

## Study of SHG and LE-O Susceptibilities of InAs Crystal: Linear Absorption Taken into Account

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**Keywords:** Nonlinear Optics, Second Harmonic Generation, Linear Electro-Optic Susceptibility Coefficient.

**Abstract:** We applied a model involving two coupled anharmonic oscillators (electronic and ionic) to estimate the Second Harmonic Generation (SHG) and Linear Electro-Optic (LE-O) susceptibilities of InAs crystal. The crystal of InAs belongs to III-V group compounds owing to the cubic zinc-blende-type structure. Linear absorption is considered for the selected spectral region 1250 nm – 390 nm. So, the contribution of the imaginary part of the involved complex linear ionic susceptibility to the resultant SHG and LE-O susceptibilities is taken into account and hence the absolute value of complex-linear ionic susceptibility i.e.  $|\chi_i^{(1)}(\omega)|$ , is used in place of  $\chi_i^{(1)}(\omega)$  in the computation of SHG and LE-O coefficients. All of the four constants (nonlinear strength factors), appearing in the model, are determined with the help of experimental data of SHG susceptibility measured in the selected region of 1076 nm -535 nm. Application of such calculated nonlinear strength factors in the concerned modelled expressions, SHG and LE-O susceptibility coefficients are computed as a function of frequency to illustrate the dispersion in the region of 1250 nm –390 nm.

### Introduction:

A number of nonlinear effects result in the interaction between laser and matter [1]-[2], are studied in Nonlinear Optics. The research object of nonlinear optics mainly involves the new phenomena and new effects in the interaction process of strong laser radiation and materials, including an in-depth understanding of the causes and the process regularity and exploration of their possible applications in the current or future development of disciplines. The interaction of a laser with a nonlinear optical material causes a modification of the optical properties of the material system, such that the next photon that arrives realizes a different material [3]. Extensive advances have been made in the understanding and application of nonlinear optical interactions since the invention of laser (around 1960). Both experimental, as well as theoretical research in the field of nonlinear optics, is represented by the determination of the absolute value of nonlinear susceptibility. An extensive theoretical study of the electronic, linear, and nonlinear optical properties of the III-V indium compound semiconductors has been done by Ali Hussain Reshak [4]. In the last two decades, a variety of studies have been performed on the Nonlinear Optical Properties (NOPs) of novel materials because of the potential of these materials in optical device applications[5], and novel materials with enhanced nonlinearities need to be identified [6].

C.G. Garrett [7] used a model with two coupled anharmonic oscillators (electronic & ionic) to predict the nonlinear susceptibilities for a simple diatomic, cubic material. With the limitation of 1-D (1-dimensional), the model should give a reasonable description of the behaviour of zinc-blende-type materials that are both diatomic and cubic. InAs is one of the III-V group compounds having a zinc-blende-type structure. The III-V group compound semiconductor InAs has attracted much attention because they possess narrow band gaps and have potential as new device materials. InAs is a good infrared (IR) photodetector like other narrow bandgap compound semiconductors [8]. Infrared detectors can be used in thermal imaging systems, free-space communication, and chemical-agent monitoring [9]. Formerly, several models are applied by different workers to compute the second-order optical properties of III-V group compounds in the different regions of

radiation. Some of such models are bond-charge model [10]-[12], charge-transfer model [13]. S.S. Jha and N. Bloembergen, [14]; C.L. Tang [15] and C. Flytzanis *et al.* [16], also, have calculated the second-order optical susceptibility coefficients such as Second Harmonic Generation (SHG) and Linear Electro-Optic (LE-O) coefficient, for III-V group compounds to which InAs belongs. Classically, none of the authors [13]-[16], had obtained a dispersion relation to estimating the second-order optical susceptibilities, involving a simultaneous contribution from linear electronic and linear ionic susceptibilities for InAs along with other III-V group semiconducting compounds. Presently, the author applied a model to the InAs crystal to compute its nonlinear optical properties (SHG and LE-O susceptibility coefficients, here) in the selected spectral region of 1250 nm – 390 nm. For this, first, the four Nonlinear Strength Factors (NSF) appearing in our modelling, are computed with the help of existing available experimental data [17]. And then, as per the objectives of the author's present work, by using such calculated parameters; the author estimated the required LE-O and SHG coefficients as a function of the frequency. This way, the dispersion in the near infra-red (NIR) region of 1250 nm- 390 nm, is illustrated.

### Theoretical Aspect

Garrett has taken one-dimensional lattice and writes the equations of motion in terms of configuration co-ordinates  $q_e$  and  $q_i$  for electronic and ionic oscillation respectively as,

$$\ddot{q}_e + \omega_e^2 q_e = \frac{e_e}{m_e} E \quad (1)$$

$$\ddot{q}_i + \omega_i^2 q_i = \frac{e_i}{\mu} E. \quad (2)$$

Here,  $m_e$  is the electronic mass,  $\mu$  is the reduced ionic mass,  $e_e$  and  $e_i$  is the charges of the order of one electronic charge and defined in terms of cation, anion core and anion shell charges.  $\omega_e$  is the resonant frequency associated with the dominant ultraviolet inter-band electronic transition responsible for the dispersion in the visible region and  $\omega_i$  is the resonant frequency associated with transverse optical (TO) phonon frequency in the infrared region.  $q_e$  is called electronic configuration co-ordinate associated with  $\omega_e$  and  $q_i$  is ionic configuration co-ordinate associated with  $\omega_i$ . The polarization,

$$P = N[e_e q_e + e_i q_i] \quad (3)$$

And the linear susceptibility is

$$\chi^{(1)} = \frac{N}{E\epsilon_0}[e_e q_e + e_i q_i] = \frac{N}{E\epsilon_0} e_e q_e + \frac{N}{E\epsilon_0} e_i q_i = \chi_e^{(1)} + \chi_i^{(1)} \quad (4)$$

where,  $\chi_e^{(1)}$  and  $\chi_i^{(1)}$  is electronic and ionic susceptibility respectively. For

$$q_e = \frac{e_e E}{m_e D_e(\omega)}, \quad (5)$$

$$\chi_e^{(1)} = \frac{N}{E\epsilon_0} e_e q_e = \frac{N e_e^2}{\epsilon_0 m_e D_e(\omega)} \quad (6)$$

where,  $D_e(\omega) = \omega_e^2 - \omega^2$ .

On taking the ionic damping effect on the harmonic oscillatory motion of the ion into account, an extra damping term is appeared in the equation of motion (2) as,

$$\ddot{q}_i + \tau \dot{q}_i + \omega_i^2 q_i = \frac{e_i}{\mu} E \quad (7)$$

It gives,

$$q_i = \frac{e_i}{\mu(-\omega^2 - i\tau\omega + \omega_i^2)} E \quad (8)$$

So,

$$\chi_i^{(1)}(\omega) = \frac{N}{E\epsilon_0} e_i q_i = \frac{N e_i^2}{\epsilon_0 \mu D_i(\omega)} \quad (9)$$

where,  $D_e(\omega) = \omega_i^2 - i\tau\omega - \omega^2$ .

where, the author has added a phenomenological damping rate  $\tau$  in the ionic response only. Cochran [18] has introduced the quadratic terms as nonlinear terms in potential as he was interested in centrosymmetric crystals. The noncentrosymmetric 1-D model necessarily possesses a unique polar axis, will be pyroelectric. So, Garrett [7] has added a cubic instead of the quadratic term to potential. So, the potential is

$$U = \frac{m_e q_e^2 \omega_e^2}{2} + \frac{\mu q_i^2 \omega_i^2}{2} + A q_i^3 + B q_i^2 q_e + C q_i q_e^2 + D q_e^3 - E(e_e q_e + e_i q_i). \quad (10)$$

Where, A, B, C, and D are constants referred to as nonlinear strength factors (NSF). So,

$$\ddot{q}_e = -\omega_e^2 q_e + \left(\frac{e_e}{m_e}\right) E - \left(\frac{3D}{m_e}\right) q_e^2 - \left(\frac{2C}{m_e}\right) q_e q_i - \left(\frac{B}{m_e}\right) q_i^2. \quad (11)$$

$$\ddot{q}_i = -\omega_i^2 q_i - \tau \dot{q}_i + \left(\frac{e_i}{\mu}\right) E - \left(\frac{C}{\mu}\right) q_e^2 - \left(\frac{2B}{\mu}\right) q_e q_i - \left(\frac{3A}{\mu}\right) q_i^2. \quad (12)$$

An applied electric field  $\underline{E}$  is assumed to be a superposition of two fields as,

$$\underline{E} = \frac{1}{2} \left[ \underline{E}_1 e^{-j\omega_1 t} + C.C. + \underline{E}_2 e^{-j\omega_2 t} + C.C. \right] \quad (13)$$

Here,  $\underline{q}_e$  and  $\underline{q}_i$  will respond to the applied electric field having components at  $\omega_1$  and  $\omega_2$  due to linear and at  $\omega_1 \pm \omega_2$ ,  $2\omega_1, 2\omega_2$  due to nonlinear behaviour. Thus,

$$q_e = q_e^{(1)} + q_e^{(2)}(0)|_{\omega_1, \omega_1} + q_e^{(2)}(0)|_{\omega_2, \omega_2} + \frac{1}{2} \left[ q_e^{(2)}(\omega_1 - \omega_2) e^{-j(\omega_1 - \omega_2)t} + q_e^{(2)}(2\omega_1) e^{-j(2\omega_1)t} + q_e^{(2)}(\omega_1 + \omega_2) e^{-j(\omega_1 + \omega_2)t} + q_e^{(2)}(2\omega_2) e^{-j(2\omega_2)t} + C.C. \right] \quad (14)$$

$$q_e^{(1)} = \frac{1}{2} \left[ q_e^{(1)}(\omega_1) e^{-j\omega_1 t} + C.C. + q_e^{(1)}(\omega_2) e^{-j\omega_2 t} + C.C. \right] \quad (15)$$

$$q_i^{(1)} = \frac{1}{2} \left[ q_i^{(1)}(\omega_1) e^{-j\omega_1 t} + C.C. + q_i^{(1)}(\omega_2) e^{-j\omega_2 t} + C.C. \right] \quad (16)$$

Using the expressions of  $\underline{q}_e$ ,  $\underline{q}_i$ , and  $\underline{E}$  into (11) and (12),  $\underline{q}_e^{(2)}$  and  $\underline{q}_i^{(2)}$  can be solved in terms of  $\underline{E}_1$ ,  $\underline{E}_2$ ,  $\underline{q}_e^{(1)}$  and  $\underline{q}_i^{(1)}$ . Second-order polarization at  $\omega_{ij}$ ,

$$\underline{P}(\omega_{ij}, \omega_i, \omega_j) = \frac{1}{2} \left[ \underline{P}^{(2)}(\omega_{ij}, \omega_i, \omega_j) e^{-j\omega_{ij} t} + C.C. \right].$$

$$\text{Or, } \underline{P}(\omega_{ij}, \omega_i, \omega_j) = \frac{1}{2} \left[ \chi^2(\omega_{ij}, \omega_i, \omega_j) \underline{E}_i \underline{E}_j e^{-j\omega_{ij} t} + C.C. \right]. \quad (17)$$

A detailed tedious calculation results in the general expression for the first-order nonlinear susceptibility,

$$\begin{aligned} \chi^{(2)}(\omega_i \pm \omega_j, \omega_i, \omega_j) | i=1, j=2 | = & -\frac{\epsilon_0^2}{2} \left\{ \left( \frac{3D}{N_e^2 e_e^3} \right) \left[ \chi_e^{(1)}(\omega_1) \cdot \chi_e^{(1)}(\omega_2) \cdot \chi_e^{(1)}(\omega_1 \pm \omega_2) \right] + \right. \\ & \left( \frac{C}{N_e N_i e_e^2 e_i} \right) \left[ \chi_e^{(1)}(\omega_1) \cdot \chi_i^{(1)}(\omega_2) \cdot \chi_e^{(1)}(\omega_1 \pm \omega_2) + \chi_i^{(1)}(\omega_1) \cdot \chi_e^{(1)}(\omega_2) \cdot \chi_e^{(1)}(\omega_1 \pm \omega_2) \right] + \\ & \left( \frac{C}{N_e^2 e_e^2 e_i} \right) \left[ \chi_e^{(1)}(\omega_1) \cdot \chi_e^{(1)}(\omega_2) \cdot \chi_i^{(1)}(\omega_1 \pm \omega_2) \right] + \left( \frac{B}{N_e N_i e_i^2 e_e} \right) \left[ \chi_e^{(1)}(\omega_1) \cdot \chi_i^{(1)}(\omega_2) \cdot \chi_i^{(1)}(\omega_1 \pm \omega_2) + \right. \\ & \left. \chi_i^{(1)}(\omega_1) \cdot \chi_e^{(1)}(\omega_2) \cdot \chi_i^{(1)}(\omega_1 \pm \omega_2) \right] + \left( \frac{B}{N_i^2 e_i^2 e_e} \right) \left[ \chi_i^{(1)}(\omega_1) \cdot \chi_i^{(1)}(\omega_2) \cdot \chi_e^{(1)}(\omega_1 \pm \omega_2) \right] + \\ & \left. \left( \frac{3A}{N_i^2 e_i^3} \right) \left[ \chi_i^{(1)}(\omega_1) \cdot \chi_i^{(1)}(\omega_2) \cdot \chi_i^{(1)}(\omega_1 \pm \omega_2) \right] \right\} \quad (18) \end{aligned}$$

### Present Modelling

The author made a realistic approach and modified Garrett's anharmonic model [7] and took the contribution of the imaginary part of the complex linear ionic susceptibility  $\chi_i^{(1)}(\omega)$ , into account along with its real part and so absolute value of  $\chi_i^{(1)}(\omega)$  i.e.  $|\chi_i^{(1)}(\omega)|$  is used in place of  $\chi_i^{(1)}(\omega)$  in the computation of SHG and LE-O coefficients for the InAs crystal, for the selected spectral range.

**SHG Susceptibility Coefficient:** For sum-frequency mode  $\omega_1 + \omega_2 = \omega + \omega = 2\omega$ , (18) gives SHG expression

$$\begin{aligned} \chi^{(2)}(2\omega, \omega, \omega) = & -\frac{\epsilon_0^2}{2} \left\{ \left( \frac{3D}{N_e^2 e_e^3} \right) [\chi_e^{(1)}(\omega) \cdot \chi_e^{(1)}(\omega) \cdot \chi_e^{(1)}(2\omega)] + \right. \\ & \left( \frac{2C}{N_e N_i e_e^2 e_i} \right) [\chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(\omega)| \cdot \chi_e^{(1)}(2\omega)] + \left( \frac{C}{N_e^2 e_e^2 e_i} \right) [\chi_e^{(1)}(\omega) \cdot \chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(2\omega)|] + \\ & \left( \frac{2B}{N_e N_i e_i^2 e_e} \right) [\chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(2\omega)|] + \left( \frac{B}{N_i^2 e_i^2 e_e} \right) [|\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(\omega)| \cdot \chi_e^{(1)}(2\omega)] + \\ & \left. \left( \frac{3A}{N_i^2 e_i^3} \right) [|\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(2\omega)|] \right\} \end{aligned} \quad (19)$$

**LE-O Susceptibility Coefficient:** For  $\omega_1 = 0$ ,  $\omega_2 = \omega$ , (18) gives the LE-O coefficient,

$$\begin{aligned} \chi^{(2)}(0 + \omega, 0, \omega) = & -\frac{\epsilon_0^2}{2} \left\{ \left( \frac{3D}{N_e^2 e_e^3} \right) [\chi_e^{(1)}(0) \cdot \chi_e^{(1)}(\omega) \cdot \chi_e^{(1)}(\omega)] + \right. \\ & \left( \frac{C}{N_e N_i e_e^2 e_i} \right) [\chi_e^{(1)}(0) \cdot |\chi_i^{(1)}(\omega)| \cdot \chi_e^{(1)}(\omega) + \chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(0)| \cdot \chi_e^{(1)}(\omega)] + \\ & \left( \frac{C}{N_e^2 e_e^2 e_i} \right) [\chi_e^{(1)}(0) \cdot \chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(\omega)|] + \left( \frac{B}{N_e N_i e_i^2 e_e} \right) [\chi_e^{(1)}(0) \cdot |\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(\omega)| + \\ & \chi_e^{(1)}(\omega) \cdot |\chi_i^{(1)}(0)| \cdot |\chi_i^{(1)}(\omega)|] + \left( \frac{B}{N_i^2 e_i^2 e_e} \right) [|\chi_i^{(1)}(0)| \cdot |\chi_i^{(1)}(\omega)| \cdot \chi_e^{(1)}(\omega)] + \\ & \left. \left( \frac{3A}{N_i^2 e_i^3} \right) [|\chi_i^{(1)}(0)| \cdot |\chi_i^{(1)}(\omega)| \cdot |\chi_i^{(1)}(\omega)|] \right\}. \end{aligned} \quad (20)$$

where Linear electronic susceptibility,

$$\chi_e^{(1)}(\omega) = \frac{N_e e_e^2}{m_e \epsilon_0 (\omega_e^2 - \omega^2)}, \leftarrow \text{Real}$$

Linear ionic susceptibility,

$$\chi_i^{(1)}(\omega) = \frac{N_i e_i^2}{\mu \epsilon_0 (\omega_i^2 - \omega^2 - i\tau\omega)}, \leftarrow \text{Complex. And}$$

$$|\chi_i^{(1)}(\omega)| = \text{Absolute value of } \chi_i^{(1)}(\omega) = \left\{ [\text{Re}\chi_i^{(1)}(\omega)]^2 + [\text{Im}\chi_i^{(1)}(\omega)]^2 \right\}^{1/2}. \quad (21)$$

Where  $\text{Re}\chi_i^{(1)}(\omega)$  = Real part of  $\chi_i^{(1)}(\omega)$  and  $\text{Im}\chi_i^{(1)}(\omega)$  = Imag. part of  $\chi_i^{(1)}(\omega)$ .

### Applications and Numerical Computations

The input parameters are listed in Table 1a. and the SHG experimental data are given in Table 1b  
**Nonlinear Strength Factors (NSF):** Using the input parameters (Table 1a) and the experimental data [17] (Table 1b), in (19), A, B, C, and D are calculated for the further applications (Table 2).

**Table 1(a).** Input Parameters [19] for calculation of Nonlinear Strength Factors A, B, C and D for InAs.

Parameter	Sym.	Value	Unit
Electronic Oscillator Density	$N_e$	1.798800E+28	$m^{-3}$
Electronic Charge **	$e_e$	-1.600000E-19	C
Electronic Mass**	$m_e$	9.109999E-31	Kg
Electronic Resonant Frequency	$\omega_e$	7.644800E+15	rad/s
Ionic Oscillator Density	$N_i$	1.798800E+28	$m^{-3}$
Reduced Mass of Electronic & Ionic Oscillator ***	$\mu$	7.526100E-26	Kg
TO Phonon Frequency	$\omega_i$	3.950000E+13	rad/s
Ionic Charge	$e_i$	1.600000E-19	C
Damping Rate	$\tau$	3.950000E+11	rad/s
The permittivity of Free Space **	$\epsilon_0$	8.854000E-12	$C^2/N.m^2$
E* $\pm$ n = x $10^{\pm n}$ ,    ** Standard data,    * ** Calculated data.			

**Table 1(b).** Input Data (Experimental) [17] for InAs.

Photon Energy,[eV]	Frequency,[xE+15 rad/s]	Normalized SHG Susc. Coefficient
1.293	1.9653	(8.20 $\pm$ 1.27)E+2
1.552	2.3584	(7.23 $\pm$ 0.99)E+2
1.707	2.5943	(3.10 $\pm$ 0.40)E+2
2.353	3.5769	(8.09 $\pm$ 0.87)E+2

**Table 2.** Calculated NSF A, B, C, and D for InAs.

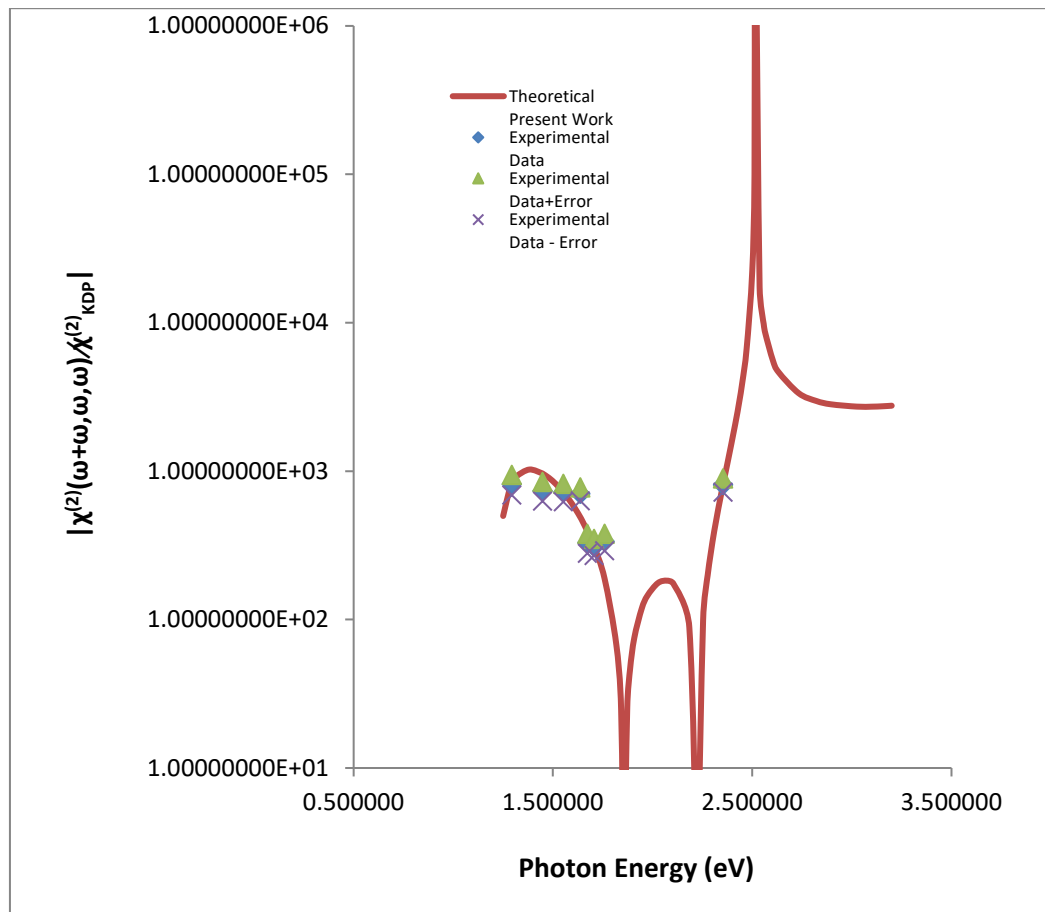
NSF	Value, [kg/ms <sup>2</sup> ]
A	3.37956805E+25
B	4.84953698E+21
C	2.84497189E+17
D	5.49731433E+12

**SHG and LE-O Coefficients:** So calculated factors A, B, C, and D (Table 2), are applied in (19) and (20) to compute SHG and LE-O susceptibility coefficients respectively at several different frequencies in the selected spectral region of 1.000 eV – 3.200 eV. The normalization of SHG results is done with  $\chi_{\text{KDP}}^{36} = 0.39 \text{ pm/V}$  (at 1064 nm) [20].

Here, the author did the computations in double precision to record the changes in the results of the dependent function.

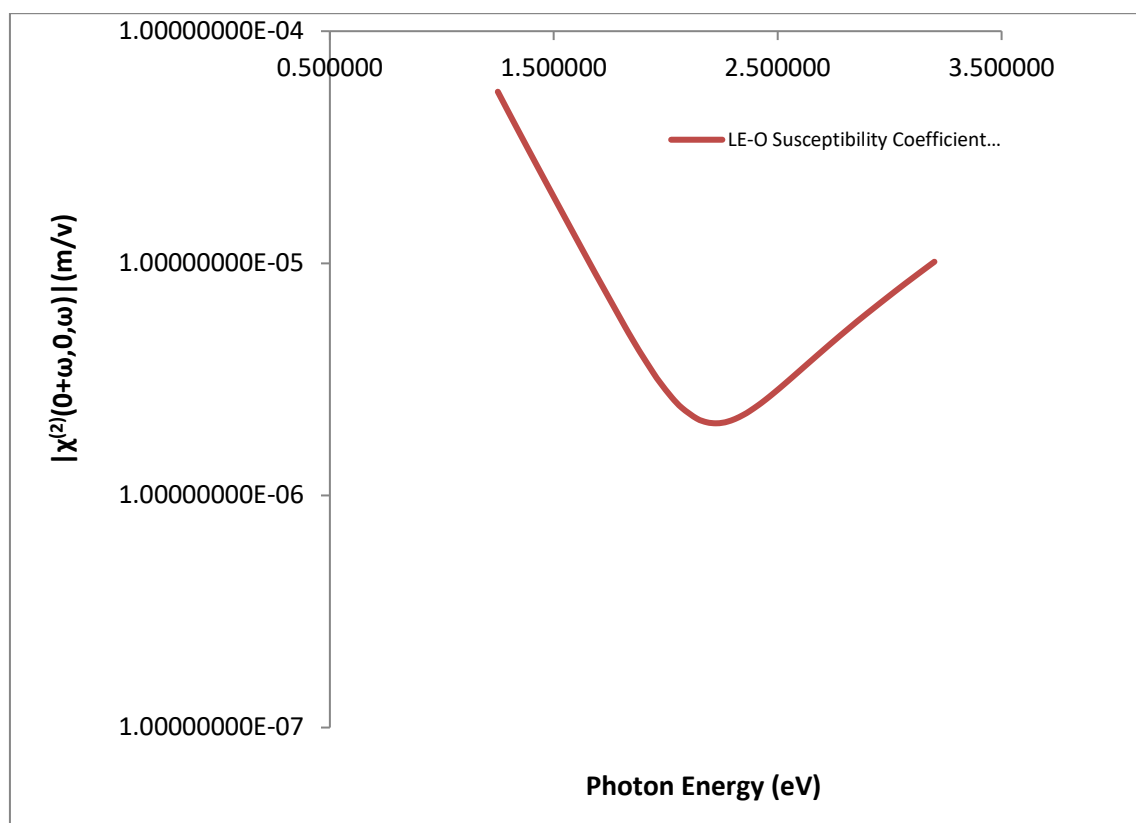
## Results and Discussion

**SHG Results:** Following the present model, the computed results of normalized SHG (absolute values) is plotted as a function of photon energy, in Fig.1. InAs shows large absolute values of SHG susceptibility for the range 1.283 eV– 1.600 eV that belongs to the NIR region. The first two dips result from the sum of +ive and –ive values of the cross terms involved in the concerned expression. Absolute SHG susceptibility goes to infinite at  $\omega_e/2 = 3.8224\text{E}+15 \text{ rad/s}$  ( $\approx 2.514957 \text{ eV}$ ) which is caused by the doubling of the applied field (fundamental) frequency (SHG process) equal to  $\omega_e/2$ , at which the electronic oscillators get in their resonance-mode and causing the maximum (infinite) absolute value of the SHG susceptibility. Near  $\omega_e/2$ , InAs shows large SHG susceptibility but it falls exponentially in the region near  $\omega_e/2$ . For 2.822 eV – 3.200 eV, InAs crystal shows the very small variation in the dispersion and hence refers to almost constant SHG response concerning this special band of frequencies.



**Figure 1.** Normalized SHG Susceptibility Coefficient (Absolute value)  $[\chi^{(2)}(\omega+\omega,\omega,\omega)/\chi^{(2)}_{\text{KDP}}]$  shows its variation with Photon Energy of radiation hitting the selected crystal of InAs. Normalization is done with  $\chi^{(2)}_{\text{KDP}}^{36} = 0.39 \text{ pm/V (at 1064 nm)}$ .

**LE-O Results:** Computed results of LE-O susceptibility coefficients are illustrated in Fig.2. InAs shows large values of absolute LE-O susceptibility coefficient in the region 1.250 eV – 1.645 eV of NIR region. Around 2.223400 eV, LE-O susceptibility has lower absolute values (including lowest at 2.223353 eV).



**Figure 2.** Linear Electro-Optic (LE-O) Susceptibility Coefficient (Absolute value)  $|\chi^{(2)}(0+\omega,0,\omega)|$  (m/V)] shows its variation with photon energy of radiation hitting the crystal of InAs.

InAs shows large absolute values of LE-O coefficient in the region 1.250 eV – 1.645 eV of the NIR region. Thus it is found that for these regions, InAs can be more useful to fabricate the SHG based NLO devices than other NLO materials.

## Conclusion

As results, obtained in the present work, are in good agreement with the experimental [17] ones, the modelling applied here, can be justified for the considered region of radiation. And hence it can be concluded that the theoretical consideration of the contribution from the imaginary part (along with the real part) of the linear ionic susceptibility to the resultant SHG coefficients, is very closely true experimentally. So the linear absorption corresponding to  $Im\chi_i^{(1)}(\omega)$  susceptibility is highly acceptable in the spectral region selected here. , the LE-O coefficient estimated in the present work shows a large absolute value in the NIR region, which indicates the potential application of InAs crystal in the fabrication of nonlinear electro-optic devices such as E-O rectifiers and Electro-Optic Modulators.

The nonlinear optical response of a material can be used to make a variety of all-optical devices. The material criteria depend on the need of each specific device. Highlights of present work are that in the present work we have tried to explain the considered theoretical model for different nonlinear optical effects (SHG & LE-O here) for III-V group compound InAs crystal in the limited spectral region which shows quite high response, especially in NIR region. The extracted knowledge from the present work may be used for fabricating suitably specific NLO devices that can be used to serve society ultimately.

In future, one may try to get information about anharmonic coefficients from data other than the nonlinear optic data. The extension of Garrett's model by Sugie and Tada [21] is yet to be tested for materials such as ZnO etc. The present work results can further be improved by making a more suitable choice of data out of the experimental data considered.



## Conflict of Interest

The author declares that there is no conflict of interest.

## Acknowledgements

The author (Chandra P. Singh) thankfully acknowledges the Department of Applied Sciences, Ch. Charan Singh University Campus, Meerut (India), where he is working as an Assistant Professor that motivated and provided the required time to the author to complete the present research work. Blessed with the valuable inspirational guidance from the esteemed Professor (Emeritus) S.P. Khare, Department of Physics, Ch. Charan Singh University, Meerut, in the present work, the author very gratefully thank him. Thanks are due to Dr S.K. Tyagi, associated with Computer Centre, Ch. Charan Singh University Campus, Meerut, India.

## Appendix-A

Following Sugie and Tada three-dimensional model, we have the anharmonic potential, for  $i^{\text{th}}$  location,

$$U = \sum_{klm} [A_{klm} q_{ik} q_{il} q_{im} + B_{klm} q_{ik} q_{il} q_{em} + C_{klm} q_{ik} q_{el} q_{em} + D_{klm} q_{ek} q_{el} q_{em}] . \quad (\text{A-1})$$

For cubic crystal like CdTe, we have the tensorial form given by Bhagvantum,

$$\begin{array}{cccccc} 0 & 0 & 0 & d_{123} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{123} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{123} \end{array}$$

So, U gets then form,

$$U = A_{123} q_{i1} q_{i2} q_{i3} + A_{123} q_{i2} q_{i3} q_{i1} + A_{123} q_{i3} q_{i1} q_{i2} + B_{123} q_{i1} q_{i2} q_{e3} + B_{123} q_{i2} q_{i3} q_{e1} + B_{123} q_{i3} q_{i1} q_{e2} + C_{123} q_{i1} q_{e2} q_{e3} + C_{123} q_{i2} q_{e3} q_{e1} + C_{123} q_{i3} q_{e1} q_{e2} + D_{123} q_{e1} q_{e2} q_{e3} + D_{123} q_{e2} q_{e3} q_{e1} + D_{123} q_{e3} q_{e1} q_{e2} . \quad (\text{A-2})$$

Now, for a cubic crystal,

$$\begin{array}{l} q_{i1} = q_{i2} = q_{i3} \\ q_{e1} = q_{e2} = q_{e3} . \end{array}$$

Taking,

$$3A_{123} = A \quad (\text{A-3.1})$$

$$3B_{123} = B \quad (\text{A-3.2})$$

$$3C_{123} = C \quad (\text{A-3.3})$$

$$\text{and, } 3D_{123} = D \quad (\text{A-3.4})$$

Now, U may take the form,

$$U = A q_i^3 + B q_i^2 q_e + C q_i q_e^2 + D q_e^3 , \quad (\text{A-4})$$

which is same as given by the Garrett. Therefore for CdTe, instead of 3-dimensional Sugie and Tada model, we can take 1-dimensional Garrett model for calculating the nonlinear susceptibilities.

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