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Some Physical Properties of Different Compositions of Alums

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Abstract

The norm of elastic constant tensor and the norms of the irreducible parts of the elastic constants of different compositions of alums (cubic systems) are calculated. The relation of the scalar parts norms and the other parts norms and the anisotropy of these alums are characterized. The norm ratios are used to study the isotropy and anisotropy of these alums.

Key words: Alums, Deuterated Alums, Isotropy, Norm, Anisotropy, Elastic Constants.

1. Introduction

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 [1-4], also the definition of norm concept and the norm ratios and the relationship between the anisotropy and the norm ratios are given in [1-5]. 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 then 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 then the material becomes more anisotropic as explained in [1-5]. We planned to study the isotropy of the alums for different compositions because when the properties of a material vary with different crystallographic orientations, the material is said to be anisotropic. Alternately, when the properties of a material are the same in all directions, the material is said to be isotropic.

2. Experimental

2.1. Data and Calculations

The elastic constants and calculations were presented in table 1-2.

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Table 1. Elastic constants (GPa) [6].

Composition[a]	C_{11}	C_{44}	C_{12}
$C(NH_2)_3VS$	35.1	5.2	22.9
CsAlS	31.15	8.39	15.39
CsAlSe	26.08	7.42	11.78
CsCrS	30.7	8.5	14.8
CsFeS	30.38	8.41	14.48
CsGaS	30.69	8.16	15.33
CsGaSe	25.30	7.56	11.3
CsInS	29.57	8.16	14.07
CsTiS	30.0	8.4	15.0
CsVS	30.4	8.0	16.0
KAlS	24.9	8.49	10.4
KAlSe	23.30	7.75	9.7
KCrS	23.8	7.49	10.0
KFeS	22.62	8.21	8.86
KGaS	23.56	8.49	9.94
KVS	26.7	7.85	13.0
NaAlS	35.14	7.7	23.02
NH_3CH_3AlS	29.71	5.84	17.32
NH_3CH_3AlSe	27.36	5.43	16.08
NH_3CH_3FeS	28.75	5.76	16.61
NH_3CH_3GaS	28.98	5.62	16.86
NH_3CH_3InS	27.03	5.54	15.51
NH_3CH_3VS	28.0	5.6	16.6
NH_3NH_2AlS	26.21	5.63	17.75
NH_3OHAlS	24.16	6.49	17.74
NH_3OHGaS	23.6	6.6	16.0
NH_4AlS	25.1	8.06	10.7
NH_4AlSe	23.84	7.52	10.40
NH_4CrS	24.9	8.0	10.7
NH_4FeS	24.13	8.02	10.23
NH_4GaS	23.95	8.05	10.29
NH_4GaSe	22.68	7.58	9.68
NH_4InS	23.51	7.85	10.11
NH_4VS	27.2	7.35	14.1
RbAlS	25.35	8.44	10.33
RbAlSe	24.26	7.78	9.96
RbCrS	24.7	8.6	10.3
RbFeS	24.5	8.5	9.9
RbGaS	24.50	8.53	9.96
RbGaSe	23.13	7.80	9.35
RbInS	23.66	8.26	9.54

RbVS	28.6	8.4	13.4
TlAlS	27.7	8.31	12.6
TlAlSe	23.50	7.33	10.46
TlGaS	24.59	8.3	11.09
TlInS	23.0	8.0	10.3
TlVS	28.5	7.8	14.4
Deuterated Alums			
CsAlS	31.18	8.55	15.36
KAlS	24.59	8.56	9.95
ND_3CD_3AlS	29.66	5.82	17.2
TlAlS	25.42	8.17	11.24

[a]Alums have the general formula $XY^*(ZO_4)_2.12H_2O$, where X is a monovalent atom or radical, Y is a tervalent atom and Z is S or Se. The composition in the above table is expressed as XYZ.

By using table 1 and the decomposition of the elastic constant tensor, the norms and the norm ratios are calculated as given in table 2.

Table 2. The norms and norm ratios.

Composition[a]	N_s	N_d	N_n	N	N_s/N	N_d/N	N_n/N
$C(NH_2)_3VS$	82.975	0	1.650	82.991	0.9998	0	0.01988
CsAlS	67.620	0	0.935	67.626	0.999904	0	0.01382
CsAlSe	55.247	0	0.495	55.249	0.99996	0	0.008958
CsCrS	66.259	0	1.008	66.266	0.99988	0	0.015214
CsFeS	65.311	0	0.843	65.317	0.999917	0	0.012909
CsGaS	66.800	0	0.8798	66.805	0.999913	0	0.01317
CsGaSe	53.725	0	1.02650	53.735	0.999818	0	0.019103
CsInS	63.512	0	0.75154	63.516	0.99993	0	0.011832
CsTiS	65.659	0	1.64973	65.679	0.999684	0	0.025118
CsVS	67.399	0	1.46642	67.415	0.999763	0	0.021752
KAlS	52.834	0	2.27296	52.883	0.999076	0	0.042981
KAlSe	49.201	0	1.74138	49.232	0.999374	0	0.035371
KCrS	49.972	0	1.08149	49.984	0.999766	0	0.021637
KFeS	47.705	0	2.43793	47.767	0.998697	0	0.051037
KGaS	50.590	0	3.07949	50.684	0.998152	0	0.060759
KVS	58.205	0	1.83303	58.234	0.999504	0	0.031477
NaAlS	**84.475**	**0**	**3.00617**	**84.528**	**0.999367**	**0**	**0.035564**
NH_3CH_3AlS	67.339	0	0.65073	67.342	0.999953	0	0.009663
NH_3CH_3AlSe	62.266	0	0.38494	62.267	0.999981	0	0.006182
NH_3CH_3FeS	64.970	0	0.56824	64.973	0.999962	0	0.008746
NH_3CH_3GaS	65.581	0	0.80653	65.586	0.999924	0	0.012297
NH_3CH_3InS	60.977	0	0.40327	60.979	0.999978	0	0.006613
NH_3CH_3VS	**63.995**	**0**	**0.18330**	**63.995**	**0.999996**	**0**	**0.002864**
NH_3NH_2AlS	63.960	0	2.56624	64.011	0.999196	0	0.04009
NH_3OHAlS	**62.063**	**0**	**6.01234**	**62.354**	**0.99534**	**0**	**0.096423**
NH_3OHGaS	58.495	0	5.13248	58.720	0.996173	0	0.087406

NH_4AlS	53.077	0	1.57641	53.100	0.999559	0	0.029687
NH_4AlSe	50.626	0	1.46642	50.647	0.999581	0	0.028954
NH_4CrS	52.780	0	1.64973	52.806	0.999512	0	0.031241
NH_4FeS	51.208	0	1.96134	51.246	0.999267	0	0.038273
NH_4GaS	51.107	0	2.23630	51.156	0.999044	0	0.043715
NH_4GaSe	48.264	0	1.97967	48.304	0.99916	0	0.040983
NH_4InS	50.130	0	2.10798	50.175	0.999117	0	0.042013
NH_4VS	60.107	0	1.46642	60.124	0.999703	0	0.02439
RbAlS	53.225	0	1.70472	53.253	0.999487	0	0.032012
RbAlSe	51.920	0	2.70372	51.99	0.998647	0	0.052005
RbCrS	52.566	0	2.56624	52.628	0.99881	0	0.048762
RbFeS	51.672	0	2.19964	51.719	0.999095	0	0.042531
RbGaS	51.785	0	2.30962	51.837	0.999007	0	0.044556
RbGaSe	48.559	0	1.66806	48.588	0.999411	0	0.034331
RbInS	49.925	0	2.19964	49.974	0.999031	0	0.044016
RbVS	61.541	0	1.46642	61.559	0.999716	0	0.023822
TlAlS	59.190	0	1.39310	59.206	0.999723	0	0.02353
TlAlSe	50.130	0	1.48475	50.152	0.999562	0	0.029605
TlGaS	53.256	0	2.84120	53.332	0.99858	0	0.053274
TlInS	49.936	0	3.0245	50.027	0.998171	0	0.060457
TlVS	62.466	0	1.37477	62.481	0.999758	0	0.022003
Deuterated Alums							
CsAlS	**67.737**	**0**	**1.17314**	**67.7472**	**0.99985**	**0**	**0.017316**
KAlS	**51.9102**	**0**	**2.27296**	**51.9599**	**0.999043**	**0**	**0.043744**
ND_3CD_3AlS	**67.0640**	**0**	**0.75154**	**67.0682**	**0.999937**	**0**	**0.011206**
TlAlS	54.342	0	1.97967	54.3785	0.999337	0	0.036406

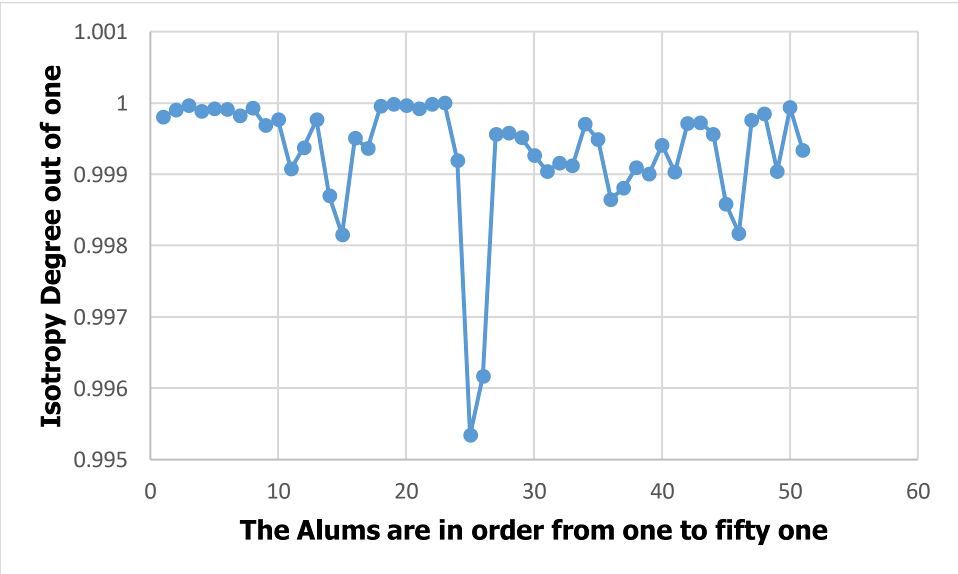

Figure 1. Isotropy degree.

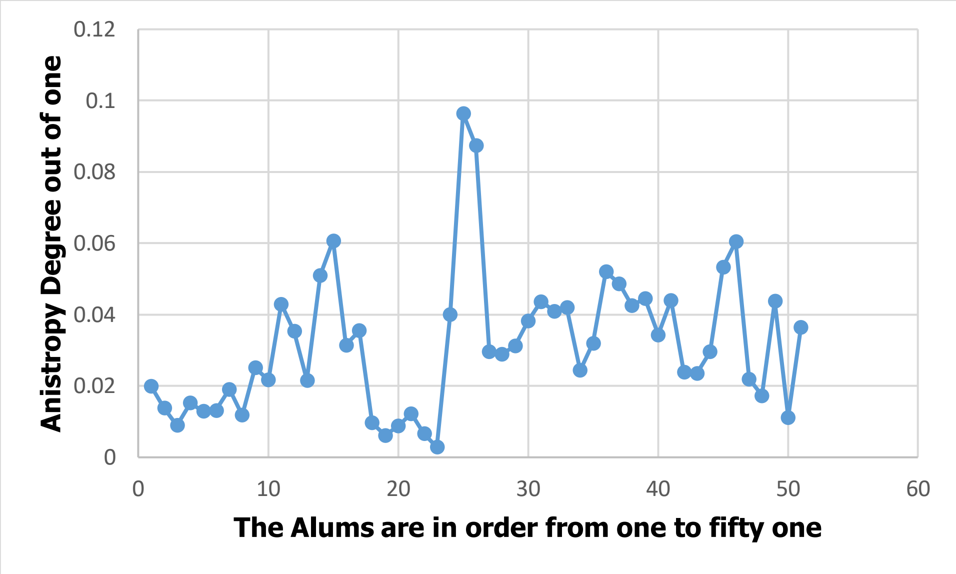

Figure 2. Anisotropy degree.

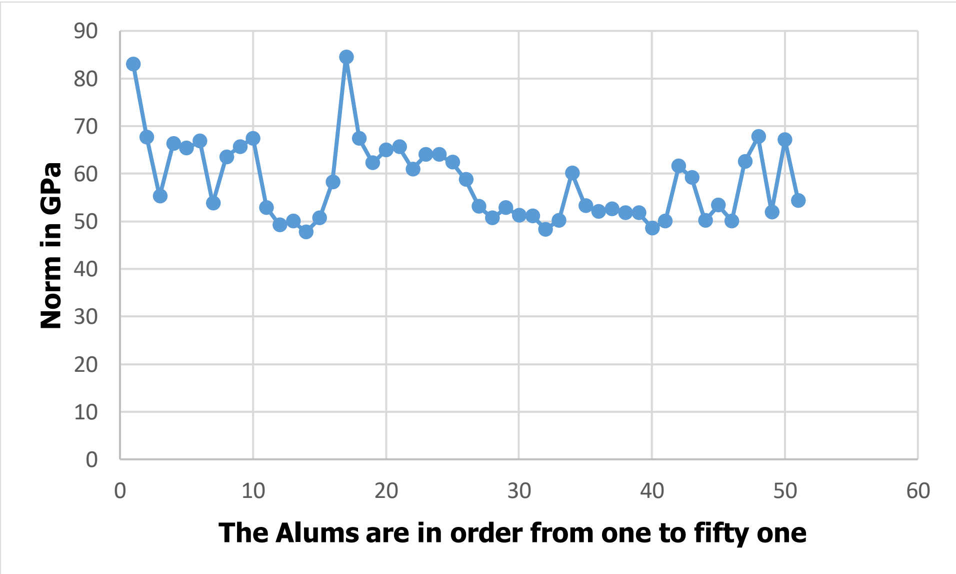

Figure 3. Elastically srong.

3. Results and Conclusion

From table 2 and the Figures (Figure 1-3) and analyzing the ratio ***N_s/N,*** we can conclude that **NH_3CH_3VS** is the most isotropic composition alum with highest value of ***N_s*** **/N** (**0.999996**) and lowest value of ***N_n*/N** (**0.002864**) and **NH_3OHAlS** is the most anisotropic composition alum with highest value of ***N_n*/N** (**0.096423**) and with lowest value of ***N_s*** **/N** (**0.99534**), because for isotropic material ***N_s*** **/N = 1** and ***N_n*** **/N = 0**. Which means that as the value of ***N_n*** **/N** increases the anisotropy increases. And also the elastically strongest composition alum is **NaAlS**, which has the highest value of **N** (**84.475**). And for Deuterated Alums, **ND_3CD_3AlS** is the most isotropic composition alum with highest value of ***N_s*/N** (**0.999937**) and lowest value of ***N_n*** **/N** (**0.011206**) and **KAlS** is the most anisotropic composition alum with highest value of ***N_n*/N** (**0.043744**) and with lowest value of ***N_s*/N** (**0.999043**) and also the elastically strongest composition alum is **CsAlS**, which has the highest value of **N** (**67.737**). In general we can say that alums are highly isotropic because of the value of ***N_s*/N** is very close to one for all compositions.

4. Conflicts of Interest

The author(s) report(s) no conflict(s) of interest(s). The author along are responsible for content and writing of the paper.

5. Acknowledgements

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