Supporting materials

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Ductile-to-brittle transition and materials' resistance to amorphization by irradiation damage

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* The shear and bulk moduli are calculated within Voigt approximation. MD represents molecular dynamics. Expt reveals that this data is from experimental findings on single crystal. Calc suggest that this data is from calculations based on DFT. EMTO is the abbreviation of exact muffin-tin orbitals (EMTO) method.

TABLE I: The calculated lattice parameters (in Å) and elastic properties (in GPa) of typical fcc and bcc metals, as well as experimental results.

	a	C_{11}	C_{12}	C_{44}	G	B	ν	G/B	Cauchy Pressure/B	Note
fcc-Zr	4.52	-	-	53						FPLAPW[1]
fcc-Zr	4.527	115	78	48	33	90	0.3373	0.3649	0.3270	This work
fcc-Al	4.04	114.3	61.92	31.62	29	79	0.3355	0.3694	0.3817	Expt[2]
fcc-Al	4.038	105.3	65.1	31	26	79	0.3506	0.3319	0.4343	This work
fcc-Au	4.079	192.3	163.1	42	28	173	0.4244	0.1592	0.7007	Expt(300K)[3]
fcc-Au	4.173	141	133	30	24	185	0.4376	0.1301	0.7545	This work
fcc-Cu	-	171.0	123.9	75.6	48	140	0.3458	0.3438	0.3444	Expt[4]
fcc-Cu	3.635	178	145	69	39	156	0.3847	0.2499	0.4876	This work
fcc-Ir	3.877	582.1	230.3	252	218	348	0.2404	0.6279	-0.0627	This work
fcc-Ir	3.829	596	252	270	225	367	0.2450	0.6146	-0.0491	Calc[5]
fcc-Ir	-	580	242	256	225	367	0.2450	0.6146	-0.0491	Expt[6]
fcc-Ag	-	124	93.4	46.1	30	104	0.3693	0.2863	0.4566	Expt[6]
fcc-Ag	-	115.8	89	40.7	26	98	0.3776	0.2665	0.4932	Calc[6]
fcc-Pd	-	227.1	176	71.73	47	193	0.3864	0.2458	0.5402	Expt[6]
fcc-Pd	-	198.1	149.7	55.2	40	166	0.3893	0.2391	0.5698	This work
fcc-Pt	-	346.7	250.7	76.5	63	283	0.3956	0.2244	0.6162	Expt[6]
fcc-Pt	-	289.9	224.9	45.9	40	247	0.4231	0.1620	0.7261	This work
fcc-Ni	-	243.6	149.4	119.6	82	181	0.3024	0.4553	0.1648	Expt[6]
fcc-Ni	-	268.2	159.7	130.2	92	196	0.2976	0.4679	0.1505	This work
bcc-Mo	3.150	496	159	107	125	265	0.2958	0.4729	0.1974	This work
bcc-Mo	-	464.7	161.5	109	124	263	0.2955	0.4736	0.2003	Expt[7]
bcc-Nb	3.322	238	143	14	24	174	0.4346	0.1368	0.7350	This work
bcc-Nb	-	246.6	133.2	28.1	37	171	0.3981	0.2185	0.6146	Expt[7]
bcc-Fe	2.870	239.55	135.75	120.75	86	170	0.2838	0.5051	0.0881	Expt[8]
bcc-Ta	3.30	266.32	158.16	87.36	72	194	0.3349	0.3711	0.3645	Expt[8]
bcc-W	3.16	532.55	204.95	163.13	163	314	0.2784	0.5200	0.1333	Expt[8]
bcc-W	-	516.6	199.7	146.7	151	305	0.2874	0.4955	0.1736	This work
bcc-V	3.03	232.4	119.36	45.95	50	157	0.3562	0.3180	0.4673	Expt[8]
bcc-Cr	-	394.1	88.5	103.75	121.2	190.4	0.2374	0.6367	-0.0801	0K[9]
bcc-Cr	-	424.9	54.5	97.4	126	178	0.2130	0.7099	-0.2410	This work
bcc-Li	3.439	15.1	13.4	12.7	7.9	13.9		0.5683	0.0493	This work*
bcc-Li	3.471	-	-	11.7		14.1				Calc[10]
bcc-Na	4.193	8.7	7.4	6.8	4.33	7.87		0.5502	0.0829	This work*
bcc-Na	4.200	-	-	6.3		7.67				Calc[10]
bcc-K	4.166	4.5	4.0	2.9	1.8	4.2		0.4286	0.2706	This work*
bcc-K	-	-	-	2.9		3.77				Calc[10]
bcc-Rb	-	-	-	2.2		3.17				Calc[10]
bcc-Rb	-	3.1	2.7	2.1	1.33	2.8		0.4750	0.2200	This work*
bcc-Cs	-	-	-	1.61	2.32					Calc[10]
Diamond-C	3.567	1079	124	578	535	442	0.069	1.2105	-1.0263	Expt[11]
Diamond-C	3.557	-	-	534						LCAO[12]
Diamond-C	3.572	1051.4	125.9	560	519	434	0.073	1.195	-1.000	This work
Diamond-Si	5.4309	-	-	-						Expt[13]
Diamond-Si	5.4345	-	-	-						PBE-HSE
Diamond-Si	5.468	153.3	56.8	75	63	89	0.2150	0.7038	-0.1996	This work
SiC	4.3596	390	142	256	191	225	0.1683	0.8518	-0.5074	Expt[14]
SiC	4.315	420	126	287	219	224	0.1308	0.9795	-0.7188	Calc[15]
SiC		383	126.6	240.2	187	212	0.1597	0.8803	-0.5355	This work
AlN	4.38	328	139	133	116	202	0.2590	0.5742	0.0297	Calc[16]
GaN	4.54	264	153	68	63	190	0.3514	0.3299	0.4474	Calc[16]
InN	5.03	172	119	37	32	137	0.3902	0.2368	0.6000	Calc[16]
Si_3N_4	-	532.6	191.2	341.0	258	305	0.1698	0.8469	-0.4911	Calc[17]
Ge_3N_4	-	395.1	165.4	234.5	176	242	0.2072	0.7277	-0.2856	Calc[17]
Nb_3Sn	-	282.4	110.1	53.8	65	168	0.3282	0.3881	0.3361	Calc[18]
TiN	-	671.01	106.4	166.22	206	295	0.2167	0.6985	-0.2030	Calc[19]
TiN	-	625	165	163	187	318	0.2542	0.5879	0.0006	Expt[19]
TiCrN	-	649.35	123.9	160.22	196	299	0.2316	0.6538	-0.1214	Calc[19]
TiZrN	-	593.89	85.07	147.15	183	255	0.2095	0.7206	-0.2436	Calc[19]
TiNbN	-	591.76	102.85	146.58	180	266	0.2236	0.6775	-0.1644	Calc[19]
TiVN	-	574.78	123.94	159.18	183	274	0.2270	0.6676	-0.1287	Calc[19]
TiWN	-	574.01	154.7	134.12	161	294	0.2694	0.5451	0.0700	Calc[19]
TiMoN	-	573.33	191.23	145.09	162	319	0.2827	0.5084	0.1450	Calc[19]
TiAlN	-	503.87	143.05	174.01	177	263	0.2261	0.6703	-0.1173	Calc[19]
Zr_3Al	-	146.45	74.27	75.67	56	98	0.2599	0.5717	-0.0142	Calc[20]
PdZr(Pm-3m)	-	152.9	141.3	34.1	17	145	0.4431	0.1183	0.7385	Calc[21]
$MgAl_2O_4$	-	266.2	148.0	148.6	103	187	0.2684	0.5479	-0.0032	Calc[17]
$MgAl_2O_4$	-	282.9	154.8	155.4	109	198	0.2671	0.5514	-0.0030	Expt[17]
Mg_2SiO_4	-	333.7	111.0	140.0	128	185	0.2196	0.6896	-0.1566	Calc[17]
Mg_2SiO_4	-	327.0	126.0	112.0	107	193	0.2656	0.5557	0.0725	Expt[17]

TABLE II: The calculated lattice parameters (in Å) and elastic properties (in GPa) of cubic structures, as well as experimental results(continued)

	a	C_{11}	C_{12}	C_{44}	G	B	ν	G/B	Cauchy Pressure/B	Note
NaCl	-	51.6	12.2	13.6	16	25	0.2421	0.6229	-0.0553	Expt[22]
NaCl	-	49.11	12.25	12.84	15	25	0.2483	0.6050	-0.0240	Expt[4]
NaCl	5.653	48.97	11.87	12.31	15	24	0.2504	0.5988	-0.0181	This work
NaCl	-	57.33	11.23	13.31	16.6	26.6	0.2415	0.6246	-0.0782	4.2K[23]
NaCl	-	56.48	11.42	13.30	16.4	26.4	0.2424	0.6221	-0.0711	80K[23]
NaCl	-	50.45	12.99	12.95	15.0	25.5	0.2537	0.5895	0.0016	240K[23]
NaCl	-	49.85	13.05	12.85	14.8	25.3	0.2548	0.5862	0.0079	260K[23]
NaCl	-	49.27	13.08	12.75	14.7	25.1	0.2557	0.5836	0.0131	280K[23]
NaCl	-	48.70	13.11	12.66	14.5	25.0	0.2566	0.5811	0.0180	300K[23]
NaCl	-	49.5	13.2	12.79	14.7	25.3	0.2564	0.5818	0.0162	300K[24]
NaCl	-	47.6	13.3	12.62	14.3	24.7	0.2580	0.5770	0.0275	350K[24]
NaCl	-	44.1	13.5	12.26	13.4	23.7	0.2622	0.5653	0.0523	450K[24]
NaCl	-	40.5	13.5	11.90	12.5	22.5	0.2654	0.5563	0.0711	550K[24]
NaCl	-	37.0	13.1	11.52	11.7	21.1	0.2659	0.5549	0.0750	650K[24]
NaCl	-	33.7	12.9	11.10	10.8	19.8	0.2693	0.5453	0.0908	750K[24]
NaF	-	108.5	22.9	28.99	34.5	51.4	0.2298	0.6591	-0.1184	4.2K*[23]
NaF	-	107.1	23.12	28.97	34.2	51.1	0.2302	0.6579	-0.1145	80K*[23]
NaF	-	98.62	24.28	28.19	31.7	49.1	0.2356	0.6419	-0.0797	260K*[23]
NaF	-	98.07	24.36	28.13	31.3	48.9	0.2360	0.6406	-0.0770	270K[23]
NaF	-	97.49	24.44	28.07	31.45	48.79	0.2365	0.6393	-0.0744	280K*[23]
NaF	-	96.90	24.52	28.01	31.0	48.6	0.2369	0.6380	-0.0717	290K[23]
NaF	-	96.3	24.59	27.94	30.9	48.5	0.2374	0.6367	-0.0691	300K[23]
NaBr	-	48.0	9.86	10.7	14.0	22.6	0.2504	0.5986	-0.0372	4.2K*[23]
NaBr	-	46.45	9.88	10.6	13.7	22.1	0.2505	0.5985	-0.0326	80K*[23]
NaBr	-	41.53	9.95	10.17	12.4	20.5	0.2525	0.5928	-0.0107	240K*[23]
NaBr	-	40.92	9.97	10.11	12.3	20.3	0.2530	0.5914	-0.0069	260K*[23]
NaBr	-	40.31	9.99	10.05	12.1	20.1	0.2535	0.5899	-0.0030	280K*[23]
NaBr	-	39.70	10.01	9.98	11.9	19.9	0.2542	0.5880	-0.0015	300K*[23]
RbBr	-	38.63	4.74	4.085	9.2	16.0	0.2583	0.5762	0.0408	4.2K*[23]
RbBr	-	38.53	4.74	4.083	9.2	16.0	0.2586	0.5755	0.0411	20K*[23]
RbBr	-	38.2	4.74	4.076	9.14	15.9	0.2588	0.5749	0.0418	40K*[23]
RbBr	-	37.75	4.74	4.068	9.04	15.7	0.2590	0.5744	0.0427	60K[23]
RbBr	-	37.25	4.74	4.05	8.9	15.6	0.2593	0.5734	0.0443	80K*[23]
RbBr	-	31.35	5.12	3.77	7.51	13.9	0.2705	0.5418	0.0971	290K*[23]
RbBr	-	31.07	5.15	3.76	7.44	13.8	0.2714	0.5395	0.1007	300K*[23]
KCl	-	40.95	7.05	6.30	9	18	0.2795	0.5169	0.0409	Expt[4]
KCl	6.364	38.7	6.9	6.5	9	18	0.2734	0.5338	0.0269	This work
KCl	-	40.1	5.45	6.35	10.7	17.0	0.2391	0.6318	-0.0530	300K[25]
KCl	-	36.9	5.40	6.21	10.0	15.9	0.2396	0.6302	-0.0509	400K[25]
KCl	-	33.8	5.15	6.11	9.40	14.7	0.2364	0.6395	-0.0653	500K[25]
KCl	-	31.1	5.0	5.96	8.8	13.7	0.2355	0.6423	-0.0700	600K[25]
KCl	-	28.2	4.8	5.79	8.2	12.6	0.2339	0.6468	-0.0786	700K[25]
KCl	-	25.5	4.5	5.57	7.5	11.5	0.2321	0.6522	-0.0930	800K[25]
KCl	-	23.5	4.6	5.57	7.1	10.9	0.2324	0.6514	-0.0890	850K[25]
LiI	6.013	33.7	13.1	13.9	12	20	0.2443	0.6164	-0.0381	This work
LiCl	-	49.27	23.1	24.95	19	32	0.2482	0.6051	-0.0581	Expt[23]
LiCl	-	51.8	21.9	23.6	20	32	0.2441	0.6171	-0.0545	This work
NaF	-	96.9	24.5	28.01	31	49	0.2368	0.6383	-0.0722	Expt[23]
NaF	-	127.4	25.6	33	39	60	0.2294	0.6604	-0.1252	This work
NaBr	-	40.0	10.0	10.02	12	20	0.2538	0.5892	-0.0009	Expt[23]
KF	-	64.9	15.2	12.32	16	32	0.2800	0.5157	0.0907	Expt[23]
RbCl	-	36.46	6.47	4.68	7.6	16.4	0.2993	0.4634	0.1087	Expt[23]
RbBr	-	31.35	5.12	3.774	6.4	13.9	0.3001	0.4612	0.0971	Expt[23]
RbI	-	25.75	3.4	2.778	5.1	10.9	0.2984	0.4658	0.0573	Expt[23]
NaH(NaCl)	-	47.3	2.5	22.5	22.5	17.4	0.0494	1.288	-1.147	Expt[26]
NaH(NaCl)	-	59.1	9.2	22.02	23.1	25.8	0.1550	0.8961	-0.4963	GGA[26]
NaH(CsCl)	-	73.02	11.9	30.11	30.3	32.3	0.1426	0.9385	-0.5642	GGA[26]
RbH(NaCl)	-	26.46	7.93	10.97	10.3	14.1	0.2072	0.7277	-0.2157	GGA[26]
RbH(CsCl)	-	42.0	1.4	12.0	14.8	14.9	0.1269	0.9933	-0.7098	GGA[26]
RbH(NaCl)	-	26.46	7.93	10.97	10.3	14.1	0.2072	0.7277	-0.2157	GGA[26]
RbH(CsCl)	-	42.0	1.4	12.0	14.8	14.9	0.1269	0.9933	-0.7098	GGA[26]
LiH(NaCl)	-	66.4	15.6	45.8	36.2	32.5	0.0946	1.1112	-0.9283	Expt[26]
LiH(NaCl)	-	84.7	14.0	48.9	42.9	37.6	0.0863	1.1423	-0.9287	this work
LiH(CsCl)	-	66.5	12.0	32.0	30.0	30.2	0.1265	0.9947	-0.6630	GGA[26]
KH(NaCl)	-	31.1	8.35	14.47	13.1	15.9	0.1766	0.8247	-0.3841	GGA[26]
KH(CsCl)	-	51.0	4.5	20.0	21.2	20.0	0.1078	1.062	-0.7750	GGA[26]
CsH(NaCl)	-	23.23	6.761	9.74	9.1	12.3	0.2021	0.7434	-0.2432	GGA[26]
CsH(CsCl)	-	38.0	3.2	6.5	9.8	14.8	0.2295	0.6599	-0.2230	GGA[26]

TABLE III: The elastic properties (in GPa) of cubic structures, as well as experimental results(continued)

	C_{11}	C_{12}	C_{44}	G	B	ν	G/B	Cauchy Pressure/B	Note
Ne	1.31	0.65	0.58	0.46	0.87	0.2742	0.5317	0.0805	This work
Ne	1.206	0.732	0.633	0.427	0.89	0.2932	0.4798	0.1112	0GPa,23.7K[27]
Ne	1.175	0.74	0.595	0.398	0.885	0.3046	0.4493	0.1638	0GPa,24.3K[28]
Ar	2.48	1.53	1.24	0.84	1.85	0.3017	0.4571	0.1570	0GPa,82K[27]
Ar	2.38	1.56	1.12	0.75	1.83	0.3202	0.4085	0.2400	82.3K[29]
Ar	16	8.4	7.5	5.7	10.9	0.2776	0.5222	0.0823	2GPa,RT[30]
Ar	32	16.3	11.6	9.9	21.5	0.3003	0.4607	0.2183	4GPa,RT[30]
Ar	48	21.9	17.6	15.6	30.6	0.2820	0.5102	0.1405	6GPa,RT[30]
Ar	74	33.3	27.1	24.2	46.9	0.2800	0.5156	0.1323	10GPa,RT[30]
Ar	109	44	41	37.4	65.7	0.2609	0.5689	0.0457	15GPa,RT[30]
Ar	142	54	54	49.8	83.3	0.2510	0.5970	0.0000	20GPa,RT[30]
Ar	178	63	68	63.6	101.3	0.2405	0.6275	-0.493	25GPa,RT[30]
Ar	211	71	80	75.8	111.7	0.2347	0.6445	-0.0765	30GPa,RT[30]
Kr	4.99	2.86	2.69	1.85	3.57	0.2785	0.5197	0.0476	This work
Kr	5.14	2.84	2.68	1.9	3.61	0.2751	0.5292	0.0444	0GPa,10K[31]
Kr	2.89	1.85	1.44	0.96	2.20	0.3097	0.4359	0.1866	0GPa,114K[27]
Kr	2.657	1.725	1.261	0.85	2.04	0.3174	0.4157	0.2279	0GPa,115.6K[32]
Kr	14	8	11	7.8	10.0	0.1905	0.7800	-0.3000	2GPa,RT[33]
Kr	36	17	21	16.4	23.3	0.2149	0.7039	-0.1714	5GPa,RT[33]
Kr	71	29	34	28.0	43.0	0.2323	0.6518	-0.1163	10GPa,RT[33]
Kr	101	46	45	36.9	64.3	0.2591	0.5741	0.0155	15GPa,RT[33]
Kr	131	62	56	50	83.3	0.2510	0.5970	0.0000	20GPa,RT[33]
Kr	160	79	64	53.3	106.0	0.2848	0.5026	0.1415	25GPa,RT[33]
Kr	184	97	70	57.8	126.0	0.3009	0.4591	0.2143	30GPa,RT[33]
Kr	205	118	73	59.3	147.0	0.3222	0.4035	0.3061	35GPa,RT[33]
Xe	5.45	3.17	2.97	2.0	3.93	0.2803	0.5148	0.0509	This work
Xe	5.27	2.82	2.95	2.1	3.64	0.2604	0.5702	-0.0357	0GPa,10K[34]
Xe	2.98	1.9	1.48	0.99	2.26	0.3092	0.4373	0.1858	0GPa,156K[35]
Xe	7.20	5.15	2.92	1.92	5.83	0.3517	0.3292	0.3823	0.45GPa,296K[36]
Xe	19.1	13.1	8.55	5.6	15.1	0.3344	0.3723	0.3013	2.11GPa,296K[36]
Xe	24.7	17.2	10.9	7.1	19.7	0.3389	0.3610	0.3198	2.96GPa,296K[36]
Xe	28.9	19.3	12.6	8.6	22.5	0.3312	0.3804	0.2978	3.73GPa,296K[36]
Xe	36.7	24.0	14.8	10.5	28.2	0.3340	0.3733	0.3259	4.95GPa,296K[36]
Xe	43.0	28.7	18.3	12.6	33.5	0.3333	0.3751	0.3108	6.08GPa,296K[36]
Xe	55.7	37.5	22.5	15.6	43.5	0.3396	0.3592	0.3443	8.04GPa,296K[36]
Xe	63.7	42.3	26.7	18.5	49.4	0.3336	0.3743	0.3156	10.6GPa,296K[36]
Al-Li0.05	103.1	60.6	42.1	31.9	74.8	0.3127	0.4280	0.2474	EMT[37]
Al-Li0.10	101.1	58.2	43.3	32.6	72.5	0.3042	0.4505	0.2055	EMTO[37]
Al-Li0.15	94.7	54.9	42.5	31.3	68.2	0.3007	0.4598	0.1819	EMTO[37]
Al-Li0.20	91.0	50.1	40.9	30.9	63.7	0.2909	0.4859	0.1444	EMTO[37]
Fe-Cr0.025	284.2	131.5	108.6	94.3	182.4	0.2795	0.5170	0.1256	EMTO[38]
Fe-Cr0.05	280.0	126.9	112.8	96.6	177.9	0.2702	0.5427	0.0792	EMTO[38]
Fe-Cr0.075	283.5	127.2	117.5	99.8	179.3	0.2653	0.5565	0.0541	EMTO[38]
Fe-Cr0.10	287.8	127.9	120.7	102.3	181.2	0.2624	0.5647	0.0397	EMTO[38]
Fe-Cr0.125	292.3	129.5	122.4	103.9	183.8	0.2621	0.5656	0.0386	EMTO[38]
Fe-Cr0.15	296.8	131.7	124.1	105.4	186.7	0.2625	0.5644	0.0407	EMTO[38]
Fe-Cr0.175	305.0	137.2	125.6	106.8	193.1	0.2665	0.5532	0.0601	EMTO[38]
Fe-Cr0.2	305.5	136.3	126.0	107.4	192.7	0.2650	0.5574	0.0535	EMTO[38]
Fe-Cr0.2	305.5	136.3	126.0	107.4	192.7	0.2650	0.5574	0.0535	EMTO[38]
Fe-Mg0.025	263.7	125.3	103.6	88.1	171.4	0.2806	0.5141	0.1266	EMTO[38]
Fe-Mg0.05	235.8	112.7	101.0	82.8	153.7	0.2717	0.5386	0.0761	EMTO[38]
Fe-Mg0.075	211.0	102.4	98.9	77.8	138.6	0.2637	0.5610	0.0253	EMTO[38]
Fe-Mg0.1	189.7	93.4	97.9	73.6	125	0.2546	0.5867	-0.0359	EMTO[38]
NiCoFeCr	271	175	189.3	109.9	207	0.2358	0.6414	-0.0691	EMTO[39]
NiCoFeCrTi	184.5	170.9	127.0	47.3	175.4	0.3044	0.4497	0.2502	EMTO[39]
CuNiCoFeCrTi0.1	219.7	152.6	160.2	109.5	174.9	0.2410	0.6261	-0.0434	EMTO[39]
CuNiCoFeCrTi0.2	213.6	152.1	155.1	105.4	172.6	0.2464	0.6104	-0.0174	EMTO[39]
CuNiCoFeCrTi0.3	209.6	151.9	154.6	104.3	171.1	0.2467	0.6095	-0.0158	EMTO[39]
CuNiCoFeCrTi0.4	207.6	151.7	150.8	101.7	170.3	0.2511	0.5968	0.0053	EMTO[39]
CuNiCoFeCrTi0.5	198.4	151.0	142.7	95.1	166.8	0.2605	0.5701	0.0498	EMTO[39]
CuNiCoFeCrTi0	227.8	154.6	165.3	113.8	179.0	0.2377	0.6359	-0.0598	EMTO[39]
CuNiCoFeCrTi1	174.3	148.6	125.0	80.1	157.2	0.2821	0.5099	0.1502	EMTO[39]

TABLE IV: The elastic properties (in GPa) of cubic structures, as well as experimental results(continued)

	C_{11}	C_{12}	C_{44}	G	B	ν	G/B	Cauchy Pressure/B	Note
ZrO_2-8mol%Y_2O_3	401.8	95.2	55.8	94.8	197.4	0.2930	0.4802	0.1996	RT*[40]
ZrO_2-11.1mol%Y_2O_3	403.5	102.4	59.9	96.2	202.8	0.2953	0.4742	0.2096	RT*[40]
ZrO_2-12.1mol%Y_2O_3	405.1	105.3	61.8	97.0	205.2	0.2957	0.4729	0.2120	RT*[40]
ZrO_2-15.5mol%Y_2O_3	397.6	108.6	65.8	97.3	204.9	0.2950	0.4749	0.2088	RT*[40]
ZrO_2-17.9mol%Y_2O_3	390.4	110.8	69.1	97.4	204.0	0.2941	0.4775	0.2044	RT*[40]
ZrO_2-11.1mol%Y_2O_3	400.2	101.8	59.0	95.1	201.3	0.2959	0.4724	0.2127	373K*[40]
ZrO_2-11.1mol%Y_2O_3	395.6	101.0	57.7	93.5	199.2	0.2971	0.4694	0.2174	473K*[40]
ZrO_2-11.1mol%Y_2O_3	389.8	99.8	56.0	91.6	196.5	0.2983	0.4662	0.2229	573K*[40]
ZrO_2-11.1mol%Y_2O_3	382.0	97.1	54.1	89.4	192.1	0.2986	0.4654	0.2239	673K*[40]
ZrO_2-11.1mol%Y_2O_3	373.1	91.2	52.2	87.7	185.2	0.2955	0.4735	0.2106	773K*[40]
ZrO_2-11.1mol%Y_2O_3	364.7	88.9	50.1	85.2	180.8	0.2964	0.4712	0.2146	873K*[40]
ZrO_2-11.1mol%Y_2O_3	356.6	86.8	48.0	82.8	176.7	0.2974	0.4686	0.2195	973K*[40]
ZrO_2-12.1mol%Y_2O_3	401.6	104.8	60.9	95.9	203.7	0.2965	0.4707	0.2155	373K*[40]
ZrO_2-12.1mol%Y_2O_3	396.6	104.3	59.5	94.2	201.7	0.2979	0.4670	0.2221	473K*[40]
ZrO_2-12.1mol%Y_2O_3	391.2	102.9	57.9	92.4	199.0	0.2990	0.4643	0.2261	573K*[40]
ZrO_2-12.1mol%Y_2O_3	385.1	100.4	56.4	90.8	195.3	0.2987	0.4649	0.2253	673K*[40]
ZrO_2-12.1mol%Y_2O_3	378.9	93.4	54.8	90.0	188.6	0.2941	0.4772	0.2047	773K*[40]
ZrO_2-12.1mol%Y_2O_3	372.1	86.9	53.2	89.0	182.0	0.2898	0.4890	0.1852	873K*[40]
ZrO_2-12.1mol%Y_2O_3	364.8	82.6	51.5	87.3	176.7	0.2879	0.4941	0.1760	973K*[40]
ZrO_2-15.5mol%Y_2O_3	394.5	108.2	64.9	96.2	203.6	0.2959	0.4725	0.2126	373K*[40]
ZrO_2-15.5mol%Y_2O_3	389.8	107.3	63.5	94.6	201.5	0.2970	0.4695	0.2174	473K*[40]
ZrO_2-15.5mol%Y_2O_3	384.7	106.4	61.9	92.8	199.2	0.2984	0.4659	0.2234	573K*[40]
ZrO_2-15.5mol%Y_2O_3	379.5	105.0	59.9	90.8	196.5	0.2998	0.4621	0.2295	673K*[40]
ZrO_2-15.5mol%Y_2O_3	373.6	102.1	57.7	88.9	192.6	0.3000	0.4616	0.2305	773K*[40]
ZrO_2-15.5mol%Y_2O_3	366.8	98.2	55.3	86.9	187.7	0.2995	0.4630	0.2285	873K*[40]
ZrO_2-15.5mol%Y_2O_3	360.2	96.3	52.6	84.3	184.3	0.3016	0.4574	0.2372	973K*[40]
ZrO_2-17.9mol%Y_2O_3	387.0	109.9	68.1	96.3	202.3	0.2946	0.4760	0.2067	373K*[40]
ZrO_2-17.9mol%Y_2O_3	382.8	108.9	66.7	94.8	200.2	0.2955	0.4735	0.2108	473K*[40]
ZrO_2-17.9mol%Y_2O_3	378.1	107.5	65.2	93.2	197.7	0.2963	0.4714	0.2140	573K*[40]
ZrO_2-17.9mol%Y_2O_3	373.4	105.6	63.3	91.5	194.9	0.2970	0.4695	0.2171	673K*[40]
ZrO_2-17.9mol%Y_2O_3	368.2	100.5	61.2	90.3	189.7	0.2946	0.4760	0.2071	773K*[40]
ZrO_2-17.9mol%Y_2O_3	361.4	98.1	58.8	87.9	185.9	0.2958	0.4728	0.2114	873K*[40]
ZrO_2-17.9mol%Y_2O_3	353.8	94.0	56.2	85.7	180.6	0.2951	0.4745	0.2093	973K*[40]
Fe-30Al	147	96.3	116.3	79.9	113.2	0.2143	0.7058	-0.1767	273K*[41]
Fe-30Al	137.2	92.4	110.4	75.2	107.3	0.2159	0.7008	-0.1677	428K*[41]
Fe-30Al	134.2	91.4	108.9	73.9	105.7	0.2165	0.6991	-0.1656	473K*[41]
Fe-30Al	131.1	90.4	107.3	72.5	104.0	0.2171	0.6973	-0.1626	523K*[41]
Fe-30Al	128.3	89.6	105.3	70.9	102.5	0.2189	0.6917	-0.1532	573K*[41]
Fe-30Al	123.4	87.3	100.6	67.6	99.3	0.2226	0.6804	-0.1339	673K*[41]
Fe-30Al	117.9	83.8	95.1	63.9	95.2	0.2258	0.6710	-0.1187	773K*[41]
Fe-30Al	111.3	79.7	89.1	59.8	90.2	0.2287	0.6625	-0.1042	873K*[41]
Fe-30Al	103.9	75.8	86.1	57.3	85.2	0.2253	0.6725	-0.1209	973K*[41]
Fe-30Al	92.3	69.3	78.5	51.7	76.9	0.2256	0.6717	-0.1195	1173K*[41]
MgO	298.96	96.42	157.13	131.8	163.9	0.1831	0.8037	-0.3703	300K[42]
MgO	292.94	97.02	155.78	129.3	162.3	0.1852	0.7968	-0.3620	400K[42]
MgO	296.92	97.64	154.33	126.8	160.7	0.1876	0.7892	-0.3527	500K[42]
MgO	280.62	98.0	152.84	124.3	158.9	0.1897	0.7824	-0.3452	600K[42]
MgO	274.47	98.43	151.31	121.8	157.1	0.1921	0.7750	-0.3366	700K[42]
MgO	268.22	98.54	149.68	119.2	155.1	0.1941	0.7685	-0.3297	800K[42]
MgO	261.94	98.62	148.1	116.6	153.1	0.1962	0.7620	-0.3233	900K[42]
MgO	255.74	98.74	146.52	114.1	151.1	0.1984	0.7550	-0.3163	1000K[42]
MgO	249.52	98.6	144.77	111.5	148.9	0.2005	0.7485	-0.3101	1100K[42]
MgO	243.32	98.38	143.06	108.9	146.7	0.2025	0.7423	-0.3046	1200K[42]
MgO	237.15	98.05	141.33	106.3	144.4	0.2044	0.7362	-0.2997	1300K[42]
MgO	230.96	97.56	139.54	103.8	142.0	0.2062	0.7306	-0.3233	1400K[42]
MgO	224.88	97.08	137.86	101.3	139.7	0.2081	0.7249	-0.2920	1500K[42]
MgO	219.04	96.44	136.24	98.9	137.3	0.2096	0.7201	-0.2899	1600K[42]
MgO	213.43	95.69	134.65	96.6	134.9	0.2110	0.7160	-0.2887	1700K[42]
MgO	208.18	95.02	133.12	94.4	132.7	0.2125	0.7115	-0.2870	1800K[42]
CaO	220.53	57.67	80.03	80.6	111.9	0.2097	0.7198	-0.1997	300K[43]
CaO	215.66	57.96	79.34	79.14	110.5	0.2110	0.7161	-0.1934	400K[43]
CaO	210.73	58.23	78.70	77.7	109.1	0.2121	0.7125	-0.1877	500K[43]
CaO	205.88	58.44	77.94	76.22	107.6	0.2134	0.7085	-0.1812	600K[43]
CaO	201.22	58.66	77.18	74.76	106.2	0.2149	0.7041	-0.1744	700K[43]
CaO	196.58	58.81	76.46	73.3	104.7	0.2162	0.7002	-0.1685	800K[43]
CaO	192.03	58.98	75.72	71.9	103.3	0.2176	0.6958	-0.1620	900K[43]
CaO	187.24	58.98	74.92	70.4	101.7	0.2189	0.6920	-0.1567	1000K[43]
CaO	182.74	58.96	74.17	68.9	100.2	0.2200	0.6884	-0.1518	1100K[43]
CaO	178.11	58.99	73.48	67.6	98.7	0.2213	0.6845	-0.1468	1200K[43]

TABLE V: The calculated lattice parameters (in Å) and elastic properties (in GPa) of hexagonal and tetragonal structure,as well as experimental results

	a	c	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
Ti	-	-	160	90	66	181	46.5	35	43	105	0.3184	0.4133	0.3548	Expt[44]
Zr	-	-	145.3	63.9	66.5	165.4	27.5	40.7	36	94	0.3322	0.3779	0.3297	Expt[44]
Sc	-	-	92.9	31.7	30.1	90.6	31.4	30.6	31	51	0.2479	0.6061	-0.0019	Calc[44]
Sc	-	-	99.3	39.7	29.4	107	27.7	29.8	31	56	0.2684	0.5478	0.1039	Expt[44]
Y	-	-	77.4	23.9	21.3	80.9	22.4	26.8	25	41	0.2427	0.6213	-0.049	Calc[44]
Y	-	-	77.9	29.2	21.0	76.9	24.7	24.4	26	43	0.2525	0.5928	0.0134	Expt[44]
Re	-	-	649	269.4	187.6	678.1	185	189.8	199	363	0.2678	0.5493	0.1134	Calc[44]
Re	-	-	634.4	266	202	701.1	169.1	184.2	189	368	0.2804	0.5145	0.1559	Expt[44]
Tb	-	-	73.8	20.3	18.1	75.2	24.1	26.8	26	37	0.2169	0.6978	-0.1677	Calc[44]
Tb	-	-	68.6	24.7	22.4	73.3	21.6	22.0	22	39	0.2580	0.5770	0.0451	Expt[44]
Tc	-	-	525.4	229.7	184.7	596.3	160	147.8	162	316	0.2807	0.5137	0.1686	Calc[44]
Ru	-	-	622.5	203	179.8	724.6	212.4	210	220	343	0.2361	0.6404	-0.0573	Calc[44]
Ru	-	-	563	188	168	624	181	187.5	191	311	0.2448	0.6149	-0.0201	Expt[44]
Gd	-	-	70.0	23.1	18.2	72.1	21.6	23.4	23	37	0.2378	0.6353	-0.0493	Calc[44]
Gd	-	-	67.8	25.6	20.7	71.2	20.8	21.1	22	38	0.2587	0.5751	0.0585	Expt[44]
Os	-	-	816.3	225.2	256.1	915	312.7	295.5	305	446	0.2218	0.6831	-0.1422	Calc[44]
Na_3Bi	5.469	9.735	35.9	13.5	4.0	40.9	7.0	11.2	10	17	0.2490	0.6029	-0.0202	This work
Na_3Bi	5.448	9.655	-	-	-	-	-	-						Expt[45]
K_3Bi	6.217	11.044	20.0	9.4	3.0	24.7	4.2	5.3	6	11	0.2735	0.5336	0.1372	This work
Graphene	2.469	8.346	896.6	176.0	23.0	104.3	40.7	360.3	136	177	0.1931	0.7715	-0.5713	This work*
Graphene	2.46	-	-	-	-	-	-	360.3						Expt
NaBi	3.443	4.886	64.6	19.7	13.6	46.7	11.5	9.1	14	29	0.2933	0.4796	0.2153	This work
AlN	-	-	345	125	120	395	118	110	117	201	0.2567	0.5807	0.0422	Expt[46]
GaN	-	-	367	135	103	405	95	116	113	202	0.2649	0.5575	0.0667	Calc[46]
GaN	-	-	390	145	106	398	105	122.5	120	210	0.2599	0.5718	0.0559	Expt[46]
InN	-	-	190	104	121	182	10	43	22	139	0.4237	0.1608	0.6175	Calc[16]
ReN	-	-	570	252	202	794	110	159	153	359	0.3133	0.4263	0.2580	Calc[47]
Re_2N	-	-	662	237	258	870	192	212.5	213	407	0.2770	0.5239	0.1111	Calc[47]
Re_3N	-	-	657	248	244	794	198	204.5	213	401	0.2742	0.5317	0.1116	Calc[47]
ZnO	-	-	210	121	105	211	43	44.5	46	144	0.3556	0.3195	0.4823	Calc[48]
ZnO	-	-	191.9	107.3	88.6	217	38.3	42.3						Calc[48]
Zr_2Al	-	-	178.08	85.16	53.25	186.68	57.19	46.4	55	103	0.2733	0.5341	0.1694	Calc[20]
Zr_4Al_3	-	-	218.20	40.11	57.23	213.16	74.6	89	80	106	0.1985	0.7546	-0.3112	Calc[20]
Zr_5Al_4	-	-	184.73	76.54	48.72	192.69	30.36	54	46	101	0.3026	0.4546	0.2024	Calc[20]
$ZrAl_2$	-	-	236.81	46.65	57.05	217.22	90.01	95.0	90	112	0.1836	0.8020	-0.3615	Calc[20]
Pd_3Zr	-	-	268	90	99	305	70	89	82	157	0.2778	0.5217	0.0955	Calc[53]
parahydrogen	-	-	0.334	0.13	0.056	0.408	0.104	0.102	82	157	0.2778	0.5217	0.0955	13.2K[49]
SnO_2	-	-	260	197	117	429	131	225	109	200	0.2703	0.5426	-0.1049	Calc[50]
SnO_2	-	-	262	177	156	449	103	207	102	212	0.2937	0.4784	0.054	Expt[50]
IrN_2	-	-	322	301	217	553	103	273	83	294	0.3705	0.2835	0.2419	Calc
V_2B	-	-	496	94	122	442	223	197	200	234	0.1673	0.8550	-0.4352	Calc[51]
Nb_2B	-	-	439	89	143	361	164	145	150	221	0.2226	0.6807	-0.1743	Calc[51]
Ta_2B	-	-	475	101	154	393	173	175	165	240	0.2207	0.6864	-0.1938	Calc[51]
V_3B_2	-	-	551	89	132	459	215	183	202	252	0.1836	0.8021	-0.3517	Calc[51]
Nb_3B_2	-	-	474	92	121	449	169	135	164	229	0.2108	0.7167	-0.1983	Calc[51]
Ta_3B_2	-	-	506	126	141	470	204	150	182	255	0.2121	0.7125	-0.1704	Calc[51]
VB_2	-	-	672	120	130	470	223	276	237	283	0.1718	0.8402	-0.4405	Calc[51]
NbB_2	-	-	602	106	186	429	218	248	209	286	0.2071	0.7279	-0.3037	Calc[51]
TaB_2	-	-	596	142	196	427	190	227	190	297	0.2362	0.6402	-0.1331	Calc[51]
C_4	-	-	932.6	172.1	58.5	1189.6	446.7	324.5	422	403	0.1121	1.046	-0.6708	Calc[52]
Sn	-	-	74.2	58	22.2	81.2	23.4	9.9	17	48	0.3388	0.3612	0.4904	Calc[18]
$ZrAl_3$	-	-	203.98	65.35	44.7	202.2	81.06	100.21	82	102	0.1824	0.8057	-0.3489	Calc[20]
Zr_5Al_3	-	-	183.2	67.59	61.27	167.57	32.65	64.61	47	101	0.2999	0.4618	0.1979	Calc[20]
$Pd_{11}Zr_9$	-	-	171	127	116	187	36	23	30	139	0.4003	0.2136	0.6641	Calc[53]
$PdZr_2$	-	-	197	86	106	149	64	47	49	126	0.3292	0.3856	0.3214	Calc[53]
$MoSi_2$	-	-	410	114.9	87.5	514	207	200	190.7	212.1	0.1541	0.8991	-0.4823	Calc[54]
WSi_2	-	-	442.8	121.7	81.0	552.3	211.6	217.5	203.5	222.4	0.1494	0.9151	-0.5089	Expt[54]
WSi_2	-	-	372	116	81.6	596	211	236	197	208	0.1401	0.9471	-0.5996	Calc[54]
$MoSi_2$	-	-	403.7	114.5	88.0	505.3	202.7	194.8	186.5	209.9	0.1572	0.8888	-0.4646	Expt[54]
$MoSi_2$	-	-	345	109	87.7	547	190	220	178.8	197.7	0.1525	0.9046	-0.5393	Calc[54]
$CrSi_2$	-	-	372.2	45.3	82.6	385.2	149.1	163.5	153	171.9	0.1563	0.8916	-0.5370	Expt[54]
$CrSi_2$	-	-	372	45.3	68.3	441	146	163	157.4	171.1	0.1481	0.9195	-0.5708	Calc[54]
VSi_2	-	-	357.8	50.6	68.1	422.3	146	153.6	152.3	167.2	0.1507	0.9108	-0.5410	Expt[54]
VSi_2	-	-	356	50.6	67.0	430	135.7	154	148.3	167.0	0.1574	0.8800	-0.5153	Calc[54]
$NbSi_2$	-	-	380.2	75.9	88.3	468	145.3	152.2	153.2	191.5	0.1843	0.7996	-0.3480	Expt[54]
$NbSi_2$	-	-	380	75.9	80.4	508	144	152	155.8	191.8	0.1803	0.8124	-0.3652	Calc[54]
$TaSi_2$	-	-	375	78.4	90.1	476.7	143.7	148.5	151.1	192.4	0.1887	0.7855	-0.3215	Expt[54]
$TaSi_2$	-	-	375	78.4	82.1	517	142	148	153.4	192.7	0.1854	0.7962	-0.3361	Calc[54]

TABLE VI: The elastic properties (in GPa) of cubic, tetragonal and orthorhombic structure,as well as experimental results.

	C_{11}	C_{12}	C_{13}	C_{23}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
$TiSi_2$	317.5	29.35	38.45	86.0	320.4	413.2	112.5	75.8	117.5	117.0	148.9	0.1887	0.7856	-0.3403	Calc[54]
$TiSi_2$	276	29.9	33.4	93.5	302	394	119	755	134	116.2	140.9	0.1765	0.8249	-0.3944	Calc[54]
$Mo(Si,Al)_2$	402.8	74.2	107.1	-	-	434.4	148.2	-	164.3	155.3	201.4	0.1932	0.7714	-0.3258	RT[55]
$Mo(Si,Al)_2$	398.0	75.2	107.8	-	-	430.6	146.4	-	161.7	153.1	200.4	0.1956	0.7638	-0.3121	400K[55]
$Mo(Si,Al)_2$	392.1	73.8	105.3	-	-	420.7	144.3	-	159.5	150.8	196.6	0.1947	0.7667	-0.3171	500K[55]
$Mo(Si,Al)_2$	388.4	73.7	105.3	-	-	416.3	142.1	-	157.6	148.7	195.3	0.1963	0.7615	-0.3090	600K[55]
$Mo(Si,Al)_2$	384.1	73.2	105.1	-	-	410.3	140.5	-	155.6	146.8	193.5	0.1973	0.7585	-0.3044	700K[55]
$Mo(Si,Al)_2$	379.8	73.4	104.3	-	-	405.9	138.6	-	153.1	144.7	191.7	0.1984	0.7549	-0.2973	800K[55]
$Mo(Si,Al)_2$	375.5	73.6	106.5	-	-	403.2	136.7	-	151.2	142.5	191.4	0.2018	0.7445	-0.2815	900K[55]
$Mo(Si,Al)_2$	371.3	73.5	106.5	-	-	398.8	135.0	-	149.3	140.6	189.9	0.2032	0.7401	-0.2745	1000K[55]
$Mo(Si,Al)_2$	366.4	73.0	106.3	-	-	393.9	132.9	-	146.7	138.3	188.1	0.2047	0.7353	-0.2666	1100K[55]
$Mo(Si,Al)_2$	361.1	71.9	105.1	-	-	385.6	130.7	-	144.8	136.0	185.3	0.2051	0.7342	-0.2658	1200K[55]
TiO_2	646	250	229	283	475	635	148	203	246	180	362	0.2869	0.4968	0.1520	Calc[56]
ZrO_2	619	176	210	224	450	632	107	178	174	160	320	0.2858	0.4998	0.1573	Calc[56]
HfO_2	664	193	236	235	575	640	137	185	165	176	355	0.2873	0.4958	0.1660	Calc[56]
FeB_2	592	185	160	136	723	574	271	198	221	230	315	0.2066	0.7296	-0.2211	Calc[57]
FeB_4	409	161	161	152	768	451	216	154	222	189	278	0.2226	0.6807	-0.1416	Calc[57]
VB	560	126	130	130	559	572	248	248	188	223	274	0.1800	0.8135	-0.3630	Calc[51]
NbB	513	119	148	148	513	505	219	219	158	192	262	0.2058	0.7321	-0.2300	Calc[51]
TaB	545	117	169	169	545	518	222	222	163	196	280	0.2155	0.7023	-0.1811	Calc[51]
V_5B_6	616	83	134	140	634	477	224	265	234	234	270	0.1646	0.8641	-0.4513	Calc[51]
Nb_5B_6	535	117	168	157	537	452	227	245	194	202	267	0.1977	0.7574	-0.2793	Calc[51]
Ta_5B_6	552	139	167	164	563	484	227	233	194	205	282	0.2078	0.7157	-0.2176	Calc[51]
V_3B_4	475	135	135	90	636	626	235	263	229	235	272	0.1644	0.8647	-0.4501	Calc[51]
Nb_3B_4	521	123	155	133	549	553	222	220	217	212	272	0.1899	0.7817	-0.3045	Calc[51]
Ta_3B_4	531	135	167	156	559	557	209	211	214	206	285	0.2086	0.7232	-0.2061	Calc[51]
V_2B_3	484	128	129	98	642	639	254	248	229	239	274	0.1621	0.8721	-0.4582	Calc[51]
Nb_2B_3	499	148	162	106	574	591	218	240	238	221	277	0.1851	0.7971	-0.3368	Calc[51]
Ta_2B_3	517	162	161	137	582	603	211	229	233	217	291	0.2019	0.7442	-0.2439	Calc[51]
TiB	411	91	107	61	524	410	189	186	193	185	206	0.1552	0.8953	-0.4992	Calc[58]
Nb_6Sn_5	266.5	83	90.4	110.6	228.2	410	210.4	65.5	62.9	54	141	0.3304	0.3824	0.3081	Calc[18]
$NbSn_2$	180.8	77.3	68.9	60.1	178.5	188.3	52.5	37.3	57.4	51	107	0.2924	0.4818	0.1847	Calc[18]
ZrAl	142.87	64.66	92.6	49.26	217.32	193.33	70.28	116.67	62.22	68	107	0.2388	0.6325	-0.1331	Calc[20]
Zr_2Al_3	226.06	46.84	48.31	67.91	203.50	203.01	74.73	76.07	56.91	72	107	0.2240	0.6766	-0.1397	Calc[20]
PdZr	169.6	108.1	134.7	126.7	230.4	229.5	70.6	67.5	16.6	42	149	0.3714	0.2813	0.4797	Calc[21]
Ti0.25Mo0.75	363.6	151.5	-	-	-	-	62	-	-	76.9	222.2	0.3447	0.3465	0.4028(207)	Calc[59]
Ti0.5Mo0.5	224.0	146.6	-	-	-	-	10.4	-	-	18.2	172.4	0.4490	0.1056	0.7900(52.8)	Calc[59]
Ti0.75Mo0.25	160.5	125.6	-	-	-	-	34.1	-	-	26.0	137.2	0.4107	0.1899	0.6667(73.5)	Calc[59]
Ti0.25Nb0.75	203.5	126.8	-	-	-	-	21.3	-	-	27.0	152.4	0.4163	0.1773	0.6924(76.5)	Calc[59]
Ti0.5Nb0.5	155.4	124.7	-	-	-	-	12.8	-	-	13.8	134.9	0.4507	0.1020	0.8293(39.9)	Calc[59]
Ti0.75Nb0.25	128.5	115.5	-	-	-	-	14.9	-	-	10.7	119.8	0.4567	0.0891	0.8395(31.1)	Calc[59]
Ti0.25Ta0.75	207.0	145.3	-	-	-	-	55.6	-	-	43.9	165.9	0.3784	0.2646	0.5408(121.0)	Calc[59]
Ti0.5Ta0.5	163.4	132.8	-	-	-	-	39.0	-	-	26.8	143.0	0.4118	0.1874	0.6559(75.7)	Calc[59]
Ti0.75Ta0.25	129.9	121.6	-	-	-	-	38.6	-	-	16.9	124.4	0.4351	0.1357	0.6674(48.4)	Calc[59]
Ti0.25V0.75	213.0	132.2	-	-	-	-	29.6	-	-	33.5	159.1	0.4016	0.2107	0.6447(93.9)	Calc[59]
Ti0.5V0.5	169.6	122.3	-	-	-	-	33.6	-	-	29.2	138.1	0.4012	0.2114	0.6424(81.8)	Calc[59]
Ti0.75V0.25	123.9	116.9	-	-	-	-	36.3	-	-	15.4	119.2	0.4380	0.1293	0.6760(44.3)	Calc[59]
Ti0.25W0.75	374.8	184.2	-	-	-	-	81.7	-	-	86.9	247.7	0.3430	0.3508	0.4138(233.4)	Calc[59]
Ti0.5W0.5	239.9	165.9	-	-	-	-	50.9	-	-	44.8	190.6	0.3910	0.2351	0.6035(124.6)	Calc[59]
Ti0.75W0.25	169.2	134.2	-	-	-	-	32.4	-	-	25.3	145.9	0.4180	0.1735	0.6979(71.8)	Calc[59]
Zr0.25Mo0.75	342.4	134.5	-	-	-	-	49.7	-	-	67.1	203.8	0.3516	0.3293	0.4161(181.4)	Calc[59]
Zr0.5Mo0.5	208.5	124.3	-	-	-	-	29.2	-	-	33.8	152.4	0.3967	0.2220	0.6242(94.5)	Calc[59]
Zr0.75Mo0.25	138.4	104.2	-	-	-	-	16.6	-	-	16.8	137.2	0.4307	0.1453	0.7578(48.1)	Calc[59]
Zr0.25Nb0.75	196.2	118.5	-	-	-	-	17.9	-	-	24.6	144.4	0.4195	0.1700	0.6967(69.7)	Calc[59]
Zr0.5Nb0.5	144.4	108.3	-	-	-	-	18.3	-	-	18.2	120.3	0.4280	0.1512	0.7479(52.0)	Calc[59]
Zr0.75Nb0.25	112.8	98.3	-	-	-	-	19.8	-	-	13.2	103.1	0.4384	0.1284	0.7612(38.1)	Calc[59]
Ag	120.5	92.0	-	-	-	-	44.6	-	-	28	101.5	0.3726	0.2785	0.4670	400K[60]
Ag	117.0	90.0	-	-	-	-	42.6	-	-	26	99	0.3753	0.2719	0.4788	500K[60]
Ag	113.5	88.0	-	-	-	-	40.7	-	-	25.6	96.5	0.3781	0.2653	0.4902	600K[60]
Ag	110.0	86.0	-	-	-	-	38.8	-	-	24	94	0.3811	0.2584	0.5021	700K[60]
Ag	106.5	84.5	-	-	-	-	36.9	-	-	22.7	91.8	0.3855	0.2480	0.5183	800K[60]
Au	189	160.5	-	-	-	-	41.0	-	-	26.8	199.9	0.4250	0.1580	0.7029	400K[60]
Au	185	158	-	-	-	-	39.7	-	-	25.8	167	0.4266	0.1544	0.7084	500K[60]
Au	182	155.5	-	-	-	-	38.3	-	-	25.0	164.3	0.4275	0.1524	0.7132	600K[60]
Au	178.5	153	-	-	-	-	36.9	-	-	24.1	161.5	0.4289	0.1493	0.7189	700K[60]
Au	175.5	150.5	-	-	-	-	35.5	-	-	23.4	158.8	0.4299	0.1472	0.7240	800K[60]

TABLE VII: The elastic properties (in GPa) of actinide and lanthanide intermetallic compounds,as well as experimental results.

	C_{11}	C_{12}	C_{13}	C_{23}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
Pu-1at%Ga	36.28	26.73	-	-	-	-	33.59	-	-	22.1	29.9	0.2039	0.7378	-0.2293	Expt[61]
α-U	215	46	22	108	199	267	124	73	74	84	113	0.2019	0.7441	-0.2799	Expt[62]
α-U	299	59	30	144	231	364	100	150	132	114	149	0.1933	0.7711	0.3343	Calc[62]
β-U	220	107	79	-	-	201	65	-	36	57	130	0.3090	0.4378	0.3271	Calc[62]
α-UH_3	217	37	-	-	-	-	65	-	-	74	97	0.1957	0.7635	-0.2887	0GPa[63]
α-UH_3	240	42	-	-	-	-	70	-	-	80	108	0.2016	0.7449	-0.2593	5GPa[63]
α-UH_3	260	45	-	-	-	-	66	-	-	80	117	0.2200	0.6885	-0.1800	10GPa[63]
α-UH_3	274	46	-	-	-	-	60	-	-	78	122	0.2370	0.6378	-0.1148	15GPa[63]
α-UH_3	297	61	-	-	-	-	60	-	-	79	140	0.2622	0.5652	-0.0072	20GPa[63]
α-UH_3	213	50	-	-	-	-	48	-	-	59	104	0.2607	0.5695	-0.0192	GGA[64]
α-UH_3	216	57	-	-	-	-	50	-	-	60	110	0.2684	0.5478	0.0636	LDA[64]
α-UH_3	221	63	-	-	-	-	53	-	-	62	116	0.2719	0.5379	0.0865	LDA+U[64]
β-UH_3	201	92	-	-	-	-	57	-	-	56	128	0.3096	0.4363	0.2727	LDA[64]
β-UH_3	222	70	-	-	-	-	58	-	-	65	121	0.2727	0.5356	0.0994	LDA+U[64]
β-UH_3	227	102	-	-	-	-	60	-	-	61	144	0.3141	0.4245	0.2923	GGA[64]
UN	423.9	98.1	-	-	-	-	75.7	-	-	103	207	0.2855	0.5004	0.1084	Expt[65]
UN	381	113	-	-	-	-	54.6	-	-	79	202	0.3273	0.3902	0.2886	AFM-SOC[66]
UN_2	495.4	137.3	-	-	-	-	65.6	-	-	99	257	0.3285	0.3874	0.2793	GGA[67]
UN_2	488.2	140.5	-	-	-	-	55.3	-	-	89	256	0.3438	0.3486	0.3438	GGA+U2[67]
UN_2	483.8	146.2	-	-	-	-	41.3	-	-	76	259	0.3667	0.2927	0.4054	GGA+U4[67]
UO_2	389.3	118.7	-	-	-	-	59.7	-	-	83	209	0.3238	0.3993	0.2824	Expt[68]
UO_2	369.4	112.5	-	-	-	-	61.7	-	-	83	198	0.3159	0.4196	0.2564	GGA[68]
UO_2	343.1	121.3	-	-	-	-	62.7	-	-	79	195	0.3218	0.4043	0.3001	GGA+U[68]
UO_2	440.6	141.3	-	-	-	-	88.1	-	-	109	241	0.3034	0.4525	0.2207	LDA[68]
UO_2	382.3	136.5	-	-	-	-	64.5	-	-	84	218	0.3300	0.3834	0.3269	LDA+U[68]
UO_2	386.4	118.0	-	-	-	-	63.9	-	-	86.4	207	0.3171	0.4166	0.2608	RT[69]
UO_2	317.9	118.3	-	-	-	-	59.8	-	-	73.5	184.8	0.3244	0.3977	0.3165	1200K[69]
UO_2	253.9	96.2	-	-	-	-	49.6	-	-	59.8	148.8	0.3228	0.4018	0.3132	2060K[69]
UO_2	233.3	80.4	-	-	-	-	48.2	-	-	58.0	131.4	0.3075	0.4417	0.2451	2250K[69]
UO_2	219.5	90.7	-	-	-	-	43.0	-	-	50.6	133.6	0.3320	0.3785	0.3569	2370K[69]
UO_2	217.3	97.2	-	-	-	-	43.0	-	-	49.2	137.2	0.3399	0.3583	0.3949	2460K[69]
UO_2	212.8	92.6	-	-	-	-	40.7	-	-	47.6	132.7	0.3398	0.3588	0.3912	2580K[69]
UO_2	196.7	94.5	-	-	-	-	36.4	-	-	41.7	128.6	0.3536	0.3244	0.4519	2670K[69]
UO_2	178.3	93.6	-	-	-	-	32.7	-	-	36.3	121.8	0.3646	0.2977	0.4999	2760K[69]
UO_2	146.1	78.7	-	-	-	-	27.5	-	-	29.8	88.5	0.3485	0.3371	0.5786	2930K[69]
UC	315	77	-	-	-	-	61	-	-	80	156	0.2815	0.5116	0.1023	Expt[70]
UC	315	136	-	-	-	-	72	-	-	79	196	0.3230	0.4015	0.3271	GGA+U3[70]
UC_2	292	154	58	-	-	512	46	-	143	87	180	0.2927	0.4812	0.0637	GGA+U3[71]
U_2C_3	383	121	-	-	-	-	91	-	-	105	208	0.2837	0.5056	0.1440	GGA+U3[71]
UB_2	450.4	58.6	102.3	-	-	497.2	262.6	-	195.9	217	213	0.1197	1.0188	-0.6986	This work
UB_4	558.4	118.9	80.9	-	-	569.1	223	-	226.4	228	250	0.1500	0.9130	-0.4998	This work
UB_{12}	488.9	118.1	-	-	-	-	254.1	-	-	224	242	0.1460	0.9267	-0.5628	This work(0GPa)
UB_{12}	673.1	212.2	-	-	-	-	329.3	-	-	285	366	0.1904	0.7802	-0.3201	This work(50GPa)
UB_{12}	807.8	295.1	-	-	-	-	392.1	-	-	331	466	0.2131	0.7096	-0.2081	This work(100GPa)
U_2Ti	293.6	81	28.2	-	-	310	133.9	-	106.3	124	130	0.1375	0.9562	-0.5037	This work
U_2Ti	285	74	28	-	-	300	129	-	105.5	121	125	0.1346	0.9661	-0.5282	Calc[72]
U_2Ti	295.1	89.4	30.1	-	-	310.8	128	-	102.9	120	133	0.1520	0.9063	-0.4182	Calc[72]
U_2Ti	464.3	189.3	71.4	-	-	489.3	167.9	-	137.5	164	231	0.2121	0.7125	0.0969	20GPa[72]
U_2Ti	603.6	285.7	117.9	-	-	657.1	200	-	159.0	197	322	0.2465	0.6101	0.0692	40GPa[72]
U_2Ti	664.3	332.1	139.3	-	-	732.1	214.3	-	166.1	210	364	0.2583	0.5764	0.1251	50GPa[72]
U_2Ti	928.6	571.4	246.4	-	-	1150	128	-	178.6	195	570	0.3468	0.3412	0.4483	100GPa[72]
NpN	402	140	-	-	-	-	38.4	-	-	64	227	0.3704	0.2837	0.4469	NM[66]
NpN	331	54.2	-	-	-	-	79.1	-	-	99	140	0.2129	0.7100	0.1783	FM[66]
NpN	341	97.7	-	-	-	-	60.8	-	-	81	170	0.2957	0.4731	0.2167	AFM[66]
NpN	359	112	-	-	-	-	50.4	-	-	73	194	0.3334	0.3748	0.3170	NM-SOC[66]
NpN	330	86.4	-	-	-	-	60.7	-	-	81	168	0.2929	0.4805	0.1533	FM-SOC[66]
NpN	339	94.2	-	-	-	-	61.8	-	-	82	176	0.2991	0.4639	0.1843	AFM-SOC[66]
PuN	280	89.6	-	-	-	-	66.2	-	-	74	147	0.2852	0.5013	0.1596	AFM-SOC[66]
Ce	28	17	-	-	-	-	15	-	-	11.2	21	0.2705	0.5419	0.0968	Calc[73]
Ce	37.9	26.4	-	-	-	-	20.9	-	-	14.8	30.2	0.2891	0.4908	0.1819	Calc[73]
CeH_2-CaF_2	84	52	-	-	-	-	27	-	-	21.9	62.7	0.3436	0.3493	0.3989	Calc[73]
CeH_2-CaF_2	87.6	55	-	-	-	-	37	-	-	26.6	65.9	0.3219	0.4043	0.2733	Expt[73]
CeH_2-FeS_2	118	31	-	-	-	-	33	-	-	36.9	60.0	0.2450	0.6144	-0.0333	Calc[73]
CeH_2-AlB_2	90	21	33	-	-	51.55	33	-	-	23.6	51.0	0.2992	0.4635	0.1128	Calc[73]
CeH_2-ReB_2	114	41	18	-	-	56.11	12	-	-	30.4	56.0	0.2705	0.5418	0.0937	Calc[73]
CeH_3-BiF_3	96	35	-	-	-	-	19	-	-	23.0	55.3	0.3175	0.4154	0.2892	Calc[73]
CeH_3-ReO_3	71	49	-	-	-	-	9	-	-	9.8	56.3	0.4181	0.1731	0.7101	Calc[73]
CeH_3-P-3C1	89	20.8	21	-	-	104	23	-	-	30.6	45.2	0.2289	0.6619	-0.1693	Calc[73]

TABLE VIII: The elastic properties (in GPa) of some intermetallic compounds under the pressure and temperature,as well as experimental results.

	C_{11}	C_{12}	C_{13}	C_{23}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
ZrB_{12}	443	129	-	-	-	-	265	-	-	215	234	0.1482	0.9193	-0.5820	Expt[74]
ZrB_{12}	437.9	146.3	-	-	-	-	256.2	-	-	204	244	0.1721	0.8392	-0.4513	0GPa[74]
ZrB_{12}	483.6	174.8	-	-	-	-	275	-	-	218	278	0.1888	0.7855	-0.3608	10Gpa[74]
ZrB_{12}	527.6	203.6	-	-	-	-	291.4	-	-	230	312	0.2036	0.7389	-0.2818	20GPaCalc[74]
ZrB_{12}	611.5	322.1	-	-	-	-	258.8	-	-	253	376	0.2255	0.6720	-0.1682	40GPaCalc[74]
ZrB_{12}	651.7	285.0	-	-	-	-	335.3	-	-	263	407	0.2341	0.6462	-0.1235	50GPaCalc[74]
HfB_{12}	436.4	156.1	-	-	-	-	250.8	-	-	199	250	0.1855	0.7958	-0.3795	0GPaCalc[74]
HfB_{12}	483.1	185.8	-	-	-	-	267.6	-	-	211	285	0.2026	0.7419	-0.2871	10GPaCalc[74]
HfB_{12}	530.1	213.9	-	-	-	-	285.1	-	-	225	315	0.2146	0.7048	-0.2230	20GPaCalc[74]
HfB_{12}	618.5	270.4	-	-	-	-	315.4	-	-	248	386	0.2353	0.6430	-0.1164	40GPaCalc[74]
HfB_{12}	661.4	296.4	-	-	-	-	328.1	-	-	259	418	0.2430	0.6202	-0.0758	50GPaCalc[74]
LuB_{12}	460.4	114.7	-	-	-	-	248	-	-	215	230	0.1441	0.9333	-0.5797	0GPaCalc[74]
LuB_{12}	504.8	138.4	-	-	-	-	268.5	-	-	230	261	0.1585	0.8842	-0.4994	10GPaCalc[74]
LuB_{12}	554.3	167.0	-	-	-	-	284.4	-	-	244	296	0.1770	0.8234	-0.3965	20GPaCalc[74]
LuB_{12}	638.9	219.0	-	-	-	-	316	-	-	268	359	0.2009	0.7472	-0.2702	40GPaCalc[74]
LuB_{12}	679.3	243.1	-	-	-	-	328.1	-	-	279	389	0.2107	0.7170	-0.2188	50GPaCalc[74]
YB_{12}	464.3	107.4	-	-	-	-	252	-	-	219	226	0.1337	0.9695	-0.6388	0GPaCalc[74]
YB_{12}	513.1	135.2	-	-	-	-	270.4	-	-	234	266	0.1600	0.8792	-0.5075	10GPaCalc[74]
YB_{12}	559.3	161.5	-	-	-	-	287.8	-	-	248	294	0.1707	0.8439	-0.4294	20GPaCalc[74]
YB_{12}	646	214.5	-	-	-	-	287.8	-	-	272	358	0.1972	0.7587	-0.2869	40GPaCalc[74]
YB_{12}	686.9	241.1	-	-	-	-	330.9	-	-	282	390	0.2081	0.7247	-0.2304	50GPaCalc[74]
γ-TiAl	186.6	75.0	75.0	-	-	182.9	108.8	-	81.2	78.3	111.8	0.2162	0.7001	-0.1789	0K[75]
γ-TiAl	182.8	75.2	75.0	-	-	176.9	103.5	-	81.2	74.5	110.3	0.2243	0.6756	-0.1351	298K[75]
γ-TiAl	179.7	75.3	75.3	-	-	173.7	100.5	-	74.4	72.3	109.4	0.2293	0.6608	-0.1110	443K[75]
γ-TiAl	178.0	75.6	75.5	-	-	172.1	99.0	-	73.3	71.1	109.0	0.2321	0.6523	-0.0972	523K[75]
γ-TiAl	172.5	75.2	75.7	-	-	167.3	94.8	-	70.6	67.9	107.3	0.2387	0.6329	-0.0676	723K[75]
γ-TiAl	150.3	76.0	76.0	-	-	152.6	81.6	-	63.8	56.9	101.0	0.2627	0.5638	0.0327	1273K[75]
S-ZnO	189.8	102.2	93.7	-	-	199.1	45.2	-	43.8	46.0	128.7	0.3402	0.3576	0.4155	Calc[76]
S-ZnO	190	110	90	-	-	196	39	-	40	42.3	128.4	0.3516	0.3293	0.4713	Expt[76]
V_O^0-1	182.0	96.8	82.7	-	-	192.8	44.5	-	42.6	45.7	120.1	0.3311	0.3807	0.3846	Calc[76]
V_O^{+2}-1	180.7	112.1	97.5	-	-	192.4	35.9	-	34.3	37.4	129.8	0.3686	0.2879	0.5371	Calc[76]
V_O^0-2	169.2	88.0	87.3	-	-	163.5	38.3	-	40.6	39.4	114.1	0.3452	0.5638	0.4224	Calc[76]
ReB_2	682	188	131	-	-	1118	290	-	247	294.1	369.6	0.1855	0.7958	-0.2949	Calc[77]
$0.32B_V$	629	167	135	-	-	1006	266	-	231	269.4	342.8	0.1887	0.7857	-0.2844	Calc[77]
$0.65B_V$	596	167	182	-	-	922	227	-	214	236.0	346.0	0.2221	0.6821	-0.1329	Calc[77]
$1.30B_V$	543	170	226	-	-	667	195	-	186	190.2	329.9	0.2582	0.5766	0.0227	Calc[77]
HA	137.2	44.5	57.8	-	-	164.8	42.3	-	46.35	44.7	83.7	0.2734	0.5337	0.0815	Calc[78]
HA	137	42.5	54.9	-	-	172	39.6	-	47.25	44.6	82.6	0.2713	0.5397	0.0639	Expt[78]
HA-V_H	129.0	27.6	69.5	-	-	158.6	47.8	-	50.7	44.8	80.4	0.2648	0.5578	-0.0087	Calc[78]
HA-V_O	113.7	43.5	47.1	-	-	163.9	39.9	-	35.1	39.5	72.9	0.2709	0.5409	0.1069	Calc[78]
HA-V_{OH}	109.0	28.4	62.7	-	-	160.1	42.1	-	40.3	39.2	72.3	0.2701	0.5429	0.0602	Calc[78]
HA-V_{Ca1}^{2+}	116.2	53.4	40.7	-	-	156.0	31.7	-	31.4	35.1	72.9	0.2925	0.4816	0.2128	Calc[78]
HA-V_{Ca2}^{2+}	77.0	21.9	70.4	-	-	119.1	34.1	-	27.55	26.5	66.5	0.3241	0.3984	0.4609	Calc[78]
Ni	246.58	147.24	-	-	-	-	124.97	-	-	94.85	180.35	0.2763	0.5259	0.1235	MD[79]
Ni-1at%H	246.74	148.04	-	-	-	-	122.56	-	-	93.28	180.94	0.2800	0.5155	0.1408	MD[79]
Ni-2at%H	246.93	148.81	-	-	-	-	120.20	-	-	91.74	181.52	0.2827	0.5082	0.1576	MD[79]
Ni-3at%H	247.13	149.57	-	-	-	-	117.83	-	-	90.21	182.09	0.2874	0.4954	0.1743	MD[79]
Ni-4at%H	247.33	150.34	-	-	-	-	115.46	-	-	88.67	182.67	0.2911	0.4854	0.1909	MD[79]
Ni-5at%H	247.53	151.1	-	-	-	-	113.10	-	-	87.15	183.24	0.2947	0.4756	0.2074	MD[79]
$PbTiO_3$	235	101	98.8	-	-	105	65	-	104	56.5	130.2	0.2853	0.5011	0.1282	Expt[80]
$BaTiO_3$	211	107	114	-	-	160	56.2	-	127	58.2	137.9	0.3152	0.4216	0.1370	Expt[80]
Ti	176.1	86.9	68.3	-	-	190.5	50.8	-	44.6	50.2	109.9	0.3020	0.4562	0.2719	4K[81]
Ti	162.4	92.0	69.0	-	-	180.7	46.7	-	35.2	43.4	107.3	0.3219	0.4042	0.3687	298K[81]
Ti	152.2	94.3	69.5	-	-	173.4	43.4	-	28.5	38.2	104.9	0.3375	0.3644	0.3749	473K[81]
Ti	129.9	99.2	68.8	-	-	157.6	33.7	-	15.4	26.1	98.9	0.3788	0.2637	0.5185	923K[81]
Ti	97.7	82.7	-	-	-	-	37.5	-	25.5	87.7	137.9	0.3675	0.2908	0.5154	1273 K[82]

TABLE IX: The elastic properties (in GPa) of potential structural materials for nuclear reactors, as well as experimental results.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
ZrC	470	100			160	-	170	223	0.1970	0.7593	-0.2687	Expt[83]
SiC	390	142			256	-	191	225	0.1683	0.8518	-0.5074	Expt[14]
SiC	420	126			287	-	219	224	0.1308	0.9795	-0.7188	Expt[15]
Ti_2SC	-	-	-	-	-	-	125	145	0.16	-	-	Expt[84]
α-Ti_3SiC_2	360	84	101	350	158	1380	142	182	0.1910	0.7784	-0.3054	FLAPW[85]
β-Ti_3SiC_2	360	86	89	348	120	1370	129	177	0.2077	0.7262	-0.2312	FLAPW[85]
Fe-19Cr-10Ni	204.6	137.7	-	-	126.2	-	89.1	160	0.2652	0.5569	0.0719	Expt[86]
Fe-12Cr-12Ni	210.9	140.3	-	-	122.5	-	88	164	0.2730	0.5349	0.1086	Expt[86]
Fe-12Cr-18Ni	233.2	162.7	-	-	122.6	-	88	168	0.2965	0.4708	0.2153	Expt[86]
Fe-18Cr-8Ni	209	133.0	-	-	121	-	88	153	0.2595	0.5727	0.0758	Expt[87]
Fe-18Cr-12Ni	191.2	117.9	-	-	138.6	-	98	142	0.2204	0.6874	-0.1454	Expt[86]
Fe-18Cr-12Ni	215.9	144.6	-	-	128.9	-	89.1	160	0.2652	0.5569	0.0719	Expt[86]
Fe-18Cr-14Ni	198	125	-	-	122	-	88	149.3	0.2542	0.5881	0.0201	Expt[86]
Fe-18Cr-19Ni	191	119	-	-	124	-	89	143	0.2428	0.6210	-0.0350	Expt[86]
Fe-19Cr-10Ni	207	132	-	-	123	-	89.1	157	0.2621	0.5656	0.0573	Expt[86]
Fe-19Cr-14Ni	205	133	-	-	127	-	91	157	0.2580	0.5771	0.0382	Expt[86]
Fe-19Cr-19Ni	204	133	-	-	126	-	89	156.7	0.2594	0.5731	0.0447	Expt[86]
Fe-19Cr-24Ni	215.2	144.0	-	-	125.8	-	90	168	0.2730	0.5350	0.1085	Expt[87]
Fe	276	173.5	-	-	136.3	-	102	208	0.2885	0.4924	0.1719	Expt[86]
Co	239.8	163.4	-	-	133.4	-	95	189	0.2841	0.5045	0.1588	Expt[86]
Ni	251.6	154.4	-	-	122.0	-	93	187	0.2873	0.4957	0.1734	Expt[86]
Fe-15Cr-15Ni	215.0	137	-	-	136	-	97.2	163	0.2513	0.5963	0.0061	195K[87]
Fe-15Cr-15Ni	214.9	137	-	-	135	-	96.6	163	0.2526	0.5926	0.0123	200K[87]
Fe-15Cr-15Ni	214.7	137	-	-	134	-	95.9	163	0.2541	0.5883	0.0184	220K[87]
Fe-15Cr-15Ni	214.6	137	-	-	133	-	95.3	162.8	0.2551	0.5739	0.0246	230K[87]
Fe-15Cr-15Ni	213.1	137	-	-	133	-	95.0	162.4	0.2552	0.5853	0.0246	240K[87]
Fe-15Cr-15Ni	213.2	137	-	-	132	-	94.4	162.4	0.2565	0.5813	0.0308	250K[87]
Fe-15Cr-15Ni	212.6	137	-	-	132	-	94.3	162.2	0.2565	0.5814	0.0308	260K[87]
Fe-15Cr-15Ni	212.1	137	-	-	132	-	94.2	162.0	0.2565	0.5815	0.0309	270K[87]
Fe-15Cr-15Ni	211.8	137	-	-	131	-	93.6	161.9	0.2576	0.5781	0.0371	280K[87]
Fe-15Cr-15Ni	211.4	137	-	-	131	-	93.5	161.8	0.2577	0.5797	0.0371	290K[87]
Fe-15Cr-15Ni	211	137	-	-	130	-	93	162	0.2591	0.5739	0.0433	295K[87]
Ti_2AlB	196.4	87.1	58.0	209.0	75.3	54.7	67	112	0.2512	0.5963	0.0674	PAW[88]
Zr_2AlB	176.7	70.0	51.4	175.7	52.0	53.4	55	97	0.2617	0.5667	0.0824	PAW[88]
Hf_2AlB	203.8	76.5	58.5	200	67.5	63.7	67	110	0.2469	0.6990	0.0172	PAW[88]
V_2AlB	285.1	85.7	97.7	278.5	138.8	99.7	111	157	0.2127	0.7108	-0.1757	PAW[88]
Nb_2AlB	283.6	91.4	101.7	249.2	125.3	96.1	101	160	0.2400	0.6280	-0.0603	PAW[88]
Ta_2AlB	325.5	96.8	113.0	276.2	140.6	114.4	118	175	0.2249	0.6735	-0.1295	PAW[88]
Cr_2AlB	298.8	81.9	129.8	289.6	157.4	108.5	121	174	0.2177	0.6954	-0.1557	PAW[88]
Mo_2AlB	316.6	105.4	151.7	268.7	161.1	105.6	118	191	0.2438	0.6199	-0.0251	PAW[88]
Sc_2AlC	179.2	65.3	34.2	194.5	45.2	57.0	56	91	0.2447	0.6154	-0.0148	PAW[88]
Ti_2AlC	304.4	65.4	64.0	269.9	105.7	119.5	112	140	0.1857	0.7953	-0.3412	PAW[88]
Zr_2AlC	259.2	64.7	63.3	225.3	85.0	97.3	90	125	0.2093	0.7212	-0.2174	PAW[88]
Hf_2AlC	291.1	74.5	72.2	255.0	99.2	108.3	102	141	0.2083	0.7243	-0.2150	PAW[88]
V_2AlC	330.2	74.3	107.1	321.1	149.3	128.0	130	173	0.1991	0.7529	-0.2771	PAW[88]
Nb_2AlC	318.9	89.4	120.8	296.5	141.2	114.8	118	177	0.2282	0.6639	-0.1291	PAW[88]
Ta_2AlC	349.0	125.3	132.2	338.2	153.3	111.9	125	202	0.2432	0.6197	-0.0191	PAW[88]
Cr_2AlC	369.8	86.1	108.7	362.5	142.9	141.9	139	190	0.2065	0.7298	-0.2370	PAW[88]
Mo_2AlC	354.4	98.0	146.6	359.0	144.4	128.2	127	205	0.2431	0.6199	-0.0683	PAW[88]
Sc_2AlN	210.3	69.6	54.0	217.7	70.9	70.4	73	110	0.2291	0.6613	-0.0802	PAW[88]
Ti_2AlN	316.2	69.7	94.7	291.3	127.9	123.3	120	160	0.2012	0.7461	-0.2709	PAW[88]
Zr_2AlN	268.8	76.9	87.2	243.5	109.1	96.0	98	1143	0.2215	0.6842	-0.3054	PAW[88]
Hf_2AlN	307.4	84.5	103.1	268.4	124.5	111.5	111	163	0.2229	0.6799	-0.1488	PAW[88]
V_2AlN	301.7	44.8	131.4	331.7	143.1	128.5	121	169	0.2105	0.7175	-0.2820	PAW[88]
Nb_2AlN	340.4	149.9	110.6	332.3	147.7	95.3	119	195	0.2468	0.6095	0.0449	PAW[88]
Ta_2AlN	351.9	174.1	142.8	372.5	160.0	88.9	119	222	0.2727	0.5359	0.1533	PAW[88]
Cr_2AlN	286.7	74.9	144.5	376.7	88.2	105.9	95	181	0.2764	0.5256	0.0599	PAW[88]
Ti_3AlC_2	368	81	76	313	130	143	135	168	0.1833	0.8029	-0.3456	PAW[89]
Zr_3AlC_2	322	73	75	270	106	124	113	151	0.2003	0.7490	-0.3385	PAW[89]
Hf_3AlC_2	357	82	83	283	126	138	127	165	0.1930	0.7722	-0.3000	PAW[89]
V_3AlC_2	415	88	113	361	163	163	156	202	0.1936	0.7701	-0.3094	PAW[89]
Nb_3AlC_2	331	131	126	321	137	100	113	194	0.2556	0.5839	0.0515	PAW[89]
Ta_3AlC_2	417	118	187	351	177	150	147	241	0.2466	0.6099	-0.0456	PAW[89]
Cr_3AlC_2	381	100	136	381	118	141	117	209	0.2649	0.5582	0.0258	PAW[89]
Mo_3AlC_2	370	159	140	361	121	105	113	220	0.2800	0.5155	0.1661	PAW[89]
W_3AlC_2	392	181	177	389	121	106	112	249	0.3047	0.4490	0.2628	PAW[89]
Ti_3SiC_2	366	94	100	352	153	136	141	186	0.1976	0.7574	-0.2557	GGA[90]
Ti_3GeC_2	357	94	97	333	143	132	133	182	0.2048	0.7350	-0.2230	GGA[90]
Ti_3SnC_2	346	92	84	313	123	127	124	169	0.2051	0.7341	-0.2187	GGA[90]
Ti_2GeC	279	99	95	283	125	90	104	158	0.2306	0.6569	-0.0666	LDA[91]

TABLE X: The elastic properties (in GPa) of potential structural materials for nuclear reactors, as well as experimental results(continued).

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
V_2GeC	282	121	144	259	160	80.5	108	182	0.2532	0.5908	0.0672	LDA[91]
Cr_2GeC	315	148	146	354	89	83.5	88	207	0.3130	0.4273	0.2937	LDA[91]
Zr_2GeC	224	105	108	243	99	59.5	74	148	0.2856	0.5004	0.1842	LDA[91]
Nb_2GeC	308	133	168	306	177	87.5	119	206	0.2590	0.5744	0.0884	LDA[91]
Mo_2GeC	331	136	184	342	123	97.5	100	223	0.3052	0.4478	0.2235	LDA[91]
Hf_2GeC	269	96	125	278	128	86.5	97	167	0.2568	0.5804	0.0194	LDA[91]
Ta_2GeC	370	147	194	389	220	111.5	149.9	243.4	0.2445	0.6161	0.0195	LDA[91]
W_2GeC	340	146	222	368	117	97.0	96.7	244	0.3963	0.3250	0.3156	LDA[91]
Ti_2GaC	314	66	59	272	122	124	121	141	0.1650	0.8627	-0.4306	LDA[92]
Nb_2GaC	374	88	135	310	149	141.5	132	197	0.2260	0.6704	-0.1713	LDA[92]
Ta_2GaC	420	101	146	333	175	159.5	150	217	0.2186	0.6929	-0.2013	LDA[92]
V_2GaC	343	67	124	312	157	138	133	181	0.2044	0.7362	-0.2877	LDA[92]
V	232.4	119.36	-	-	45.95	-	50	157	0.3563	0.3179	0.4675	4.2K[93]
V	227.95	118.75	-	-	42.55	-	47	155	0.3624	0.3031	0.4911	300K[93]
Ta	267.95	162.4	-	-	86.75	-	71	198	0.3394	0.3597	0.3829	4.2K[94]
Ta	266.86	162.17	-	-	85.49	-	70	197	0.3407	0.3563	0.3891	100K[94]
Ta	264.82	161.29	-	-	83.32	-	69	195.8	0.3426	0.3516	0.3982	200K[94]
Ta	262.77	160.88	-	-	81.44	-	67	194.8	0.3448	0.3463	0.4077	300K[94]
Ta90W10	287.98	162.11	-	-	87.21	-	76.5	204	0.3333	0.3750	0.3670	4.2K[94]
Ta90W10	286.78	161.98	-	-	86.28	-	75.8	203.6	0.3344	0.3722	0.3718	100K[94]
Ta90W10	284.73	161.73	-	-	84.68	-	74.5	202.7	0.3363	0.3675	0.3801	200K[94]
Ta90W10	282.51	161.24	-	-	83.15	-	73.3	201.7	0.3380	0.3633	0.3872	300K[94]
Ta70W30	325.95	173.26	-	-	87.31	-	82.7	224.1	0.3357	0.3691	0.3834	4.2K[94]
Ta70W30	325.10	172.67	-	-	86.93	-	82.5	223.5	0.3357	0.3690	0.3837	100K[94]
Ta70W30	323.12	171.60	-	-	86.23	-	81.9	222.1	0.3359	0.3686	0.3844	200K[94]
Ta70W30	321.13	170.42	-	-	85.56	-	81.3	222.6	0.3359	0.3685	0.3846	300K[94]
Ta50W50	371.14	185.65	-	-	86.72	-	89.1	247.5	0.3393	0.3599	0.3997	4.2K[94]
Ta50W50	370.38	185.19	-	-	87.07	-	89.2	246.9	0.3387	0.3614	0.3974	100K[94]
Ta50W50	368.59	183.85	-	-	87.49	-	89.4	245.4	0.3376	0.3643	0.3926	200K[94]
Ta50W50	366.51	182.23	-	-	88.03	-	89.7	243.7	0.3361	0.3679	0.3866	300K[94]
Ta33W67	434.65	191.29	-	-	114.43	-	117.3	272.4	0.3118	0.4305	0.2821	4.2K[94]
Ta33W67	433.50	191.13	-	-	114.30	-	117.0	271.9	0.3118	0.4303	0.2825	100K[94]
Ta33W67	430.52	190.88	-	-	114.05	-	116.3	270.8	0.3121	0.4296	0.2838	200K[94]
Ta33W67	426.86	189.97	-	-	113.84	-	115.7	268.9	0.3119	0.4300	0.2831	300K[94]
Ta17W83	481.68	196.41	-	-	139.32	-	140.6	291.5	0.2922	0.4825	0.1958	4.2K[94]
Ta17W83	480.49	196.21	-	-	139.07	-	140.3	290.9	0.2923	0.4821	0.1964	100K[94]
Ta17W83	476.94	196.42	-	-	138.34	-	139.1	289.9	0.2932	0.4798	0.2003	200K[94]
Ta17W83	473.12	196.72	-	-	137.68	-	137.9	288.9	0.2941	0.4774	0.2044	300K[94]
W	530.25	201.90	-	-	160.92	-	162.2	311.4	0.2780	0.5210	0.1316	4.2K[94]
W	529.81	199.98	-	-	160.83	-	162.5	309.9	0.2769	0.5242	0.1263	100K[94]
W	526.42	200.75	-	-	159.58	-	160.9	309.3	0.2784	0.5201	0.1331	200K[94]
W	521.48	201.01	-	-	158.50	-	159.2	307.8	0.2795	0.5171	0.1381	300K[94]
V	237	122	-	-	47.08	-	82.7	224.1	0.3357	0.3691	0.3834	4.2K[95]
V	236.09	121.09	-	-	46.145	-	50.4	159.4	0.3570	0.3161	0.4701	100K[95]
V	233.38	120.72	-	-	44.800	-	49.1	158.3	0.3594	0.3102	0.4797	200K[95]
V	230.98	120.17	-	-	43.768	-	48	157	0.3611	0.3062	0.4863	300K[95]
V	281.72	124.63	-	-	36.09	-	49.6	177.0	0.3716	0.2800	0.5002	EMTO[96]
V-2.5Cr	285.81	125.15	-	-	35.38	-	49.5	178.7	0.3733	0.2768	0.5023	EMTO[96]
V-5Cr	289.59	125.48	-	-	34.37	-	19.1	180.2	0.3751	0.2726	0.5057	EMTO[96]
V-7.5Cr	292.85	125.84	-	-	33.20	-	48.5	181.5	0.3773	0.2674	0.5104	EMTO[96]
V10Cr	296.66	125.79	-	-	32.15	-	48.2	182.7	0.3789	0.2635	0.5124	EMTO[96]
V-2.5Ti	275.2	123.49	-	-	36.60	-	49.2	174.1	0.3708	0.2828	0.4992	EMTO[96]
V-5Ti	269.21	122.40	-	-	37.03	-	48.9	171.3	0.3697	0.2853	0.4983	EMTO[96]
V-7.5Ti	263.45	121.55	-	-	37.72	-	48.7	168.9	0.3684	0.2885	0.4965	EMTO[96]
V-10Ti	257.71	120.55	-	-	38.32	-	48.5	166.3	0.3671	0.2916	0.4946	EMTO[96]
V-2.5Cr-2.5Ti	279.76	123.82	-	-	36.11	-	49.4	175.8	0.3715	0.2811	0.4989	EMTO[96]
V-2.5Cr-5Ti	273.49	122.72	-	-	36.76	-	49.2	173.0	0.3700	0.2846	0.4969	EMTO[96]
V-2.5Cr-7.5Ti	267.53	121.67	-	-	37.27	-	48.9	170.3	0.3689	0.2874	0.4956	EMTO[96]
V-2.5Cr-10Ti	261.76	120.70	-	-	37.94	-	48.8	167.7	0.3675	0.2907	0.4934	EMTO[96]
V-4Cr-4Ti	278.56	123.34	-	-	36.16	-	49.4	175.1	0.3711	0.2819	0.4979	EMTO[96]
V-5Cr-2.5Ti	283.72	124.23	-	-	35.47	-	49.4	177.4	0.3726	0.2784	0.5004	EMTO[96]
V-5Cr-5Ti	277.78	123.02	-	-	36.24	-	49.4	174.6	0.3708	0.2827	0.4970	EMTO[96]
V-5Cr-7.5Ti	271.64	121.97	-	-	36.85	-	49.1	171.9	0.3695	0.2859	0.4953	EMTO[96]
V-5Cr-10Ti	265.81	120.92	-	-	37.53	-	48.9	169.2	0.3680	0.2895	0.4928	EMTO[96]
V-7.5Cr-2.5Ti	287.22	124.30	-	-	34.62	-	49.2	178.6	0.3739	0.2752	0.5021	EMTO[96]
V-7.5Cr-5Ti	282.71	122.87	-	-	35.68	-	49.6	176.2	0.3713	0.2816	0.4950	EMTO[96]
V-7.5Cr-7.5Ti	275.88	122.25	-	-	36.51	-	49.4	173.5	0.3699	0.2849	0.4943	EMTO[96]
V-7.5Cr-10Ti	269.97	121.12	-	-	37.17	-	49.3	170.7	0.3684	0.2886	0.4917	EMTO[96]
V-10Cr-2.5Ti	291.44	124.77	-	-	33.76	-	53.9	179.4	0.3635	0.3004	0.5037	EMTO[96]
V-10Cr-5Ti	285.66	123.62	-	-	35.03	-	53.4	177.6	0.3633	0.3008	0.4987	EMTO[96]

TABLE XI: The elastic properties (in GPa) of potential structural materials for nuclear reactors, as well as experimental results(continued).

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	G	B	ν	G/B	Cauchy Pressure/B	Note
V-10Cr-7.5Ti	280.81	122.13	-	-	36.05	-	50	175	0.3702	0.2842	0.4918	EMTO[96]
V-10Cr-10Ti	274.07	121.35	-	-	36.90	-	50	172	0.3686	0.2879	0.4903	EMTO[96]
Nb	244.1	130	-	-	27.8	-	37.2	168.0	0.3968	0.2216	0.6082	300K[97]
Nb90Zr10	229.2	124.8	-	-	27.0	-	35.3	159.6	0.3971	0.2210	0.6128	300K[97]
Nb80Zr20	203	114	-	-	27.1	-	33.0	143.6	0.3930	0.2303	0.6049	300K[97]
Nb70Zr30	180.8	106.4	-	-	28.6	-	31.7	131.2	0.3879	0.2422	0.5930	300K[97]
Nb60Zr40	164.9	100.0	-	-	30.0	-	31.0	121.6	0.3827	0.2545	0.5755	300K[97]
Nb50Zr50	151.8	96.6	-	-	31.8	-	30.0	115.0	0.3798	0.2613	0.5635	300K[97]
Nb30Zr70	124.4	88.2	-	-	33.6	-	26.2	100.3	0.3798	0.2614	0.5445	300K[97]
Nb	220.1	124.4	-	-	34.7	-	39.5	156.3	0.3835	0.2525	0.5739	1500K[97]
Nb90Zr10	204.2	119.2	-	-	34.6	-	37.6	147.5	0.3826	0.2547	0.5734	1500K[97]
Nb80Zr20	177.4	108.1	-	-	33.4	-	33.9	131.2	0.3811	0.2583	0.5694	1500K[97]
Nb70Zr30	156.9	101.5	-	-	33.1	-	30.8	119.9	0.3817	0.2569	0.5702	1500K[97]
Nb60Zr40	144.9	96.4	-	-	31.4	-	28.3	112.6	0.3840	0.2515	0.5774	1500K[97]
Nb50Zr50	131.3	92.6	-	-	30.5	-	25.5	105.4	0.3885	0.2409	0.5886	1500K[97]
Nb30Zr70	111.9	84.0	-	-	28.7	-	21.5	93.3	0.3931	0.2303	0.5927	1500K[97]
Nb50Zr50	155.6	96.9	-	-	33.2	-	31.6	116.5	0.3756	0.2713	0.5469	5K[97]
Nb50Zr50	149	95.9	-	-	31.9	-	29.6	113.6	0.3799	0.2609	0.5634	500K[97]
Nb50Zr50	141.2	94.5	-	-	31.4	-	27.9	110.1	0.3832	0.2534	0.5733	1000K[97]
Nb50Zr50	132	92.5	-	-	30.7	-	25.7	105.7	0.3874	0.2434	0.5849	1500K[97]
Cr-0.67%V	379.6	78.2	-	-	102.73	-	119.8	178.7	0.2259	0.6706	-0.1373	80K[98]
Cr-0.67%V	378.8	78.1	-	-	102.64	-	119.6	178.3	0.2259	0.6709	-0.1376	100K[98]
Cr-0.67%V	375.3	77.5	-	-	102.23	-	118.9	176.8	0.2253	0.6726	-0.1399	150K[98]
Cr-0.67%V	370.3	76.1	-	-	101.76	-	118.0	174.2	0.2237	0.6774	-0.1473	200K[98]
Cr-0.67%V	366.1	74.3	-	-	101.41	-	117.4	171.6	0.2215	0.6840	-0.1580	230K[98]
Cr-0.67%V	363.9	72.9	-	-	101.30	-	117.1	169.9	0.2197	0.6895	-0.1672	240K[98]
Cr-0.67%V	362.8	71.9	-	-	101.27	-	117.1	168.9	0.2184	0.6935	-0.1739	245K[98]
Cr-0.67%V	369.0	78.5	-	-	101.22	-	117.0	175.3	0.2270	0.6674	-0.1296	250K[98]
Cr-0.67%V	372.8	82.9	-	-	101.12	-	116.8	179.5	0.2326	0.6508	-0.1015	260K[98]
Cr-0.67%V	373.2	85.9	-	-	100.72	-	116.1	181.7	0.2365	0.6393	-0.0816	300K[98]
Cr-0.67%V	371.8	88.0	-	-	100.23	-	115.2	182.6	0.2393	0.6313	-0.0670	350K[98]
Cr-1.5%V	383.4	102.2	-	-	102.10	-	116.1	195.9	0.2526	0.5924	0.0005	80K[98]
Cr-1.5%V	382.4	102.1	-	-	101.97	-	115.8	195.5	0.2526	0.5924	0.0007	100K[98]
Cr-1.5%V	380.1	101.6	-	-	101.59	-	115.3	194.4	0.2525	0.5929	0.0001	130K[98]
Cr-1.5%V	378.5	101.5	-	-	101.33	-	114.9	193.8	0.2526	0.5926	0.0009	150K[98]
Cr-1.5%V	377.7	101.6	-	-	101.20	-	114.6	193.6	0.2528	0.5919	0.0021	160K[98]
Cr-1.5%V	377.3	101.4	-	-	101.13	-	114.5	193.4	0.2527	0.5923	0.0014	165K[98]
Cr-1.5%V	380.7	104.8	-	-	110.17	-	120.6	196.8	0.2456	0.6127	-0.0273	170K[98]
Cr-1.5%V	382.1	106.4	-	-	101.02	-	114.4	198.3	0.2580	0.5771	0.0271	175K[98]
Cr-1.5%V	382.0	106.6	-	-	101.00	-	114.4	198.4	0.2582	0.5764	0.0282	180K[98]
Cr-1.5%V	381.9	107.1	-	-	100.91	-	114.2	198.7	0.2588	0.5748	0.0312	190K[98]
Cr-1.5%V	381.5	107.2	-	-	100.83	-	114.1	198.6	0.2590	0.5743	0.0321	200K[98]
Cr-1.5%V	379.5	108.2	-	-	100.36	-	113.2	198.6	0.2605	0.5701	0.0395	250K[98]
Cr-1.5%V	376.4	107.9	-	-	99.88	-	112.5	197.4	0.2606	0.5697	0.0406	300K[98]
Cr-1.5%V	373.4	108.2	-	-	99.42	-	111.6	196.6	0.2614	0.5676	0.0447	350K[98]
Cr	394.1	88.5	-	-	103.75	-	121.2	190.4	0.2374	0.6367	-0.0801	0K[9]
Cr	393.2	88.2	-	-	103.73	-	121.1	189.9	0.2370	0.6378	-0.0818	50K[9]
Cr	389.8	87.4	-	-	103.28	-	120.4	188.2	0.2364	0.6395	-0.0844	100K[9]
Cr	389.4	87.4	-	-	103.04	-	120.1	188.1	0.2367	0.6388	-0.0832	110K[9]
Cr	388.0	87.2	-	-	102.35	-	119.5	187.5	0.2372	0.6372	-0.0808	120K[9]
Cr	386.5	95.3	-	-	101.33	-	117.2	192.4	0.2468	0.6092	-0.0313	125K[9]
Cr	380.4	91.0	-	-	101.93	-	117.3	187.5	0.2411	0.6258	-0.0583	130K[9]
Cr	380.3	92.7	-	-	102.28	-	117.3	188.6	0.2425	0.6219	-0.0508	135K[9]
Cr	378.7	92.9	-	-	102.35	-	117.0	188.2	0.2425	0.6219	-0.0502	140K[9]
Cr	378.5	94.5	-	-	102.38	-	116.7	189.2	0.2441	0.6171	-0.0417	145K[9]
Cr	374.7	99.9	-	-	101.99	-	114.9	191.5	0.2499	0.6002	-0.0109	185K[9]
Cr	372.9	99.3	-	-	101.80	-	114.6	190.5	0.2494	0.6016	-0.0131	200K[9]
Cr	364.7	90.9	-	-	101.15	-	114.2	182.2	0.2407	0.6269	-0.0563	250K[9]
Cr	348.4	70.2	-	-	100.71	-	114.6	162.9	0.2150	0.7036	-0.1873	300K[9]
Cr	345.1	66.3	-	-	100.67	-	114.7	159.2	0.2096	0.7204	-0.2158	305K[9]
Cr	337.2	57.4	-	-	100.70	-	114.9	150.7	0.1960	0.7626	-0.2874	310K[9]
Cr	354.2	72.4	-	-	100.67	-	115.2	166.3	0.2186	0.6926	-0.1699	315K[9]
Cr	356.4	75.0	-	-	100.64	-	115.1	168.8	0.2222	0.6820	-0.1519	320K[9]
Cr	358.4	77.4	-	-	100.53	-	114.9	171.1	0.2254	0.6721	-0.1352	330K[9]

TABLE XII: The calculated Eigenvalue of Hessian matrix at critical points and $\triangle\rho$.

	CP class	Eigenvalue1	Eigenvalue2	Eigenvalue3	$\triangle\rho$	charge density
Diamond-C	Bond	-4.731E-1	-4.731E-1	3.796E-1	-5.667E-1	2.404E-1
Diamond-C	Ring	-1.694E-2	6.183E-2	6.244E-2	1.073E-1	2.123E-2
Diamond-C	Cage	2.500E-2	2.500E-2	2.500E-2	7.499E-2	1.312E-2
Diamond-Si	Bond	-7.280E-2	-7.280E-2	2.156E-2	-1.240E-1	8.340E-2
Diamond-Si	Ring	-2.078E-3	7.253E-3	7.314E-3	1.249E-2	5.366E-3
Diamond-Si	Cage	2.742E-3	2.742E-3	2.742E-3	8.226E-3	3.115E-3
Diamond-Si-HSE	Bond	-7.747E-2	-7.747E-2	1.714E-2	-1.378E-1	8.6857E-2
Diamond-Si-HSE	Ring	-2.196E-3	7.674E-3	7.674E-3	1.315E-2	5.575E-3
Diamond-Si-HSE	Cage	2.896E-3	2.896E-3	2.896E-3	8.6868E-3	3.1847E-3
fcc-Ti	Nuclei	-1.360E-03	-1.360E-03	-1.360E-03	-4.080E-03	2.972E-02
fcc-Ti	Bond	-2.493E-03	-2.493E-03	1.750E-03	-3.092E-03	2.971E-02
fcc-Ti	Ring	-5.504E-03	3.656E-03	3.243E-02	3.058E-02	2.797E-02
fcc-Ti	Cage	4.806E-04	4.806E-04	4.806E-04	1.442E-03	2.459E-02
fcc-Zr	Nuclei	-4.237E-04	-4.237E-04	-4.237E-04	-1.271E-03	2.640E-02
fcc-Zr	Bond	-8.591E-04	-8.591E-04	6.080E-04	-1.110E-03	2.640E-02
fcc-Zr	Ring	-5.331E-03	2.253E-03	2.830E-02	2.523E-02	2.533E-02
fcc-Zr	Cage	1.066E-03	1.066E-03	1.066E-03	2.039E-02	3.199E-03
fcc-Al	Bond	-1.045E-2	-2.570E-03	1.313E-02	1.147E-4	3.007E-2
fcc-Al	Ring	-2.602E-03	4.778E-03	4.778E-03	6.954E-03	2.817E-2
fcc-Al	O-site	7.652E-03	7.652E-03	7.652E-03	2.296E-02	1.690E-2
fcc-Al	T-site	2.511E-03	2.511E-03	2.511E-03	7.532E-03	2.808E-2
fcc-Cu	Bond	-2.077E-02	-1.516E-02	1.002E-01	6.423E-02	3.824E-02
fcc-Cu	Ring	-9.679E-03	2.190E-02	2.190E-02	3.411E-02	3.142E-02
fcc-Cu	O-site	9.909E-03	9.909E-03	9.909E-03	2.973E-02	2.089E-02
fcc-Cu	T-site	1.095E-02	1.095E-02	1.095E-02	3.285E-02	3.044E-02
fcc-Au	Bond	-2.014E-02	-1.991E-02	1.148E-01	7.472E-02	3.708E-02
fcc-Au	Ring	-1.059E-02	2.766E-02	2.939E-02	4.646E-02	2.578E-02
fcc-Au	O-site	8.820E-03	8.820E-03	8.820E-03	2.646E-02	1.310E-02
fcc-Au	T-site	1.488E-02	1.488E-02	1.488E-02	4.463E-02	2.371E-02
bcc-Mo	Bond	-0.0225	-0.0223	0.0796	0.035	0.050
bcc-Mo	Ring	-0.0044	0.0095	0.0095	0.015	0.037
bcc-Mo	Cage	0.0048	0.0048	0.0057	0.015	0.035
bcc-Nb	Bond	-0.0158	-0.0158	0.0900	0.0584	0.0414
bcc-Nb	Ring	-0.0016	0.0082	0.0082	0.0148	0.0307
bcc-Nb	Cage	0.0029	0.0029	0.0134	0.0191	0.0296
hcp-Ti	Nuclei	-0.0016	0.0082	0.0082	-0.0065	0.0335
hcp-Ti	Bond1	0.0029	0.0029	0.0134	-8.074E-5	0.0311
hcp-Ti	Bond2	0.0029	0.0029	0.0134	-0.0062	0.0335
NaCl	Bond1	-2.291E-3	-1.158E-3	1.537E-2	1.192E-2	4.630E-3
NaCl	Bond2	-1.098E-2	-1.097E-2	7.881E-2	5.686E-2	1.180E-2
NaCl	Ring	-2.207E-3	4.412E-3	1.103E-2	1.324E-2	4.270E-3
NaCl	Cage	1.520E-3	1.520E-3	1.520E-3	4.561E-3	1.877E-3
KCl	Bond	-8.756E-03	-8.755E-03	5.886E-02	4.135E-02	1.139E-02
KCl	Ring	-9.270E-04	2.892E-04	6.398E-03	5.760E-03	2.146E-03
KCl	Cage	6.080E-04	6.080E-04	6.080E-04	1.824E-03	7.640E-04
Graphene	Bond	-2.821E-04	-2.810E-04	4.757E-03	4.194E-03	1.307E-03
Diamond-C	Bond	-4.731E-1	-4.731E-1	3.796E-1	-5.667E-1	2.404E-1
Diamond-Si	Bond	-7.280E-2	-7.280E-2	2.156E-2	-1.240E-1	8.340E-2
Diamond-Si-HSE	Bond	-7.747E-2	-7.747E-2	1.714E-2	-1.378E-1	8.6857E-2
fcc-Ti	Bond	-2.493E-03	-2.493E-03	1.750E-03	-3.092E-03	2.971E-02
fcc-Zr	Bond	-8.591E-04	-8.591E-04	6.080E-04	-1.110E-03	2.640E-02
fcc-Al	Bond	-1.045E-2	-2.570E-03	1.313E-02	1.147E-4	3.007E-2
fcc-Cu	Bond	-2.077E-02	-1.516E-02	1.002E-01	6.423E-02	3.824E-02
fcc-Au	Bond	-2.014E-02	-1.991E-02	1.148E-01	7.472E-02	3.708E-02
bcc-Mo	Bond	-0.0225	-0.0223	0.0796	0.035	0.050
bcc-Nb	Bond	-0.0158	-0.0158	0.0900	0.0584	0.0414
hcp-Ti	Bond1	0.0029	0.0029	0.0134	-8.074E-5	0.0311
hcp-Ti	Bond2	0.0029	0.0029	0.0134	-0.0062	0.0335
NaCl	Bond1	-2.291E-3	-1.158E-3	1.537E-2	1.192E-2	4.630E-3
NaCl	Bond2	-1.098E-2	-1.097E-2	7.881E-2	5.686E-2	1.180E-2
KCl	Bond	-8.756E-03	-8.755E-03	5.886E-02	4.135E-02	1.139E-02

TABLE XIII: The charge density (in electrons per Bohr^3), laplacian of charge density (in electrons per Bohr^5) at bonding critical points, shear modulus (in GPa), bulk modulus (in GPa), G/B and Poisson's ratio for fcc and bcc metals.

	ρ_b	$\triangle\rho$	θ	$< tan(\theta) >$	G	B	G/B	ν
fcc-Au	3.708E-2	7.472E-2	22.67	0.4177	24	185	0.1301	0.4376
fcc-Pt	5.185E-2	9.207E-2	24.35	0.4526	40	247	0.1620	0.4231
fcc-Pd	4.034E-2	7.732E-2	23.45	0.4338	40	166	0.2391	0.3893
fcc-Cu	3.824E-2	6.423E-2	22.95	0.4235	39	156	0.2499	0.3847
fcc-Al	3.007E-2	1.147E-4	35.15	0.7040	26	79	0.3319	0.3506
fcc-Ir	6.300E-2	8.789E-2	25.90	0.4857	218	348	0.6279	0.2404
bcc-Nb	4.140E-2	5.844E-2	22.72	0.4188	24	174	0.1368	0.4346
bcc-V	4.291E-2	6.023E-2	21.22	0.3884	41	184	0.2251	0.3953
bcc-Ta	4.792E-2	8.588E-2	21.61	0.3963	64	196	0.3262	0.3529
bcc-Mo	5.423E-2	7.932E-2	24.67	0.4595	125	265	0.4729	0.2958
bcc-W	6.054E-2	7.371E-1	24.10	0.4474	151	305	0.4955	0.2874
bcc-Cr	5.570E-2	7.866E-2	24.53	0.4564	137	256	0.5330	0.2737
Diamond-Si	8.340E-2	-1.240E-2	61.45	1.8476	63	89	0.7038	0.2150
Diamond	2.404E-1	-5.667E-1	48.15	1.1164	519	434	1.195	0.073
SiC	1.185E-01	3.001E-2	34.04	0.676	187	212	0.8803	0.1597
ZnS	6.809E-02	8.202E-02	28.99	0.554	32	70	0.4562	0.3020

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