$$n(E) = -\frac{1}{\pi}\left(\frac{[(E - V_1)^2 - 4V_1^2 - V_2^2\,][E - V_1]}{2V_1^2 V_2^2}\right) \mathrm{Im}\, I_{\mathrm{fcc}}\left(\frac{[(E - V_1)^2 - 4V_1^2 - V_2^2]^2}{4V_1^2 V_2^2 - 1}\right). \tag{B6}$$

Notice that adding a small imaginary part to ϵ is equivalent to adding a small imaginary part to E, apart from a possible sign change. However, this sign change is exactly compensated for by the factor in curly brackets in (B6) with the result that the density of states is always positive. In a recent paper, Joyce[20] has expressed the integrals $I_{\mathrm{fcc}}(\epsilon)$ in terms of complete elliptic integrals of the first kind. We refer the reader to Joyce's paper for this further reduction. The density of states (B6) is shown in Fig. 12 together with the δ functions at $-V_1 \pm V_2$.

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Charge-Transfer Model of the Nonlinear Susceptibilities of Polar Semiconductors*

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The second-order optical susceptibilities of III-V and II-VI compounds are calculated on the basis of a charge-transfer model and shown to be in close agreement with the experimental values. The importance of the d-electron contributions to the determination of the sign of the nonlinear susceptibilities of polar semiconductors and other compounds is also discussed.

In the optical transparency region, the behavior of the second-order susceptibilities $\chi^{(2)}$ in dielectrics is closely related to the characteristics of the valence electronic distribution. For simple structures this quantity can be calculated now by molecular-orbital methods.[1,2] For polar diatomic semiconductors simpler methods,[3-6] based upon the prescriptions of Phillips and van Vechten, have also been used to describe[7] the macroscopic electric susceptibility for sp^3-bonded III-V and II-VI compounds. The bond-charge model[4,5] yields results apparently in good agreement with experiments. However, the adjustable parameters and assumptions used are not easily justified.

Here we want to show that exactly the same results can be obtained simply, without any of the troublesome assumptions about the bond charge, by a completely different model that sheds more

light on the Phillips–van Vechten expression for the macroscopic electric susceptibility and at the same time shows the importance of including the d-electron contributions. Instead of the point bonding charge, we stress what we believe to be the essential characteristics of the bond, its spatial extension and its asymmetry, and emphasize explicitly that the second-order susceptibility $\chi^{(2)}$ arises from the asymmetry and the extension of the valence-charge distribution.[2]

The macroscopic electric susceptibility in zinc-blende compounds with sp^3 character can be well represented in terms of a single average energy gap E_g which consists of a homopolar part E_h and a heteropolar part C such that $E_g^2 = E_h^2 + C^2$. The heteropolar part of the energy gap C, or the electronegativity difference,[7] is well fitted by

$$C = 4be^{-kR}\left(\frac{\zeta_A}{r_A} - \frac{\zeta_B}{r_B}\right)e^2 ,\qquad (1)$$

where b is a constant close to 1.5; R is the interatomic distance; e^{-kR} is the Thomas-Fermi screening factor; $\zeta_i = Z_i/4$, and Z_i is the number of valence electrons on atom $i = A, B$; r_i is the corresponding covalent radius; and e is the magnitude of the electronic charge.

The valence electronic distribution in these compounds is well described in terms of bonds tetrahedrally distributed around each atom. Each of these bonds possesses axial symmetry and C characterizes the asymmetry of the valence charge along the bond in the absence of any applied electric field. Associating the electronic charges $-\zeta_A e$ and $-\zeta_B e$, respectively, with the end points A and B of the bond, one can define an electronic dipole moment (or the first moment of the valence charge distribution in the bond), $\vec{\mu}$, with respect to an origin chosen at the midpoint of the bond that reflects mainly the asymmetry of the valence-charge distribution. The polarity of this dipole moment of the bond is directed from A to B,[8] if ζ_A is greater than ζ_B; there are two electrons per bond or $\zeta_A + \zeta_B = 2$. When an electric field $\vec{\mathscr{E}}$ is applied, an additional redistribution of valence charge will result and the dipole moment will change. Defining a field-dependent bond polarizability $\overset{\leftrightarrow}{\alpha}(\vec{\mathscr{E}})$, which can further be expanded in powers of $\vec{\mathscr{E}}$ with the conventional bond polarizabilities $\overset{\leftrightarrow}{\alpha}$ and $\underline{\beta}$ as the coefficients, this change in the electronic dipole moment of the bond $\Delta\vec{\mu}$ can be expressed as

$$\Delta\vec{\mu} = \overset{\leftrightarrow}{\alpha}(\vec{\mathscr{E}})\cdot\vec{\mathscr{E}} = \overset{\leftrightarrow}{\alpha}\cdot\vec{\mathscr{E}} + \underline{\beta}:\vec{\mathscr{E}}\vec{\mathscr{E}} + \cdots . \qquad (2)$$

In terms of these polarizabilities, the macroscopic linear and second-order susceptibilities, $\chi^{(1)}$ and $\chi^{(2)}_{14}$, respectively, are given by[2,9]

$$\chi^{(1)} = \tfrac{4}{3}N(\alpha_\parallel + 2\alpha_\perp) , \qquad (3)$$

$$\chi^{(2)}_{14} = (4/3\sqrt{3})N(\beta_\parallel - 3\beta_\perp) , \qquad (4)$$

where $N = 3\sqrt{3}/16R^3$ is the number of unit cells per unit volume; $\alpha_\parallel$ and $\alpha_\perp$ are, respectively, the longitudinal and transverse components of the linear bond polarizability $\overset{\leftrightarrow}{\alpha}$; similarly, $\beta_\parallel$ and $\beta_\perp$ are the corresponding components of the second-order bond polarizability β. Since $\beta_\parallel$ is much larger[2,10] than $\beta_\perp$ and $\beta_\parallel = \partial\alpha_\parallel(\vec{\mathscr{E}})/\partial\mathscr{E}_\parallel$, where $\mathscr{E}_\parallel$ is the component of $\vec{\mathscr{E}}$ along the bond axis, $\alpha_\parallel(\vec{\mathscr{E}})$ is of primary interest.

Using the Phillips–van Vechten expression[7] for the macroscopic linear susceptibility $\chi^{(1)}$ and Eq. (3), one obtains

$$\alpha_\parallel = \frac{3}{4N}\frac{1}{1+2\kappa}\frac{1}{4\pi}\frac{(\hbar\Omega_p)^2}{E_h^2 + C^2} , \qquad (5)$$

where Ω_p is the plasma frequency corresponding to the valence charge density and $\kappa = \alpha_\perp/\alpha_\parallel$ characterizes the anisotropy of the bond polarizability.

Clearly $\alpha_\parallel$ depends on the spatial extension of the bond along its axis. In the picture of redistribution of charge then, when an electric field $\vec{\mathscr{E}}$ is applied along the bond from atom B to atom A,[8] the first-order induced dipole moment can be interpreted as arising from the transfer of an additional amount of charge $\Delta\zeta e$ (>0) from atom B to atom A within the bond or

$$\alpha_\parallel\mathscr{E} = \Delta\zeta e R_e , \qquad (6)$$

where R_e is the effective length of the bond over which the two electrons of the bond are polarizable; more precisely,

$$R_e = R - r_{iA} - r_{iB} , \qquad (6')$$

where r_{iA} and r_{iB} are the ionic or core radii of the elements A and B, respectively. Due to this additional transfer of charge induced by the applied electric field, ζ_A and ζ_B in Eq. (1) are replaced by $\zeta_A - \Delta\zeta$ and $\zeta_B + \Delta\zeta$, respectively, and the electronegativity difference changes from C to $C + \Delta C$:

$$C + \Delta C = 4be^{-kR}\left(\frac{\zeta_A - \Delta\zeta}{r_A} - \frac{\zeta_B + \Delta\zeta}{r_B}\right)e^2 ; \qquad (7)$$

or the change of the electronegativity difference is

$$\Delta C = -4be^{-kR}\left(\frac{1}{r_A} + \frac{1}{r_B}\right)e^2\Delta\zeta . \qquad (8)$$

Thus, in analogy with Eq. (5), the field-dependent bond polarizability $\alpha_\parallel(\mathscr{E})$ becomes

$$\alpha_\parallel(\mathscr{E}) = \alpha_\parallel + \beta_\parallel\mathscr{E} + \cdots$$
$$= \frac{3}{4N}\frac{1}{1+2\kappa}\frac{1}{4\pi}\frac{(\hbar\Omega_p)^2}{E_h^2 + (C+\Delta C)^2} . \qquad (9)$$

Expanding the last expression in powers of $\mathscr{E}$, one obtains the expression for $\beta_\parallel$ and from Eq. (4) that of the second-order susceptibility $\chi^{(2)}_{14}$ or

$$\chi_{14}^{(2)} = \frac{2}{(1+2\kappa)^2} \left(\frac{R}{R_e}\right) \frac{C}{E_g^2} \frac{\Gamma e R}{\sqrt{3}} (\chi^{(1)})^2 , \qquad (10)$$

where

$$\Gamma = \frac{16 b R}{\sqrt{3}} e^{-kR} \left(\frac{1}{r_A} + \frac{1}{r_B}\right) . \qquad (11)$$

In obtaining Eq. (10), we have made use of the fact that[2,10] $\beta_{\parallel} \gg \beta_{\perp}$.

For sp^3 bonds,[11] $\kappa \simeq \frac{1}{2}$ to $\simeq \frac{2}{3}$ and $2R_e \simeq R$ from Eq. (6'); this gives the factor $[2/(1+2\kappa)^2](R/R_e)$ $\simeq 1$ in Eq. (10). Using this value along with the tabulated values of the other parameters in Eqs. (10) and (11) we obtain the tabulated values for Γ and $\chi_{14}^{(2)}$ shown in Table I; note that Γ is very nearly constant for all the materials. The agreement with experiment in magnitude is particularly gratifying, since it is consistent with the prevailing view that the covalent bond is partially anisotropic.

It is interesting to obtain the expression for the Miller coefficient $\delta = \chi_{14}^{(2)}/(\chi^{(1)})^3$ or

$$\delta = \frac{4\pi\Gamma}{\sqrt{3}} \frac{2}{(1+2\kappa)^2} \left(\frac{R}{R_e}\right) \frac{C}{(\hbar\Omega_p)^2} ; \qquad (12)$$

it can be put in the approximate form[3]

$$\delta = D(Z - \Delta) e R \frac{R^2}{e^2 a_0} + O(Z^2, \Delta^2), \qquad (13)$$

where $Z = (Z_A - Z_B)/(Z_A + Z_B)$ and $\Delta = (r_B - r_A)/(r_B + r_A)$; a_0 is the Bohr radius; $D \simeq 0.7$ is a constant that is almost the same for all compounds.

TABLE I. Calculated charge-transfer contribution to the nonlinear optical susceptibility $\chi_{14}^{(2)} = 2d_{123}$ and the measured values of $\chi_{14}^{(2)}$ (both in units of 10^{-7} esu) for various semiconductors of zinc-blende structure. The values of Γ calculated directly on the basis of Eq. (11) are also shown.

Compound	Γ	$\chi_{14}^{(2)}$ (10^{-7} esu)	
		Calc	Expt[a]
InSb	4.03	40	33[b]
InAs	4.03	24	20[c]
GaSb	4.04	36	30[c]
GaAs	4.00	10	9[c]
GaP	4.03	6.2	5.2[c]
CdTe	4.00	7.1	8.0[d]
ZnTe	4.01	7.3	7.3[e]
ZnSe	4.01	3.0	2.2[e]
ZnS	4.04	1.7	1.7[e]

[a]The experimental error in the most favorable case is 20%.

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This last expression clearly shows how δ varies within a vertical family of compounds (III-V or II-VI) where Z is constant and Δ varies or within a horizontal (isoelectronic) series where mainly Z changes. The interplay of these two asymmetries determines δ for the sp^3 bonded compounds.

Putting now $C/E_h = X$, the expression (10) for $\chi_{14}^{(2)}$ can be written

$$\chi_{14}^{(2)} \sim \frac{X}{(1+X^2)^3} \qquad (14)$$

for an isoelectronic series, E_h is fixed, and only C varies. The maximum of (14) occurs at $X = \frac{1}{5}$ which corresponds to an ionicity[7] of $f_i \simeq 0.17$, near to that for the III-V compound. The experimental values confirm this. This method for identifying within a family of bonds that bond which has the maximum nonlinearity may well be applicable to more complicated polarizable units where both charge asymmetry and geometrical factors determine $\chi^{(2)}$; it may, therefore, be useful for finding materials with high values of $\chi^{(2)}$.

The numerical results shown in Table I could also be obtained with the bond-charge model.[4] The dielectric properties of the crystals are attributed in this model to the rigid movement of the point bond charge which is assumed located at the intersection of the covalent radii and its magnitude must be taken arbitraily the same for all the materials. The bonds are further assumed to be isotropic and the magnitude of this fictitious bonding charge is supposedly chosen to fit the linear properties of the crystal. The results were best fitted with the value $-0.5e$ for this charge,[12] which has, however, no relation to the bonding charge introduced by Phillips.[13] Since, however, this charge is taken as an adjustable parameter, the same results could be obtained for all compounds if its value was calculated by fitting the experimental value of $\chi_{14}^{(2)}$ for one compound. In the charge-transfer model presented here, the contribution due to the true bonding charge is negligibly small. Any relationship between the present charge-transfer model and the bonding charge model, if any, is perhaps due fortuitously to what may be called the Mulliken-Lowdin approximation[14] in the molecular-orbital description of the bonds. The rigid movement of the bonding charge also determines the sign of $\chi^{(2)}$ without any reference to the actual polarity or charge distribution of the bond. In order then to explain the reversal of the sign of $\chi^{(2)}$ observed[15] in compounds such as ZnO, additional adjustable parameters and assumptions had to be introduced.[5]

In the present approach, the sign of $\chi^{(2)}$ is determined by the actual over-all unperturbed valence charge distribution. For sp^3-bonded compounds considered above, the eight s and p electrons per unit cell contribute to the susceptibilities. More

valence charge within the bond is near atom A than atom B (metal atom) or the polarity of the static electronic dipole moment $\vec{\mu}$ due to charge transfer along the bond is pointed in the direction from A to B opposite to that of the applied electric field; therefore, the signs of C and ΔC in Eq. (9) are opposite to each other and the sign of $\chi_{14}^{(2)}$, which is proportional to $(-C\Delta C)$, is positive. This is consistent with the known molecular-orbital result[2,12] that the nonlinear bond polarizability $\beta_{\parallel}$ is positive if the polarity of the bond is opposite to the direction of the applied field.

However, this situation may change if d hybridization occurs; this will be the case when the atoms forming the bond are very different and in particular when one of the atoms is of the first or second row while the other is of the third or fourth row. The former have no d-core states near the sp^3 state while the latter do. In such a compound a situation analogous to the one encountered in crystal field or ligand theory will occur.[16] Because the energy separation between the d and the s, p states in third and fourth row atoms is small and the potential due to the first or second row atom is large the d-electron contribution in the third or fourth row atom will be enhanced. The d-core electrons of these atoms will be promoted to the valence level increasing the effective number of electrons which contribute to the dielectric properties of the compound in the frequency range considered. These additional electrons, however, will be localized mainly around the atom from which they originate. The addition of d-electron contribution on one atom but not the other leads to an added dipole moment along the bond pointed toward the other atom and will thus modify $\beta_{\parallel}$.

If in the bond AB atom A is of the third or fourth row, then the d electrons contribute to the dipole moment of the bond with the same sign as that due to the sp^3 states and similarly to the nonlinear susceptibilities; this will be the case for compounds such as BAs or AlSb. However, if atom B is of the third or fourth row then the polarity of the d-electron contribution will be opposite to that of the sp^3

states and may even reverse the sign of the polarity[17] and, hence, the sign of $\chi^{(2)}$; this appears to be the situation in the very skew compound ZnO.[18] It may also occur in the very ionic compound CuCl,[11] and may even, to a lesser extent, in InN and GaN.[19] In the case of CuCl, there is evidence for the contribution of the d states to the valence electron distribution on the basis of exciton spectrum studies.[20] There is no such evidence for the other compounds. It is likely also that the presence of d-core states, on only one of the atoms forming the bonds, with symmetry properties different from those of the sp^3 states will tend to favor instead structures distorted with respect to the zinc-blende structure. In particular the d-core electron contribution will be important to account for $\chi^{(2)}$ in the more complex structures like LiGaO$_2$[15] or other oxygen-bonded compounds.

No attempt is made here to evaluate the d-electron contributions to $\chi^{(2)}$. This would be a rather difficult problem and it can perhaps only be done on the basis of the molecular orbitals along the lines of the method outlined in Ref. 2. In fact the inclusion of the d electrons in the Phillips-van Vechten theory is still not well understood. This is reflected in particular in the deviations of the values of the parameters used there [e.g., b in Eq. (1)] for some of the compounds compiled by van Vechten.[7] One way to include the d-core electrons then seems to be to modify the ζ_i occurring in Eq. (1); another is to add one more oscillator strength in $\chi^{(1)}$ or writing $\chi^{(1)} = \chi_{sp}^{(1)} + \chi_d^{(1)}$. The sensitiveness of $\chi^{(2)}$ to the d hybridization makes this quantity a useful tool for testing various approaches. Furthermore, $\chi^{(2)}$ provides information about the polarity of the bonds.

The approach outlined here may well be relevant to the calculation of second-order polarizabilities of molecules both in their ground and excited states or conversely, from an experimental study of β to define an electronegativity difference or polarity of such states.

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(Oxford U. P., Oxford, England, 1961), Sec. 4.9; Ref. 2, Fig. 2. Atom B represents the metal atom and the positive direction of the reference axis is directed from B to A.

[9]Here we do not include explicitly the effective field correction; part of this correction is contained implicitly in the macroscopic parameters in the final expression for $\chi^{(2)}$. To allow for it completely is difficult in the present simple model.

[10]See Ref. 2; $\beta_{\parallel} \gg \beta_{\perp}$ reflects the fact that the electronic distribution of the atoms forming the bond changes mainly along the bond axis while the charge distribution transversally to the bond axis tends to retain that of the atom with spherical symmetry. For an isolated atom $\beta \equiv 0$.

[11]J. Ducuing and Chr. Flytzanis, in *Optical Properties of Solids*, edited by F. Abeles (North-Holland, Amsterdam, 1970), Sec. 3.3 and the appendices; for CuCl see Sec. 3.3.

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[19]In all these compounds (ZnO, CuCl, InN, and GaN) the electronegativity difference ΔX (Pauling) is larger than unity or $\Delta X > 1$; for the zinc-blende compounds considered in Table I on the other hand $\Delta X < 1$. This separation in two classes with $\chi^{(2)} < 0$ if $\Delta X > 1$ and $\chi^{(2)} > 0$ if $\Delta X < 1$, however, seems to be more general (compare BeO).

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Analytical Solutions of the Boltzmann Transport Equation. I. Carrier Transport Phenomena in Nondegenerate Semiconductors at Low Fields

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By expressing the carrier distribution function in a power series, a self-consistent method is presented for solving analytically the Boltzmann transport equation. Using an iterative technique, this method enables the calculation of carrier mobilities in nondegenerate semiconductors to any desired degree of accuracy at fields of any strengths. A "mesh" diagram is proposed for the calculation of the low-field mobilities governed by polar-optical scattering. It is shown that the results obtained by relaxation-time approximation under some conditions are rather poor. The effect of applied magnetic field is also discussed in some detail.

I. INTRODUCTION

The theory of carrier transport phenomena in semiconductors lies on the determination of the carrier distribution function f which is governed by the applied field $\vec{\xi}$, and the scattering of the carriers with the carriers and the lattice vibrations. In the steady state these effects are balanced in accordance with the Boltzmann equation

$$e\vec{\xi} \cdot \frac{\partial f(\vec{p})}{\partial \vec{p}} + \sum_{\vec{p}} W(\vec{p} \to \vec{p}')f(\vec{p}) - \sum_{\vec{p}'} W(\vec{p}' \to \vec{p})f(\vec{p}')$$

$$+ L_{ee} f(\vec{p}) = 0 , \qquad (1)$$

where e is the electronic charge, $W(\vec{p} \to \vec{p}')$ is the transition probability per unit time of a carrier in

a state with momentum $\vec{p}$ being scattered into a state with momentum $\vec{p}'$ by the lattice vibrations, and L_{ee} is the probability per unit time of a carrier being scattered by another carrier. Thus each term in this equation represents a rate of change of f; the term $e\vec{\xi} \cdot \partial f(\vec{p})/\partial \vec{p}$ is due to the applied field $\vec{\xi}$, the terms $\sum_{\vec{p}'} W(\vec{p} \to \vec{p}')f(\vec{p})$ and $\sum_{\vec{p}'} W(\vec{p}' \to \vec{p})f(\vec{p}')$ are, respectively, due to the carriers being scattered out of and into state $\vec{p}$ through the absorption or emission of phonons, and the term $L_{ee} f(\vec{p})$ is due to the carrier-carrier scattering. Since there is no net carrier transport in the absence of external fields, the equilibrium distribution function can be assumed to be the Maxwell-Boltzmann function for nondegenerate semiconductors when $\vec{\xi} = 0$.