Concentration-dependent dielectric response of $Ga_{1-x}Al_xAs$

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The dielectric properties of the semiconductor $Ga_{1-x}Al_xAs$ are of importance in the study of electronic states and charge conduction. In this paper we present analytical composition-dependent spatial dielectric functions for $Ga_{1-x}Al_xAs$ involving compositions from $x=0.05$ to $x=0.45$ in steps of 0.05. The spatial dielectric functions we present describe the response of $Ga_{1-x}Al_xAs$ to charges of $Z=\pm1, \pm2$ (in atomic units) embedded in the semiconductor.

I. INTRODUCTION

The semiconductor $Ga_{1-x}Al_xAs$ has received and continues to receive a great deal of attention. The reason is that, in conjunction with GaAs, superlattices can be formed which present a unique opportunity for the study of electronic states[1] and charge conduction.[2] For this reason the dielectric properties of $Ga_{1-x}Al_xAs$ are of fundamental importance. In this paper we present analytical composition-dependent spatial dielectric functions for this semiconductor. We have considered the composition of $x=0.05$ to $x=0.45$ in steps of 0.05, and the response to charges of $Z=\pm1, \pm2$ (in atomic units).

II. THEORETICAL BACKGROUND

The spatial dielectric function of an undoped semiconductor describes the response of the valence electrons to a point charge placed into the crystal lattice. The response consists of a rearrangement of the valence electrons that results in the shielding of the potential of the charge.

A few years ago Resta[3] formulated a Thomas-Fermi (TF) approach for obtaining an isotropic spatial dielectric function of a semiconductor. In a subsequent work Cornolti and Resta[4] have numerically solved the nonlinear TF equation for the potential and presented the spatial dielectric functions in the form of graphs for point charges $Z=\pm1, \pm4$ embedded in undoped diamond, Si, and Ge.

In order to obtain analytical spatial dielectric functions, Csavinszky and Brownstein[5] formulated a variational approach by which the nonlinear TF equation can be solved approximately. In their work they have considered point charges $Z=+1, +2, +3$, and $+4$ in undoped diamond, Si, and Ge. In a subsequent work, Csavinszky and Brownstein[6] extended their variational approach to point charges $Z=-1, -2, -3$, and -4, again in undoped diamond, Si, and Ge. In another paper,[7] the variational approaches of Refs. 5 and 6 have been applied to GaAs, and site-dependent spatial dielectric functions have been obtained. In the above work, point charges $Z=\pm0.16, \pm1.16$, and ±0.84 have been considered. The charges $Z=+0.16$ and $Z=-0.16$ are the effective charges[8] due to the partial ionicity of the chemical bonds on a Ga and As site, respectively. The charge $Z=+0.84$ corresponds to a column VI donor on an As site, that of $Z=+1.16$ to a column IV donor on a Ga site. Similarly, the charge $Z=-1.16$ corresponds to a column IV acceptor on an As site, that of $Z=-0.84$ to a column II acceptor on a Ga site.

In the present work, the site dependence of the spatial dielectric function of $Ga_{1-x}Al_xAs$ is not considered since, to our knowledge, no data are available on the composition-dependent partial ionicity of the sites in $Ga_{1-x}Al_xAs$. In what follows, atomic units ($\hbar=1$, $m=1$, $e^2=1$) will be used. In Sec. II A we discuss positive point charges, and in Sec. II B negative point charges.

A. Positive point charges

The spatial dielectric function $\bar{\epsilon}_n(r)$ is defined[3] by

$$V(r)=-\frac{Z}{\bar{\epsilon}_n(r)r}, \quad 0<r\leq R_n , \tag{1}$$

where R_n is a screening radius beyond which the screening of the charge is complete, and $V(r)$, the potential energy of the charge, is the solution[4] of

$$\nabla^2 V(r)=\begin{cases} a\{E_F^{3/2}-[E_F+A-V(r)]^{3/2}\}, & 0<r\leq R_n \\ 0, & R_n\leq r<\infty \end{cases} . \tag{2}$$

The boundary conditions that V must obey are discussed elsewhere.[4] In Eqs. (1) and (2) the subscript n refers to the word nonlinear, while in Eq. (2) the constants a and A are defined[3] by $a=2^{7/2}/3\pi$ and $A=V(R_n)$. The quantity E_F denotes the valence Fermi energy, which is related to the valence Fermi momentum k_F by $E_F=k_F^2/2$. The latter is calculated from $k_F=(3\pi^2 n_0)^{1/3}$, where n_0 is the density of the valence electrons. In our calculation of n_0, due to lack of data, we have neglected the very slight composition dependence of the size of the $Ga_{1-x}Al_xAs$ unit cube, i.e., we have assumed that $Ga_{1-x}Al_xAs$ has the same size unit cube as GaAs. In calculating n_0 we have used a unit cube side[9] of $10.684a_B$ (a_B is the Bohr radius), and considered that it contains eight atoms,[10] with a Ga or an Al atom contributing three electrons, and an As atom contributing five electrons. The value of the valence Fermi momentum used in our calculations is $k_F=0.92a_B^{-1}$.

In the variational approach of Csavinszky and Brownstein,[5] Eq. (1) is rewritten by the substitution

$$\psi(r)=r[V(r)-A] . \tag{3}$$

The resulting differential equation,

$$\psi''=\begin{cases} a[rE_F^{3/2}-r(E_F-\psi/r)^{3/2}], & 0<r\leq R_n \\ 0, & R_n\leq r<\infty \end{cases} , \tag{4}$$

is then solved by an equivalent variational principle. As before,[5] in the $0<r\leq R_n$ interval we have used the trial

TABLE I. Parameters entering into the spatial dielectric function of $Ga_{1-x}Al_xAs$ for the case of $Z=+1$.

x	$\epsilon(0)$	R_n (a.u.)	r_0 (a.u.)	λ
0.05	12.95	4.27	0.25	0.15
0.10	12.80	4.26	0.25	0.15
0.15	12.65	4.25	0.25	0.15
0.20	12.50	4.24	0.25	0.15
0.25	12.35	4.22	0.25	0.15
0.30	12.20	4.21	0.25	0.15
0.35	12.05	4.19	0.25	0.15
0.40	11.90	4.17	0.25	0.15
0.45	11.75	4.16	0.25	0.15

function

$$\psi(r)=[(1-\lambda)+\lambda e^{-r/r_0}]\left[-\frac{Z\sinh[q(R_n-r)]}{\sinh(qR_n)}\right], \quad (5)$$

where $q=(4k_F/\pi)^{1/2}$, and r_0 and R_n are variational parameters. As shown elsewhere,[5] the parameter λ is obtained by imposing a matching condition of $\psi'(r)$ at $r=R_n$. This leads to the expression

$$\lambda=\left[1-\frac{\sinh(qR_n)}{\epsilon(0)qR_n}\right]\frac{1}{1-e^{-R_n/r_0}}, \quad (6)$$

where $\epsilon(0)$ is the static dielectric constant of $Ga_{1-x}Al_xAs$. This quantity is given[1] by

$$\epsilon(0)=13.1(1-x)+10.1x . \quad (7)$$

Finally, the spatial dielectric function $\bar{\epsilon}_n(r)$, as defined by Eqs. (1) and (3), is given by

$$\bar{\epsilon}_n(r)=-\frac{Z}{\psi(r)+rA} . \quad (8)$$

Using $A=V(R_n)$, and Eq. (6), we find that Eq. (8) becomes

$$\bar{\epsilon}_n(r)=\left\{[(1-\lambda)+\lambda e^{-r/r_0}]\left[\frac{\sinh[q(R_n-r)]}{\sinh(qR_n)}+\frac{r}{\epsilon(0)R_n}\right]\right\}^{-1} . \quad (9)$$

The values of the parameters $\epsilon(0)$, λ, R_n, and r_0, for charges $Z=+1$, $+2$, for different values of x, are listed in Tables I and II.

TABLE II. Parameters entering into the spatial dielectric function of $Ga_{1-x}Al_xAs$ for the case of $Z=+2$.

x	$\epsilon(0)$	R_n (a.u.)	r_0 (a.u.)	λ
0.05	12.95	4.17	0.25	0.22
0.10	12.80	4.15	0.25	0.22
0.15	12.65	4.14	0.25	0.22
0.20	12.50	4.13	0.25	0.22
0.25	12.35	4.11	0.25	0.22
0.30	12.20	4.10	0.25	0.22
0.35	12.05	4.08	0.25	0.22
0.40	11.90	4.07	0.25	0.22
0.45	11.75	4.05	0.25	0.22

TABLE III. Parameters entering into the spatial dielectric function of $Ga_{1-x}Al_xAs$ for the case of $Z=-1$.

x	$\epsilon(0)$	R_n (a.u.)	r_0 (a.u.)	λ	R_c (a.u.)
0.05	12.95	4.89	0.86	−0.45	1.03
0.10	12.80	4.89	0.90	−0.47	1.03
0.15	12.65	4.89	0.94	−0.49	1.03
0.20	12.50	4.89	0.98	−0.51	1.03
0.25	12.35	4.88	0.99	−0.51	1.03
0.30	12.20	4.88	1.04	−0.53	1.03
0.35	12.05	4.87	1.04	−0.53	1.03
0.40	11.90	4.85	1.04	−0.53	1.03
0.45	11.75	4.84	1.05	−0.54	1.03

B. Negative point charges

The spatial dielectric function $\bar{\epsilon}_n(r)$ is defined again by Eq. (1), where $V(r)$ is now the solution[4] of

$$\nabla^2 V(r)=\begin{cases} aE_F^{3/2}, & 0<r\leq R_c \\ a\{E_F^{3/2}-[E_F+A-V(r)]^{3/2}\}, & R_c\leq r\leq R_n \\ 0, & R_n\leq r<\infty . \end{cases} \quad (10)$$

The boundary conditions that V must obey are discussed elsewhere.[4] In Eq. (10) the quantity R_c denotes the radius of the Coulomb hole, determined[4] from

$$E_F+A-V(R_c)=0 , \quad (11)$$

while the other quantities have their previous meaning.

In the variational approach of Csavinszky and Brownstein[6], Eq. (10) is rewritten with the aid of Eq. (3) as

$$\psi''=\begin{cases} arE_F^{3/2}, & 0<r\leq R_c \\ a[rE_F^{3/2}-r(E_F-\psi/r)^{3/2}], & R_c\leq r\leq R_n \\ 0, & R_n\leq r<\infty , \end{cases} \quad (12)$$

and solved by an equivalent variational principle.

As before,[6] in the $0<r\leq R_n$ interval, we have used the trial function displayed in Eq. (5). A matching condition on

TABLE IV. Parameters entering into the spatial dielectric function of $Ga_{1-x}Al_xAs$ for the case of $Z=-2$.

x	$\epsilon(0)$	R_n (a.u.)	r_0 (a.u.)	λ	R_c (a.u.)
0.05	12.95	5.29	1.76	−1.14	1.52
0.10	12.80	5.29	1.81	−1.15	1.52
0.15	12.65	5.29	1.87	−1.21	1.52
0.20	12.50	5.29	1.92	−1.22	1.52
0.25	12.35	5.29	1.98	−1.28	1.52
0.30	12.20	5.29	2.05	−1.31	1.52
0.35	12.05	5.29	2.11	−1.35	1.52
0.40	11.90	5.29	2.18	−1.39	1.52
0.45	11.75	5.29	2.26	−1.39	1.52

$\psi'(r)$ at $r = R_n$ leads again to Eq. (6).

The values of the parameters $\epsilon(0)$, λ, R_n, r_0, and R_c, for charges $Z = -1, -2$, for different values of x, are displayed in Tables III and IV.

III. CONCLUDING REMARKS

Inspection of Tables I–IV shows that, with the exception of Table IV, the screening radius R_n is a slowly decreasing function of x. Inspection of Tables I and II shows that the other variational parameter r_0 is not affected by x, and it is the same for charges $Z = +1$ and $+2$. In contrast to this, comparison of Tables III and IV reveals that r_0 for $Z = -1$ is quite different from r_0 for $Z = -2$, and that in each case the r_0 values show a dependence on x. It is also seen from Tables III and IV that the R_c values are quite different for different negative charges, but in each case they do not show an x dependence.

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