.675	2.556	2.475	2.464	25.342
7.0	2.340	2.323	2.653	2.553	2.467	2.457	25.104
8.0	2.335	2.320	2.634	2.550	2.460	2.449	24.878
9.0	2.330	2.317	2.617	2.546	2.452	2.443	24.664
10.0	2.325	2.314	2.601	2.542	2.445	2.436	24.460
11.0	2.320	2.311	2.586	2.537	2.439	2.429	24.266
12.0	2.315	2.308	2.573	2.532	2.432	2.423	24.078
13.0	2.311	2.306	2.560	2.527	2.426	2.417	23.898
14.0	2.306	2.303	2.548	2.522	2.420	2.411	23.725
15.0	2.301	2.300	2.537	2.517	2.414	2.406	23.557
16.0	2.296	2.298	2.526	2.512	2.408	2.400	23.396
17.0	2.292	2.295	2.516	2.506	2.402	2.395	23.238
18.0	2.287	2.293	2.507	2.501	2.397	2.389	23.089
19.0	2.283	2.290	2.498	2.496	2.392	2.384	22.941
20.0	2.278	2.288	2.489	2.490	2.386	2.379	22.798
21.0	2.274	2.286	2.480	2.485	2.381	2.374	22.659
22.0	2.269	2.283	2.473	2.480	2.376	2.370	22.525
23.0	2.265	2.281	2.464	2.475	2.371	2.365	22.392
24.0	2.261	2.279	2.457	2.470	2.367	2.360	22.265
25.0	2.257	2.277	2.450	2.465	2.362	2.356	22.141

Table 4: Variation in bond lengths in the M2 polyhedron with pressure