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Study of Refractive Index Profile near the Surface of YVO4 Waveguide using Point Dipole Approach

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Abstract : Yttrium Ortho Vanadate (YVO₄) is a positive uniaxial, wide transparency range optical fiber material with large birefringence. The variation of refractive indices near the surface of YVO_4 optical fibers is observed. The "Local" fields experienced by ions near the surface of fiber material are different from those in the interior. Using theoretical Point Dipole Approximation (PDA), one can calculate refractive index variation near the surface of the material. In thin films and optical waveguides, this variation can alter the propagation characteristics. The variation of ordinary and extraordinary refractive indices n_o and n_e from the surface to a depth of 71.2Å near the surface for Z-cut and X-cut YVO₄ waveguides are evaluated using PDA. For a Z-cut waveguide, n_o is found to increase from surface to the interior whereas n_e is found to decrease from surface to the interior. For an X-cut, Z-propagation waveguide, n_o is found to decrease from the surface to the interior whereas, n_e is found to increase from the surface to the interior. It is observed that the refractive indices n_o , and n_e variation and also the birefringence (dn= n_e - n_o) variation with depth near the surface for both the cases are quite opposite in nature.

IndexTerms - Point Diople Approximation, refractive index, birefriengence, YVO4 waveguide, thin film.

I. INTRODUCTION

Extensive research work has been carried out on rare earth Orthovanadate, as it is significant oxide in material science and technology (Baogeng Xie, 2020, Chinh, 2019 and Naveen, 2018). Particularly, Yttrium Orthovanadate (YVO₄) has immense applications in fields such as laser host material (Banal, 2014 and Huang, 2011) and polarizer (Chen, 2006 and Lagatsky, 2005). Because of its large birefringence ($\Delta n = 0.2225$ at 6328Å), it has high damage threshold, high conductivity, good mechanical properties and chemical stability (Shuai Wang ,2021, Huang, 2012 and Milev, 2007). It is also widely used as optical isolator and beam displacer (Tang, 2007 and Wang, 2009). The compound attracted many researchers for its large birefringence, non-linear coefficients, and effectively no infrared absorption from 2.5 to 15mm (Mey, 2012 and Messekine, 2010). It can be considered as the oldest laser host crystal for Nd⁺³ ions (Kaminskii, 1969 and O'Conner, 1966) and EU⁺³:YVO₄ acts as highly efficient red emitting phosphor. In the characterization of optical devices the Refractive Index is an important parameter and understanding of this from atomic point of view is very essential. Present day interest in every field is to assess the behavior of the sample at nano-scale. Hence the proposed work is aimed at calculating the Refractive Indices values at atomic level.

II. EXPRESSIONS FOR REFRACTIVE INDICES - A POINT DIPOLE APPROACH

In the Point Dipole Approach (PDA) method, the ions in YVO_4 waveguide are polarizable points that can accurately approximate the response of a continuum target in the bulk. Each ion can be treated as a point dipole oscillating under the electric field of the incident e.m. radiation. The sum of external field and the field due to all the oscillating dipoles around the ion represents the total field acting on each ion. The Clausius-Mossotti relation, eqn.(1)-eqn.(3), helps us to evaluate the electronic polarizabilities of ions at a given wavelength say 6328Å by using the refractive indices values from the experimental data (DeShazer, 1987).

$$\chi_{x} = \frac{P_{x}}{E_{x}} = \frac{\varepsilon_{x} - 1}{4\pi} = \frac{n_{x}^{2} - 1}{4\pi} = \frac{\sum_{j} N_{j} \alpha_{j} [1 + \sum_{i} D_{ij} \alpha_{i}]}{1 - \sum_{j} N_{j} \alpha_{j} [1 + \sum_{i} D_{ij} \alpha_{i}] K_{x}}$$
(1)

$$\frac{n_y^2 - 1}{4\pi} = \frac{\sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i]}{1 - \sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i] K_y}$$
(2)

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$$\frac{n_z^2 - 1}{4\pi} = \frac{\sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i]}{1 - \sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i] K_z}$$
(3)

where $\sum_{j} \sum_{i} D_{x_{ij}} = \sum_{j} \sum_{i} \frac{3x_i^2 - r_i^2}{r_i^5}$ is a measure of the lattice anisotropy factor or geometric anisotropy in the X-direction for

all the i^{th} ions with j^{th} ion at the center and $K_x = K_y = K_z = 4\pi/3$ is the depolarization factor for spherical cavity.

From eqn. (1) to eqn. (3) one can evaluate, electronic polarizabilities of ions by using the lattice anisotropy factors summations for various ions in the core of the YVO_4 waveguide along the cartesian axes. The lattice anisotropy factors cartesian components are calculated at a depth of 10 times of lattice constant 'a=7.12Å' inside the core of YVO_4 waveguide and are shown in Table 2.

As Refractive Index is due to the dipole moments of the ions which can be expressed in terms of the effective local fields at the site of the ions and the polarizability of the ions. The ions on the surface and near the surface have a different effective local field as compared to the ions well within the medium. This is because an ion near the surface sees a different environment when compared to an ion well within the lattice. There will be, consequently a variation in electrical field from ion to ion is observed as we move from the surface to the interior of the waveguide. Thus the geometric anisotropy factors $\sum_i \sum_i D_{ij}$'s would also vary from the surface to the interior and a gradation of refractive index n_o or n_e from the surface to interior results.

Let us consider a YVO₄ waveguide placed in an external electric field E_0 of the incident light wave. Each atom of the

waveguide becomes a dipole under the action of the electric field. Thus dipole moments could be attributed to these atoms and are treated as point dipoles at the appropriate lattice sites. The Lorentz fields are then evaluated at different lattice sites in the unit cell caused due to different atomic dipoles surrounding them by PDA method which is used so far by (Praveena, 1989, Ramesh, 1993, Ramesh, 1994, Manoher, 2015, Satyanarayan Reddy, 2016 and Suhasini, 2021).

III. CALCULATIONS

For the purpose of calculation, the X-cut and Z-cut waveguides are considered separately, with propagation directions coinciding with the normals to the faces cut. For an X-cut waveguide, the direction of propagation is chosen along X direction so that the electric vector of light oscillates in the YZ plane. For a Y-cut waveguide, the direction of propagation is chosen along Y direction so that the electric vector of light oscillates in the XZ plane. For a Z-cut waveguide, the direction of propagation is chosen along Y direction so that the electric vector of light oscillates in the XZ plane. For a Z-cut waveguide, the direction of propagation is chosen along Y direction so that the electric vector of light oscillates in the XZ plane. For a Z-cut waveguide, the direction of propagation is chosen along Z direction so that the electric vector of light oscillates in the XZ plane. For a Z-cut waveguide, the direction of propagation is chosen along z direction so that the electric vector of light oscillates in the XZ plane. For a Z-cut waveguide, the direction of propagation is chosen along z direction so that the electric vector of light oscillates in the XZ plane. Table 1 lists various cuts of a given waveguide along with cartesian propagation directions to know n_o or n_e .

For YVO₄ waveguide which is uniaxial (a=b=7.12Å and c=6.289Å), only two cuts are possible i.e. X-cut and Z-cut. Y-cut is same as X-cut. Only one optic axis is observed i.e along crystallographic c-axis. If light propagates along c-axis, the electric vibration is uniform in the XY plane. So n_e is observed along crystallographic c-axis or Cartesian Z-axis.

An iterative programme is written in C++ to calculate n_x , n_y and n_z and by using equation (1), equation (2) and equation (3) for the electric vector vibrating along the X, Y and Z axes by varying the values of polarizabilities α_i in small increments, one at a time within the range of their practically observed values. The local anisotropic factors ' $\Sigma_j \Sigma_i D_{ij}$'s' are calculated and given in Table 2 The polarizability values tuned to fit the calculated refractive indices with the experimental values (DeShazer, 1987) are shown in Table 3.

Table 1: n_o and n_e representation	tions along cartesian a	ixes for X, Y and Z-cu	t waveguides
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Crystal Axis Cartesian Axis	n_x	n_{y}	nz	Configuration Names
c-axis X-axis	n _e	no	no	<i>Y</i> -cut, <i>X</i> -propagation <i>Z</i> -cut, <i>X</i> -propagation
c-axis Y-axis	no	ne	no	X-cut, Y-propagation Z-cut, Y-propagation
c-axis Z-axis	no	no	ne	X-cut, Z-propagation Y-cut, Z-propagation

Table 2: Lattice Anisotropy Factors $\left(\sum_{j}\sum_{i} D_{X_{ij}} / \sum_{j}\sum_{i} D_{Z_{ij}}\right) \times 10^{-24}$ cm³ values obtained using PDA within the Core of YVO₄ Optical Waveguide at λ =6328Å along Cartesian *X* and *Z*-axes

Effect On \rightarrow Effect due to \downarrow	$\sum_{j} \sum_{i} D_{j}$	$x_{ij} = \sum_{j} \sum_{i} \frac{2}{j}$	$\frac{3x_i^2 - r_i^2}{r_i^5}$	$\sum_{j} \sum_{i} D_{Z_{ij}} = \sum_{j} \sum_{i} \frac{3z_{i}^{2} - r_{i}^{2}}{r_{i}^{5}}$		
· ·	Yj	\mathbf{V}_{j}	O_j	Y_j	V_j	Oj
Yi	0.042625	0.156712	0.016186	-0.085249	0.313424	0.032371
V_i	0.156712	0.042625	-0.344646	0.313424	-0.085249	0.689293
O_i	-0.016186	-0.344646	0.161745	0.032371	0.689293	0.323490

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Table 3: Electronic polarizability tuned values for various constituent ions of YVO_4 waveguide at λ =6328Å

Electronic Polarizability		Refractive Indices			$e (\Delta n = n_e - n_o)$
$\alpha \times 10^{-24} \text{cm}^3$	п	Calculated	Experimental	Calculated	Experimental
$\alpha_{Y} = 0.55$ $\alpha_{V} = 0.5515$ $\alpha_{O} = 2.1998$	$n_x = n_o$ $n_y = n_o$ $n_z = n_e$	1.9929 1.9929 2.2154	1.9929 1.9929 2.2154	0.2225	0.2225

I. VARIATION OF REFRACTIVE INDICES AND BIREFRINGENCE NEAR THE SURFACE OF A Z-CUT, X-**PROPAGATION YVO4 WAVEGUIDE**

Here the cartesian X-axis of the unit cell coincides with the Z-axis of the waveguide (See Table-1). To calculate the variation of the Refractive Indices near the surface, the waveguide is divided into regions of one-unit cell dimensions normal to the surface. A unit cell of YVO₄ touching the surface of the waveguide is considered. This unit cell is represented as 0th unit cell. The local field effects at the different lattice sites with this position of the sphere are evaluated. The centre is then shifted to 1st unit cell below the surface and local fields are evaluated. This procedure is continued until the radius of the sphere of influence is 71.2Å which corresponds to 10 times the lattice constant 'a'.

Table 4: Lattice Anisotropy Factors ($\sum_{j} \sum_{i} D_{X_{ij}} / \sum_{j} \sum_{i} D_{Z_{ij}}$) × 10⁻²⁴cm³ for Z-Cut, X-Propagation YVO₄ Waveguide at various Depths for λ =6328Å

	150				10.00		
Effect On \rightarrow			$3x^2 - r^2$	$\sum \sum 3z_i^2 - r_i^2$			
	$\sum_{j} \sum_{i} D_{j}$	$X_{ij} = \sum_{j} \sum_{i} -$	r ⁵	$\sum_{j} \sum_{i} D_{j}$	$z_{ij} = \sum_{j} \sum_{i} -$	r ⁵	
Effect due to \downarrow	V O	N 1	I_i		N.	I_i	
	Y _j			Y_j	Vj	Oj	
V	0.140860	o 256146	the Surface	(0A - 7.12A))	0.207251	
Y _i	-0.149860	-0.356146	-0.753163	0.001911	0.416929	0.397351	
V _i	-0.356146	-0.149860	-1.124412	0.416929	0.001911	1.088151	
Ui	-0.838662	-1.21/130	-2.961399	0.303985	0.912475	1./06319	
	1 st Unit	Cell below the	he Surface (7	.12A – 14.24	-A)		
Y_i	-0.120413	-0.319962	-0.653823	-0.003812	0.395080	0.351261	
Vi	-0.319962	-0.120413	-0.982470	0.395080	-0.003812	1.008274	
Oi	-0.684569	-1.013359	-2.773758	0.366561	1.023710	1.629409	
1	2 nd Unit	Cell below th	ne Surface (1-	4.24Å – 21.3	6Å)		
Yi	-0.090152	-0.289728	-0.533610	-0.018923	0.379981	0.291116	
Vi	-0.289728	-0.090152	-0.862147	0.379981	-0.018923	0.947998	
Oi	-0.563134	-0.891686	-2.290427	0.305928	0.962831	1.387509	
	3 rd Unit	Cell below th	e Surface (2	1.36Å – 28.4	8Å)		
Yi	-0.061489	-0.261095	-0.419970	-0.033229	0.365641	0.234283	
Vi	-0.261095	-0.061489	-0.748476	0.365641	-0.033229	0.891245	
Oi	-0.447611	-0.776116	-1.832146	0.248088	0.905026	1.158343	
	4 th Unit	Cell below th	e Surface (2)	8.48Å – 35.6	0Å)		
Yi	-0.035035	-0.234651	-0.315519	-0.046424	0.352350	0.182034	
Vi	-0.234651	-0.035035	-0.644047	0.352350	-0.046424	0.839012	
Oi	-0.340637	-0.669153	-1.409016	0.194594	0.851583	0.946919	
	5 th Unit	Cell below th	e Surface (3:	5.60Å – 42.72	2Å)	1	
Y _i	-0.011430	-0.211058	-0.222676	-0.058209	0.340580	0.135589	
Vi	-0.211058	-0.011430	-0.551222	0.340580	-0.058209	0.792583	
Oi	-0.244651	-0.573198	-1.031385	0.146591	0.803577	0.758232	
	6 th Unit	Cell below th	e Surface (42	2.72Å – 49.84	4Å)	I	
Yi	0.008711	-0.190918	-0.144046	-0.068283	0.330559	0.096218	
V_i	-0.190918	0.008711	-0.472591	0.330559	-0.068283	0.753257	
Oi	-0.162236	-0.490778	-0.709305	0.105306	0.762340	0.597197	
	7 th Unit	Cell below th	e Surface (49	9.84Å – 56.9	6Å)	1	
Yi	0.024735	-0.174848	-0.082097	-0.076290	0.322495	0.065327	
Vi	-0.174848	0.024735	-0.410740	0.322495	-0.076290	0.722352	
Oi	-0.095875	-0.424475	-0.452929	0.072197	0.729242	0.469107	
	8 th Unit	Cell below th	e Surface (5	6.96Å – 64.0	8Å)		
Yi	0.035988	-0.163532	-0.039315	-0.081927	0.316841	0.043935	
V_i	-0.163532	0.035988	-0.368100	0.316841	-0.081927	0.701010	
Oi	-0.048077	-0.376833	-0.272190	0.048320	0.705380	0.378715	
	9 th Unit	Cell below th	e Surface (64	4.08Å – 71.20	0Å)	1	
Yi	0.041857	-0.157515	-0.018422	-0.084863	0.313826	0.033489	
Vi	-0.157515	0.041857	-0.346994	0.313826	-0.084863	0.690464	
Oi	-0.021428	-0.350118	-0.177646	0.034989	0.692020	0.331458	

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	10 th Unit	Cell below the	he Surface (7	1.20Å – 78.3	32Å)		
Yi	0.042625	-0.156712	-0.016186	-0.085249	0.313424	0.032371	
\mathbf{V}_{i}	-0.156712	0.042625	-0.344646	0.313424	-0.085249	0.689293	
O_i	-0.016186	-0.344646	-0.161745	0.032371	0.689293	0.323490	

The local anisotropic factors ' $\Sigma_i \Sigma_i D_{ij}$'s are given in Table 4. The values given in these tables represent the 'local field' as seen by each of the species of Y, V and O atoms. The values of Refractive Indices and Birefringence are given in Table 5.

Table 5: n_o , n_e and Δn variation near the surface for Z-cut, X-propagation waveguide at λ =6328Å.

Depth	Refractiv	e Indices	Birefringence
(in Å)	no	n _e	$(\Delta n = n_e - n_o)$
$0 \times a = 0$	1.44352	2.68995	1.24643
$1 \times a = 7.12$	1.48653	2.66718	1.18065
$2 \times a = 14.24$	1.56618	2.56999	1.00382
$3 \times a = 21.36$	1.64647	2.48444	0.83797
$4 \times a = 28.48$	1.72540	2.41047	0.68507
$5 \times a = 35.60$	1.80036	2.34802	0.54766
$6 \times a = 42.72$	1.86814	2.29716	0.42902
$7 \times a = 49.84$	1.92495	2.25819	0.33324
$8 \times a = 56.96$	1.96667	2.23142	0.26474
$9 \times a = 64.08$	1.98913	2.21763	0.22850
$10 \times a = 71.20$	1.99290	2.21535	0.22245

*a = 7.12Å is the lattice constant along *a*-axis.

II. VARIATION OF REFRACTIVE INDICES AND BIREFRINGENCE NEAR THE SURFACE FOR AN X-CUT, Z-**PROPAGATION YVO4 WAVEGUIDE**

In Table 1, n_o and n_e directions for various crystal cuts in various Cartesian propagation directions are listed. For an open type X-cut YVO₄ waveguide, with the light propagation direction along Z-axis the c-axis of the unit cell coincides with the X-axis of the waveguide. The electric vector of light is considered to be along X and Z directions leading to evaluation of n_e and n_o in the waveguide.

Table 6: Lattice Anisotropy Factors ($\sum_{j} \sum_{i} D_{X_{ij}} / \sum_{j} \sum_{i} D_{Z_{ij}}$) × 10⁻²⁴cm³ for an X-Cut, Z-Propagation YVO₄ Waveguide for

		p2 - 8			TA N		
Effect On			$3x_i^2 - r_i^2$	$\Sigma \Sigma D$	$\Sigma \Sigma D = \Sigma \Sigma \frac{3z_i^2 - r_i^2}{2}$		
\rightarrow Effect due to \downarrow		^K ij [–] <u>L</u> j <u>L</u> i	r_i^5		$Z_{ij} = \sum_j \sum_i $	r_i^5	
	Yi	Vi	Oi	Yi	Vi	O _i	
	0 th Ui	nit Cell below	v the Surface	(0Å – 6.289)	Å)	J	
Yi	0.144196	-0.068155	0.445151	-0.218486	0.066405	-0.728737	
V_i	-0.068155	0.144196	-0.327417	0.066405	-0.218486	-0.071507	
Oi	0.445151	-0.327417	1.216041	-0.728737	-0.071507	-2.436921	
	1 st Unit	Cell below th	e Surface (6.	289Å – 12.5	78Å)		
Yi	0.127201	-0.072475	0.321114	-0.254003	0.144552	-0.641710	
V_i	-0.072475	0.127201	-0.007304	0.144552	-0.254003	0.014110	
Oi	0.321114	-0.007304	1.188470	-0.641710	0.014110	-2.375668	
	2 nd Unit	Cell below th	e Surface (12	2.578Å – 18.8	367Å)		
Yi	0.113598	-0.085835	0.267304	-0.227176	0.171650	-0.534661	
\mathbf{V}_{i}	-0.085835	0.113598	-0.061255	0.171650	-0.227176	0.122523	
Oi	0.267304	-0.061255	0.972587	-0.534661	0.122523	-1.945298	
	3 rd Unit	Cell below th	e Surface (18	3.867Å - 25.1	.56Å)		
Y _i	0.100670	-0.098738	0.215602	-0.201299	0.197434	-0.431190	
\mathbf{V}_{i}	-0.098738	0.100670	-0.112945	0.197434	-0.201299	0.225861	
Oi	0.215602	-0.112945	0.765848	0.431190	0.225861	-1.531488	
	4 th Unit (Cell below the	e Surface (25	5.156Å – 31.4	45Å)		
Yi	0.088434	-0.110854	0.166970	-0.176910	0.221749	-0.333867	
V_i	-0.110854	0.088434	-0.161610	0.221749	-0.176910	0.323209	
Oi	0.166970	-0.161610	0.570886	-0.333867	0.323209	-1.141730	
	5 th Unit (Cell below the	e Surface (31	.445Å – 37.7	/34Å)		
Y_i	0.077251	-0.122063	0.122194	-0.154493	0.244118	-0.244329	
\mathbf{V}_{i}	-0.122063	0.077251	-0.206381	0.244118	-0.154493	0.412749	
Oi	0.122194	-0.206381	0.391757	-0.244329	0.412749	-0.783477	
6 th Unit Cell below the Surface (37.734Å – 44.023Å)							

Various Depths at $\lambda = 6328$ Å.

www.jetir.org (ISSN-2349-5162) 0.067240 -0.132057 0.082152 -0.134490 0.264125 -0.164361 Yi 0.067240 -0.134490 Vi -0.132057 -0.246347 0.264125 0.492745 Oi 0.082152 -0.246347 0.231760 -0.164361 0.492745 -0.463557 7th Unit Cell below the Surface $(44.023\text{\AA} - 50.312\text{\AA})$ Yi 0.058672 -0.140657 0.047856 -0.117326 0.281296 -0.095682 -0.140657 0.058672 -0.280725 0.281296 Vi -0.1173260.561426 -0.095682 0.047856 -0.280725 0.094479 0.561426 -0.188918 Oi 8^{th} Unit Cell below the Surface (50.312Å – 56.601Å) Yi 0.051703 -0.147623 0.020021 -0.103380 0.295219 -0.040030 Vi -0.147623 0.051703 -0.308565 0.295219 -0.103380 0.617081 O_i 0.020021 -0.308565 -0.016919 -0.040030 0.617081 0.033815 9th Unit Cell below the Surface (56.601Å - 62.89Å) Yi 0.046599 -0.152763 -0.000370 -0.093196 0.305523 0.000757 Vi -0.152763 0.046599 -0.328967 0.305523 -0.093196 0.657928 -0.328967 -0.098531 0.000757 0.657928 0.197027 Oi -0.000370 10th Unit Cell below the Surface (62.89Å - 69.179Å) Yi 0.311626 0.043570 -0.155813 -0.012562 -0.087140 0.025118 Vi -0.155813 0.043570 -0.341129 0.311626 -0.0871400.682255 Oi -0.012562 -0.341129 -0.147078 0.025118 0.682255 0.294183 11th Unit Cell below the Surface (69.315Å – 83.178Å) Yi 0.032283 0.042641 -0.156696 -0.016141 -0.085282 0.313391 Vi -0.156696 0.042641 -0.344597 0.313391 -0.085282 0.689194 O_i -0.016141 -0.344597 -0.161523 0.032283 0.689194 0.323046

In order to calculate the variation of the Refractive Indices near the surface, the waveguide is divided into regions of one-unit cell dimensions normal to the surface. As the Z-axis of the unit cell coincides with the X-axis of the waveguide. The 0th unit cell covers up to a depth of c=6.289Å, 1st unit cell depth is of 2c, 2^{nd} unit cell depth is of 3c, 3^{rd} unit cell depth is of 4c and so on and 10th unit cell depth is of 11c below the surface, which covers the core radius or depth.

Table 7: n_a , n_e and Δn variation near the surface for X-cut, Z-propagation YVO₄ waveguide at λ =6328Å.

2.1

Depth	Refractive	e Indices	Birefringence				
(in A)	no	ne	$(\Delta n = n_e - n_o)$				
$0 \times c = 0$	2.35305	1.5927	-0.76035				
$1 \times c = 6.289$	2.37063	1.6138	-0.75683				
$2 \times c = 12.578$	2.30172	1.6921	-0.60962				
$3 \times c = 18.867$	2.29459	1.7007	-0.59389				
$4 \times c = 25.156$	2.23282	1.7809	-0.45192				
$5 \times c = 31.445$	2 <mark>.1774</mark> 8	1.8613	-0.31618				
$6 \times c = 37.734$	2. <mark>0912</mark> 8	2.0071	-0.08418				
$7 \times c = 44.023$	2.05603	2.0758	0.01977				
$8 \times c = 50.312$	2.02817	2.1345	0.10633				
$9 \times c = 56.601$	2.00816	2.1794	0.17124				
$10 \times c = 62.890$	1.99290	2.2154	0.22250				
$11 \times c = 69.179$	1.99290	2.2154	0.22250				
$10 \times a = 71.200$	1.99290	2.2154	0.22250				
a = 7.12Å is the lattice constant along <i>a</i> -axis.							

*c = 6.289Å is the lattice constant along *a*-axis.

To calculate the refractive indices on the surface, a unit cell of YVO₄ touching the surface of the waveguide is considered. This unit cell is represented as 0^{th} unit cell. The Local field effects are within a radius of $6.289A^{\circ}$ for different lattice sites with this position are evaluated. The centre is then shifted to 1st unit cell below the surface and local fields are evaluated. This procedure is continued to to ten times the lattice constant 'c' where the radius of the sphere of influence is 62.89Å. At this position all the sphere of local field is totally within the core of the waveguide.

The local anisotropic factors $\Sigma_i \Sigma_i D_{ij}$'s' are given in Table 6. The values given in these tables represent the 'local field' as seen by each of the species of Y, V and O atoms. The values of Refractive Indices and Birefringence are given in Table 7.



Figure 1: Variation of n_o and n_e near the Surface of an Z-cut, X-propagation YVO₄ Waveguide at $\lambda = 6328$ Å.



Figure 2: Variation of Birefringence near the Surface of an Z-cut, X-propagation YVO₄ Waveguide at $\lambda = 6328$ Å.



Figure 3. Variation of n_o and n_e near the Surface of a X-cut, Z-propagation YVO₄ Waveguide at $\lambda = 6328$ Å.



Figure 4. Variation of Birefringence near the Surface of a X-cut, Z-propagation YVO₄ Waveguide at $\lambda = 6328$ Å.

VI. RESULTS AND DISCUSSION

The calculations are carried out for YVO₄ optical waveguide at wavelength 6328Å. For an X-cut, Z-propagation YVO₄ waveguide, n_o is found to increase from 1.44 on the surface to 1.99 in the interior, whereas n_e is found to decrease from 2.69 on the surface to 2.22 in the interior of the waveguide. For a Z-cut waveguide, n_o is found to increase from 1.44 to 1.99 whereas n_e is found to decrease from 2.69 to 2.22. The opposite behavior in the variation of *no* and *ne* near the surface of the X-cut, and Z-cut waveguides are primarily due to the dipole orientation in the lattice being different for the two directions of the electric vectors of light.

Variation of the refractive index near the surface is to be considered in the studies involving the propagation mechanisms of light through all such waveguides.

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