Anısotropy of Some Haxagonal Systems

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Abstract:

The norm of elastic constant tensor and the norms of the irreducible parts of the elastic constants of some hexagonal systems (Apatite Fluor apatite, Hydroxyapatite, Beryl, Beryllium, Beryllium oxide, Biotite, Cadmium, Cadmium selenide, Cadmium sulfide, Cadmium telluride, Cesium copper chloride, Calcium-magnesium, Cancrinite, Cerium fluoride, Cobalt, Cobalt nickel, Co – 32 wt % Ni, Copper chloride, Dunite, Dysprosium, Erbium, Gadolinium, Gadolinium-yttrium, Gd – 40 at % Y, Gallium selenide, Graphite, Hafnium, Holmium, Indium bismuth, Indium selenide, Lead germinate vanadate, Lithium iodate, Lithium iodate, Yttrium, Zinc oxide (Zincite), Zinc selenide,and Zinc telluride) are calculated. The relation of the scalar parts norm and the other parts norms and the anisotropy of the materials are presented. The norm ratios are used as a criterion to present the anisotropy degree of the properties of these materials.

Key Words: Norm, Anisotropy, Elastic Constant, Irreducible, and hexagonal systems.

1 – Introduction:

The hexagonal system has four crystallographic axes consisting of three equal horizontal, or equilateral axes at 120 degrees to each other, as well as one vertical axis which is perpendicular to the other three. The decomposition procedure and the decomposition of elastic constant tensor (Elastic constant tensor can be decomposed into two scalar parts, two deviator parts and one nonor part) is given in [1,2,3,4], also the definition of norm concept and the norm ratios and the relationship between the anisotropy and the norm ratios are given in [1,2,3,4]. As the ratio N_s / N (Norm of the scalar part of the elastic constant tensor/Norm of the elastic constant tensor) becomes close to one the material becomes more isotropic, and as the sum of the ratios N_d / N (Norm of the deviator part of the elastic constant tensor/Norm of the elastic constant tensor) and N_n / N (Norm of the nonor part of the elastic constant tensor/Norm of the elastic constant tensor) becomes close to one the material becomes more anisotropic as explained in [1,2,3,4].

2 – Calculations:

The elastic constants of Hexagonal Systems Materials are given in the following table, [5].

Table 1. Elastic constants in GPa

Material	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}
Apatite Fluor apatite $Ca_{10}(PO_4)_6F_2$	139	178	44.3	45	56
Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$	139.9	179.5	36.2	12.9	69.0
Beryl, $Be_2Al_2Si_6O_{18}$	290	257	67.7	107	83
Material	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}

Beryllium , Be	292	349	163	24	6
Beryllium oxide, (piezoel), BeO	470	494	153	168	119
Biotite $K(Mg,Fe)_3AlSi_3O_{10}(OH,F)_2$	186	54	5.8	32	12
Cadmium, Cd	116	50.9	19.6	42	41
Cadmium selenide, (piezoel), CdSe	74.1	84.3	13.4	45.2	38.9
Cadmium sulfide, (piezoel), CdS	87.0	94.1	14.9	54.6	47.5
Cadmium telluride, (piezoel), CdTe	62.2	68.9	11.6	35.9	29.1
Cesium copper chloride (piezoel), $CsCuCl_3$	29.0	46.6	5.49	11.3	10.3
Calcium-magnesium $CaMg_3$	56.2	61.6	18.0	15.9	15
Cancrinite (piezoel), $(Na_2Ca)_4(AlSiO_4)_6CO_3.nH_2O$	52	83	24	2	12
Cerium fluoride, CeF_3	180	225	34.2	88	64
Cobalt, Co	295	335	71.0	159	111
Cobalt nickel Co – 32 wt % Ni	326	358	74.0	161	95
Copper chloride, CuCl	52.5	61.6	7.0	41.3	32.2
Dunite	198	238	67	76	96
Dysprosium, Dy	74.0	78.6	24.3	25.5	21.8
Erbium, Er	84.1	84.7	27.4	29.4	22.6
Gadolinium, Gd	66.7	71.9	20.1	25.0	21.3
Gadolinium-yttrium Gd – 40 at % Y	67.9	72.6	22.5	25.1	16.2
Gallium selenide (piezoel), GaSe	111	35.3	10.2	33	12
Graphite, C	1060	36.5	4	180	15
Hafnium, Hf	181	197	55.7	77	66
Holmium, Ho	76.5	79.6	25.9	25.6	21.0
Indium bismuth, In_2Bi	49.2	54.1	9.66	39.6	29.0
Indium selenide, InSe	118	38.2	11.7	47.5	32
Lead germinate vanadate $Pb_5(GeO_4)(VO_4)_2$	71	84	17	21	33
Lead silicate vanadate $Pb_5(SiO_4)(VO_4)_2$	77	92	21	25	36

Material	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}

Lithium iodate (piezoel) $LiIO3$	81.2	52.9	17.8	31.8	9.2
Yttrium, Y	77.9	76.9	24.3	29.2	20
Zinc oxide (Zincite) (piezoel), ZnO	209	218	44.1	120	104
Zinc selenide, ZnSe	107	116	25.0	45	35
Zinc telluride, ZnTe	86	93	20.2	37	30

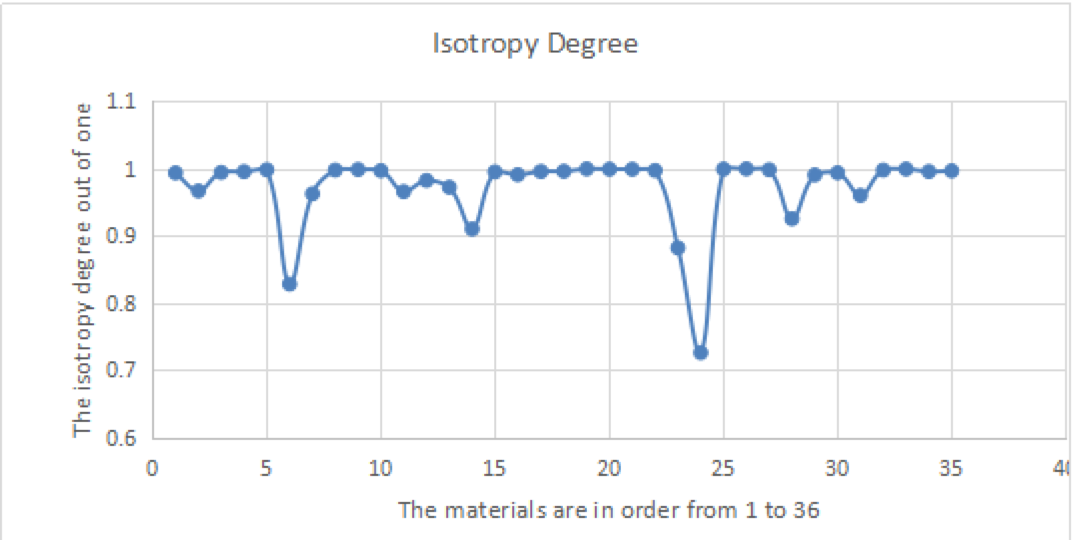
By using table 1, the decomposition of the elastic constant tensor and the norm concept we can calculate the norms and the norm ratios of the given materials as in the following table.

Table 2. The norms and norm ratios (the anisotropy degree)

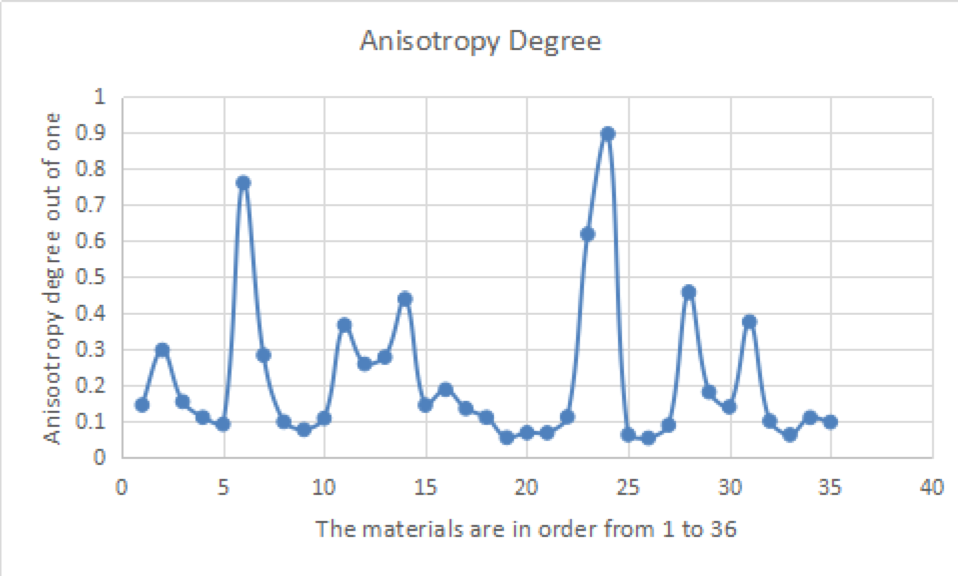
Material	N_s	N_d	N_n	N	N_s / N	N_d / N	N_n / N	Sum of 7th and 8th columns
Apatite Fluor apatite $Ca_{10}(PO_4)_6F_2$	300.3863	33.43556	10.68602	302.4303	0.993242	0.110556	0.035334	0.14589
Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$	299.055	78.27699	14.06865	309.4497	0.966409	0.252955	0.045463	0.298418
Beryl, $Be_2Al_2Si_6O_{18}$	536.9017	41.44993	42.3597	540.1629	0.993963	0.076736	0.07842	0.155156
Beryllium , Be	604.7319	58.88834	8.840953	607.6567	0.995187	0.096911	0.014549	0.11146
Beryllium oxide, (piezoel), BeO	917.5332	41.10415	43.82038	919.4982	0.997863	0.044703	0.047657	0.09236
Biotite $K(Mg,Fe)_3AlSi_3O_{10}(OH,F)_2$	227.867	135.3358	74.11025	275.1935	0.828025	0.491784	0.269302	0.761086
Cadmium, Cd	196.6168	55.56432	2.49853	204.3326	0.962239	0.271931	0.012228	0.284159
Cadmium selenide, (piezoel), CdSe	167.6308	6.327031	10.37851	168.0709	0.997381	0.037645	0.061751	0.099396
Cadmium sulfide, (piezoel), CdS	197.4217	5.107657	10.18632	197.7503	0.998338	0.025829	0.051511	0.07734
Cadmium telluride,	135.2464	4.59444	10.18632	135.7072	0.996604	0.033856	0.075061	0.108917

(piezoel), CdTe								
Cesium copper chloride (piezoel), $CsCuCl_3$	63.28701	11.41405	12.70022	65.55014	0.965475	0.174127	0.193748	0.367875
Calcium-magnesium $CaMg_3$	100.5101	10.11704	16.45186	102.3489	0.982034	0.098849	0.160743	0.259592
Cancrinite (piezoel), $(Na_2Ca)_4(AlSiO_4)_6CO_3.nH_2O$	115.7857	27.43403	5.765839	119.131	0.971919	0.230284	0.048399	0.278683
Cerium fluoride, CeF_3	289.0439	131.5104	8.264369	317.6628	0.909908	0.413994	0.026016	0.44001
Cobalt, Co	619.3554	42.89665	47.66427	622.6662	0.994683	0.068892	0.076549	0.145441
Cobalt nickel Co – 32 wt % Ni	644.0702	46.5475	76.10907	650.2197	0.990542	0.071587	0.117051	0.188638
Copper chloride, CuCl	128.7497	9.246621	8.341247	129.3505	0.995355	0.071485	0.064486	0.135971
Dunite	443.0747	40.34747	9.225342	445.0036	0.995665	0.090668	0.020731	0.111399
Dysprosium, Dy	147.3096	3.616671	4.535793	147.4238	0.999225	0.024532	0.030767	0.055299
Erbium, Er	163.6616	5.901553	5.38145	163.8563	0.998811	0.036017	0.032842	0.068859
Gadolinium, Gd	133.8473	3.198517	5.996472	134.0197	0.998713	0.023866	0.044743	0.068609
Gadolinium-yttrium Gd – 40 at % Y	132.7145	8.074449	6.957446	133.1419	0.996791	0.060645	0.052256	0.112901
Gallium selenide (piezoel), GaSe	149.4059	73.47677	31.32772	169.4178	0.881878	0.433702	0.184914	0.618616
Graphite, C	1125.582	986.3977	403.8009	**1550.151**	**0.726111**	0.636323	0.260491	**0.896814**
Hafnium, Hf	374.9283	14.79342	8.917831	375.326	0.99894	0.039415	0.02376	0.063175
Holmium, Ho	150.7527	4.12977	4.036087	150.8633	**0.999267**	0.027374	0.026753	**0.054127**
Indium bismuth, In_2Bi	131.3914	6.713308	5.127753	131.6627	0.99794	0.050989	0.038946	0.089935
Indium selenide, InSe	181.8634	72.56688	17.45127	196.5828	0.925124	0.369142	0.088773	0.457915

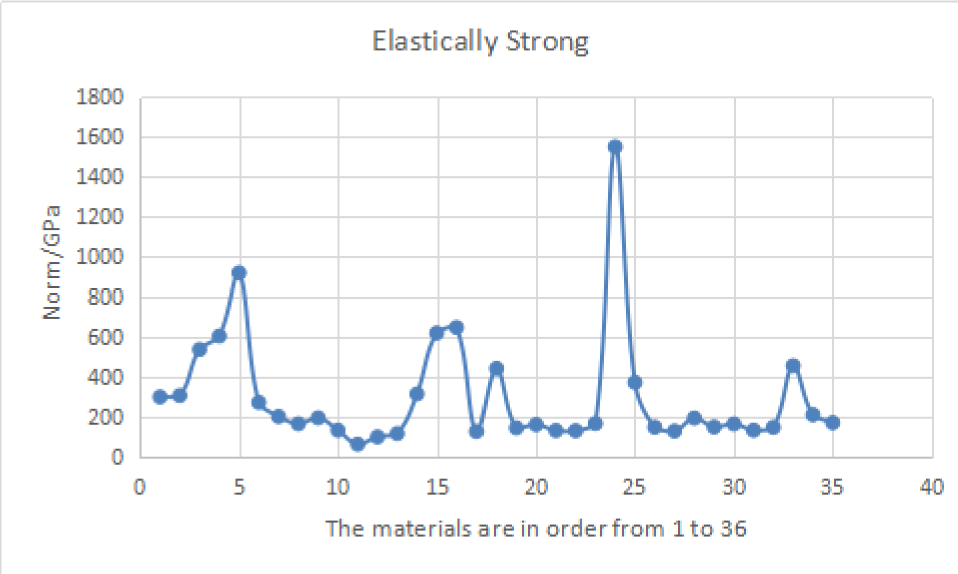
Lead germinate vanadate $Pb_5(GeO_4)(VO_4)_2$	150.5311	19.5789	8.072174	152.0136	0.990248	0.128797	0.053102	0.181899
Lead silicate vanadate $Pb_5(SiO_4)(VO_4)_2$	166.1418	18.49729	4.99706	167.243	0.993416	0.110601	0.029879	0.14048
Lithium iodate (piezoel) $LiIO_3$	130.1032	33.95166	17.10532	135.5439	0.95986	0.250485	0.126198	0.376683
Yttrium, Y	149.8293	8.478225	6.765251	150.2214	0.99739	0.056438	0.045035	0.101473
Zinc oxide (Zincite) (piezoel), ZnO	458.0924	12.58058	16.37498	458.5576	0.998986	0.027435	0.03571	0.063145
Zinc selenide, ZnSe	212.3666	3.297082	20.37263	213.367	0.995311	0.015453	0.095482	0.110935
Zinc telluride, ZnTe	172.7437	2.377703	14.68367	173.383	0.996313	0.013714	0.084689	0.098403



Graph 1. The Isotropy Degree of the Given Materials.



Graph 2. The Anisotropy Degree of the Given Materials.



Graph 3. The Elastically Strong of the Given Materials.

3 - Results and Conclusion:

From table 2 and the Graphs (Graph 1 to Graph 3), and analyzing the ratio N_s / N we can conclude that Holmium, Ho is the most isotropic material with highest value of N_s / N (0.999267) and lowest sum value of N_d / N and N_n / N (0.054227), and Graphite, C is the most anisotropic material with highest sum value of N_d / N and N_n / N (0.896814) and with lowest value of N_s / N (0.726111), because for isotropic material N_s / N = 1, and N_d / N = 0 and N_n / N = 0. Which means that as values of N_d / N and N_n / N increase the anisotropy increases. And also the elastically strongest material is Graphite, C, which has the highest value of. N (1550.151).

4 – References:

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