Supplementary Material

Valence electron concentration as an indicator for mechanical properties in rocksalt structure nitrides, carbides and carbonitrides

Karthik Balasubramanian, Sanjay V. Khare and Daniel Gall

This supplementary document provides the numerical values of the calculated mechanical properties of binary nitrides (Table 1) and carbides (Table 2). The tables include Poisson's ratio v, Pugh's ratio k, elastic constants C_{11} and C_{12} and C_{44}, bulk modulus B, isotropic elastic modulus E, Tian's Hardness H, Cauchy pressure p_C, and a column that indicates if the compound is mechanically stable. The numbers in parenthesis are C_{44} values for magnetic phases. The hyphen "-" denotes values that have not been calculated and/or are not defined because of mechanical instability which is either due to $C_{44} < 0$ or $C_{12} > C_{11}$ in accordance to the Born-Huang criterion[1,2] for mechanical stability of crystal structures.

References:

[1] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices Oxford Classic Texts in the Physical Sciences* (Clarendon Press: Oxford, 1988).

[2] F. Mouhat and F. Coudert, Phys. Rev. B **90**, 224104 (2014).

Table 1: Mechanical properties rock-salt structure nitrides

Phase	VEC	v	k	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	E (GPa)	H (GPa)	p_C (GPa)	Mech. Stable
TiN	9	0.22	0.69	590	169	164	309	463	25	5	Yes
ZrN	9	0.25	0.59	546	164	126	291	403	19	38	Yes
HfN	9	0.24	0.63	602	163	120	309	392	20	43	Yes
VN	10	0.28	0.5	623	251	122	375	406	15	129	Yes
NbN	10	0.32	0.41	639	164	78	322	335	10	86	Yes
TaN	10	0.33	0.36	719	194	59	369	319	8	135	Yes
CrN	11	0.44	0.14	582	270	8 (126)	373	45	2	262	Yes
MoN	11	-	-	582	248	-40	359	-55	-	288	No
WN	11	-	-	680	202	-86	361	-285	-	288	No
MnN	12	-	-	-	-	-9 (122)	-	-	-	-	No
TcN	12	-	-	-	-	-161	-	-	-	-	No
ReN	12	-	-	-	-	-275	-	-	-	-	No
FeN	13	-	-	-	-	-44 (69)	-	-	-	-	No
RuN	13	-	-	-	-	-149	-	-	-	-	No
OsN	13	-	-	-	-	-239	-	-	-	-	No
CoN	14	0.38	0.27	510	230	55	320	220	4	175	Yes
RhN	14	-	-	-	-	-43	-	-	-	-	No
IrN	14	-	-	-	-	-128	-	-	-	-	No
NiN	15	0.36	0.29	368	214	80	265	215	5	134	Yes
PdN	15	0.39	0.23	301	185	48	224	143	3	137	Yes
PtN	15	0.44	0.12	264	223	34	237	79	1	189	Yes
CuN	16	0.37	0.28	305	176	61	219	170	4	115	Yes
AgN	16	0.40	0.22	233	135	30	168	102	2	130	Yes
AuN	16	0.42	0.16	231	162	26	185	83	1	136	Yes
ZnN	17	0.34	0.33	245	134	59	171	155	5	75	Yes
CdN	17	0.35	0.32	211	109	43	143	124	4	66	Yes
HgN	17	0.43	0.19	165	132	36	143	74	1	96	Yes

Table 2: Mechanical properties of rock-salt structure carbides

Phase	VEC	ν	k	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	E (GPa)	H (GPa)	p_C (GPa)	Mech. Stable
TiC	8	0.21	0.71	509	146	168	267	431	24	-22	Yes
ZrC	8	0.19	0.77	468	123	152	238	444	27	-29	Yes
HfC	8	0.20	0.74	520	133	172	262	395	24	-39	Yes
VC	9	0.21	0.7	648	170	189	329	520	27	-19	Yes
NbC	9	0.22	0.68	666	117	171	300	504	26	-54	Yes
TaC	9	0.22	0.68	722	157	176	345	533	26	-19	Yes
CrC	10	0.29	0.47	645	177	132 (89)	333	413	14	45	Yes
MoC	10	0.29	0.47	659	226	116	370	407	14	110	Yes
WC	10	0.29	0.46	741	222	122	395	445	14	100	Yes
MnC	11	0.36	0.3	501	269	101 (100)	346	289	7	168	Yes
TcC	11	-	-	-	-	-48	-	-	-	-	No
ReC	11	-	-	-	-	-80	-	-	-	-	No
FeC	12	0.41	0.19	566	282	79	377	275	5	203	Yes
RuC	12	0.44	0.12	509	239	12	329	40	1	237	Yes
OsC	12	-	-	-	-	-87	-	-	-	-	No
CoC	13	0.45	0.1	543	205	28	318	177	3	177	Yes
RhC	13	-	-	-	-	-40	-	-	-	-	No
IrC	13	-	-	-	-	-129	-	-	-	-	No
NiC	14	0.42	0.16	316	242	50	267	125	2	192	Yes
PdC	14	0.39	0.22	287	182	43	217	130	2	139	Yes
PtC	14	-	-	277	297	48	290	-	-	249	No
CuC	15	0.42	0.15	252	172	27	199	90	1	145	Yes
AgC	15	0.46	0.29	181	120	31	140	86	2	89	Yes
AuC	15	-	-	161	191	35	181	-	-	156	No
ZnC	16	0.42	0.17	220	143	23	169	80	1	120	Yes
CdC	16	0.4	0.21	166	92	19	117	69	2	73	Yes
HgC	16	0.38	0.23	143	98	24	113	65	2	74	Yes