PHYSICAL REVIEW B VOLUME 29, NUMBER 4 15 FEBRUARY 1984

# Reflectivity of a nonlocal dielectric with an excitonic surface potential

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(Received 11 July 1983)

The reflectivity of a semi-infinite nonlocal dielectric is investigated theoretically, including the effect of the surface potential and without invoking the simplifying dead-layer approximation. This is achieved by integrating the exciton equation of motion in the presence of the repulsive, spatially varying, surface potential together with Maxwell's equations. The method is developed for both $s$ and $p$ polarizations, and the results of numerical calculations of the reflectivity of CdS and ZnSe are presented.

## I. INTRODUCTION

In their discussion of the optical properties of nonlocal dielectrics Hopfield and Thomas[1] suggested that the effect of the surface could be represented by a repulsive potential $U(z)$ which acts on the exciton in the vicinity of the surface. The geometry of a semi-infinite spatially dispersive dielectric at $z>0$ is assumed. Since they found the solution of the resulting differential equations containing a spatially varying term $U(z)$ to be difficult, Hopfield and Thomas replaced the potential by an infinite potential barrier a finite distance $d$ inside the crystal. With this simplifying assumption there are three spatial regions in which one has to solve the equations: Outside the dielectric ($z<0$), in the exciton-free layer ($0<z<d$), and in the spatially dispersive region ($z>d$). After obtaining the solutions in the three regions one has to match fields at the boundaries. At $z=0$ the usual Maxwell boundary conditions suffice, but at $z=d$ additional boundary conditions (ABC's) have to be specified. Much effort has been invested in discussions of the merits or deficiencies of the various possible choices of these ABC's.[2-16] Some of the arguments were based on pure theoretical considerations (e.g., energy conservation) and some relied on fitting experimental data from optical experiments. In many works the further simplification of ignoring the dead layer altogether has been invoked and the ABC's were applied directly at $z=0$.

Our purpose here is to return to the original formulation of Hopfield and Thomas[1] and to solve the exciton equation of motion together with Maxwell's equations without replacing the spatially varying potential $U(z)$ by a step function. In this way we dispense with the need of specifying the ABC's at a fictitious interface as is done in the dead-layer approximation at $z=d$. We perform a direct integration of the set of differential equations, starting at some large $z$ deep in the bulk and advancing towards the surface of the dielectric, $z=0$. At this surface we will still need an ABC, but here, in view of the repulsive nature of the potential $U(z)$, the obvious choice is the vanishing of the excitonic polarization, i.e., the Pekar ABC.

Since Hopfield and Thomas have explicitly stated that the theory of excitons in the surface region must be completed by actually solving the differential equations with a spatially varying potential $U(z)$, it is somewhat surprising that this approach has almost been neglected, while numerous works were devoted to the ABC problem. Important exceptions are the recent works of Sakoda,[17] Kiselev,[18] and Balslev,[19,20] in which various forms of surface potentials were included in the calculations. However, in these investigations only the case of $s$ polarization was considered and reflectivity calculations were performed for normal incidence only. Perhaps this was due to the fact that Hopfield and Thomas[1] formulated the basic system of differential equations containing the surface potential for $s$ polarization only. We develop here an analogous set of equations for the more complex case of $p$ polarization. We then present a systematic method for integrating the equations for both polarizations and for calculating the corresponding reflectivities at oblique incidence.

## II. BULK SOLUTIONS

We now define the model dielectric and recall some of the well-known properties of its bulk solutions, i.e., the exciton-polariton modes of the infinite homogeneous solid. Starting from these solutions we will subsequently build up the solutions for the semi-infinite dielectric.

The dielectric under consideration has a dielectric constant

$$\epsilon(\omega,q)=\epsilon_0+\frac{\omega_p^2}{\omega_T^2-\omega^2+Dq^2-i\omega\gamma} . \tag{1}$$

Here $\epsilon_0$ is the background dielectric constant, $\omega_T$ is the frequency of the transverse resonance, $\omega_p$ is a measure of the oscillator strength, and $\gamma$ is the damping constant. Spatial dispersion enters through the term $Dq^2$, with $D=\hbar\omega_T/M$, where $M$ is the exciton mass.

At any given frequency $\omega$ there exist three different modes. There are two transverse modes, which are obtained from the dispersion relation

$$c^2q^2/\omega^2=\epsilon(\omega,q) . \tag{2}$$

We assume, without loss of generality, that the exciton-polariton wave vector lies in the $x$-$z$ plane so that $q^2=q_x^2+q_z^2$. For given $\omega$ and $q_x$, (2) is a quadratic equation in $q_z^2$. The roots, which will be denoted by $q_1$ and $q_2$, are given by

 

$$q_{1,2}^2=\tfrac{1}{2}\left\{\Gamma_B^2+\epsilon_0\frac{\omega^2}{c^2}-q_x^2 \pm\left[\left[\Gamma_B^2-\epsilon_0\frac{\omega^2}{c^2}+q_x^2\right]^2+\frac{4\omega_p^2\omega^2}{c^2D}\right]^{1/2}\right\}, \tag{3}$$

where

$$\Gamma_B^2=(\omega^2-\omega_T^2-Dq_x^2+i\omega\gamma)/D . \tag{4}$$

The third bulk mode is longitudinal, defined by

$$\epsilon(\omega,q)=0 . \tag{5}$$

For given $\omega$ and $q_x$ we can obtain $q_z$ from (5). The solution, which will be denoted by $q_L$, is given by

$$q_L^2=\Gamma_B^2-\frac{\omega_p^2}{\epsilon_0 D} . \tag{6}$$

## III. REFLECTIVITY OF SEMI-INFINITE DIELECTRIC

We now consider the semi-infinite dielectric occupying the half-space $z>0$. The effects of the surface will be represented by a repulsive potential $U(z)$ acting on the exciton. The exciton equation of motion in the presence of this potential is[1]

$$\left[\omega^2-\omega_T^2+i\omega\gamma+D\nabla^2-2\frac{\omega_T U(z)}{\hbar}\right]\vec{P}=-\frac{\omega_p^2}{4\pi}\vec{E} . \tag{7}$$

Assuming an $\exp(iq_x x)$ $x$ dependence of the fields this assumes the form

$$\left[\frac{\partial^2}{\partial z^2}+\Gamma^2(z)\right]\vec{P}(z)=-\frac{\omega_p^2}{4\pi D}\vec{E}(z) , \tag{8}$$

where only the $z$-dependent parts of the fields have been retained. Here

$$\Gamma^2(z)=\left[\omega^2-\omega_T^2-Dq_x^2+i\omega\gamma-2\frac{\omega_T U(z)}{\hbar}\right]\Big/D . \tag{9}$$

If we discard the surface potential term, $\Gamma^2(z)$ reduces to the bulk value $\Gamma_B^2$ of Eq. (4).

We will solve the exciton equation of motion (8) together with Maxwell's equations and then match the internal solutions with the fields outside the dielectric to obtain the reflectivity. The external fields consist of incident and reflected waves. The angle of incidence is denoted by $\theta$ and the wave vector of the incident field is again assumed to lie in the $x$-$z$ plane, so that its components are $k_x=k\sin\theta$ and $k_z=k\cos\theta$, where $k=\omega/c$. Of course, the wave-vector component parallel to the surface is conserved, so that $k_x=q_x$, and all the fields have a common $\exp(iq_x x)$ factor.

By eliminating $\vec{H}$ from the Maxwell equations

$$\vec{\nabla}\times\vec{H}=-i\frac{\omega}{c}\vec{D} , \tag{10}$$

$$\vec{\nabla}\times\vec{E}=i\frac{\omega}{c}\vec{H} , \tag{11}$$

and using the relation

$$\vec{D}=\epsilon_0\vec{E}+4\pi\vec{P} , \tag{12}$$

we obtain

$$\vec{\nabla}\times\vec{\nabla}\times\vec{E}=\frac{\omega^2}{c^2}(\epsilon_0\vec{E}+4\pi\vec{P}) . \tag{13}$$

Equations (8) and (13) form the system of differential equations to be solved. We now describe the method of solution for the two independent polarizations.

### A. *s* polarization

The excitonic polarization and the corresponding electric field have $y$ components only and Eqs. (8) and (13) reduce to

$$\left[\frac{\partial^2}{\partial z^2}+\Gamma^2(z)\right]P_y(z)=-\frac{\omega_p^2}{4\pi D}E_y(z) , \tag{14}$$

$$\left[q_x^2-\epsilon_0\frac{\omega^2}{c^2}-\frac{\partial^2}{\partial z^2}\right]E_y(z)=4\pi\frac{\omega^2}{c^2}P_y(z) . \tag{15}$$

We integrate these two equations numerically, starting from some large enough $z=z_0$ outside the range of the surface potential $U(z)$ and advancing toward the surface $z=0$. As discussed above, there exist in the bulk two independent $s$-polarized exciton-polariton modes. We therefore perform the integration twice with two different sets of initial conditions at $z=z_0$. The first set is derived from bulk fields

$$P_y(z)=e^{iq_1z} , \tag{16}$$

$$E_y(z)=\frac{4\pi D}{\omega_p^2}(q_1^2-\Gamma_B^2)e^{iq_1z} , \tag{17}$$

and the second one is derived from

$$P_y(z)=e^{iq_2z} , \tag{18}$$

$$E_y(z)=\frac{4\pi D}{\omega_p^2}(q_2^2-\Gamma_B^2)e^{iq_2z} . \tag{19}$$

Here $q_1$ and $q_2$ are the two bulk values of $q_z$ defined by Eq. (3), and $\Gamma_B^2$, given by (4), is the bulk value of $\Gamma^2(z)$.

We denote the solutions which have an $e^{iq_1z}$ behavior in the bulk by $P_{y1}(z)$ and $E_{y1}(z)$, and those with an $e^{iq_2z}$ bulk behavior we denote by $P_{y2}(z)$ and $E_{y2}(z)$. The general solution will be a combination of the form

$$P_y(z)=A_1P_{y1}(z)+A_2P_{y2}(z) , \tag{20}$$

$$E_y(z)=A_1E_{y1}(z)+A_2E_{y2}(z) . \tag{21}$$

We determine the ratio $A_1/A_2$ numerically by applying the Pekar[21] ABC, $P_y(0)=0$, at the surface of the solid. This is the natural choice of an ABC at a surface near which there exists a repulsive potential.[19] The boundary condition gives

$$\frac{A_1}{A_2}=-\frac{P_{y2}(0)}{P_{y1}(0)} . \tag{22}$$

The incident and reflected fields outside the dielectric are of the form

$$E_y^i=E_0e^{i(k_xx+k_zz)} , \tag{23}$$

$$E_y^r = E_R e^{i(k_x x - k_z z)} . \quad (24)$$

Applying the usual continuity conditions on the tangential components of the electric and magnetic fields at $z=0$ we obtain

$$E_0 + E_R = A_1 E_{y1}(0) + A_2 E_{y2}(0) , \quad (25)$$

$$ik_z(E_0 - E_R) = A_1 E'_{y1}(0) + A_2 E'_{y2}(0) , \quad (26)$$

from which it follows that

$$\frac{E_R}{E_0} = \frac{ik_z\left[\frac{A_1}{A_2}E_{y1}(0)+E_{y2}(0)\right] - \left[\frac{A_1}{A_2}E'_{y1}(0)+E'_{y2}(0)\right]}{ik_z\left[\frac{A_1}{A_2}E_{y1}(0)+E_{y2}(0)\right] + \left[\frac{A_1}{A_2}E'_{y1}(0)+E'_{y2}(0)\right]} . \quad (27)$$

Thus, once we have performed the numerical integration of Eqs. (14) and (15), we get the reflectivity

$$R = |E_R/E_0|^2 \quad (28)$$

from (27) and (22).

### B. $p$ polarization

In this case the nonvanishing components of the excitonic polarization and the electric field are $P_x$, $P_z$, $E_x$, and $E_z$. The $x$ and $z$ components of Eqs. (8) and (13) are

$$E_x = -\frac{4\pi D}{\omega_p^2}\left[\frac{\partial^2}{\partial z^2} + \Gamma^2(z)\right] P_x , \quad (29)$$

$$E_z = -\frac{4\pi D}{\omega_p^2}\left[\frac{\partial^2}{\partial z^2} + \Gamma^2(z)\right] P_z , \quad (30)$$

$$iq_x \frac{\partial E_z}{\partial z} - \left[\frac{\partial^2}{\partial z^2} + \epsilon_0 \frac{\omega^2}{c^2}\right] E_x - 4\pi \frac{\omega^2}{c^2} P_x = 0 , \quad (31)$$

$$iq_x \frac{\partial E_x}{\partial z} + \left[q_x^2 - \epsilon_0 \frac{\omega^2}{c^2}\right] E_z - 4\pi \frac{\omega^2}{c^2} P_z = 0 . \quad (32)$$

These four equations can be reduced to two equations for $P_x$ and $P_z$, which can readily be integrated numerically by substituting $E_x$ and $E_z$ from (29) and (30) into (31) and (32). This gives

$$\frac{\partial^4 P_x}{\partial z^4} + \left[\Gamma^2(z) + \epsilon_0 \frac{\omega^2}{c^2}\right] \frac{\partial^2 P_x}{\partial z^2} + 2\frac{\partial \Gamma^2}{\partial z}\frac{\partial P_x}{\partial z} + \left[\epsilon_0 \frac{\omega^2}{c^2}\Gamma^2(z) + \frac{\partial^2 \Gamma^2}{\partial z^2} - \frac{\omega^2 \omega_p^2}{Dc^2}\right] P_x - iq_x \left[\frac{\partial^3 P_z}{\partial z^3} + \Gamma^2(z)\frac{\partial P_z}{\partial z} + \frac{\partial \Gamma^2}{\partial z} P_z\right] = 0 , \quad (33)$$

$$iq_x \left[\frac{\partial^3 P_x}{\partial z^3} + \frac{\partial \Gamma^2}{\partial z} P_x + \Gamma^2(z) \frac{\partial P_x}{\partial z}\right] + \left[q_x^2 - \epsilon_0 \frac{\omega^2}{c^2}\right] \frac{\partial^2 P_z}{\partial z^2} + \left[\frac{\omega^2 \omega_p^2}{Dc^2} + \left[q_x^2 - \epsilon_0 \frac{\omega^2}{c^2}\right] \Gamma^2(z)\right] P_z = 0 . \quad (34)$$

We integrate these two coupled equations numerically three times, starting with three different initial conditions at $z=z_0$ in the bulk. We obtain two transverse solutions by using the initial conditions corresponding to

$$\vec{P}(z) = (q_i, 0, -q_x) e^{iq_i z} , \quad i = 1,2 \quad (35)$$

where $q_i$ are again the bulk values given by (3). We obtain a longitudinal solution by starting at $z_0$ with the longitudinal bulk mode

$$\vec{P}(z) = (q_x, 0, q_L) e^{iq_L z} , \quad (36)$$

where $q_L$ is given by (6).

We denote the solution with an $e^{iq_1 z}$ bulk behavior by $\vec{P}_1(z) = (P_{x1}, 0, P_{z1})$, the solution with an $e^{iq_2 z}$ behavior by $\vec{P}_2(z) = (P_{x2}, 0, P_{z2})$ and the longitudinal solution by $\vec{P}_L(z) = (P_{xL}, 0, P_{zL})$. The general solution will be a combination of the form

$$\vec{P}(z) = A_1 \vec{P}_1(z) + A_2 \vec{P}_2(z) + A_L \vec{P}_L(z) . \quad (37)$$

Applying the Pekar ABC $\vec{P}(0) = 0$ we obtain the two amplitude ratios

$$\frac{A_2}{A_1} = \frac{P_{z1}(0)P_{xL}(0) - P_{x1}(0)P_{zL}(0)}{P_{x2}(0)P_{zL}(0) - P_{z2}(0)P_{xL}(0)} , \quad (38)$$

$$\frac{A_L}{A_1} = \frac{P_{z2}(0)P_{x1}(0) - P_{x2}(0)P_{z1}(0)}{P_{x2}(0)P_{zL}(0) - P_{z2}(0)P_{xL}(0)} . \quad (39)$$

The $p$-polarized external fields are given by the sum of an incident and a reflected wave of the form

$$\vec{E}^i = E_0 \left[1, 0, -\frac{k_x}{k_z}\right] e^{i(k_x x + k_z z)} , \quad (40)$$

$$\vec{E}^r = E_R \left[1, 0, \frac{k_x}{k_z}\right] e^{i(k_x x - k_z z)} . \quad (41)$$

The Maxwell boundary conditions at the surface give

$$E_0 + E_R = A_1 E_{x1}(0) + A_2 E_{x2}(0) + A_L E_{xL}(0) , \quad (42)$$

$$ik^2(E_0 - E_R) = k_z\{A_1 E'_{x1}(0) + A_2 E'_{x2}(0) - ik_x[A_1 E_{z1}(0) + A_2 E_{z2}(0)]\} , \quad (43)$$

so that the ratio of reflected to incident amplitudes is

$$\frac{E_R}{E_0} = \frac{ik^2\left[\frac{A_2}{A_1}E_{x2}(0) + E_{x1}(0) + \frac{A_L}{A_1}(E_{xL}(0)\right] - k_z\left[\frac{A_2}{A_1}E'_{x2}(0) + E'_{x1}(0) - ik_x\left[\frac{A_2}{A_1}E_{z2}(0) + E_{z1}(0)\right]\right]}{ik^2\left[\frac{A_2}{A_1}E_{x2}(0) + E_{x1}(0) + \frac{A_L}{A_1}E_{xL}(0)\right] + k_z\left[\frac{A_2}{A_1}E'_{x2}(0) + E'_{x1}(0) - ik_x\left[\frac{A_2}{A_1}E_{z2}(0) + E_{z1}(0)\right]\right]} . \quad (44)$$

The components of the electric fields and their derivatives appearing in the last equation are calculated by (29) and (30) from the corresponding components of the polarizations which follow from the numerical integration of Eqs. (33) and (34).

## IV. NUMERICAL CALCULATIONS

We have performed reflectivity calculations using the method developed in Sec. III. For the repulsive potential we have used the simple exponential form

$$U(z)=\hbar\omega_B e^{-z/a} . \tag{45}$$

This potential is characterized by two parameters: $\hbar\omega_B$, the height at $z=0$, and $a$, which provides a measure of its spatial extent. As discussed by Balslev, $\omega_B$ is taken to be of the order of $\omega_{LT}=\omega_L-\omega_T$, the longitudinal-transverse splitting of the excitons of zero wave vector, and $a$ will be of the order of 50 Å.

In the numerical integration of the differential equations we start from a point $z=z_0$ inside the solid, at which the effect of the potential $U(z)$ is negligible. In our numerical work we have found that the calculated reflectivities were practically independent of the choice of $z_0$ provided that $z_0>5a$.

First, we calculated the normal incidence reflectivity for the $A_{n=1}$ exciton of CdS. The values used for $\omega_T$ and $\omega_L$ were those measured by Yu and Evangelisti[22] by the Brillouin scattering technique. These were converted to energies by Halevi and Hernandez-Cocoletzi,[16] who carefully included the index of refraction of air to obtain $\omega_T=2.5520$ eV and $\omega_L=2.5538$ eV. Other CdS data used in the calculation are[23] $M=0.94m$, $\epsilon_0=8.0$, $\gamma=0.15$ meV. We have chosen $\omega_B/\omega_T=0.003$ for the strength of the surface potential and varied the parameter $a$, which characterizes the width of the surface barrier. The calculated reflectivities for $a=40$ and 60 Å are shown in Fig. 1, in which the reflectivity of the homogeneous semi-infinite dielectric [(i.e., with $U(z)=0$] is also shown, for

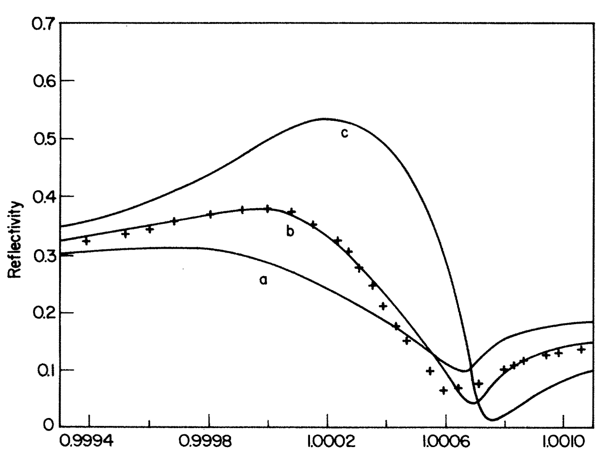


FIG. 1. Normal incidence reflectivity of CdS: $a$, with $\omega_B/\omega_T=0.003$, $a=60$ Å; $b$, with $\omega_b/\omega_T=0.003$, $a=40$ Å; $c$, without a surface potential. Crosses denote the experimental data of Patella *et al.* (Ref. 9).

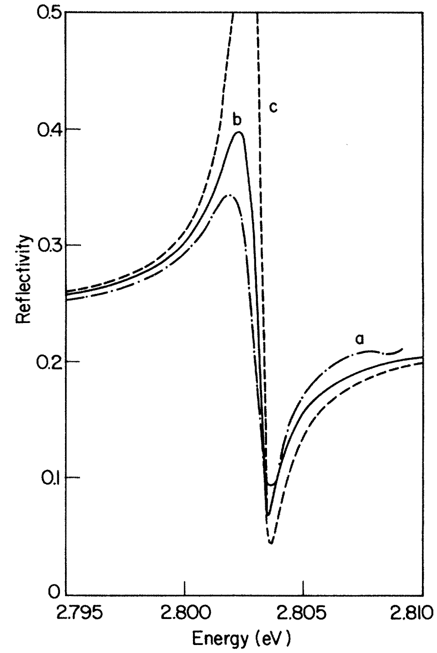


FIG. 2. Normal incidence reflectivity of ZnSe: $a$, experimental data of Tokura *et al.* (Ref. 24); $b$, calculated without a surface potential; $c$, calculated by the local theory.

comparison. The measured reflectivity data of Patella *et al.*[9] are shown by the crosses. We find that the choice of $a=40$ Å yields good agreement with the experimental results.

All further calculations in the present work will refer to ZnSe, which is isotropic and hence convenient for calculations of the reflectivity at nonnormal incidence. For the optical parameters of ZnSe we use the values[23,24] $\omega_T=2.8022$ eV, $\omega_L=2.8034$ eV, $\gamma=0.4$ meV,

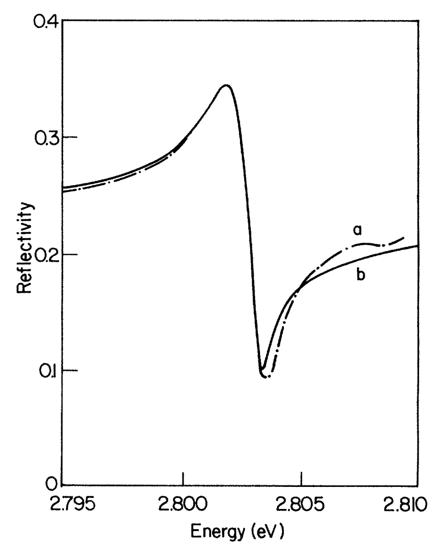


FIG. 3. Normal incidence reflectivity of ZnSe: $a$, experimental data of Tokura *et al.* (Ref. 24); $b$, calculated with $\omega_B/\omega_T=0.8\times10^{-3}$, $a=50$ Å.

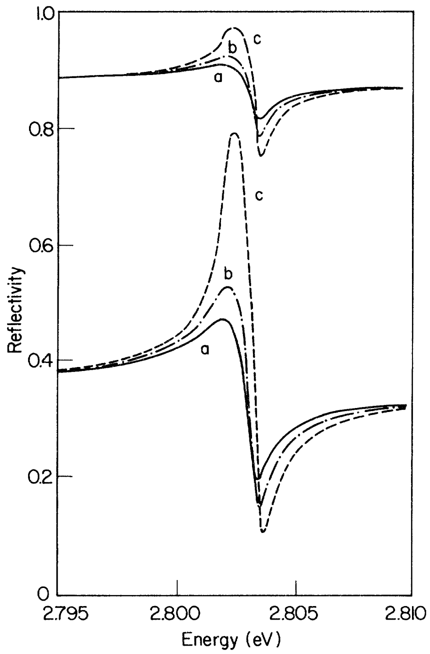


FIG. 4. Calculated reflectivity of ZnSe for $s$ polarization. Angle of incidence is 45° for the lower curves and 85° for the upper curves. $a$, with $\omega_B/\omega_T=0.8\times10^{-3}$, $a=50$ Å; $b$, without a surface potential; $c$, calculated by the local theory.

$M=0.92m$, and $\epsilon_0=8.1$. The normal incidence reflectivity of ZnSe, as measured by Tokura *et al.*[24] is shown in curve $a$ of Fig. 2. Curve $c$ was calculated from the local theory, i.e., neglecting spatial dispersion. Curve $b$ was obtained from the nonlocal theory, but without a surface potential, i.e., assuming $U(z)=0$ and using the Pekar ABC. The reflectivity obtained by the method described in Sec.

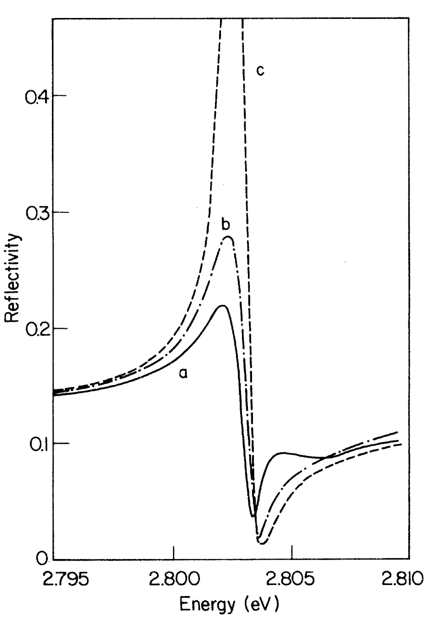


FIG. 5. Calculated reflectivity of ZnSe for $p$ polarization. Angle of incidence is 45°. $a$, with $\omega_B/\omega_T=0.8\times10^{-3}$, $a=50$ Å; $b$, without a surface potential; $c$, calculated by the local theory.

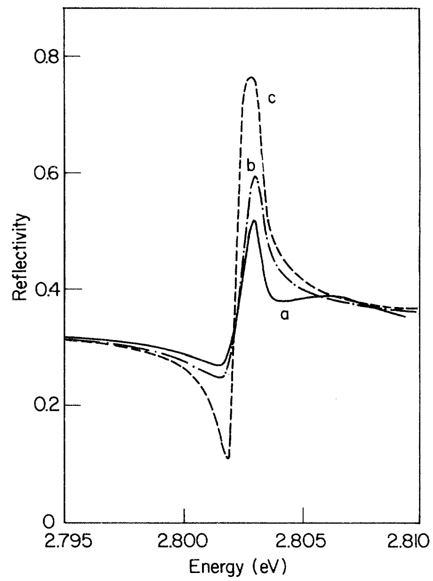


FIG. 6. Calculated reflectivity of ZnSe for $p$ polarization. Angle of incidence is 85°. $a$, with $\omega_B/\omega_T=0.8\times10^{-3}$, $a=50$ Å; $b$, without a surface potential; $c$, calculated by the local theory.

III using a surface potential of the form (45) with $\omega_B/\omega_T=0.8\times10^{-3}$ and $a=50$ Å is given by curve $b$ of Fig. 3, in which $a$ is again the experimental spectrum. The calculated reflectivity agrees well with the experimental reflectivity at energies up to about half-way between $\omega_T$ and $\omega_L$, but does not reproduce the structure at higher energies. This discrepancy will be discussed in Sec. V. Nevertheless, we will use the values $\omega_B/\omega_T=0.8\times10^{-3}$ and $a=50$ Å in the following reflectivity calculations, which demonstrate the ready applicability of our method to the case of oblique incidence and for both $s$ and $p$ polarizations.

The calculated reflectivity for $s$ polarization and angles of incidence of 45° and 85° is shown in Fig. 4. It is compared with the results of the local theory and of the nonlocal Pekar theory without a surface potential. We see that the main effect of the surface potential is the reduction of the intensities of the relative maximum and minimum of the spectrum, accompanied by a slight shift of these extrema toward the lower-energy side. The analogous reflectivities for the case of $p$ polarization are shown in Figs. 5 and 6. In addition to the effects which occur for $s$ polarization there also appears a secondary reflectivity maximum above $\omega_L$.

## V. DISCUSSION

We have presented a method for calculating the reflectivity of a semi-infinite dielectric, in which the effect of the surface on the excitons is represented by a continuous surface potential instead of the discontinuous potential which is used in the dead-layer approximation. The sample calculation performed for CdS (Fig. 1) demonstrates that with a reasonable choice of the surface potential parameters, the experimentally measured reflectivity can be reproduced. For this case the agreement with the measured data does not fall short of that which has been achieved by Halevi and Hernandez-Cocoletzi[16] with the dead-layer approximation.

In the case of ZnSe we could not reproduce the full structure of the experimental spectrum (Fig. 3). This may be due to the over simplified form of the surface potential (45). It is possible that the surface potential also has to contain a well, i.e., a region in which $U(z)<0$, as suggested by Kiselev[18] and Lagois.[23] In any case, as correctly noted by Kiselev,[18] whereas the reflectivity of a crystal with a given surface potential is uniquely defined, the reverse problem, that of reconstructing the potential from a given reflectivity spectrum does not have a unique solution. Additional information, such as reflectivity data at various angles of incidence for both $s$ and $p$ polarizations will be useful for defining the correct shape and magnitude of the surface potential. The method presented here provides a step in this direction, because it is applicable to arbitrary polarization and angle of incidence, and can thus be combined with a systematic set of optical measurements on a given sample. Here the importance of using one and the same sample for a large number of experiments should be stressed. This is because different samples of the same material can have different surface potentials for the excitons, depending on the preparation of the crystal. This has been shown, e.g., by Tokura *et al.*,[24] who have presented two clearly different reflectivity spectra of two ZnSe samples. Furthermore, Lagois has also measured the reflectivity of ZnSe and his data[23] differ considerably from those of Tokura *et al.*[24]

An important additional source of information which will yield information about the surface potential is the dispersion relation of the surface polaritons, which can be traced experimentally by the method of attenuated total reflection (ATR). Lagois[23] has performed ATR calculations for ZnO using a three-layer model to approximate the surface potential (or depth-dependent exciton eigenenergy in his nomenclature). In his calculations, however, a dead layer was also assumed, so that his model still involves an inherently discontinuous potential. The application of the present method to ATR calculations is now being investigated and will be discussed elsewhere.

## ACKNOWLEDGMENTS

The author is much indebted to Professor R. Englman for many useful discussions which led to this work. Helpful correspondence with Professor P. Halevi is also acknowledged.

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