Supplementary Materials for

The elastic properties of *hcp*-Fe alloys under the conditions of the Earth's inner core

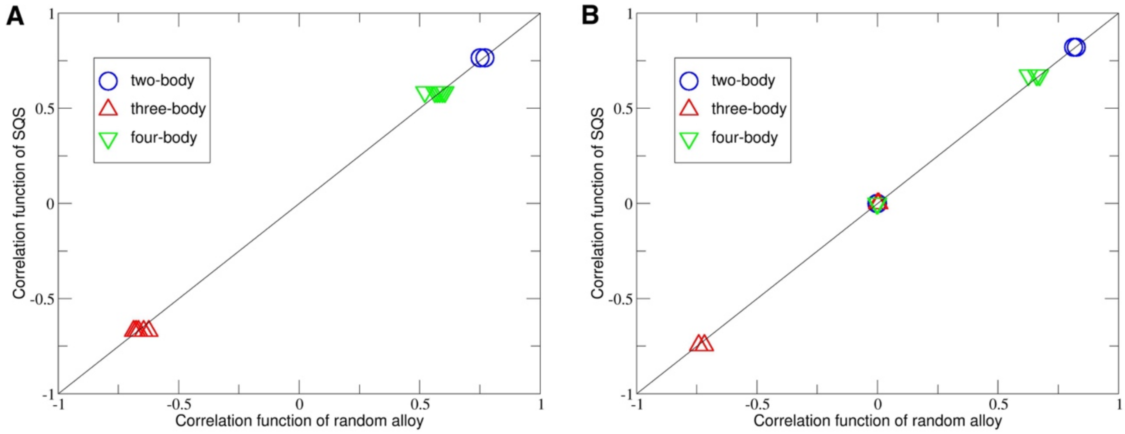
Yunguo Li[1]*, Lidunka Vočadlo[1], and John P. Brodholt[1]

[1]Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, United Kingdom

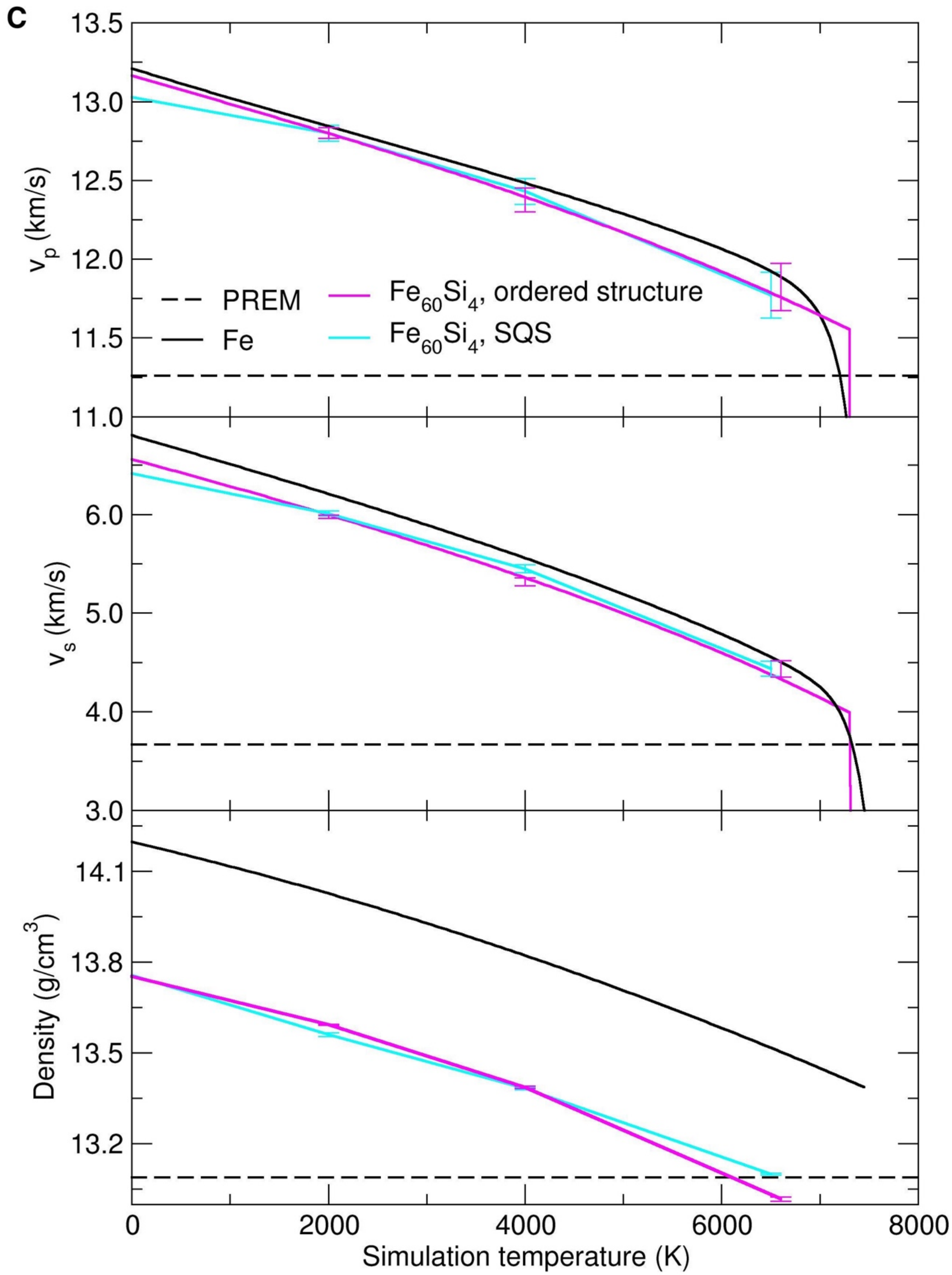
*Correspondence to: Yunguo Li (email:yunguo.li@ucl.ac.uk).

This PDF file includes:

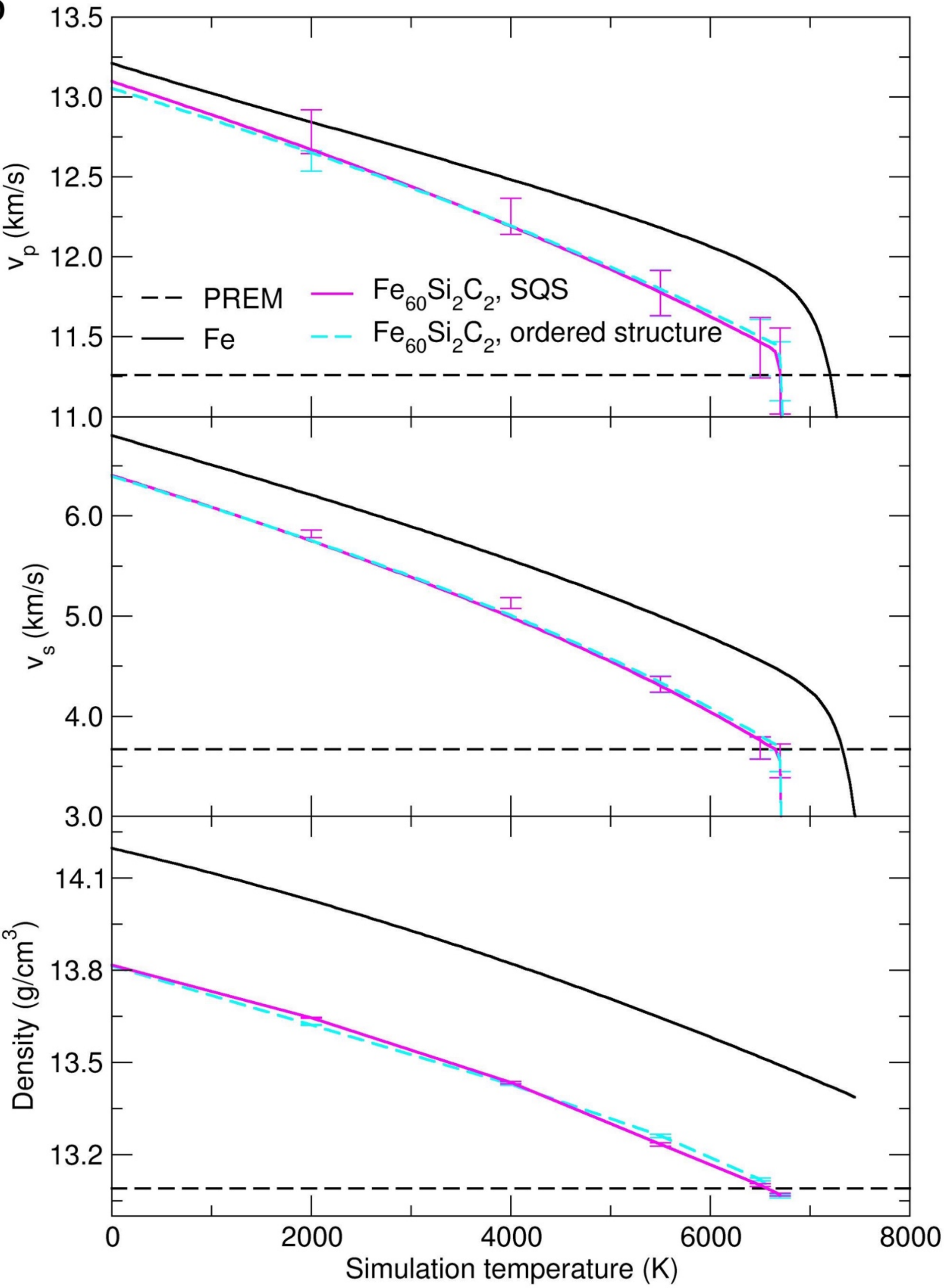
Fig. S1
Tables S1 to S5
Fortran code for the solid solution model



A
B
two-body
three-body
four-body
Correlation function of SQS
Correlation function of random alloy
1
0.5
0
-0.5
-1


c
PREM
Fe
$Fe_{60}Si_4$, ordered structure
$Fe_{60}Si_4$, SQS
v_p (km/s)
v_s (km/s)
Density (g/cm^3)
Simulation temperature (K)
13.5
13.0
12.5
12.0
11.5
11.0
6.0
5.0
4.0
3.0
14.1
13.8
13.5
13.2
0
2000
4000
6000
8000

D


13.5
13.0
12.5
12.0
11.5
11.0
v_p (km/s)
PREM
Fe
$Fe_{60}Si_2C_2$, SQS
$Fe_{60}Si_2C_2$, ordered structure
6.0
5.0
4.0
3.0
v_s (km/s)
14.1
13.8
13.5
13.2
Density (g/cm^3)
0
2000
4000
6000
8000
Simulation temperature (K)

E

Lattice parameter	a	b	c
	8.4499	8.4418	6.7673
	α	β	γ
	90.074	90.033	120.005
Structure parameter	x	y	z
Fe	0.0001	0.0003	0.9996
Fe	0.2501	0.0002	0.0000
Fe	0.4995	0.9996	0.0001
Fe	0.7494	0.9997	0.9992
Fe	0.9994	0.2491	0.9998
Fe	0.2499	0.2490	0.9982
Fe	0.4999	0.2505	0.9992
Fe	0.7502	0.2501	0.0003
Fe	0.9992	0.4999	0.0006
Fe	0.2498	0.4999	0.0003
Fe	0.5003	0.4996	0.0004
Fe	0.7503	0.4996	0.0012
Fe	0.0005	0.7499	0.9988
Fe	0.2502	0.7505	0.9995
Fe	0.5003	0.7506	0.9993
Fe	0.7502	0.7498	0.0027
Fe	0.0008	0.0015	0.4992
Fe	0.2500	0.0001	0.4993
Fe	0.5000	0.0004	0.4994
Fe	0.7501	0.0013	0.4998
Fe	0.9997	0.2500	0.5004
Fe	0.2509	0.2498	0.5022
Fe	0.5010	0.2518	0.5015
Fe	0.7501	0.2509	0.5001
Fe	0.9998	0.5000	0.5003
Fe	0.5023	0.5022	0.5009
Fe	0.7513	0.5021	0.5005
Fe	0.0018	0.7503	0.4997
Fe	0.2505	0.7509	0.5004
Fe	0.4991	0.7510	0.4992
Fe	0.1664	0.0834	0.2500
Fe	0.4167	0.0833	0.2499
Fe	0.6664	0.0835	0.2495
Fe	0.9164	0.0836	0.2495
Fe	0.1660	0.3334	0.2482
Fe	0.6672	0.3343	0.2502
Fe	0.9162	0.3329	0.2499
Fe	0.1666	0.5831	0.2486
Fe	0.4159	0.5840	0.2488
Fe	0.6680	0.5839	0.2483
Fe	0.9171	0.5836	0.2510
Fe	0.1668	0.8332	0.2494
Fe	0.4167	0.8332	0.2496
Fe	0.6663	0.8333	0.2492
Fe	0.9182	0.8340	0.2479
Fe	0.1651	0.0815	0.7492
Fe	0.4161	0.0828	0.7503
Fe	0.6664	0.0828	0.7498
Fe	0.9155	0.0820	0.7501
Fe	0.1661	0.3328	0.7516
Fe	0.4160	0.3320	0.7507
Fe	0.6662	0.3319	0.7507
Fe	0.9161	0.3329	0.7508
Fe	0.1662	0.5823	0.7520
Fe	0.4146	0.5834	0.7515
Fe	0.9178	0.5829	0.7507
Fe	0.1668	0.8334	0.7497
Fe	0.4172	0.8332	0.7501
Fe	0.6657	0.8304	0.7496
Fe	0.9156	0.8312	0.7506
Si	0.2500	0.4999	0.4999
Si	0.7520	0.7528	0.4972
Si	0.4165	0.3343	0.2507
Si	0.6652	0.5810	0.7525

F

Lattice parameter	a	b	c
	8.4102	8.3954	6.7300
	α	β	γ
	90.158	89.956	119.803
Structure parameter	x	y	z
Fe	0.9994	0.0019	0.0012
Fe	0.2505	0.0003	0.0022
Fe	0.5049	0.0023	0.0075
Fe	0.7493	0.0043	0.0042
Fe	0.0022	0.2606	0.9997
Fe	0.2495	0.2506	0.0001
Fe	0.5008	0.2503	0.0004
Fe	0.7525	0.2510	0.0052
Fe	0.2490	0.5009	0.9993
Fe	0.5007	0.5000	0.9996
Fe	0.7534	0.4979	0.9998
Fe	0.0015	0.7480	0.9997
Fe	0.2477	0.7487	0.9997
Fe	0.4998	0.7497	0.9982
Fe	0.7500	0.7502	0.0004
Fe	0.9989	0.9997	0.5000
Fe	0.2505	0.9998	0.4982
Fe	0.5043	0.0007	0.4927
Fe	0.7488	0.0018	0.4980
Fe	0.0001	0.2508	0.5034
Fe	0.2504	0.2504	0.5008
Fe	0.5004	0.2495	0.5001
Fe	0.7496	0.2443	0.4939
Fe	0.0003	0.4991	0.5014
Fe	0.2499	0.5013	0.4993
Fe	0.5005	0.4996	0.5002
Fe	0.7519	0.4991	0.4978
Fe	0.9982	0.7475	0.4994
Fe	0.2496	0.7480	0.4991
Fe	0.4995	0.7490	0.5016
Fe	0.7495	0.7498	0.4992
Fe	0.1641	0.0835	0.2508
Fe	0.4191	0.0832	0.2505
Fe	0.9109	0.0851	0.2503
Fe	0.1675	0.3334	0.2515
Fe	0.4162	0.3326	0.2499
Fe	0.6656	0.3259	0.2510
Fe	0.1625	0.5810	0.2426
Fe	0.4168	0.5835	0.2496
Fe	0.6672	0.5819	0.2492
Fe	0.9186	0.5797	0.2426
Fe	0.1659	0.8332	0.2515
Fe	0.4170	0.8327	0.2494
Fe	0.6652	0.8375	0.2502
Fe	0.9160	0.8330	0.2490
Fe	0.1661	0.0836	0.7500
Fe	0.6682	0.0848	0.7508
Fe	0.9161	0.0837	0.7522
Fe	0.1675	0.3339	0.7499
Fe	0.4168	0.3334	0.7501
Fe	0.6681	0.3323	0.7487
Fe	0.9166	0.3370	0.7535
Fe	0.1630	0.5824	0.7555
Fe	0.4168	0.5836	0.7497
Fe	0.6677	0.5826	0.7498
Fe	0.9187	0.5818	0.7552
Fe	0.1663	0.8340	0.7481
Fe	0.4160	0.8346	0.7503
Fe	0.6677	0.8351	0.7505
Fe	0.9169	0.8335	0.7507
Si	0.9157	0.3333	0.2482
Si	0.4175	0.0817	0.7502
C	0.0026	0.5044	0.9975
C	0.6590	0.0779	0.2487

Fig. S1

Comparison of the elastic properties of the SQS and ordered structures. Pair and multisite correlation functions of the SQS structure plotted against that of random structure for **(A)** *hcp*-$Fe_{60}Si_4$ and for (**B**) *hcp*-$Fe_{60}Si_2C_2$. Calculated elastic properties of the SQS and ordered structures for (**C**) *hcp*-$Fe_{60}Si_4$, and for (**D**) *hcp*-$Fe_{60}Si_2C_2$. Crystallographic information of the SQS structures for (**E**) *hcp*-$Fe_{60}Si_4$, and for (**F**) *hcp*-$Fe_{60}Si_2C_2$.

Table S1.

Calculated isothermal elastic properties of the alloys at 360 GPa.

	T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	ρ (g/cm^3)	B_s (GPa)	G (GPa)	V_s (km/s)	V_p (km/s)	V_D (km/s)	ν
hcp-Fe	0	2522	1229	1065	2777	576	14.19	1615	657	6.80	13.25	7.65	0.32
	2000	2279	1267	1087	2495	462	14.03	1595	527	6.13	12.79	6.89	0.35
	4000	2076	1274	1101	2187	404	13.82	1565	433	5.60	12.45	6.31	0.37
	6700	1780	1247	1059	1956	237	13.49	1497	291	4.65	11.82	5.27	0.41
$Fe_{62}C_2$ (ordered)	0	2424	1300	1117	2674	495	14.11	1621	576	6.39	13.02	7.18	0.34
	2000	2182	1331	1120	2444	384	13.87	1597	454	5.72	12.60	6.45	0.37
	4000	1964	1377	1091	2175	277	13.65	1557	339	4.98	12.13	5.64	0.40
	5500	1806	1337	1086	1882	252	13.43	1505	280	4.56	11.82	5.18	0.41
	6400	1700	1344	1057	1741	172	13.36	1468	217	4.03	11.47	4.58	0.43
$Fe_{60}C_4$ (ordered)	0	2286	1361	1153	2586	419	13.88	1610	493	5.96	12.78	6.71	0.36
	2000	2115	1346	1159	2307	318	13.69	1587	396	5.38	12.43	6.07	0.38
	4000	1844	1383	1147	2055	237	13.45	1562	279	4.55	11.93	5.16	0.41
	4500	1787	1381	1140	1978	198	13.38	1527	246	4.29	11.78	4.87	0.42
	5000	1689	1370	1148	1913	170	13.34	1508	208	3.95	11.57	4.49	0.43
$Fe_{62}S_2$ (ordered)	0	2458	1246	1095	2688	550	14.04	1608	619	6.64	13.17	7.45	0.33
	2000	2259	1287	1112	2420	435	13.86	1598	500	6.00	12.78	6.76	0.36
	4000	2046	1266	1102	2192	343	13.65	1558	403	5.43	12.39	6.13	0.38
	5500	1892	1292	1061	2009	251	13.47	1518	319	4.86	12.01	5.51	0.40
	6600	1724	1293	1074	1889	199	13.34	1493	249	4.32	11.70	4.90	0.42
$Fe_{60}S_4$ (ordered)	0	2424	1262	1111	2653	508	13.89	1608	587	6.50	13.12	7.30	0.34
	2000	2228	1308	1085	2472	421	13.71	1589	490	5.95	12.79	6.74	0.36
	4000	1981	1278	1118	2155	300	13.49	1548	364	5.19	12.28	5.87	0.39
	5500	1790	1282	1079	1935	232	13.29	1491	282	4.61	11.85	5.22	0.41
	6000	1706	1291	1081	1864	216	13.22	1475	250	4.34	11.69	4.93	0.42
	6500	1635	1315	1063	1823	191	13.15	1460	218	4.08	11.54	4.63	0.43
$Fe_{60}Si_4$ (ordered)	0	2401	1262	1092	2631	509	13.75	1592	583	6.51	13.13	7.31	0.34
	2000	2221	1323	1066	2459	415	13.59	1580	485	5.98	12.80	6.73	0.36
	4000	2002	1300	1072	2232	306	13.39	1546	379	5.32	12.38	6.01	0.39
	6600	1723	1301	1036	1914	204	13.02	1478	256	4.44	11.82	5.04	0.42
$Fe_{60}Si_4$ (SQS)	0	2349	1283	1088	2609	507	13.76	1581	566	6.41	13.03	7.20	0.34
	2000	2202	1295	1075	2410	436	13.56	1569	490	6.01	12.80	6.76	0.36
	4000	1991	1274	1057	2298	332	13.38	1539	398	5.45	12.43	6.15	0.38
	6500	1756	1322	1045	1897	204	13.10	1471	258	4.44	11.77	5.04	0.42
$Fe_{56}Si_8$ (ordered)	0	2263	1369	1090	2581	441	13.35	1578	503	6.14	12.98	6.91	0.36
	2000	2177	1348	1070	2425	379	13.20	1574	454	5.87	12.85	6.61	0.37
	4000	1926	1338	1077	2220	272	13.00	1537	340	5.11	12.37	5.78	0.40
	6500	1675	1324	1085	1843	174	12.68	1486	218	4.15	11.84	4.71	0.43
$Fe_{60}Si_3C_1$ (SQS)	0	2378	1293	1134	2685	498	13.79	1618	566	6.41	13.12	7.20	0.34
	2000	2203	1324	1062	2338	403	13.53	1561	469	5.89	12.71	6.63	0.36
	4000	2013	1320	1065	2206	314	13.35	1547	381	5.34	12.40	6.03	0.39
	5500	1826	1329	1072	1949	252	13.20	1509	292	4.70	11.99	5.33	0.41
	6500	1750	1345	1046	1828	211	13.11	1487	251	4.38	11.79	4.97	0.42
	7000	1637	1295	1072	1632	188	13.04	1446	207	3.99	11.49	4.53	0.43
	7200	1598	1362	1030	1576	179	13.02	1430	185	3.77	11.35	4.29	0.44
$Fe_{60}Si_3C_1$ (ordered)	0	2369	1288	1114	2601	479	13.78	1597	554	6.34	13.02	7.13	0.34
	2000	2197	1295	1105	2408	389	13.62	1581	466	5.85	12.71	6.59	0.37
	4000	2037	1313	1069	2190	298	13.41	1551	379	5.32	12.38	6.01	0.39
	5500	1842	1292	1066	1973	217	13.20	1504	291	4.69	11.97	5.32	0.41
	6500	1685	1302	1073	1826	169	13.07	1475	223	4.13	11.64	4.69	0.43
	6700	1628	1333	1069	1807	165	13.03	1468	202	3.93	11.55	4.47	0.43
	7000	1589	1343	1033	1783	142	12.99	1446	185	3.77	11.41	4.29	0.44
$Fe_{60}Si_2C_2$ (SQS)	0	2349	1295	1126	2613	486	13.82	1601	551	6.31	13.00	7.09	0.35
	2000	2208	1317	1158	2411	401	13.60	1613	462	5.82	12.78	6.56	0.37
	4000	1950	1291	1113	2190	291	13.43	1546	354	5.13	12.25	5.80	0.39
	5500	1749	1339	1105	1923	202	13.23	1506	247	4.32	11.77	4.90	0.42
	6500	1547	1360	1117	1811	179	13.10	1475	178	3.68	11.43	4.19	0.44
	6700	1468	1333	1098	1818	174	13.07	1444	165	3.55	11.28	4.05	0.44
$Fe_{60}Si_2C_2$ (ordered)	0	2328	1335	1123	2598	460	13.81	1602	528	6.18	12.92	6.95	0.35
	2000	2146	1306	1135	2339	378	13.62	1577	439	5.68	12.60	6.40	0.37
	4000	1943	1331	1108	2159	274	13.43	1547	337	5.01	12.19	5.67	0.40
	5500	1701	1414	1086	2024	177	13.26	1515	222	4.09	11.69	4.65	0.43
	6500	1597	1403	1085	1804	164	13.12	1481	180	3.70	11.45	4.22	0.44
	6700	1562	1382	1085	1767	157	13.06	1467	170	3.61	11.39	4.11	0.44
$Fe_{60}S_3C_1$ (ordered)	0	2361	1301	1126	2617	494	13.88	1605	556	6.33	13.00	7.11	0.34
	2000	2190	1302	1144	2361	375	13.71	1593	449	5.72	12.65	6.45	0.37
	4000	1932	1332	1117	2160	301	13.49	1549	322	5.05	12.20	5.72	0.40
	5500	1774	1354	1079	1944	192	13.27	1505	251	4.35	11.77	4.94	0.42
	6000	1740	1346	1044	1877	167	13.19	1481	234	4.21	11.66	4.79	0.42
	6200	1712	1299	1045	1760	156	13.17	1453	224	4.12	11.53	4.68	0.43
$Fe_{60}S_2C_2$ (ordered)	0	2362	1285	1151	2579	464	13.88	1609	541	6.24	12.96	7.02	0.35
	2000	2176	1289	1146	2372	371	13.70	1589	447	5.71	12.63	6.44	0.37
	4000	1944	1125	1288	2142	266	13.48	1582	344	5.05	12.30	5.72	0.40
$Fe_{60}S_3Si_1$ (ordered)	0	2426	1263	1106	2635	513	13.85	1604	589	6.52	13.14	7.32	0.34
	2000	2220	1279	1106	2433	416	13.68	1586	486	5.96	12.78	6.71	0.36
	4000	2000	1363	1079	2160	324	13.47	1555	369	5.24	12.33	5.92	0.39

	5500	1832	1410	1072	1980	246	13.26	1534	280	4.60	12.00	5.21	0.41
	6000	1772	1408	1070	1896	214	13.19	1518	248	4.33	11.84	4.92	0.42
	6500	1745	1388	1066	1813	179	13.07	1505	226	4.16	11.76	4.73	0.43
$Fe_{60}S_2Si_2$ (ordered)	0	2414	1276	1097	1635	507	13.82	1600	582	6.49	13.12	7.29	0.34
	2000	2205	1243	1099	2423	408	13.65	1569	485	5.96	12.74	6.71	0.36
	4000	2030	1297	1084	2173	318	13.43	1551	385	5.35	12.40	6.05	0.39
	5500	1831	1278	1064	2010	227	13.23	1502	297	4.74	11.98	5.37	0.41
	6500	1715	1347	1045	1846	183	13.07	1482	233	4.22	11.71	4.79	0.43

Table S2.

Calculated adiabatic elastic properties of the alloys at 360 GPa**.** The adiabatic elastic constants (C_{ij}^{S}) were calculated from the isothermal elastic constants (C_{ij}^{T}) via the thermodynamic equation $C_{ij}^{S} = C_{ij}^{T} + T \cdot V \left(\frac{\partial \sigma_i}{\partial T}\right)_{\eta} \left(\frac{\partial \sigma_j}{\partial T}\right)_{\eta} / C_{\eta}$, where T is temperature, V is volume, C_{η} is specific heat at configuration η, and σ_i and σ_j are the thermal stress tensors (Wallace, 1998).

	T (K)	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{33} (GPa)	C_{44} (GPa)	ρ (g/cm^3)	B_s (GPa)	G (GPa)	V_s (km/s)	V_p (km/s)	V_D (km/s)	ν
hcp-Fe	0	2522	1229	1065	2777	576	14.19	1615	657	6.80	13.25	7.65	0.32
	2000	2279	1267	1087	2495	462	14.03	1595	527	6.13	12.80	6.89	0.35
	4000	2125	1323	1164	2268	404	13.82	1536	433	5.60	12.36	6.31	0.37
	6700	1890	1359	1212	2168	237	13.49	1502	292	4.65	11.84	5.28	0.41
$Fe_{62}C_2$ (ordered)	0	2424	1300	1117	2674	495	14.11	1621	576	6.39	13.02	7.18	0.34
	2000	2233	1376	1179	2513	384	13.87	1605	456	5.73	12.63	6.46	0.37
	4000	2040	1452	1191	2308	277	13.65	1562	340	4.99	12.15	5.65	0.40
	5500	1914	1447	1234	2085	252	13.43	1527	281	4.57	11.90	5.18	0.41
	6400	1700	1344	1057	1741	172	13.36	1340	217	4.03	11.04	4.57	0.42
$Fe_{60}C_4$ (ordered)	0	2286	1361	1153	2586	419	13.88	1610	493	5.96	12.78	6.71	0.36
	2000	2165	1394	1211	2361	318	13.69	1591	396	5.38	12.44	6.08	0.39
	4000	1939	1481	1246	2158	237	13.45	1554	278	4.55	11.96	5.16	0.42
	4500	1899	1499	1256	2098	198	13.38	1546	245	4.28	11.83	4.86	0.42
	5000	1811	1498	1274	2043	170	13.34	1529	208	3.95	11.64	4.49	0.43
$Fe_{62}S_2$ (ordered)	0	2458	1246	1095	2688	550	14.04	1608	619	6.64	13.17	7.45	0.33
	2000	2282	1311	1142	2459	435	13.86	1579	500	6.00	12.73	6.76	0.36
	4000	2100	1321	1178	2298	343	13.65	1539	403	5.43	12.33	6.13	0.38
	5500	1979	1385	1175	2157	251	13.47	1509	318	4.86	11.98	5.51	0.40
	6600	1832	1411	1229	2111	199	13.34	1501	249	4.32	11.72	4.90	0.42
$Fe_{60}S_4$ (ordered)	0	2424	1262	1111	2653	508	13.89	1608	587	6.50	13.12	7.30	0.34
	2000	2254	1335	1121	2520	421	13.71	1576	490	5.98	12.75	6.73	0.36
	4000	2044	1344	1204	2272	300	13.49	1540	364	5.19	12.25	5.87	0.39
	5500	1885	1401	1237	2159	232	13.29	1520	278	4.57	11.93	5.19	0.41
	6000	1805	1400	1229	2078	216	13.22	1490	250	4.35	11.74	4.93	0.42
	6500	1755	1436	1233	2048	191	13.15	1485	219	4.08	11.62	4.64	0.43
$Fe_{60}Si_4$ (ordered)	0	2401	1262	1092	2631	509	13.75	1592	583	6.51	13.13	7.31	0.34
	2000	2253	1356	1100	2496	415	13.59	1568	485	5.98	12.77	6.73	0.36
	4000	2069	1368	1138	2297	306	13.39	1525	379	5.32	12.31	6.01	0.39
	6600	1858	1425	1195	2125	204	13.02	1497	260	4.47	11.90	5.07	0.42
$Fe_{56}Si_8$ (ordered)	0	2263	1369	1090	2581	441	13.35	1578	503	6.14	12.98	6.91	0.36
	2000	2247	1432	1166	2557	379	13.20	1620	452	5.85	12.98	6.60	0.37
	4000	2017	1443	1208	2407	272	13.00	1573	338	5.10	12.48	5.77	0.40
	6500	1795	1479	1230	2098	174	12.68	1507	218	4.14	11.91	4.76	0.43
$Fe_{60}Si_3C_1$ (ordered)	0	2369	1288	1114	2601	479	13.78	1597	554	6.34	13.02	7.13	0.34
	2000	2226	1324	1141	2453	389	16.62	1569	466	5.85	12.68	6.59	0.36
	4000	2105	1380	1155	2298	298	13.41	1543	380	5.32	12.36	6.01	0.40
	5500	1966	1421	1219	2163	217	14.20	1535	290	4.69	12.07	5.32	0.41
	6500	1814	1443	1249	2066	169	13.07	1508	222	4.12	11.75	4.67	0.43
	6700	1786	1505	1283	2097	165	13.03	1535	201	3.92	11.76	4.46	0.44
	7000	1729	1504	1230	2063	142	12.99	1494	183	3.75	11.57	4.27	0.44
$Fe_{60}Si_2C_2$ (ordered)	0	2328	1335	1123	2598	460	13.81	1602	528	6.18	12.92	6.95	0.35
	2000	2174	1335	1172	2387	378	13.62	1566	439	5.68	12.57	6.40	0.37
	4000	2004	1394	1196	2286	274	13.43	1541	338	5.02	12.18	5.68	0.40
	5500	1799	1514	1226	2221	177	13.26	1528	223	4.10	11.73	4.66	0.43
	6500	1712	1530	1263	2066	164	13.12	1511	179	3.70	11.55	4.21	0.44
	6700	1685	1518	1284	2032	157	13.06	1508	167	3.58	11.51	4.08	0.45
$Fe_{60}S_3C_1$ (ordered)	0	2361	1301	1126	2617	494	13.88	1605	556	6.33	13.00	7.11	0.34
	2000	2216	1330	1181	2414	375	13.71	1581	449	5.72	12.61	6.45	0.37
	4000	1994	1398	1207	2290	301	13.49	1545	344	5.05	12.19	5.72	0.40
	5500	1870	1465	1220	2152	192	13.27	1522	250	4.34	11.82	4.93	0.42
	6000	1850	1473	1206	2117	167	13.19	1510	233	4.21	11.75	4.78	0.43
	6200	1826	1435	1214	2011	156	13.17	1488	222	4.10	11.64	4.66	0.43
$Fe_{60}S_2C_2$ (ordered)	0	2362	1285	1151	2579	464	13.88	1609	541	6.24	12.96	7.02	0.35
	2000	2206	1319	1184	2422	371	13.70	1579	447	5.71	12.60	6.44	0.37
	4000	2010	1194	1379	2268	266	13.48	1577	344	5.05	12.29	5.72	0.39
$Fe_{60}S_3Si_1$ (ordered)	0	2426	1263	1106	2635	513	13.85	1604	589	6.52	13.14	7.32	0.34
	2000	2247	1307	1139	2475	416	13.68	1571	486	5.96	12.74	6.71	0.36
	4000	2063	1428	1162	2269	324	13.47	1544	369	5.24	12.30	5.92	0.39
	5500	1927	1520	1191	2151	246	13.26	1534	279	4.59	11.99	5.21	0.41
	6000	1887	1531	1197	2091	214	13.19	1524	251	4.36	11.87	4.95	0.42
	6500	1872	1528	1213	2030	179	13.07	1520	227	4.17	11.81	4.74	0.43
$Fe_{60}S_2Si_2$ (ordered)	0	2414	1276	1097	2635	507	13.82	1600	582	6.49	13.12	7.29	0.34
	2000	2232	1271	1171	2464	408	13.65	1573	480	5.93	12.73	6.68	0.36
	4000	2091	1360	1167	2285	318	13.43	1539	385	5.36	12.36	6.05	0.38
	5500	1928	1381	1198	2195	227	13.23	1512	297	4.74	12.01	5.37	0.41
	6500	1831	1485	1214	2091	183	13.07	1509	230	4.20	11.79	4.77	0.43

Table S3.

The statistical errors of the calculated elastic properties of the alloys at 360 GPa.

	T (K)	ΔC_{11} (GPa)	ΔC_{12} (GPa)	ΔC_{13} (GPa)	ΔC_{33} (GPa)	ΔC_{44} (GPa)	$\Delta \rho$ (g/cm^3)	ΔB_s (GPa)	ΔG (GPa)	ΔV_s (km/s)	ΔV_p (km/s)
hcp-Fe	0	0	0	0	0	0	0	0	0	0	0
	2000	7.2	7.2	6.4	5.3	3.3	0.02	8.4	2.6	0.015	0.033
	4000	13.2	13.1	13.1	10.6	6.5	0.05	16.9	5.0	0.032	0.068
	6700	21.8	25.7	23.8	21.7	11.3	0.07	33	8.8	0.070	0.142
$Fe_{62}C_2$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.8	9.9	9.1	7.2	5.8	0.01	11.69	3.9	0.025	0.048
	4000	17.6	18.1	15.7	14.7	9.2	0.04	22.36	6.7	0.049	0.095
	5500	23.7	24.6	24.1	21.1	13.4	0.04	32.7	9.4	0.077	0.145
	6400	25.8	27.0	25.7	24.3	14.4	0.07	36.7	10.2	0.095	0.171
$Fe_{60}C_4$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	11.2	11.9	11.2	9.2	6.7	0.02	14.6	4.5	0.031	0.061
	4000	17.0	17.8	16.2	14.2	11.0	0.06	22.1	7.0	0.058	0.101
	4500	22.3	22.5	20.3	17.4	12.3	0.09	27.4	8.6	0.075	0.129
	5000	24.5	24.8	25.1	23.0	13.5	0.07	35.1	9.6	0.091	0.162
$Fe_{62}S_2$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.1	8.9	7.4	5.3	4.0	0.01	9.0	3.2	0.019	0.038
	4000	15.1	15.2	13.7	12.4	7.1	0.04	19.1	5.6	0.038	0.079
	5500	19.7	20.9	19.6	17.7	9.7	0.06	27.2	7.5	0.057	0.116
	6600	23.6	23.1	23.5	21.8	12.3	0.01	33.1	9.0	0.078	0.148
$Fe_{60}S_4$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.1	9.3	8.1	6.8	4.2	0.02	10.8	3.3	0.020	0.043
	4000	15.9	15.7	14.5	714.3	7.8	0.04	21.3	5.9	0.042	0.088
	5500	20.6	21.6	21.2	19.3	10.7	0.06	29.5	8.0	0.065	0.129
	6000	21.7	24.1	23.1	23.6	12.5	0.07	34.7	8.9	0.077	0.153
	6500	25.6	27.1	26.9	24.8	13.4	0.07	37.7	10.0	0.094	0.174
$Fe_{60}Si_4$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	7.5	7.7	7.4	5.0	3.4	0.01	8.6	2.8	0.017	0.035
	4000	15.8	16.3	13.0	10.9	7.2	0.04	17.4	5.7	0.040	0.076
	6600	24.2	25.4	23.9	20.7	12.0	0.08	32.3	9.2	0.083	0.151
$Fe_{60}Si_4$ (SQS)	0	0	0	0	0	0	0	0	0	0	0
	2000	12.7	12.4	10.6	6.2	4.8	0.07	11.5	4.3	0.027	0.050
	4000	15.0	14.8	14.6	12.2	7.4	0.05	19.3	5.6	0.039	0.081
	6500	23.9	23.3	22.4	21.2	11.6	0.03	32.1	8.9	0.076	0.145
$Fe_{56}Si_8$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	10.3	10.8	7.4	5.2	4.0	0.02	9.1	3.6	0.023	0.041
	4000	16.2	16.5	14.6	12.6	7.4	0.04	19.8	5.9	0.045	0.087
	6500	23.7	24.4	24.2	20.8	12.8	0.06	32.4	9.3	0.088	0.156
$Fe_{60}Si_3C_1$ (SQS)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.1	9.2	8.2	6.5	5.0	0.01	10.5	3.5	0.022	0.044
	4000	17.6	17.3	16.8	15.4	9.1	0.05	23.5	6.7	0.047	0.098
	5500	20.5	20.6	20.5	18.6	11.0	0.06	28.5	8.0	0.064	0.125
	6500	26.2	29.0	27.8	27.7	14.2	0.05	32.6	9.2	0.081	0.150
	7000	28.0	27.2	25.9	24.2	14.7	0.06	36.7	10.6	0.103	0.179
	7200	26.2	29.0	27.8	27.7	14.2	0.05	41.0	10.5	0.107	0.194
$Fe_{60}Si_3C_1$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	8.9	9.2	8.2	6.5	5.0	0.01	10.5	3.5	0.022	0.044
	4000	15.1	16.1	14.1	12.4	8.5	0.04	19.3	6.0	0.042	0.082
	5500	20.5	20.6	20.5	18.6	11.0	0.06	28.5	8.0	0.064	0.125
	6500	24.1	27.8	25.8	24.7	13.3	0.01	37.0	9.8	0.091	0.170
	6700	28.0	27.2	26.0	24.2	14.7	0.06	36.7	10.6	0.103	0.179
	7000	26.2	29.0	27.8	27.7	14.3	0.05	41.0	10.5	0.107	0.194
$Fe_{60}Si_2C_2$ (SQS)	0	0	0	0	0	0	0	0	0	0	0
	2000	11.2	10.9	27.4	26.3	7.0	0.01	38.7	5.9	0.037	0.137
	4000	19.5	20.3	20.1	16.6	11.4	0.04	26.3	7.8	0.057	0.113
	5500	23.6	24.2	22.6	20.0	12.0	0.06	30.7	9.0	0.078	0.142
	6500	27.6	28.5	27.0	25.6	15.1	0.05	38.6	10.8	0.112	0.190
	6700	39.0	45.2	37.6	31.9	21.8	0.05	50.4	15.7	0.169	0.269
$Fe_{60}Si_2C_2$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	12.9	13.4	11.4	9.4	7.7	0.01	15.1	5.1	0.033	0.064
	4000	19.5	20.3	20.1	16.6	11.4	0.04	26.3	7.8	0.058	0.113
	5500	23.6	24.2	22.6	19.8	12.0	0.06	30.7	9.0	0.083	0.144

	6500	27.8	27.3	25.5	22.4	14.3	0.05	34.9	10.5	0.108	0.176
	6700	25.9	26.7	26.2	25.5	13.6	0.07	38.1	10.1	0.107	0.185
$Fe_{60}S_3C_1$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.3	9.3	8.7	7.2	5.2	0.02	11.4	3.6	0.023	0.047
	4000	16.3	16.6	15.3	12.7	9.3	0.04	20.1	6.4	0.047	0.088
	5500	22.7	22.3	21.7	19.6	12.1	0.06	30.1	8.7	0.074	0.137
	6000	23.8	24.3	25.2	23.8	13.1	0.06	35.8	9.4	0.085	0.161
	6200	25.8	28.5	26.8	27.1	14.5	0.07	40.0	10.4	0.096	0.182
$Fe_{60}S_2C_2$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.9	9.9	8.6	7.1	5.8	0.02	11.3	3.9	0.025	0.048
	4000	16.2	16.4	16.2	14.7	9.8	0.04	22.5	6.5	0.048	0.095
$Fe_{60}S_3Si_1$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	8.1	8.3	8.2	7.9	4.1	0.02	11.8	3.11	0.019	0.046
	4000	15.3	15.8	14.6	11.6	7.6	0.04	18.8	5.8	0.041	0.080
	5500	23.3	24.6	25.3	23.5	12.4	0.07	35.6	9.2	0.076	0152
	6000	23.2	22.2	22.1	20.7	11.6	0.06	31.4	8.7	0.076	0.141
	6500	23.9	25.8	24.2	22.8	12.2	0.08	34.4	9.3	0.085	0.157
$Fe_{60}S_2Si_2$ (ordered)	0	0	0	0	0	0	0	0	0	0	0
	2000	9.1	9.1	7.5	5.1	4.4	0.01	8.9	3.3	0.020	0.039
	4000	15.7	15.6	14.5	12.8	7.5	0.04	19.8	5.8	0.040	0.083
	5500	19.4	19.8	18.2	17.3	10.6	0.06	26.2	7.5	0.060	0.116
	6500	22.2	24.0	22.1	20.7	11.9	0.07	31.4	8.7	0.079	0.145

Table S4

The original calculated data used for the solid solution model. The data for *hcp*-$Fe_{60}C_4$ are fitted from the Nadal-Le Poac model based on the data at 0, 2000, 4000, 4500 and 5000 K, imposing T_m=6550 K).

Temperature (K)	Material	ρ (g/cm^3)	B_s (GPa)	G (GPa)
5500	*hcp*-Fe	13.645	1526	353
	hcp-$Fe_{62}C_2$	13.452	1503	265
	hcp-$Fe_{60}C_4$	13.262	1495	188
	hcp-$Fe_{60}Si_4$	13.255	1521	304
	hcp-$Fe_{56}Si_8$	12.814	1513	272
	hcp-$Fe_{62}S_2$	13.475	1523	317
	hcp-$Fe_{60}S_4$	13.293	1496	281
6000	*hcp*-Fe	13.582	1513	325
	hcp-$Fe_{62}C_2$	13.391	1487	240
	hcp-$Fe_{60}C_4$	13.195	1474	159
	hcp-$Fe_{60}Si_4$	13.112	1494	277
	hcp-$Fe_{56}Si_8$	12.747	1499	248
	hcp-$Fe_{62}S_2$	13.412	1509	289
	hcp-$Fe_{60}S_4$	13.223	1478	251
6500	*hcp*-Fe	13.518	1503	298
	hcp-$Fe_{62}C_2$	13.329	1470	211
	hcp-$Fe_{60}C_4$	13.126	1456	130
	hcp-$Fe_{60}Si_4$	13.035	1478	250
	hcp-$Fe_{56}Si_8$	12.676	1482	224
	hcp-$Fe_{62}S_2$	13.348	1493	257
	hcp-$Fe_{60}S_4$	13.150	1459	218

Table S5

The standard deviations of G, B_s, and ρ for the solid solution model.

Temperature (K)	ρ (g/cm^3)	B_s (GPa)	G (GPa)
5500	0.012	4.2	8.3
6000	0.012	5.8	6.6
6500	0.015	6.3	7.5

Code

Fortran code to calculate the elastic properties of *hcp*-Fe-Si-C-S alloys based on the solid solution model.

```
PROGRAM SCAN
!!
!! units: density(kg/m^3), vs&vp (km/s), G & Ks (GPa)
!!
IMPLICIT NONE

INTEGER, PARAMETER :: ap = selected_real_kind(15,300)
INTEGER :: n,i,j,k,T

REAL(ap) :: g,ks,vs,vp,rho,vol,mol_max, mol_step,vol_fe,vol_si,vol_c,vol_s
REAL(ap), PARAMETER :: prem_vs_h=3.6678, prem_vp_h=11.2622, prem_rho_h=13.0886,&
                       prem_vs_l=3.5645, prem_vp_l=11.2409, prem_rho_l=13.0122,&
                       tolerance_vs=0.143,tolerance_vp=0.204,tolerance_rho=0.1

REAL(ap), DIMENSION(:), ALLOCATABLE :: frac_fe,frac_si,frac_c,frac_s
REAL(ap),DIMENSION(:),ALLOCATABLE :: delta,c,average

WRITE(*,*) 'Temperature: 5500 K, 6000 K, or 6500 K?'
READ(*,*) T
IF(T.EQ.5500) THEN
  vol_fe=6.79610076; vol_si=6.68112; vol_c=4.45947; vol_s=6.68479
ELSE IF(T.EQ.6000) THEN
  vol_fe=6.8276244; vol_si=6.88148; vol_c=4.51388; vol_s=6.77503
ELSE IF(T.EQ.6500) THEN
  vol_fe=6.859441887; vol_si=6.98134; vol_c=4.5305; vol_s=6.88616
ELSE
  WRITE(*,*) 'Temperature ',T, ' not considered!'
  STOP
ENDIF

WRITE(*,*) 'Molar fraction limit of light element:'
READ(*,*) mol_max

WRITE(*,*) 'The accuracy of mole fraction:'
READ(*,*) mol_step


n=mol_max/mol_step
ALLOCATE(frac_fe(n+1))
ALLOCATE(frac_si(n+1))
ALLOCATE(frac_c(n+1))
ALLOCATE(frac_s(n+1))

DO i=1, n+1
  frac_si(i)= (i-1)*mol_step
  DO j=1,n
    frac_c(j)= (j-1)*mol_step
    DO k=1,n
      frac_s(k)= (k-1)*mol_step
      frac_fe(k)= 1 - frac_s(k) - frac_c(j)- frac_si(i)
      vol=frac_fe(k)*vol_fe+frac_si(i)*vol_si+frac_c(j)*vol_c+frac_s(k)*vol_s
      IF(T.EQ.5500) THEN
        g=1/( frac_fe(k)*vol_fe/353.35/vol+frac_si(i)*vol_si/116.029097/vol &
        +frac_c(j)*vol_c/17.71045/vol+frac_s(k)*vol_s/69.825025/vol )
        ks=1/( frac_fe(k)*vol_fe/1526/vol+frac_si(i)*vol_si/1432.29162/vol &
        +frac_c(j)*vol_c/987.56876/vol+frac_s(k)*vol_s/1198.33955/vol )
        rho=1/( frac_fe(k)*vol_fe/13645/vol+frac_si(i)*vol_si/9000.748/vol &
        +frac_c(j)*vol_c/8075.44008/vol+frac_s(k)*vol_s/9545.51222/vol )
      ELSE IF(T.EQ.6000) THEN
```

```
        g=1/( frac_fe(k)*vol_fe/324.66/vol+frac_si(i)*vol_si/91.90891/vol &
        +frac_c(j)*vol_c/14.611754/vol+frac_s(k)*vol_s/58.987033/vol )
        ks=1/( frac_fe(k)*vol_fe/1513/vol+frac_si(i)*vol_si/1372.26679/vol &
        +frac_c(j)*vol_c/932.48769/vol+frac_s(k)*vol_s/1146.72943/vol )
        rho=1/( frac_fe(k)*vol_fe/13582/vol+frac_si(i)*vol_si/8869.94317/vol &
        +frac_c(j)*vol_c/8025.4563/vol+frac_s(k)*vol_s/9487.7715/vol )
      ELSE
        g=1/( frac_fe(k)*vol_fe/297.5/vol+frac_si(i)*vol_si/80.2961098/vol &
        +frac_c(j)*vol_c/11.3411737/vol+frac_s(k)*vol_s/45.4935391/vol )
        ks=1/( frac_fe(k)*vol_fe/1503/vol+frac_si(i)*vol_si/1314.7287/vol &
        +frac_c(j)*vol_c/818.818535/vol+frac_s(k)*vol_s/1056.78405/vol )
        rho=1/( frac_fe(k)*vol_fe/13518/vol+frac_si(i)*vol_si/8797.79612/vol &
        +frac_c(j)*vol_c/7941.21864/vol+frac_s(k)*vol_s/9405.95708/vol )
      ENDIF
      vs=SQRT(g/rho*1E3)
      vp=SQRT((ks+G*4/3)/rho*1E3)

      IF(i==1.and.j==1.and.k==1) WRITE(*,'(A94)') 'x_Fe      x_Si      &
      x_C       x_S    r(g/cm^3) Vs(km/s) Vp(km/s) d_r(%)   d_Vs(%)  d_Vp(%)   '
      IF((rho/1000)>(prem_rho_l-tolerance_rho) .and. &
         (rho/1000)<(prem_rho_h+tolerance_rho) .and. &
         vs>(prem_vs_l-tolerance_vs) .and. vs<prem_vs_h+tolerance_vs .and. &
         vp>(prem_vp_l-tolerance_vp) .and. vp<(prem_vp_h+tolerance_vp))  THEN
         WRITE(*,'(4(F7.5,3x),3(F6.3,3x),3(F4.2,5x))') frac_fe(k),frac_si(i), &
         frac_c(j),frac_s(k),rho/1000,vs,vp,abs((rho-13090))/130.9, &
         abs((vs-3.67))/3.67*100,abs((vp-11.26))/11.26*100
      END IF
    END DO
  END DO
END DO

DEALLOCATE(frac_fe)
DEALLOCATE(frac_si)
DEALLOCATE(frac_c)
DEALLOCATE(frac_s)

END PROGRAM SCAN
```