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Some properties of alkali halides

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ABSTRACT

The norm of elastic constant tensor and the norms of the irreducible parts of the elastic constants of Alkali Halides are calculated. The relation of the scalar parts norm and the other parts norms and the anisotropy of these compounds are presented. The norm ratios are used to study anisotropy of these compounds.

Key words: Alkali Halides , Isotropy, Norm, Anisotropy, and Elastic Constants.

INTRODUCTION

The decomposition procedure and the decomposition of elastic constant tensor is given in [1,2,3] and in the appendix, 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] and in the appendix. As the ratio N_s/N becomes close to one the material becomes more isotropic, and as the ratio N_n/N becomes close to one the material becomes more anisotropic as explained in [1,2,3] and in the appendix.

CALCULATIONS

Table 1, Elastic Constants (GPa), [4]

Cubic System	C_{11}	C_{44}	C_{12}
LiF	112.0	63.5	46.0
LiCl	49.1	24.8	22.0
LiBr	39.4	19.1	18.9
LiI	28.5	13.5	14.0
NaF	97.0	28.1	24.2
NaCl	49.1	12.8	12.8
NaBr	40.0	9.96	10.6
NaI	30.2	7.36	9.0
KF	65.0	12.5	15.0
KCl	40.5	6.27	6.9
KBr	34.5	5.10	5.5
KI	27.4	3.70	4.3
RbF	55.2	9.25	14.0
RbCl	36.4	4.7	6.3
RbBr	31.5	3.82	4.8
RbI	25.6	2.79	3.7

By using table 1 and the decomposition of the elastic constant tensor, we have calculated the norms and the norm ratios as is shown in table 2.

Table 2, the norms and norm ratios

Cubic System	N_s	N_d	N_n	N	$\frac{N_s}{N}$	$\frac{N_d}{N}$	$\frac{N_n}{N}$
LiF	265.640	0	55.907	271.459	0.9786	0	0.2060
LiCl	114.894	0	20.622	116.730	0.9843	0	0.1767
LiBr	92.861	0	16.222	94.267	0.9851	0	0.1721
LiI	67.255	0	11.456	68.224	0.9858	0	0.1679
NaF	178.887	0	15.214	179.533	0.9964	0	0.0847
NaCl	89.640	0	9.807	90.175	0.9941	0	0.1088
NaBr	72.744	0	8.689	73.261	0.9929	0	0.1186
NaI	56.102	0	5.939	56.415	0.9944	0	0.1053
KF	111.327	0	22.913	113.661	0.9795	0	0.2016
KCl	64.476	0	19.302	67.303	0.9580	0	0.2868
KBr	54.164	0	17.23	56.839	0.9529	0	0.3031
KI	42.552	0	14.389	44.919	0.9473	0	0.3203
RbF	94.942	0	20.805	97.195	0.9768	0	0.2141
RbCl	57.102	0	18.972	60.171	0.9490	0	0.3153
RbBr	48.269	0	17.469	51.333	0.9403	0	0.3403
RbI	38.6285	0	14.958	41.423	0.9325	0	0.3611

CONCLUSION

We can conclude from table 2, by considering the ratio $\frac{N_s}{N}$ that the compounds of sodium have the highest ratios, so we can say that the compounds of sodium (**NaF, NaI, NaCl,** and **NaBr**) are the most isotropic compounds among these compounds and also we can notice that NaF is the most isotropic compound which has the highest ratio $\frac{N_s}{N}$ and the lowest ratio $\frac{N_n}{N}$, and we can notice that **RbI** has the lowest ratio $\frac{N_s}{N}$ and the highest ratio $\frac{N_n}{N}$, so we can say that **RbI** is the most anisotropic compound among these compounds, and by considering the value of N we found that this value is the highest in the case of **LiF** (271.459) so we can say that **LiF** elastically is strongest, and this value is the lowest in the case of **RbI** (41.423) so we can say that **RbI** is elastically the least strong.

APPENDIX

ELASTIC CONSTANT TENSOR DECOMPOSITION

The constitutive relation characterizing linear anisotropic solids is the generalized Hook's law (Nye, 1964):

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}\,,\ \varepsilon_{ij} = S_{ijkl}\sigma_{kl} \qquad (1)$$

Where σ_{ij} and ε_{kl} are the symmetric second rank stress and strain tensors, respectively C_{ijkl} is the fourth-rank elastic stiffness tensor (here after we call it elastic constant tensor) and S_{ijkl} is the elastic compliance tensor.

There are three index symmetry restrictions on these tensors. These conditions are:

$$C_{ijkl} = C_{jikl}\,,\ C_{ijkl} = C_{ijlk}\,,\ C_{ijkl} = C_{klij} \qquad (2)$$

Which the first equality comes from the symmetry of stress tensor, the second one from the symmetry of strain tensor, and the third one is due to the presence of a deformation potential. In general, a fourth-rank tensor has 81 elements. The index symmetry conditions (2) reduce this number to 21. Consequently, for most asymmetric materials (triclinic symmetry) the elastic constant tensor has 21 independent components.

Elastic compliance tensor S_{ijkl} possesses the same symmetry properties as the elastic constant tensor C_{ijkl} and their connection is given by [1,2,3,5,6,7,8].

$$C_{ijkl}S_{klmn} = \frac{1}{2}\left(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right) \tag{3}$$

Where δ_{ij} is the Kronecker delta. The Einstein summation convention over repeated indices is used and indices run from 1 to 3 unless otherwise stated.

By applying the symmetry conditions (2) to the decomposition results obtained for a general fourth-rank tensor, the following reduction spectrum for the elastic constant tensor is obtained. It contains two scalars, two deviators, and one-nonor parts:

$$C_{ijkl} = C_{ijkl}^{(0;1)} + C_{ijkl}^{(0;2)} + C_{ijkl}^{(2;1)} + C_{ijkl}^{(2;2)} + C_{ijkl}^{(4;1)} \tag{4}$$

Where:

$$C_{ijkl}^{(0;1)} = \frac{1}{9}\delta_{ij}\delta_{kl}C_{ppqq}, \tag{5}$$

$$C_{ijkl}^{(0;2)} = \frac{1}{90}\left(3\delta_{ik}\delta_{jl} + 3\delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}\right)\left(3C_{pqpq} - C_{ppqq}\right) \tag{6}$$

$$C_{ijkl}^{(2;1)} = \frac{1}{5}\left(\delta_{ik}C_{jplp} + \delta_{jk}C_{iplp} + \delta_{il}C_{jpkp} + \delta_{jl}C_{ipkp}\right)$$
$$-\frac{2}{15}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)C_{pqpq} \tag{7}$$

$$C_{ijkl}^{(2;2)} = \frac{1}{7}\delta_{ij}\left(5C_{klpp} - 4C_{kplp}\right) + \frac{1}{7}\delta_{kl}\left(5C_{ijpp} - 4C_{ipjp}\right)$$
$$-\frac{2}{35}\delta_{ik}\left(5C_{jlpp} - 4C_{jplp}\right) - \frac{2}{35}\delta_{jl}\left(5C_{ikpp} - 4C_{ipkp}\right)$$
$$-\frac{2}{35}\delta_{il}\left(5C_{jkpp} - 4C_{iplp}\right) - \frac{2}{35}\delta_{jk}\left(5C_{ilpp} - 4C_{iplp}\right)$$
$$+\frac{2}{105}\left(2\delta_{jk}\delta_{il} + 2\delta_{ik}\delta_{jl} - 5\delta_{ij}\delta_{kl}\right)\left(5C_{ppqq} - 4C_{pqpq}\right) \tag{8}$$

$$C_{ijkl}^{(4;1)} = \frac{1}{3}(C_{ijkl} + C_{ikjl} + C_{iljk})$$
$$-\frac{1}{21}[\delta_{ij}\left(C_{klpp} + 2C_{kplp}\right) + \delta_{ik}\left(C_{jlpp} + 2C_{jplp}\right)$$
$$+\delta_{il}\left(C_{jkpp} + 2C_{jpkp}\right) + \delta_{jk}\left(C_{ilpp} + 2C_{iplp}\right) + \delta_{jl}\left(C_{ikpp} + 2C_{ipkp}\right)$$
$$+\delta_{kl}\left(C_{ijpp} + 2C_{ipjp}\right) +]$$

$$\frac{1}{105}\left[\left(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\left(C_{ppqq}+2C_{pqpq}\right)\right] \tag{9}$$

These parts are orthonormal to each other. Using Voigt's notation [5] for C_{ijkl}, can be expressed in 6 by 6 reduced matrix notation, where the matrix coefficients $c_{\mu\lambda}$ are connected with the tensor components C_{ijkl} by the recalculation rules:

$$c_{\mu\lambda}=C_{ijkl}\,; \quad (ij\leftrightarrow\mu=1,....,6, kl\leftrightarrow\lambda=1,....,6)$$

That is: $11\leftrightarrow 1, 22\leftrightarrow 2, 33\leftrightarrow 3, 23=32\leftrightarrow 4\; 31=13\leftrightarrow 5, 12=21\leftrightarrow 6$.

THE NORM CONCEPT

Generalizing the concept of the modulus of a vector, norm of a Cartesian tensor (or the modulus of a tensor) is defined as the square root of the contracted product over all indices with itself:

$$N=\|T\|=\left\{T_{ijkl..........}.T_{ijkl..........}\right\}^{1/2}$$

Denoting rank-n Cartesian $T_{ijkl..........}$, by T_n, the square of the norm is expressed as [7].

$$N^2=\|T\|^2=\sum_{j,q}\left\|T^{(j;q)}\right\|^2=\sum_{(n)}T_{(n)}T_{(n)}=\sum_{(n),j,q}T_{(n)}^{(j;q)}T_{(n)}^{(j,q)}$$

This definition is consistent with the reduction of the tensor in tensor in Cartesian formulation when all the irreducible parts are embedded in the original rank-n tensor space.

Since the norm of a Cartesian tensor is an invariant quantity, we suggest the following:

Rule1. The norm of a Cartesian tensor may be used as a criterion for representing and comparing the overall effect of a certain property of the same or different symmetry. The larger the norm value, the more effective the property is. It is known that the anisotropy of the materials, i.e., the symmetry group of the material and the anisotropy of the measured property depicted in the same materials may be quite different. Obviously, the property, tensor must show, at least, the symmetry of the material. For example, a property, which is measured in a material, can almost be isotropic but the material symmetry group itself may have very few symmetry elements. We know that, for isotropic materials, the elastic compliance tensor has two irreducible parts, i.e., two scalar parts, so the norm of the elastic compliance tensor for isotropic materials depends only on the norm of the scalar parts, i.e. $N=N_s$, Hence, the ratio $\frac{N_s}{N}=1$ for isotropic materials. For anisotropic materials, the elastic constant tensor additionally contains two deviator parts and one nonor part, so we can define $\frac{N_d}{N}$ for the deviator irreducible parts and $\frac{N_n}{N}$ for nonor parts. Generalizing this to irreducible tensors up to rank four, we can define the following norm ratios: $\frac{N_s}{N}$ for scalar parts, $\frac{N_v}{N}$ for vector parts, $\frac{N_d}{N}$ for deviator parts, $\frac{N_{sc}}{N}$ for septor parts, and $\frac{N_n}{N}$ for nonor parts. Norm ratios of different irreducible parts represent the anisotropy of that particular irreducible part they can also be used to assess the anisotropy degree of a material property as a whole, we suggest the following two more rules:

Rule 2. When N_s is dominating among norms of irreducible parts: the closer the norm ratio $\frac{N_s}{N}$ is to one, the closer the material property is isotropic.

Rule3. When N_s is not dominating or not present, norms of the other irreducible parts can be used as a criterion. But in this case the situation is reverse; the larger the norm ratio value we have, the more anisotropic the material property is.

The square of the norm of the elastic stiffness tensor (elastic constant tensor) C_{mn} is:

$$\|N\|^2 = \sum_{mn}\left(C_{mn}^{(0;1)}\right)^2 + \sum_{mn}\left(C_{mn}^{(0;2)}\right)^2 + 2\sum_{mn}\left(C_{mn}^{(0;1)}.C_{mn}^{(0;2)}\right) + \sum_{mn}\left(C_{mn}^{(2;1)}\right)^2 + \sum\left(C_{mn}^{(2;2)}\right)^2 + 2\sum_{mn}\left(C_{mn}^{(2;1)}.C_{mn}^{(2;2)}\right) + \sum_{mn}\left(C_{mn}^{(4;1)}\right)^2 \tag{10}$$

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