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## Calculation of the nonlinear optical coefficient of the $\text{NdAl}_3(\text{BO}_3)_4$ crystal

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**Abstract.** For the first time, we present the calculation of the nonlinear optical coefficient of the  $\text{NdAl}_3(\text{BO}_3)_4$  (NAB) crystal from a systematic and quantitative standpoint. Based on the dielectric theory of complex crystals and the Levine bond charge model, the method of calculation of the second-order nonlinear optical tensor coefficients of complex crystals has been given systematically. The chemical bond parameters and linear and nonlinear susceptibilities of the NAB crystal have been calculated in detail, and the calculated value of  $d_{11}^{NAB}$  is  $-5.81 \times 10^{-9}$  esu, which agrees with the measured value of  $4.06 \times 10^{-9}$  esu.

### Introduction

At the end of the 1960s people paid great attention to the studies of laser nonlinear multifunction crystals. Neodymium aluminium borate,  $\text{NdAl}_3(\text{BO}_3)_4$ , appeared in 1974 and has been studied ever since then [1–6], for it had many desirable features, such as a low laser threshold, a high gain, a linearly polarized output, a small beam divergence, high  $\text{Nd}^{3+}$  concentration and excellent physical and chemical properties. Nevertheless, it is extremely difficult to grow single crystals of high optical quality and large enough for cutting into laser rods [7]. Therefore, small NAB samples were used, and another laser system was employed as a pumping system in almost all of the reports published [3] of NAB lasing experiments. Efforts have been made to search for a best technique for the growth of NAB crystals and a satisfactory flux system is found, which is suitable for the growth of NAB single crystals by using a rotating seed. As a result, crystals with sizes up to 45 mm were obtained, which can be cut into laser rods in dimensions of  $3.2 \text{ mm} \times 23.7 \text{ mm}$  with high optical homogeneity [3]. The success in growing large NAB crystals with good optical quality has given the possibility of producing a xenon-lamp-pumping NAB crystal minilaser system with useful output characteristics.

NAB differs from most known stoichiometric Nd laser materials in that it is a high-Nd-concentration laser crystal with an accentric space group. The lack of inversion symmetry should allow second-order nonlinear optical process (e.g., second-harmonic generation) as well as linear electrooptical modulation to be carried out directly in the laser crystal [8].

In this paper, we, for the first time, quantitatively analysed the optical nonlinearity in the NAB crystal, by using the method we have set up to deal with complex compounds [9], which, based on the Phillips–Van Vechten (PV) dielectric theory [10] and the Levine bond charge model [11], theoretically predicted the value of the nonlinear optical tensor coefficient  $d_{11}^{NAB}$ .

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## 1. Theory

In order to solve the problems of the chemical bond of complex crystals, we must separate the multibond into single bonds, and the problem converts into separating the crystal formula into bond subformula. The relation between the crystal formula and all of its constitutive bond subformulae can be expressed as the subformula equation (bond–valence equation) [9], which shows that the crystal formula is a linear combination of all types of constitutive bond subformula. The subformula of any kind of chemical bond A–B in multibond crystal  $A_aB_bD_dG_g \dots$  can be acquired by the following formula

$$[N(B-A)a/N_{CA}]A[N(A-B)b/N_{CB}]B. \quad (1.1)$$

In the formula, A, B, D, G, ... represent the different elements or the different sites of the same elements in the crystal formula, and  $a, b, d, g, \dots$  represent the numbers of the corresponding elements,  $N(I-J)$  represents the number of  $I$  ions in the coordination group of a  $J$  ion and  $N_{CA}$  and  $N_{CB}, \dots$  represent the nearest coordination numbers of each elements in the crystal.

After listing the subformula equation of a complex crystal, we can calculate each type of subformula by using the PV theory [10]; the parameters in the calculation do not have the same meanings as the original ones: these parameters need to be modified according to the presented charge of ions in the chemical bond. In a complex crystal the numbers of valence electrons associated with a particular bond,  $\mu$ , between A and B ions are  $Z_A^\mu$  and  $Z_B^\mu$  respectively, the nearest coordination numbers are  $N_{CA}^\mu$  and  $N_{CB}^\mu$  respectively and the effective charges of each valence electron of A and B ions are  $q_A^\mu$  and  $q_B^\mu$  (whose values can be determined by using the presented approach [9]), respectively. Here, we can obtain the number of effective valence electrons of A and B ions

$$(Z_A^\mu)^* = Z_A^\mu q_A^\mu \quad (1.2)$$

$$(Z_B^\mu)^* = Z_B^\mu q_B^\mu. \quad (1.3)$$

The number of effective valence electrons per  $\mu$  bond is

$$(n_e^\mu)^* = (Z_A^\mu)^*/N_{CA}^\mu + (Z_B^\mu)^*/N_{CB}^\mu. \quad (1.4)$$

The bond volumes  $v_b^\mu$  for the bonds of type  $\mu$  is as expected proportional to  $(d^\mu)^3(v_b^\mu \propto (d^\mu)^3)$ , where  $d^\mu$  is the nearest-neighbour distance; in the case of the multibond, it is defined as

$$v_b^\mu = (d^\mu)^3 / \sum_v (d^\mu)^3 N_b^v \quad (1.5)$$

where  $N_b^v$  is the number of bonds of type  $v$  per cubic centimetre, which can be obtained from the structure data of the crystal, where the denominator is the normalized factor and the sum over  $v$  runs over all the different types of bond.

The effective valence electron density associated with the bond  $\mu$  is

$$(N_e^\mu)^* = (n_e^\mu)^*/v_b^\mu. \quad (1.6)$$

According to the PV theory, the susceptibility of any bond is written as

$$\chi^\mu = (4\pi)^{-1} (\hbar \Omega_p^\mu / E_g^\mu)^2 \quad (1.7)$$

where  $E_g^\mu$  is the average energy gap between the bonding and the antibonding states,  $\Omega_p^\mu$  is the plasma frequency

$$(\Omega_p^\mu)^2 = [4\pi (N_e^\mu)^* e^2 / m] D_\mu A_\mu \quad (1.8)$$

where  $D_\mu$  and  $A_\mu$  are the correction factors [12],

$$D_\mu = \Delta_A^\mu \Delta_B^\mu - (\delta_A^\mu \delta_B^\mu - 1)[(Z_A^\mu)^* - (Z_B^\mu)^*]^2 \quad (1.9)$$

$$A_\mu = 1 - (E_g^\mu/4E_F^\mu) + (E_g^\mu/4E_F^\mu)^2/3 \quad (1.10)$$

where  $\Delta$  and  $\delta$  are constant parameters which depend on the rows of the periodic table to which elements A and B belong.  $E_F^\mu$  is the Fermi energy of the bond  $\mu$

$$E_F^\mu = (\hbar k_F^\mu)^2/2m \quad (1.11)$$

$$k_F^\mu = [3\pi^2(N_e^\mu)^*]^{1/3}. \quad (1.12)$$

We can separate  $E_g^\mu$  into homopolar  $E_h^\mu$  and heteropolar  $C^\mu$  parts

$$(E_g^\mu)^2 = (E_h^\mu)^2 + (C^\mu)^2 \quad (1.13)$$

and

$$E_h^\mu = 39.74/(d^\mu)^{2.48} \quad (1.14)$$

$$C^\mu = 14.4b^\mu \exp(-k_s^\mu r_0^\mu)[(Z_A^\mu)^*/r_0^\mu - n(Z_B^\mu)^*/r_0^\mu] \quad (1.15)$$

where

$$k_s^\mu = (4k_F^\mu/\pi a_B)^{1/2} \quad (1.16)$$

and  $r_0^\mu$  is the average radius of A and B in ångströms, which is equal to a half of the nearest-neighbour distance

$$r_0^\mu = d^\mu/2 \quad (1.17)$$

$a_B$  is the Bohr radius,  $n$  is the ratio of the two elements in the subformula,  $n > 1$ ,  $\exp(-k_s^\mu r_0^\mu)$  is the Thomas–Fermi screening factor and  $b^\mu$  is a correction factor that is proportional to the square of the average coordination number  $N_C^\mu$

$$b^\mu = \beta(N_C^\mu)^2 \quad (1.18)$$

$$N_C^\mu = N_{CA}^\mu/(1+n) + nN_{CB}^\mu/(1+n). \quad (1.19)$$

This correction factor  $b^\mu$  depends on a given crystal structure; in the simple type of  $A^nB^{8-n}$  it is approximately constant and equal to 0.089 [13]. If the index of refraction or the dielectric constant for the crystal is known, the value of  $\beta$  can be obtained from the above equations.

If the crystal is composed of different types of bond (labelled  $\mu$ ), then the total  $\chi$  can be resolved into contributions  $\chi^\mu$  from the various types of bond,

$$\chi = \sum_\mu F^\mu \chi^\mu = \sum_\mu N_b^\mu \chi_b^\mu \quad (1.20)$$

where  $\chi^\mu$  is the total macroscopic susceptibility which a crystal composed entirely of bonds of type  $\mu$  would have.  $F^\mu$  is the fraction of bonds of type  $\mu$  composing the actual crystal,  $\chi_b^\mu$  is the susceptibility of a single bond of type  $\mu$ , and  $N_b^\mu$  is the number of bonds per cubic centimetre.

We can determinate the fractional ionicity  $f_i^\mu$  and covalency  $f_c^\mu$  of the individual bonds,

$$f_i^\mu = (C^\mu)^2/(E_g^\mu)^2 \quad f_c^\mu = (E_h^\mu)^2/(E_g^\mu)^2. \quad (1.21)$$

The bond nonlinearities had been evaluated on the basis of the linear results by means of the bond charge model of Levine [11]. The corresponding macroscopic properties are the second-harmonic generation (SHG) coefficients  $d_{ijk}$ , and the Miller delta  $\Delta_{ijk}$ . The complete expression for the total nonlinear susceptibility  $d_{ijk}$  can be written as

$$d_{ijk} = \sum_\mu F^\mu d_{ijk}^\mu = \sum_\mu F^\mu [d_{ijk}^\mu(C) + d_{ijk}^\mu(E_h)] \quad (1.22)$$

where  $d_{ijk}^\mu$  is the total macroscopic nonlinearity which a crystal composed entirely of bonds of type  $\mu$  would have,  $d_{ijk}^\mu(C)$  the ionic fraction of the nonlinear optical coefficient,  $d_{ijk}^\mu(E_h)$  the covalent fraction,

$$F^\mu d_{ijk}^\mu(C) = G_{ijk}^\mu N_b^\mu (14.4) b^\mu \exp(-k_s^\mu r_0^\mu) [(Z_A^\mu)^* + n(Z_B^\mu)^*] (\chi_b^\mu)^2 C^\mu / (E_g)^2 (d^\mu)^2 q^\mu \quad (1.23)$$

$$F^\mu d_{ijk}^\mu(E_h) = G_{ijk}^\mu N_b^\mu (2s - 1) [r_0^\mu / (r_0^\mu - r_c^\mu)]^2 f_c^\mu (\chi_b^\mu)^2 \rho^\mu / d^\mu q^\mu. \quad (1.24)$$

$G_{ijk}^\mu$  is the geometrical contribution of the bonds of type  $\mu$ , which can simply be calculated from

$$G_{ijk}^\mu = 1/n_b^\mu \sum_\lambda \alpha_i^\mu(\lambda) \alpha_k^\mu(\lambda) \quad (1.25)$$

where the sum on  $\lambda$  is over all  $n_b^\mu$  bonds of type  $\mu$  in the unit cell, and  $\alpha_i^\mu(\lambda)$  is the direction cosine with respect to the  $i$ th coordinate axis of the  $\lambda$ th bond of type  $\mu$  in the unit cell, the difference in the atomic sizes  $\rho^\mu = (r_A^\mu - r_B^\mu)/(r_A^\mu + r_B^\mu)$ ,  $r_A^\mu$  and  $r_B^\mu$  are the covalent radii of atoms A and B; their values are taken from [14].  $r_0^\mu$  is the averaged radius of A and B in ångströms,  $r_c^\mu$  the core radius, and  $r_c^\mu = 0.35r_0^\mu$ .  $q^\mu$  is the bond charge of the  $\mu$ th bond,

$$q^\mu = (n_e^\mu)^* [1/(\chi^\mu + 1) + K f_c^\mu] e. \quad (1.26)$$

$K$  is a function of the average covalency  $F_c$  and of the coordination number  $N_{cat}$  of the central cation, which is expressed as

$$K = (2^{F_c} - 1.1)/N_{cat} \quad (1.27)$$

where  $F_c$  is defined as

$$F_c = \sum_\mu N_b^\mu f_c^\mu. \quad (1.28)$$

Since Miller's  $\Delta_{ijk}$  [15] is normalized to the linear susceptibility, it is more closely related to the intrinsic crystalline anisotropy than  $d_{ijk}$  is, and  $\Delta_{ijk}$  is therefore a useful representation for the nonlinear susceptibility. It is defined by [15]

$$\Delta_{ijk} = d_{ijk} / \chi_i(2\omega_i) \chi_j(\omega_j) \chi_k(\omega_k) \quad (1.29)$$

where  $\omega_i$  are the appropriate optical frequencies involved, and  $\chi_i(2\omega_i)$  is the appropriate susceptibility at  $2\omega_i$ . The approximate form of the expression for  $\Delta_{ijk}$  is always introduced as follows:

$$\Delta_{ijk} = d_{ijk} / \chi_i(\omega_i) \chi_j(\omega_j) \chi_k(\omega_k). \quad (1.30)$$

Further, we have

$$\Delta_{ijk} = \sum_\mu F^\mu \Delta_{ijk}^\mu = \sum_\mu G_{ijk}^\mu N_b^\mu \Delta_\beta^\mu \quad (1.31)$$

where  $\Delta_\beta^\mu$  is the Miller's  $\Delta$  for the bond  $\mu$ , i.e.,

$$\Delta_\beta^\mu = F^\mu \Delta_{ijk}^\mu / G_{ijk}^\mu N_b^\mu. \quad (1.32)$$

Further, we have

$$\Delta_{ijk} = \sum_\mu F^\mu [\Delta_{ijk}^\mu(C) + \Delta_{ijk}^\mu(E_h)] \quad (1.33)$$

$$F^\mu \Delta_{ijk}^\mu(C) = G_{ijk}^\mu N_b^\mu (14.4) b^\mu \exp(-k_s^\mu r_0^\mu) [(Z_A^\mu)^* + n(Z_B^\mu)^*] (\chi_b^\mu)^2 C^\mu / (E_g)^2 (d^\mu)^2 q^\mu \chi^3 \quad (1.34)$$

$$F^\mu \Delta_{ijk}^\mu(E_h) = G_{ijk}^\mu N_b^\mu (2s - 1) [r_0^\mu / (r_0^\mu - r_c^\mu)]^2 f_c^\mu (\chi_b^\mu)^2 \rho^\mu / d^\mu q^\mu \chi^3. \quad (1.35)$$

In the denominators of (1.34) and (1.35),  $\chi$  is the total macroscopic susceptibility. This  $\Delta_{ijk}$  formulation is useful since in our calculation we use the extrapolated low-frequency electronic susceptibility  $\chi$ , whereas the experimentally measured nonlinearity may include a significant amount of dispersion.

## 2. Results and discussion

The structure of NAB was first reported by Mills in 1962 as hexagonal with space group  $R32$  [16]. Hong and Dwight [1] also claimed that it was an accentric space group  $R32$ , with cell parameters  $a = 9.3416(6) \text{ \AA}$ ,  $c = 7.3066(8) \text{ \AA}$  and  $Z = 3$ . The rhombohedral structure, which was further supported [8, 17], had been disputed by Lutz and Huber [18], and was reported to crystallize in two monoclinic space groups  $C2/c$  and  $C2$ . Jarchow *et al* [19] have described the crystal group of NAB as either rhombohedral or monoclinic depending on the growth conditions. According to the applications and the behaviours in the laser performance of NAB crystals developed in the Fujian Institute of Research on the Structure of Matter, its structure should be the rhombohedral space group  $R32$ .

According to the cell parameters [1], we have calculated the coordination numbers of each ion and the values of the bond length of each bond in the NAB crystal, and the calculated results reveal that the bond length of the Al–O(2) bond should be  $1.947 \text{ \AA}$ , not the value of  $2.948 \text{ \AA}$  presented in [1].

The structure of NAB is composed of two sets of isolated  $(\text{BO}_3)^{3-}$  triangles, one ( $B_1$ ) perpendicular, the other ( $B_2$ ) nearly so, to the  $c$ -axis. The  $\text{Al}^{3+}$  and  $\text{Nd}^{3+}$  ions occupy O octahedra and trigonal prisms respectively. Edge-shared  $\text{Al}^{3+}$  octahedra form helices along the  $c$ -axis. Isolated  $\text{Nd}^{3+}$  trigonal prisms alternate along the  $c$ -axis with the  $(\text{BO}_3)^{3-}$  triangles ( $B_1$ ) that are perpendicular to the  $c$ -axis. The slightly distorted Nd trigonal prisms ( $2 \times 2.3715 \text{ \AA}$ ,  $2 \times 2.3712 \text{ \AA}$ ,  $2 \times 2.3708 \text{ \AA}$ ) have six nearest Nd atoms at a distance of  $5.912 \text{ \AA}$  and are connected alternately by the B(2) and Al atoms.

In view of its accentric space group  $R32$ , NAB ought to be optically nonlinear. The restrictions imposed by the crystal symmetry (32 symmetry) and the Kleinman symmetry conditions [20] on the nonlinear optical coefficients mean that only one allowed independent coefficient  $d_{11}$  exists in the NAB crystal.

According to the detailed structure information on the NAB crystal and the method of the separation on the multinary crystal formula [9], we can write its subformula equation as

$$\begin{aligned} \text{NdAl}_3(\text{BO}_3)_4 &= 1/3\text{NdO}(3)_2 + 1/3\text{NdO}(3')_2 + 1/3\text{NdO}(3'')_2 \\ &+ \text{AlO}(1)_2 + \text{AlO}(2)_2 + \text{AlO}(3)_2 \\ &+ 1/3\text{B}(1)\text{O}(1) + 2/3\text{B}(1)\text{O}(1') + \text{B}(2)\text{O}(2) + 2\text{B}(2)\text{O}(3) \end{aligned}$$

where  $\text{NdO}(3)_2$ ,  $\text{NdO}(3')_2$  and  $\text{NdO}(3'')_2$  represent the different types of Nd–O(3) bond with the same bond length and different geometrical factors  $G_{11}^{\mu}$ ; 2 represents the ratio of the element numbers of O(3) to Nd.

The effective valence electron number of cations in each type of bond above is  $Z_{\text{Nd}}^* = Z_{\text{Al}}^* = Z_{\text{B}}^* = 3$ , but the numbers of the effective valence electrons of O anions in each type of bond are not equal: they are  $Z_0^* = 4.5$  in the Nd–O bond and Al–O bond, and  $Z_0^* = 9$  in the B–O bond. These values reflect the different ambience of each O ion. Using the known long-wavelength refractive index of NAB,  $n = 1.75$ , at  $1.06 \mu\text{m}$  [2], the detailed bond parameters and linear and nonlinear susceptibilities of each type of bond can be obtained; their values are listed in table 1.

The calculated results for the total SHG tensor coefficient  $d_{11}^{\text{NAB}}$  and the Miller delta  $\Delta_{11}^{\text{NAB}}$  are listed in table 1. There have been no reports of the value for  $d_{11}^{\text{NAB}}$  so far



in the experimental literature. However, the nonlinear effects of the neodymium yttrium aluminium borate  $\text{Nd}_x\text{Y}_{1-x}\text{Al}_3(\text{BO}_3)_4$  (NYAB) crystal have been reported [21], and the nonlinear coefficient  $d_{11}$  of the NYAB crystal has been measured to be  $4.06 \times 10^{-9}$  esu (at  $1.06 \mu\text{m}$ ). Comparing our results with the related crystal (NYAB), we can see that our result for the nonlinear coefficient  $d_{11}$  of the NAB crystal ( $d_{11}^{NAB} = -5.81 \times 10^{-9}$  esu) is quite reasonable.

In the calculation for the geometrical factor  $G_{11}^{Nd-O(3)}$ , we find that in Nd–O(3) bonds, there are three different values of  $G_{11}^\mu$ , although they have the same bond length. So, we can distinguish between the bonds by using Nd–O(3), Nd–O(3') and Nd–O(3''); each of these represents a different kind of bond with a different  $G_{11}^\mu$  value. When we calculate the values for  $G_{11}^{Al-O}$  and  $G_{11}^{B(2)-O}$  in the unit cell, we find that each type of bond has the three different values of  $G_{11}^\mu$ , e.g., Al–O(1) bonds have the values of  $G_{11}^{Al-O}$ ;  $3 \times 0.0006$ ,  $6 \times 0.2467$  and  $6 \times -0.3577$ , and the value  $G_{11}^{Al-O(1)}$  listed in table 1 is their average. From the different values for  $G_{11}^\mu$  of the same bond (e.g., in the  $\text{AlO}_6$  octahedra and  $\text{B(2)O}_3$  triangles), we can see that there is an orientation disorder of the chemical bonds existing in the NAB crystal, and it is just these disorders that make the contribution of the geometrical factor  $G_{11}^\mu$  to the total nonlinearity quite large. It is these structural disorders (in the  $\text{AlO}_6$  octahedra and  $\text{B(2)O}_3$  triangles) that contribute to the optical nonlinearity of the NAB crystal.

The results show that the most of the linear susceptibility exists in the B–O bond in the NAB crystal. In the  $\text{B(1)O}_3$  group, because the signs for  $G_{11}^{B(1)-O(1)}$  and  $G_{11}^{B(1)-O(1')}$  are opposite, and the cancellations between  $F^\mu \Delta_{11}(C)$  and  $F^\mu \Delta_{11}(E_h)$  lead to quite low nonlinearities, the group does not make the dominant contributions to the total nonlinearity of the NAB crystal. On the contrary, the  $\text{B(2)O}_3$  group makes the dominant contributions to the total nonlinear tensor coefficient  $d_{11}^{NAB}$ , because of the advantageous  $G_{11}^\mu$  and lack of strong cancellation between the two parts ( $F^\mu \Delta_{11}(C)$  and  $F^\mu \Delta_{11}(E_h)$ ).

### 3. Conclusion

An investigation of the second-order optical nonlinearity in the NAB crystal revealed its nonlinearity is closely related to the strict  $D_{3h}$  symmetry of  $\text{BO}_3$  groups. Rigorously speaking, the  $\text{B(2)O}_3$  groups give the NAB crystal quite a large value of the nonlinear coefficient. We theoretically point out, therefore, for the first time, that the self-active laser crystal NAB is at the same time a self-frequency-doubling laser crystal with a quite large nonlinear coefficient  $d_{11}^{NAB} = -5.8 \times 10^{-9}$  esu. The experimental work has demonstrated that the NAB crystals have many good features, which makes it a good material for a minilaser system which may have military, civilian, educational and scientific research applications. The work we have done shows that the NAB crystal is also a good candidate material for a high-quality self-frequency-doubling minilaser.

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