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Physical properties of Sodium Niobate ($NaNbO_3$) at different phase transitions

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Abstract: *Sodium Niobate ($NaNbO_3$) solid single crystal, it shows different phase transitions Cubic to Tetragonal, Tetragonal to Orthorhombic and Orthorhombic to Rhombohedral with various temperatures. In this paper, physical properties of $NaNbO_3$ at different phase transitions are calculated.*
Key words: *Sodium Niobate, Ferro-elastic, Ferro-electric, Magneto-electric Polarizability, Tensor pairs, domain pairs, double coset decomposition,*

I. INTRODUCTION

The various ABO_3 compounds Na_{1-x} K_x Nbo_3 (NKN) solid Solutions have received a special attention to its relatively dielectric constant, high electromechanical coupling coefficients especially near the equimolar composition. These properties make this material desirable for certain solid an ultrasonic delay line application, which requires the use of thin – section transducers.

$NaNbO_3$ and $KNbo_3$ are peroviskite materials of antiferroelectric and Ferroelectrics respectively. Among these peroviskite materials $NaNbO_3$ has maximal phase transistions and existing sequence structural phase –transistions cubic to Tetrangonal, Tetragonal to Orthorhombic and Orthorhombic to Rhombohedral at distinct temperatures has been widely investigated by various experimental techniques such as electric conductivity and dielectric permitting, X-Ray diffraction, Raman Spectroscopy, Inelastic neutron scattering etc.. At certain temperatures between 480^0C to 373^0C and 373^0C to -100^0C the $NaNbO_3$ exhibits antiferroelectric properties. Below -100^0 C a Rhombohedral ferroelectric form occurs in NaNbO3. However, Observed that NaNbO3 may exist in two other phases between the room temperature and 280^0 C when subjected to an electric field or droped with 2 percent (mol) of potassium content (K, $KNbo_3$ is ferroelectric with constant temperature 435^0 C) at Sodium site, above room temperature at 200 and 420^0C respectively (I. Lefkowitzk, et.al) This phase must be ferroelectric and undergoes phase transistions completely different from earlier phase heating. All these indicate structural phase transition states of NaNbO3 in (Na, k) Nbo_3 or NKN solid solutions.

Also, $kNbo_3$ is a widely studied peroviskite material for ferroelectric phase transitions at different temperatures. Temperatures at above curie point 428^0C, $KNbO_3$ is Cubic (C) phase and shows Para electric property. The temperature cooled down KNbo3 becomes ferroelectric and Transforms to Tetragonal (T), orthorhombic (O) and Rhombohedral (R) at 428^0C, 215^0C -63^0C respectively. Thus, the dielectric properties of NKN crystals were considered by using group theory techniques. So, here Ferro-electric, Ferro-elastic and Magneto-Electric polarizability domain pairs by using coset and double coset decomposition respectively for the NaNbO3 solid solution are calculated. While considering Ferro –electric and Ferro-elastic properties only ordinary point group m3m is considered as prototypic point group, since they are non Magnetic properties. In case of magneto electric polarizability grey group $m3m1^1$ is taken prototypic point group.

Ferro-Elastic Domain pairs for $NaNbO_3$ in the Ferroic State m3m F 4/mmm:

Consider the ferroic species m3m F 4/mmm , Where m3m is a prototypic point group and 4/mmm is Ferroic point group. The numbers of distinct domain elements is 3. The coset decomposition of m3m with respect to the group 4/mmm is given by
$G = m3m = E(4/mmm) + C^+_{31}\ (4/mmm) + C^-_{31}\ (4/mmm)$
The coset elements are E, C_{31}^+ and C_{31}^-

Table 1.1: Domains pairs for the ferroic species m3m F 4/ mmm

Domain pairs	
E	(xx + yy)/2, zz)
C_{31}^+	(zz + xx)/2, yy)
C_{31}^-	(yy + zz)/2, xx)

Ferro-Elastic Domain pairs for $NaNbO_3$ in the Ferroic State m3m F mmm:

Consider the ferroic species m3m F mmm , where m3m is a prototypic point group and mmm is a ferroic point group .The number of distinct domain pair classes is 3. The coset decomposition of m3m with respect to the group mmm is given by

$G = m3m = E (mmm) + C_{2a} (mmm) + C_{31}^{+} (mmm) + C_{4y}^{--} (mmm) + C_{31}^{-} (mmm) + \sigma_{df} (mmm)$

The coset elements are E, C_{2a}, C_{31}^{+} , C_{4y}^{--} , C_{31}^{-} and σ_{df}

Table 1.2 domain pairs for ferroic species m3m F mmm

Domain pairs	
(E, C_{2a})	(xx, yy, zz) (yy, xx, zz)
$(C_{31}^{+}, C_{4y}^{--})$	(zz ,xx, yy) (zz ,yy, xx)
$(C_{31}^{-}, \sigma_{df})$	(yy, zz ,xx,) (xx ,zz ,yy)

Ferro-Elastic Domain pairs for $NaNbO_3$ in the Ferroic State m3m F 3m:

Consider the ferroic species m3m F 3m, where m3m is prototypic point group and 3m is a ferroic point group.the number of distinct domains is 8 and distinct domain pair classes are 4.The coset decompastion of m3m with respect to the group 3m is given by

$G = m3m\ F\ 3m = E(3m) + C_{2x}(3m) + C_{32}^{+}(3m) + S_{61}^{-}(3m) + S_{34}^{--}(3m) + S_{64}^{+}(3m) + C_{2d}(3m) + C_{4x}^{+}(3m)$

The coset elements are E, C_{2x}, C_{32}^{+}, S_{61}^{--}, S_{34}^{--}, S_{64}^{+}, C_{2d} & C_{4x}^{+}

Table 1.3: Domains pairs for the ferroic species

Domain pairs	
(E, C_{2x})	(xx + yy + zz/3 , xx+ yy + zz/3)
$(C_{32}^{+}, S_{61}^{--})$	(+zz + xx+ yy /3 , +zz + xx+ yy/3)
$(S_{34}^{--}, S_{64}^{+})$	(yy + zz +xx/3 , yy +zz+ xx /3)
(C_{2d}, C_{4x}^{+})	(+xx + zz +yy /3 , xx +zz +yy /3)

II. (a) Ferro-Elastic Tensor pairs for $NaNbO_3$ in the Ferroic State m3m F 4/mmm:

Consider the ferroic species **m3m F 4/mmm**, where m3m is prototypic point group and **4/mmm** is a ferroic point group and the stabilizer is **4/mmm**. The numbers of distinct tensor pair classes is 2.The double coset decompastion of m3m with respect to the stabilizer is **4/mmm** is given by

$G = m3m = (4/mmm)\ E\ (4/mmm) + (4/mmm)\ C_{31}^{+}(4/mmm)$

Table 1.4: Tensor pairs for the ferroic species

Double Coset Representatives	**Tensor pairs**
(E,E)	((xx+yy)/2,zz) ((xx+yy/2),zz)
(E, C_{31}^{+})	((xx+yy)/2,zz) ((zz+xx/2),yy)

(b) Ferro-Elastic Tensor pairs for $NaNbO_3$ in the Ferroic State m3m F mmm:

Consider the ferroic species **m3m F mmm**, where m3m is prototypic point group and **mmm** is a ferroic point group and the stabilizer is **mmm**. The numbers of distinct tensor pair classes is 6.The double coset decomposition of m3m with respect to the stabilizer is **mmm** is given by

$G = m3m = (mmm)\ E\ (mmm) + (mmm)\ C_{31}^{+}(mmm) + (mmm)\ C_{31}^{--}(mmm) + (mmm)\ C_{2a}(mmm) + (mmm)\ C_{4y}^{--}(mmm) + (mmm)\ C_{4x}^{+}(mmm)$

Table 1.5: Domains pairs for the ferroic species

Double Coset Representatives	**Tensor pairs**
(E,E)	(xx, yy, zz) (xx, yy, zz)
(E, C_{31}^{+})	(xx, yy, zz) (zz ,xx, yy)
(E, C_{31}^{--})	(xx, yy, zz) (yy , zz, xx)
(E, C_{2a})	(xx, yy, zz) (yy , xx, zz)
(E, C_{4y}^{--})	(xx, yy, zz) (zz , yy xx)
(E, C_{4x}^{+})	(xx, yy, zz) (xx ,zz , yy)

(c)Ferro-Elastic Tensor pairs for $NaNbO_3$ in the Ferroic State m3m F 3m:

Consider the ferroic species **m3m F 3m**, where m3m is prototypic point group and **3m** is a ferroic point group and the stabilizer is **3m**. The number of distinct tensor pair classes is 4.The double coset decomposition of m3m with respect to the stabilizer **3m** is given by

$G = m3m\ F\ 3m = (3m)\ E\ (3m) + (3m)\ C_{2x}\ (3m) + (3m)\ S_{61}^{-}(3m) + (3m)\ C_{4x}^{+}\ (3m)$

Table 1.6: Tensor pairs for the ferroic species

Double Coset Representatives	**Tensor pairs**
(E,E)	(xx+ yy+ zz)/3 (xx+ yy+ zz)/3
(E, S^{--}_{61})	(xx+ yy+ zz)/3 (zz +xx,+yy)/3
(E, C_{4x}^{+})	(xx+yy+zz)/3 (xx + zz +yy)/3
(E, C_{2x})	(xx+yy+zz)/3 (xx + yy +zz)/3

III. Ferro-Electric domain pairs for $NaNbO_3$ in the Ferroic State m3m F 3m:

Consider the ferroic species **m3m F 3m**, where m3m is prototypic point group and **3m** is a ferroic point group.The number of distinct domain pair classes is 4.The coset decomposition of m3m with respect to the group **3m** is given by

$G = m3m = E\ (3m) + C_{2x}\ (3m) + C_{32}^{+}(3m) + S_{61}^{--}(3m) + C_{34}^{--}(3m) + S_{64}^{+}(3m) + C_{2d}(3m) + C_{4x}^{+}(3m)$

The coset elements are E, C_{2x}, C_{32}^{+}, S_{61}^{--}, C_{34}^{--}, S_{64}^{+}, C_{2d} and C_{4x}^{+}

Table 1.7: Domains pairs for the ferroic species m3m F 3m

Domain pairs	
(E, C_{2x})	(x + y + z)/3 ,(x- y – z)/3
(C_{32}^{+}, S_{61}^{--})	(-z + x - y) /3 , (-z – x- y)/3
(C_{34}^{--}, S_{64}^{+})	(-y - z +x)/3 , (y +z- x /3)
(C_{2d} ,C_{4x}^{+})	(x + z +y) /3 , (x -z +y /3)

(b) Ferro- Electric Tensor pairs for $NaNbO_3$ in the Ferroic State m3m F 3m:

Consider the ferroic species **m3m F 3m**, where m3m is prototypic point group and **3m** is a ferroic point group and the stabilizer is **3m** .The number of distinct tensor pair classes is 4.The double coset decomposition of m3m with respect to the stabilizer **3m** is given by

$G = m3m = (3m)\ E\ (3m) + (3m)\ C_{2x}\ (3m) + (3m)\ S_{61}^{-}(3m) + (3m)\ C_{4x}^{+}\ (3m)$

Double coset Representatives	**Tensor pairs**
(E,E)	(x+y +z)/3, (x+y+z)/3
(E, C_{2x})	(x+y +z)/3, (x-y-z)/3
(E, S_{61}^{--})	(x+y +z)/3, (-z-x-y)/3
(E, C_{4x}^{+})	(x+y +z)/3, (x-z+y)/3

IV. The magento-Electric polarizability Domain pairs for $NaNbO_3$ in the Ferroic State $m3m_1^1$ F 3m

Consider the ferroic species **$m3m_1^1$ F 3m**, where **$m3m_1^1$** is prototypic point group and **3m** is a ferroic point group. The number of distinct domain pairs is 8.The coset decomposition of **$m3m_1^1$** with respect to the group **3m** is given by

G = **$m3m_1^1$** $= E\,(3m) + R_2\,(3m) + C_{2x}\,(3m) + R_2\,C_{2x}\,(3m) + C_{32}^{+}(3m) + R_2C_{32}^{+}(3m) + S_{61}^{--}(3m) + R_2S_{61}^{--}(3m) + C_{34}^{--}(3m) + R_2C_{34}^{--}(3m) + S_{64}^{+}(3m) + R_2S_{64}^{+}(3m) + C_{2d}(3m) + R_2C_{2d}(3m) + C_{4x}^{+}(3m) + R_2C_{4x}^{+}(3m)$

The coset elements are E, R_2 ,C_{2x} ,R_2 C_{2x} ,C_{32}^{+} ,$R_2C_{32}^{+}$, S_{61}^{--},,$R_2S_{61}^{--}$, C_{34}^{-},$R_2C_{34}^{--}$,S_{64}^{+},$R_2S_{64}^{+}$,C_{2d}, ,R_2C_{2d} and C_{4x}^{+},$R_2C_{4x}^{+}$

Double Coset Representatives	**Domain pairs**
(E, R_2)	$(xy^1+yz^1+zx^1+xz^1+zy^1+yx^1)/6$, $(-xy^1-yz^1-zx^1-xz^1-zy^1-yx^1)/6$
(C_{2x} ,R_2 C_{2x})	$(-xy^1+yz^1-zx^1-xz^1+zy^1-yx^1)/6$, $(xy^1-yz^1+zx^1+xz^1-zy^1+yx^1)/6$
(C_{32}^{+} ,$R_2C_{32}^{+}$)	$(-zx^1-xy^1+yz^1+zy^1-yx^1-xz^1)/6$, $(zx^1+xy^1-yz^1-zy^1+yx^1+xz^1)/6$
(S_{61}^{--},,$R_2S_{61}^{--}$)	$(zx^1-xy^1+yz^1+zy^1+yx^1+xz^1)/6$, $(-zx^1-xy^1-yz^1-zy^1-yx^1-xz^1)/6$
(C_{34}^{-},$R_2C_{34}^{--}$)	$(yz^1-zx^1-xy^1-yx^1-xz^1+zy^1)/6$, $(-yz^1+zx^1+xy^1+yx^1+xz^1-zy^1)/6$
(S_{64}^{+},$R_2S_{64}^{+}$)	$(yz^1-zx^1-xy^1-yx^1-xz^1+zy^1)/6$, $(-yz^1+zx^1+xy^1+yx^1+xz^1-zy^1)/6$
(C_{2d}, ,R_2C_{2d})	$(-xz^1+zy^1-yx^1-xy^1+yz^1-zx^1)/6$, $(xz^1-zy^1+yx^1+xy^1-yz^1+zx^1)/6$
(C_{4x}^{+},$R_2C_{4x}^{+}$)	$(-xz^1-zy^1+yx^1+xy^1-yz^1-zx^1)/6$, $(xz^1+zy^1-yx^1-xy^1+yz^1+zx^1)/6$

(b) The magento-Electric polarizability Tensor pairs for $NaNbO_3$ in the Ferroic State $m3m_1^1$ F 3m:

Consider the ferroic species **$m3m_1^1$ F 3m**, where **$m3m_1^1$** is prototypic point group and **3m** is a ferroic point group and the stabilizer is **m^13m^1**. The number of distinct tensor pair classes is 2.The double coset decomposition of **$m3m_1^1$** with respect to the stabilizer is **m^13m^1** is given by

$G = m3m_1^1 = (m^13m^{1)}\,E\,(m^13m^1) + (\,m^13m^1\,)\,R_2\,(m^13m^1)$

Double Coset Representatives	**Tensor pairs**
(E,E)	$(xy^1+yz^1+zx^1+zx^1+xz^1+zy^1+yx^1)/6$, $(xy^1+yz^1+zx^1+xz^1+zy^1+yx^1)/6$
(E, R_2)	$(xy^1+yz^1+zx^1+xz^1+zy^1+yx^1)/6$, $(-xy^1-yz^1-zx^1-xz^1-zy^1-yx^1)/6$

V. CONCLUSION

The Na $_{1-x}$ KxNbo$_3$ (NKN) solid Solutions of the $NaNbO_3$ anti ferroelectric and KNbo3 ferroelectric with a peroviskite Structure which exhibits various phase transitions is widely used in ceramic capacitors and microelectronic technologies. Now a day's niobates are creating a new trend in Nano-technology also.

Sodium Niobate ($NaNbO_3$) is a solid single crystal. Here Ferroelectric, Ferroelastic and Magneto electric polarizability properties of Sodium Niobate ($NaNbO_3$) are calculated in different phase transitions by using group theoretical techniques both domain pairs and tensor pairs are calculated for these ferroic properties. While considering Ferroelectric, Ferro elastic properties only ordinary point group is considered as prototypic point group. In the case of Magneto electric polarizability grey group is taken prototypic point group.

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