International Journal of Engineering Research and Development
e-ISSN: 2278-067X, **p**-ISSN : 2278-800X
Volume 5, Issue 4 (December 2012), PP. 47-51

Physical Properties of Sodium Nibate (Nanbo3) At Nano Structure

[1]M.Vijaya Laxmi, [2]S.Uma Devi
[1] PhD scholar, [2]Professor Department of Engineering Mathematics, Andhra University, Visakhapatnam

Abstract:- Change in Crystallographic Symmetry is canned by nanostructing materials Sodium Niobate (NaNbo3) Solid nano crystal has a nano structure $P2_1ma$ (C_{2v} point group). Crystal point group Symmetry analysis explains a deeper understanding of Phase-matching abilities of nano Crystal materials in Non-Linear optics. In this paper a brief account of group theoretical methods of the effect of symmetry on Physical properties of Sodium niobate (NaNbo3) in the nano state are calculated.

Keywords:- Sodium Niobate (NaNbo3), Grey Groups, Nano State, Tensor, Ferroic Point group,Tensor, Tensor pairs and Double coset decomposition.

I. INTRODUCTION

Sodium Niobate (NaNbo3), discovered by Matthias in 1949, is an Oxygen perovskite with the largest number of phase transitions (B.T.Mathias), NaNbo3 (Sodium Niobate) is the most complex cubic perovskite (R.Machado, 2000). The high temperature phase is simple prototype cubic structure as in the other ABO_3 Perovskites. Below 913k, Sodium Niobate (NaNbo3), exhibits at least six more phase transitions(R.Machado,2000)

The successive phases are cubic to tetragonal, tetragonal to orthorhombic and the final phase is Rhembohedral by various experimental techniques (S.K. Mishra)

$NaNbO_3$ is a solid nano single crystals, NaNbO3 is also used in enhancing non linear optical properties and find applications in hologram recording materials. High quality $NaNbO_3$ nano wires can be grown by hydro thermal method at low temperature and can be poled by an electric field at room temperature. NaNbO3 nano wires should be quite useful for the large scale Lead free piezo electric nano generator applications.

$NaNb_2O_6$ – H_2O nano wires successively transform into NaNbO3 nano wires by X ray diffraction measurement (Jong Hoon Jung , et al, 2011), NaNbO3 nanowires have several tens of µm in length and ~ 200nm in diameter , the NaNbO3 nanocube have 0.5 ~1.0µm in lengths. By X- ray diffraction and electron diffraction lattice parameters and symmetry of P21ma for both nano wires and nano cubes are obtained. NaNbO3 nano structures is cubical for nano generator application having a $p2_1ma$ (C_{2V}) ferro electric symmetry ratherthan Pbcm (D^{11}_{2h}) anti ferroelctric symmetry. The anti ferroelectric symmetry Pbcm symmetry is changed into ferro electric P21ma symmetry the applying electric field (Jong Hoon Jung , et al, 2011), especially the anti ferro electric Pcm symmetry in buck changes into the feerro electric $P2_1ma$ symmetry in sub micron size NaNbO3 (shiratori , et , al)

So Sodium Niobite NaNbO3 nano structures is P21ma (C22V obtained by perform the rietveld analysis for high resolution X- ray diffraction pattern (Jong Hoon Jung , et al, 2011),

Physical prosperities of substances generally express the relation between the two quantities. The transformation properties of the quantities involved in a physical relation the basis for the classification of crystal properties, thus distinguishing scalar- scalar relations scalar-vector relations, vector-vector relations and tensor –tensor relations and so on .Each of these relations requires a member of independent co-efficient connecting the components of the quantities involved, and without assuming any symmetry of the crystal, the number of independent co-efficient in the case of linear relations is the product of the number of independent coefficients of the quantities being related. In crystals with symmetry elements, this maximum number of coefficients will be reduced. Aizu[1] defined a ferroic crystal and its properties on the basis of orientation states and ferroic operation.

Aizu species characterization and schmids classification of species ensembles to include ferrotoroidic crystals by including the domain state distinguishability by spontaneous toroidal moment. A fourth type of primary ferroic crystals, a ferrotoroidic crystal, as been recently observed (van aken e.t.al,2007) similarly in the same manner the fourth types of primary and secondary ferroic physical properties are given by D.B.Litvin[3].Tensor pairs of Sodium Niobate (NaNbo3) at different phase transitions are calculated (S.Uma devi et.al) . In this paper this work is extended nano state ($P2_1ma$) of Sodium Niobate (NaNbo3) tensor properties are calculated.

The primary and secondary physical properties are given in Table.1

Where "V" denotes a polar vector, and "e" and "a" denotes zero rank tensors that change signs under spatial inversion and time inversion respectively

The first column gives serial number,the second column gives physical properties , the third and fourth columns give ferroic type and jahn notation.

S.No	Physical Property	Ferroictype	Jahn notation
1	Spontaneous polarization	Ferroelectric	V
2	Spontaneous Magnetization	Ferromagnetic	aev
3	Spontaneous Strain	Ferroelastic	[V2]
4	Spontaneous Toroidal moment	Ferrrotoroidic	av
5	Electric Susceptibility	Ferrobielectric	[V2]
6	Magnetic Susceptibility	Ferrobimagnetic	[V2]
7	Toroidic Susceptibility	Ferrobitoroidic	[V2]
8	Magnetoeletric Coefficient	Ferromagneto electric	aev2
9	Magneto toroidic Coefficient	Ferromagneto toroidic	ev^2
10	Electrotoroidic Coefficient	Ferroelectrotoroidic	av^2

Tensor properties of Sodium Niobate (NaNbo3) at nano structure in the ferroic state $m3m1^1Fmm2$, m3mFmm2: Sodium Niobate (NaNbo3) solid single nano crystal, has a nano structure $P2_1ma$ (point group C_{2v}). Here tensor properties of Sodium Niobate (NaNbo3) at nano structure are calculated .also tensor pairs of Sodium Niobate (NaNbo3) at different phase transition are calculated are calculated by (S.Uma devi e.t.al) , this work is extended to calculate tensor properties of Sodium Niobate (NaNbo3) in the nano state, by using double coset elements. Here for ordinary point group m3m is taken as prototypic point groups, in case of magntic point groups and grey group $m3m1^1$ is taken as prototypic point groups. Physical properties are given in table 2.

The first column gives serial number,the second column gives physical properties , the third column gives stabilizer,and final four columns gives tensor,tensor representatives and tensor pairs.

S. No	Physical Property	Stabilizer	Double Coset elements	Tensor	Tensor pair Representatives	Tensor Pairs
1	Spontaneous polarization(v)	4mm	E, C_{31}^+, C_{2a}	$\begin{pmatrix}0\\0\\T3\end{pmatrix}$	(E,E) (E, C_{31}^+) (E, C_{2a})	$\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}0\\0\\T3\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}T3\\0\\0\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}0\\0\\-T3\end{pmatrix}$
2	Spontaneous Magnetization	Does not Exhibit				
3	Spontaneous Toroidal moment (av)	4mm	E, C_{31}^+, C_{2a} $R_2, R_2C_{31}^+, R_2C_{2a}$	$\begin{pmatrix}0\\0\\T3\end{pmatrix}$	(E,E) (E, C_{31}^+) (E, C_{2a}) (E, R_2C_{2a}) $(E, R_2C_{31}^+)$ (E, R_2)	$\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}0\\0\\T3\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}T3\\0\\0\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}0\\0\\-T3\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}\begin{pmatrix}0\\0\\T3\end{pmatrix}$

						$\begin{pmatrix}0\\0\\T3\end{pmatrix}$ $\begin{pmatrix}T3\\0\\0\end{pmatrix}$ $\begin{pmatrix}0\\0\\T3\end{pmatrix}$ $\begin{pmatrix}0\\0\\-T3\end{pmatrix}$
4	(i)Spontaneou strain (ii)Electric Susceptibility (iii)Magnetic Susceptibility (iv)Toroidic Susceptibility	4/mmm	E, C_{31}^{+}	$\begin{pmatrix}0&0&0\\0&T22&0\\0&0&T33\end{pmatrix}$	(E,E) (E, C_{31}^{+})	$\begin{pmatrix}0&0&0\\0&T22&0\\0&0&T33\end{pmatrix}\begin{pmatrix}0&0&0\\0&T22&0\\0&0&T3\end{pmatrix}$ $\begin{pmatrix}0&0&0\\0&T22&0\\0&0&T33\end{pmatrix}\begin{pmatrix}0&0&0\\0&T11&0\\0&0&T2\end{pmatrix}$
5	Magnetoelectric Coefficient	mm2	E, C_{2x}, C_{2a}, C_{31}^{+}, C_{2c}, C_{2d}, C_{4z}^{+}, S_{61}^{+}, R_2, R_2C_{2x}, $R_2C_{31}^{+}$, R_2C_{2a}, R_2C_{2c}, R_2C_{2d}, $R_2C_{4z}^{+}$, $R_2S_{61}^{+}$	$\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}$	(E,E) (E, R_2) (E, C_{2x}) (E, R_2C_{2x}) (E, C_{31}^{+}) (E, $R_2C_{31}^{+}$) (E, C_{2a}) (E, R_2C_{2a}) (E, C_{2c}) (E, R_2C_{2c}) (E, C_{2d}) (E, R_2C_{2d}) (E, C_{4z}^{+}) (E, $R_2C_{4z}^{+}$) (E, S_{61}^{+}) (E, $R_2S_{61}^{+}$)	$\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T12\\T21&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T1\\-T21&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T1\\-T21&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T12\\T21&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T31\\T13&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T3\\-T13&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T21\\T12&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T2\\-T12&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T3\\-T23&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T32\\T23&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T1\\-T31&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T13\\T31&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&-T2\\-T12&0\\0&0\end{pmatrix}$ $\begin{pmatrix}0&T12&0\\T21&0&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&T21\\T12&0\\0&0\end{pmatrix}$

						$\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & T23 \\ T32 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & -T2 \\ -T32 & 0 \\ 0 & 0 \end{pmatrix}$
6	Electrotoroidic Coefficient	mmm	E, C_{2a}, C_{31}^+, C_{4x}^+, C_{31}^-, C_{2c}, R_2, $R_2C_{31}^+$, R_2C_{2a}, $R_2C_{4x}^+$, $R_2C_{31}^-$ R_2C_{2c}	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T3 \end{pmatrix}$	(E,E) (E, C_{31}^+) (E, C_{2a}) (E, C_{4x}^+) (E, C_{31}^-) (E, R_2E) (E, $R_2C_{31}^+$) (E, R_2C_{2a}) (E, $R_2C_{4x}^+$) (E, $R_2C_{31}^-$)	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T3 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & T11 & 0 \\ 0 & 0 & T2 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & T11 & 0 \\ 0 & 0 & T3 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & T33 & 0 \\ 0 & 0 & T2 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 & 0 \\ 0 & T33 & 0 \\ 0 & 0 & T1 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & -T22 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & -T11 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & -T11 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & -T33 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 & 0 \\ 0 & T22 & 0 \\ 0 & 0 & T33 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & -T33 \\ 0 & 0 \end{pmatrix}$
7	Magneto toroidic Coefficient	mm2	E, C_{2x}, C_{2a}, C_{31}^+, C_{2c}, C_{2d}, C_{4z}^+, S_{61}^+,	$\begin{pmatrix} 0 & T12 \\ T21 & 0 \\ 0 & 0 \end{pmatrix}$	(E,E) (E, C_{2x}) (E, C_{31}^+) (E, C_{2a}) (E, C_{2c}) (E, C_{2d}) (E, C_{4z}^+) (E, S_{61}^+)	$\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & T12 \\ T21 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & -T1 \\ -T21 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & T31 \\ T13 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & T21 \\ T12 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & -T3 \\ -T23 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & -T1 \\ -T31 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & -T2 \\ -T12 & 0 \\ 0 & 0 \end{pmatrix}$

						$\begin{pmatrix} 0 & T12 & 0 \\ T21 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & T23 \\ T32 & 0 \\ 0 & 0 \end{pmatrix}$

II. CONCLUSION

Sodium Niobate, (NaNbo3) Solid single Crystal, shows sequence of different phase transitions at different temperatures, by X-ray diffraction measurement sodium Niobate nano state is $P2_1ma$. Aizu defined a ferroic crystal and its properties on the basis of orientation states and Ferroic operations [1]. And this work is extended by D.B.Litvin. He introduced fourth types of primary and secondary physical properties. In this paper tensor properties of Sodium Niobate (NaNbo3) in the nano state for both primary and secondary physical properties, are calculated.

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