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Vibrational, dielectric and scintillation properties of $YAlO_3$

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Abstract

Vibrational and dielectric properties of $YAlO_3$ are investigated within the framework of density functional perturbation theory. The calculated zone center phonon frequencies and dielectric constants are in good agreement with available experimental data. Based on the theoretical values of the dielectric constants and the highest longitudinal IR phonon energy and using the phenomenological model of Lempicki and Wojtowicz, we investigate the scintillation properties of the $YAlO_3$.

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Keywords: $YAlO_3$; Phonon modes; Dielectric permittivity; Scintillation

1. Introduction

The $YAlO_3$ crystals with the D_{2h}^{16} space symmetry group belong to a group of materials serving as the basic materials of the laser technique, optical recording media and the substrate materials for thin films of high-temperature superconductors [1–3]. $YAlO_3$ doped with Cerium has remarkable scintillation properties [4,5]. It is an interesting insulator, which exhibits fast scintillation, high light yield and very good mechanical and chemical properties.

Investigations of $YAlO_3$ optical parameters such as refractive index and band gap have been already described [6,7]. Density functional calculation of its electronic band structure was also presented [8]. However, little is known about its vibrational properties, particularly, the IR-active phonon modes. The knowledge of the vibrational and dielectric properties of the host is crucial in order to understand the optoelectronic processes such as scintillation. The Raman experiment for $YAlO_3$ was performed by Udagawa et al. [9]. Also, Gupta and Ashdhir [10] have applied a short-range force constant model to evaluate the zone center phonon modes of $YAlO_3$. However, there is a significant discrepancy between their calculated and the experimental value of the lowest Raman frequencies.

This paper presents results of calculations based on the density functional perturbation theory that is performed to obtain the zone center phonon modes and dielectric permittivity tensors. The calculated Raman frequencies are in very good agreement with the available experimental data. Also, the frequencies of IR modes are presented, which can be used in mode assignment of $YAlO_3$. The calculated high frequency and static dielectric permittivity tensors are in good agreement to available experimental data. Then, these physical values are used to evaluate scintillation properties of $YAlO_3$, using Lempicki and Wojtowicz's formulation [11,12]. This procedure is already implemented by Mikami et al. [13] for evaluation of light output of Y_2O_2S.

The paper is organized as follows. Section 2 gives some technical details of density functional calculation and presents results and discussions on vibrational and dielectric properties of $YAlO_3$. Section 3 describes scintillation properties of the $YAlO_3$, based on Lempicki and Wojtowicz's formulation. Section 4 concludes the paper.

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2. Vibrational and dielectric properties

Density functional perturbation theory [14–17] has been used to investigate the vibrational and dielectric properties of $YAlO_3$. Calculations are performed within the local density approximation [18], thanks to ABINIT code [19]. The exchange-correlation energy is evaluated by using Ceperley–Alder homogeneous electron gas data [20]. All the electron potentials are replaced by norm-conserving pseudopotentials [21–23] with Y(4s, 4p, 4d, 5s), Al(3s, 3p), O(2s, 2p) levels treated as valence states. The wave functions are expanded in plane waves up to a kinetic energy cutoff of 50 Ha. The conjugate gradient minimization technique [24] is employed to minimize the total energy with respect to both electronic and ionic degrees of freedom. The Brillouin zone is sampled by a $3\times3\times2$ Monkhorst–Pack [25] mesh of K-points.

First, we look into the structural parameters of $YAlO_3$. It has a conventional unit cell that is orthorhombic (space group D_{2h}^{16}) and contains four formula units per unit cell. Table 1 presents the lattice constants and four independent atoms positions that obtained from structural relaxation as well as results of experimental work [26] for comparison. The calculated structural parameters are in good agreement with experimental data. The close agreement with the experimental values provides a good confirmation of the reliability of the calculations.

We now investigate the zone center phonon frequencies. Since there are 20 atoms in the unit cell, there are 57 optical modes and three acoustic modes. From factor group analysis for this unit cell, the optical modes at the zone center are classified as $\Gamma_{op}=7A_g+5B_{1g}+7B_{2g}+5B_{3g}+8A_u+9B_{1u}+7B_{2u}+9B_{3u}$. Of the 57 modes, 24 modes ($7A_g+5B_{1g}+7B_{2g}+5B_{3g}$) are Raman active and 25 modes ($9B_{1u}+7B_{2u}+9B_{3u}$) are IR active and $8A_u$ modes are silent. The first principles calculations give phonon frequencies and allow us to perform for each mode a detailed analysis of the associated displacement pattern, character and symmetry. Using the calculated results together with the factor group analysis, we can assign to each mode a symmetry character.

The calculated Raman frequencies are summarized in Table 2, along with the previous experimental data [9,27]. The present calculation gives nine Raman frequencies that could not be detected experimentally. Overall, the agreement between the calculated and available experimental values is very good. However, the discrepancy is due both to systematic errors in the first principles calculations, in particular the local density approximation, and to the fact that the experimental results are at room temperature and not zero temperature. For lowest Raman frequencies, the agreement between our calculation and experiment is very good, unlike the results of Ref. [10]. However, the present calculations do not give any frequency of B_{1g} symmetry close to the experimental value [27] of $555\,cm^{-1}$. By contrast, the present calculation identifies three B_{1g} modes at 233.8, 464.2 and $675.9\,cm^{-1}$. We also obtain silent modes, inactive for both IR and Raman experiments. They are found to range from 132.7 to $480.5\,cm^{-1}$.

The calculated frequencies of the transverse and longitudinal IR (TO and LO, respectively) modes are given in Table 3. Experimental wave numbers of the IR modes are not available in the literature. However, they can play an important role in mode assignment of $YAlO_3$.

The high frequency and static dielectric tensor components are also evaluated (Table 4). The calculated orientationally averaged value of high-frequency dielectric constant $\varepsilon_{ave}^{\infty}=4.13$ is very close to experimental value

Table 1
The calculated lattice constants and atomic positions of $YAlO_3$ compared to experimental values

Lattice constants		Calculated			Experimental [26]		
a		5.13			5.18		
b		5.27			5.33		
c		7.29			7.37		
Atomic coordinates	Position	*x*	*y*	*z*	*x*	*y*	*z*
Y	4(*c*)	−0.0121	0.0532	0.25	−0.0104	0.0526	0.25
Al	4(*b*)	0.5	0	0	0.5	0	0
O(1)	4(*c*)	0.083	0.479	0.25	0.086	0.475	0.25
O(2)	8(*d*)	−0.293	0.293	0.044	−0.297	0.293	0.044

Lattice constants *a*, *b*, *c* are in Å and atomic coordinates *x*, *y*, and *z* are dimensionless.

Table 2
The calculated and experimental Raman frequencies (in cm^{-1}) of $YAlO_3$

	Calculated	Experimental [9,27]
A_g	147.3	150
	196.4	197
	277.7	278
	342.1	345
	409.3	412
	469.0	—
	547.4	553
B_{1g}	233.8	—
	259.7	270
	406.4	403
	464.2	555
	675.9	—
B_{2g}	157.9	157
	216.1	219
	283.6	283
	418.0	—
	536.1	—
	581.3	552
	697.7	—
B_{3g}	198.0	197
	394.4	—
	470.8	470
	531.0	540
	731.5	