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Optical absorption and collective modes of surface space-charge layers on (110) and (111) silicon

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The electronic properties of surface space-charge layers on semiconductors whose constant-energy surfaces are ellipsoids arbitrarily oriented with respect to the surface are investigated. Optical absorption and its relation to collective modes of the system are examined within a framework of energy-functional perturbation theory. Linear-response theory of a quasi-two-dimensional system is applied to study the polarization dependence of the intersubband absorption spectra for Si(111) and Si(110) surface inversion layers. Both the normal (six- or fourfold) valley occupancy and a reduced (twofold) valley occupancy are considered. The resonance frequencies and their strengths are calculated for both *p*- and *s*-polarized incident light. Resonances occur at frequencies which are shifted from the quasiparticle energy separations by an amount which depends upon the polarization of the light and valley occupancy of the system. In general, the resonance strength depends upon the angle of incidence and the thickness of the oxide layer and the gate electrode. Results are compared with existing theories and experiments.

I. INTRODUCTION

The one-dimensional potential well formed when an attractive electric field is applied normal to the surface of a semiconductor can quantize the motion of an electron normal to the surface. For sufficiently large electric fields, this electronic system is quasi-two dimensional in the sense that the electrons are confined to the lowest quantized level of the surface potential. Although the electronic wave function is of finite extent, the degree of freedom associated with the direction normal to the surface is frozen out by the quantization at low temperatures.

Following the first pioneering theoretical investigations of the subband structure of semiconducting surface space-charge layers,[1] more sophisticated calculations[2–4] have shown that the exchange-correlation effects modify the subband energies substantially. The Hartree energy separations are of the order of 10 meV and it turns out that correlation effects can be as large or even larger.

In recent years there has been a great deal of interest in resonant light scattering and far-infrared optical studies on semiconducting space-charge layers.[5,6] It was pointed out that in an optical-absorption experiment one would not observe the resonant peaks at the radiation frequencies associated with the quasiparticle energy separations.[7] In order to compare the optical-absorption experiment with the calculated quasiparticle energy separations two additional effects must be taken into account in the theoretical calculations.

(i) The depolarization shift (or resonant screening effect) arises due to a finite thickness of the system normal to the surface, whence enabling the system of electrons to be polarized and screen the external electromagnetic relation.[8,9]

(ii) The other correction is the final-state interaction between the charged carrier excited to the higher subband and the hole left behind in the ground subband. Both of these effects were studied theoretically for the space-charge layers with isotropic constant-energy surfaces.[10]

Ando has made an assumption that the exchange-correlation potential of the static local density-functional approach can be used to study the dynamic response of the system, which has not been justified rigorously. However, it turns out that the positions of intersubband resonances are shifted from the corresponding quasiparticle energy separation by only a small amount due to a fortuitous near cancellation between the two effects for the case of Si(100) inversion layers.

Quite recently it has been suggested that the observed resonances in far-infrared absorption in space-charge layers occur at the frequencies associated with intersubband collective modes determined by the self-consistent response function.[11]

A complete theory of the optical absorption for the semiconducting space-charge layers is desirable in order to make a meaningful comparison with experimental results. In this paper we examine the electronic properties of semiconducting space-charge layers related to the optical-absorption and collective modes. For a system with isotropic effective mass the motions in x, y, and z directions are not coupled, and hence only the normal component of the electric field in p-polarized incident light can induce intersubband transitions. We concentrate on the system of electrons in silicon inversion layers, one of the systems presently most commonly investigated by the experimentalists. The multivalley structure of the conduction band in silicon introduces unusual and controversial properties such as possible instabilities of the ground state,[12] the problem of valley occupancy[13,14] and the valley-occupancy phase transitions,[15] and the peculiar transport properties,[16] etc. For the system with tilted constant-energy ellipsoids, such as Si(111) and Si(110), the absorption spectra are much more intricate due to couplings among motions in different directions. In general, the spectra for different polarizations of the incident light should be distinguished from one another through the anisotropy of the effective mass of the system. In addition, since the total microscopic conductivity is strongly related to valley occupancy of the system, the valley occupancy of a given system should be reflected in its absorption spectrum.

In Sec. II we investigate the relationship between the optical-absorption and the collective modes. We examine the polarization dependence of the absorption spectra for the intersubband transitions in silicon surface inversion layers in Sec. III. The effect of the final-state interaction on the resonance absorption is discussed in Sec. IV. We conclude in Sec. V by comparing our results with the existing models and experiments.

II. COLLECTIVE MODES AND OPTICAL-ABSORPTION

In this section we investigate the relationship between the collective modes and the resonance absorption of the quasi-two-dimensional semiconducting space-charge layers within the framework of a self-consistent energy-functional perturbation theory.

A. Condition for collective modes

Collective modes of the system are determined from the poles of the appropriate response function which gives the response of the system to an external radiation field. We will employ a self-consistent energy-functional perturbation theory to obtain the response function of the system. Here we choose an electrostatic gauge ($\vec{A}=0$) for simplicity.[17]

We begin with the total Hamiltonian in the presence of the self-consistent field set up by the external radiation

$$H=H_0+H_1\ . \tag{2.1}$$

Here the unperturbed Hamiltonian H_0 is defined by[18]

$$H_0(\vec{x})=\frac{1}{2m}\vec{p}\cdot\underline{\alpha}\cdot\vec{p}+V_{\text{eff}}(z)\ , \tag{2.2}$$

and the perturbing Hamiltonian is given by

$$H_1(\vec{x})=-e\phi(\vec{x})\ , \tag{2.3}$$

where the position vector $\vec{x}$ is assumed to denote (x,y,z).

In the remainder of this paper wave vector $\vec{k}$ and position vector $\vec{r}$ are assumed to denote two-dimensional vectors parallel to the plane $z=0$ (the z axis is normal to the system). The eigenstates of H_0 are characterized by[1,19] $H_0\,|\nu\rangle=E_\nu\,|\nu\rangle$, where $E_\nu=E_n(k)$ and

$$|\nu\rangle\equiv|n,k\rangle=e^{i(\vec{k}\cdot\vec{r}-\gamma_k z)}\zeta_n(z)\ .$$

Here we have introduced the symbol

$$\gamma_k=\frac{k_x\alpha_{xz}+k_y\alpha_{yz}}{\alpha_{zz}}\ .$$

In Eq. (2.3) $\phi(\vec{x})$ is the self-consistent potential and is the sum of the three contributions:

$$\phi(\vec{x})=\phi_0(\vec{x})+\phi_H(\vec{x})+\phi_{\text{xc}}(\vec{x})\ . \tag{2.4}$$

$\phi_H(\vec{x})$ and $\phi_{\text{xc}}(\vec{x})$ are the change in the Hartree and the exchange-correlation potentials, respectively, caused by the external potential ϕ_0. The change in the Hartree potential is given by the solution to Poisson's equation,

$$\nabla^2\phi_H(\vec{x})=-\frac{4\pi e}{\epsilon_{\text{sc}}}\delta n(\vec{x})\ , \tag{2.5}$$

where δn is the change in density induced by the self-consistent field and ϵ_{sc} is the background dielectric constant of the semiconductor. We assume ϕ_H (also ϕ_0 and δn) to be of the form,

$$\phi_H(\vec{x},t)=\phi_H(z)e^{i\omega t-i\vec{q}\cdot\vec{r}}\ ,$$

where ω and $\vec{q}$ are the angular frequency and the wave vector parallel to the surface of the perturbation, respectively. The solution of Poisson's equation can be written,

$$\phi_H(z)=-\frac{2\pi e}{\epsilon_{\text{sc}}}\frac{1}{q}\int_0^\infty dz'e^{-q|z-z'|}\delta n(z')\ . \tag{2.6}$$

On the other hand, $\phi_{\text{xc}}(\vec{x})$ is assumed to be

$$-e\phi_{\text{xc}}(\vec{x})=\frac{\delta v_{\text{xc}}[n(\vec{x})]}{\delta n(\vec{x})}\delta n(\vec{x})\ . \tag{2.7}$$

where $v_{\text{xc}}[n(\vec{x})]$ is the exchange-correlation contribution to V_{eff}. We recall that $v_{\text{xc}}[n(z)]$ is a functional of the local electron density $n(z)$.

By using the eigenfunctions and eigenvalues of Eq. (2.2), we obtain the matrix elements,

$$-e\langle nk\,|\,\phi_H(\vec{x})\,|\,n'k'\rangle=\frac{2\pi e^2}{\epsilon_{sc}q}\int_0^\infty dz\,\zeta_n(z)\zeta_{n'}(z)e^{-i\gamma_q z}\int_0^\infty dz' e^{-q|z-z'|}\delta n(z')\delta(\vec{k}'-\vec{k}-\vec{q})\;, \tag{2.8}$$

and

$$-e\langle nk\,|\,\phi_{xc}(\vec{x})\,|\,n'k'\rangle=\int_0^\infty dz\,\zeta_n(z)\zeta_{n'}(z)e^{-i\gamma_q z}\frac{\delta v_{xc}}{\delta n}\delta n(z)\delta(\vec{k}'-\vec{k}-\vec{q})\;. \tag{2.9}$$

The induced electron density $\delta n(\vec{x})=\delta n(z)e^{i\omega t-i\vec{q}\cdot\vec{r}}$, and $\delta n(z)$ turns out to be given by

$$\delta n(z)=-\sum_{nn'}\pi_{n'n}(q,\omega)\zeta_n(z)\zeta_{n'}(z)e^{i\gamma_q z}\int_0^\infty dz'\zeta_n(z')\zeta_{n'}(z')H_1(z')e^{-i\gamma_q z'}\;. \tag{2.10}$$

The quantity $\pi_{n'n}(q,\omega)$ is defined by

$$\pi_{n'n}(q,\omega)=n_v n_\sigma\sum_k f^0(E_n(k))\frac{2E_{n'n}(k+q,k)}{E_{n'n}^2(k+q,k)-\hbar^2\omega^2}\;, \tag{2.11}$$

where $E_{n'n}(k',k)=E_{n'}(k')-E_n(k)$ and n_v and n_σ are the valley and spin occupancies. We have introduced a self-consistent potential $\phi(\vec{x},t)$ of the form

$$\phi(\vec{x},t)=\phi(z)e^{i\omega t-i\vec{q}\cdot\vec{r}}\;. \tag{2.12}$$

We see that $\phi_H(\vec{x})$ and $\phi_{xc}(\vec{x})$ can be related to $\phi_0(\vec{x})$ through the induced electron density $\delta n(z)$. Combining Eqs. (2.8), (2.9), and (2.4) we obtain the relation between ϕ and ϕ_0. In the electric quantum limit, where only the $n=0$ subband is occupied, we have

$$\langle 0,k\,|\,H^{ext}(q,z)\,|\,n,k+q\rangle=\sum_m\langle 0,k\,|\,H_1(q,z)\,|\,m,k+q\rangle M_{mn}(q,\omega)\;. \tag{2.13}$$

In Eq. (2.13) $M_{mn}(q,\omega)$ is defined by

$$M_{mn}(q,\omega)=\delta_{nm}-\pi_{n0}(q,\omega)[\widetilde{R}_{nm}(q)+T_{nm}]\;. \tag{2.14}$$

Here $\widetilde{R}_{nm}(q)$ and $T_{nm}(q)$ are given by

$$\widetilde{R}_{nm}(q)=-\frac{2\pi e^2}{\epsilon_{sc}q}\int\int dz\,dz'\zeta_0(z)\zeta_n(z)e^{-q|z-z'|}\zeta_m(z')\zeta_0(z')e^{-i\gamma_q(z-z')} \tag{2.15}$$

and

$$T_{nm}(q)=-\int_0^\infty dz\,\zeta_0(z)\zeta_n(z)\frac{\delta v_{xc}}{\delta n}\zeta_m(z)\zeta_0(z)\;. \tag{2.16}$$

Since we are interested in the long-wavelength limit ($q\rightarrow 0$), which is relevant in optical-absorption experiments, $\pi_{n0}(q,\omega)$ can be evaluated for small q,

$$\pi_{n0}(q,\omega)\simeq\frac{2N_{inv}}{\hbar}\frac{\omega_{n0}+\dfrac{\hbar q^2}{2m_x}}{\omega^2-\left[\omega_{n0}+\dfrac{\hbar q^2}{2m_x}\right]^2}\left\{1+\frac{q^2}{2m_x}\epsilon_f\frac{3\omega^2+\left[\omega_{n0}+\dfrac{\hbar q^2}{2m_x}\right]^2}{\left[\omega^2-\left[\omega_{n0}+\dfrac{\hbar q^2}{2m_x}\right]^2\right]^2}\right\}, \tag{2.17}$$

where N_{inv} is the inversion-layer electron concentration per unit area. This result is correct up to terms of the order of q^2. In obtaining Eq. (2.17) we have assumed that the wave vector $\vec{q}$ is parallel to one of the principal axes of the two-dimensional constant-energy ellipse; $\vec{q}=(q,0,0)$.

The matrix $\underline{M}(q,\omega)$ is the function which determines the response of the system to the external perturbation. The zeros of the determinant of $\underline{M}(q,\omega)$ give the collective modes of the system,

$$\det\underline{M}(q,\omega)=0\;, \tag{2.18}$$

i.e., Eq. (2.18) is the condition for the collective modes in the system.

If we only consider the ground subband, the condition $M_{00}(q,\omega)=0$ gives us the intrasubband (ground subband) collective modes. On the other hand, the intersubband ($0\leftrightarrow 1$, $0\leftrightarrow 2$, etc.) collective modes could be obtained by solving the corresponding higher-order determinantal equations.

B. Optical absorption

The intersubband and intrasubband resonances are associated with the peaks in the expression for the power absorbed by the inversion layer. The power absorption per unit area is defined by

$$P(q,\omega)=\tfrac{1}{2}\mathrm{Re}\int_0^\infty dz\,\vec{\mathrm{j}}_{\mathrm{ind}}(z)\cdot\vec{\mathrm{E}}^{*\prime}(z)\,. \tag{2.19}$$

The fields inside the system ($z>0$) are indicated with primes. Since the total electric field $\vec{\mathrm{E}}'(z)$ is given by

$$\vec{\mathrm{E}}'(z)=\frac{1}{\epsilon_{\mathrm{sc}}}\vec{\mathrm{D}}'(z)+i\frac{4\pi}{\epsilon_{\mathrm{sc}}\omega}\vec{\mathrm{j}}_{\mathrm{ind}}(z)\,, \tag{2.20}$$

Eq. (2.19) reduces to

$$P(q,\omega)=\frac{1}{2\epsilon_{\mathrm{sc}}}\mathrm{Re}\int_0^\infty dz'\,\vec{\mathrm{j}}_{\mathrm{ind}}(z)\cdot\vec{\mathrm{D}}^{*\prime}(z)\,. \tag{2.21}$$

For simplicity we assume the electric field of the incident light wave to be independent of the coordinate z normal to the surface $\vec{\mathrm{D}}(z)=\vec{\mathrm{D}}$. If we consider the electric quantum limit, the induced current, in the electrostatic gauge is given by[17]

$$\vec{\mathrm{j}}_{\mathrm{ind}}(z)=-\frac{\hbar e^2}{m}n_v n_\sigma\sum_{nk}\frac{\hbar\omega f^0(E_0(k))}{E_{n0}^2(k+q,k)-\hbar^2\omega^2}\underline{\alpha}\cdot\vec{\mathrm{f}}_{n0}(k,q,z)\langle n\,|\,\phi(z')e^{-i\gamma_q z'}\,|\,0\rangle\,, \tag{2.22}$$

where

$$\langle n\,|\,\phi(z')e^{-i\gamma_q z'}\,|\,0\rangle=\int_0^\infty dz'\zeta_n(z')\zeta_0(z')e^{-i\gamma_q z'}\phi(z') \tag{2.23}$$

and $\vec{\mathrm{f}}_{n0}(k,q,z)$ is given by

$$\vec{\mathrm{f}}_{n0}(k,q,z)=\{[2\vec{\mathrm{k}}+\vec{\mathrm{q}}-\hat{z}(2\gamma_k+\gamma_q)]\zeta_n(z)\zeta_0(z)-i\hat{z}[\zeta_0(z)\zeta_n'(z)-\zeta_n(z)\zeta_0'(z)]\}e^{i\gamma_q z}\,. \tag{2.24}$$

Here we recall that in Eq. (2.13),

$$\langle n\,|\,\phi_0 e^{-i\gamma_q z'}\,|\,0\rangle=\sum_m M_{nm}(q,\omega)\langle m\,|\,\phi(z')e^{-i\gamma_q z'}\,|\,0\rangle\,. \tag{2.25}$$

We formally invert the expression for $\langle n\,|\,\phi(z')e^{-i\gamma_q z'}\,|\,0\rangle$ to obtain

$$\langle n\,|\,\phi(z')e^{-i\gamma_q z'}\,|\,0\rangle=\sum_m M_{nm}^{-1}(q,\omega)\langle m\,|\,\phi_0 e^{-i\gamma_q z'}\,|\,0\rangle\,. \tag{2.26}$$

Substituting Eq. (2.26) into Eq. (2.22) gives

$$\vec{\mathrm{j}}_{\mathrm{ind}}(z)=-\frac{e^2\hbar}{m}n_v n_\sigma\sum_{nmk}\frac{\hbar\omega f^0(E_0(k))}{E_{n0}^2(k+q,k)-\hbar^2\omega^2}\underline{\alpha}\cdot\vec{\mathrm{f}}_{n0}(k,q,z)M_{nm}^{-1}(q,\omega)\langle m\,|\,\phi_0 e^{-i\gamma_q z'}\,|\,0\rangle\,. \tag{2.27}$$

Since the power absorption is proportional to $\int dz\,\vec{\mathrm{j}}(z)\cdot\vec{\mathrm{D}}^{*\prime}$, clearly the condition for the resonance absorption is $\det\underline{M}(q,\omega)=0$, which is the same as the condition for the collective modes of the system. Therefore, we understand that the resonances observed in far-infrared optical studies of semiconducting space-charge layers occur at the values of the frequency associated with intersubband collective modes. In the long-wavelength limit ($q\rightarrow 0$), if we consider the lowest two subbands only, $M_{11}(q,\omega)$ becomes

$$M_{11}(q,\omega)\simeq\frac{\omega^2-\omega_{10}^2\left[1+\alpha_{11}-\beta_{11}+q\dfrac{4\pi e^2}{\epsilon_{\mathrm{sc}}\hbar\omega_{10}}(z_{10})^2(1-\gamma_x^2)\right]}{\omega^2-\omega_{10}^2}\,, \tag{2.28}$$

where γ_i, α_{nm}, and β_{nm} are defined by

$$\gamma_i=\frac{\alpha_{iz}}{\alpha_{zz}}\,, \tag{2.29}$$

$$\alpha_{nm}=\frac{8\pi e^2}{\epsilon_{\mathrm{sc}}\hbar}N_{\mathrm{inv}}L_{nm}(\omega_{n0}\omega_{m0})^{-1/2}$$

$$=-\frac{2N_{\mathrm{inv}}}{\hbar}\frac{\tilde{R}_{nm}(q\rightarrow 0)}{(\omega_{n0}\omega_{m0})^{1/2}}\,, \tag{2.30}$$

and

$$\beta_{nm}=\frac{2N_{\rm inv}}{\hbar}\frac{T_{nm}}{(\omega_{n0}\omega_{m0})^{1/2}} . \tag{2.31}$$

The symbol L_{nm} is defined by

$$L_{nm}=\int_0^\infty dz \int_0^z dz'\zeta_0(z')\zeta_n(z') \times \int_0^z dz''\zeta_0(z'')\zeta_m(z'') . \tag{2.32}$$

Hence in the same limit we have

$$\int_0^\infty dz\, \vec{j}_i(z)=-i\frac{e^2}{\hbar}N_{\rm inv}\gamma_i \times \frac{2\omega\omega_{10}(z_{10})^2D_z}{\omega^2-\omega_{10}^2[1+\alpha_{11}-\beta_{11}+O(q)]} , \tag{2.33}$$

where a homogeneous external field is assumed along the direction normal to the surface, i.e.,

$$\phi_0(z)=-zD_z .$$

In this case the resonance absorption occurs at the frequency $\omega_{\rm res}$,

$$\omega_{\rm res}\simeq\omega_{10}(1+\alpha_{11}-\beta_{11})^{1/2} . \tag{2.34}$$

The shift in the resonance frequency is due to the depolarization of the system (the term with α_{11}) and the change in the exchange-correlation potential (the term with β_{11}) in the presence of the external perturbation. This result agrees with that of Ando[10] for the isotropic case where $\underline{\alpha}$ is equal to the unit matrix. We also note that the above result resumes those obtained by others[20] for the case of $\beta_{11}=0$.

III. POLARIZATION DEPENDENCE OF THE RESONANCE ABSORPTION

In this section we examine the dependence of the absorption spectra upon the polarization of the incident radiation field. The polarization dependence of the absorption spectra for the intersubband transitions is examined explicitly for a system with a isotropic constant-energy surface, and for Si(111) and Si(110) surface inversion layers. The effect of the external radiation field on the system is expected to be different depending upon the polarization and the valley occupancy of the ground state. We have focused our attention on the qualitative difference in the spectra with different polarization and with different valley occupancy.

The motion of electrons parallel and normal to the surface can be coupled to one another through off-diagonal elements of the anisotropic effective-mass tensor associated with the silicon conduction band. Hence intersubband transition can be induced with the incident electric field polarized parallel to the surface ($D_{\parallel}$) as well as in the case where the field has a component normal to the surface ($D_{\perp}$). The former configuration of the field is the so-called *s* polarization and the latter, *p* polarization.

The absorption spectra with a given perturbing field can be obtained by combining Eq. (2.21) with the microscopic-induced current density.[17] Collision of electrons with impurities or lattice imperfection is known to affect the linewidth of the spectra.[8,17,21] In actual calculation we have taken the collisionless limit and ignored the nonintersubband part in the conductivity tensor.

For a single occupied valley $\sigma_{ij}^{(v)}$ is given by

$$\sigma_{ij}^{(v)}=-\frac{e^2\hbar}{im^2\omega}4\sum_k f^0(E_0(k))[\beta_{xi}\beta_{xj}k_x^2+\beta_{yi}\beta_{yj}k_y^2+(\beta_{xj}\beta_{yi}+\beta_{xi}\beta_{yj})k_xk_y] \times\sum_n\frac{\omega_{n0}}{\omega_{n0}^2-\omega^2}\zeta_0(z)\zeta_n(z)\zeta_0(z')\zeta_n(z')+\frac{e^2\hbar}{2im^2\omega}N_{\rm inv}^{(v)}\alpha_{zz}\sum_n\frac{\beta_{ij}\omega_{n0}^2-\alpha_{ij}\omega^2}{\omega_{n0}(\omega_{n0}^2-\omega^2)}F_n(z)F_n(z') , \tag{3.1}$$

where values of α_{ij} and β_{ij} depend explicitly upon the orientation of valley v relative to the coordinates. (See Appendix.) The definition of $F_n(z)$ is

$$F_n(z)=\zeta_0(z)\zeta_n'(z)-\zeta_n(z)\zeta_0'(z) . \tag{3.2}$$

By recalling the definition of β_{ij}, one can demonstrate that

$$\sigma_{iz}^{(v)}=\gamma_i\sigma_{zz}^{(v)} . \tag{3.3}$$

In order to obtain the total conductivity σ_{ij} for a given valley occupancy, one should sum $\sigma_{ij}^{(v)}$ over all occupied valleys. In the remainder of this work we take the following configurations for the polarization of the incident light:

For *p* polarization,

$$\vec{D}=(0,D_y,D_z)e^{i\omega t-i(q_yy+q_zz)} , \tag{3.4}$$

and for *s* polarization,

$$\vec{D}=(D_x,0,0)e^{i\omega t-i(q_yy+q_zz)} . \tag{3.5}$$

Then, in general, the expressions of the power absorption for *p* and *s* polarizations reduce, respectively, to

$$P_p = \frac{1}{2\epsilon_{\text{sc}}} \text{Re} \int \int dz\, dz' \sum_i^{x,y,z} (D_y^{*\prime} \sigma_{yi} E_i' + D_z^{*\prime} \sigma_{zi} E_i') \tag{3.6}$$

and

$$P_s = \frac{1}{2\epsilon_{\text{sc}}} \text{Re} \int \int dz\, dz' \sum_i^{x,y,z} D_x^{*\prime} \sigma_{xi} E_i' \ . \tag{3.7}$$

Equations (3.6) and (3.7) can further be simplified depending upon the surface orientation and the valley occupancy. We make use of the following boundary conditions for the fields at the interfaces: The tangential components of $\vec{E}$ and the normal component of $\vec{D}$ are continuous across a semiconductor-oxide interface ($z=0$). In the remainder of this section we investigate the absorption spectra for a system with isotropic effective mass as well as for Si (111) and (110) surface inversion layers, both with normal[13,14,22] and with reduced valley occupancies. The effect of the final-state interactions on the absorption spectra is not included in this section and will be considered in Sec. IV.

A. System with isotropic effective mass

Let us consider a system with a spherical constant-energy surface. The σ_{zz} is the only component which involves the intersubband term, since $\underline{\alpha} = \underline{\mathbb{1}}$ in this case,

$$\sigma_{xx} = \sigma_{yy}$$
$$= \frac{e^2}{im\omega} N_{\text{inv}} \sum_n \left[1 + \frac{\omega_{n0}\epsilon_f/\hbar}{\omega^2 - \omega_{n0}^2} \right] \zeta_0(z)\zeta_n(z)$$
$$\times \zeta_0(z')\zeta_n(z') \ , \tag{3.8}$$

$$\sigma_{zz} = \frac{e^2\hbar}{2im^2\omega} N_{\text{inv}} \sum_n \frac{\omega^2}{\omega_{n0}(\omega^2 - \omega_{n0}^2)} F_n(z) F_n(z') \ . \tag{3.9}$$

Because there are no intersubband components in σ_{xx} and σ_{yy}, only D_z can induce intersubband transition, which is described by

$$P_p = \frac{1}{2\epsilon_{\text{sc}}} \text{Re} \int \int dz\, dz' D_z^{*\prime} \sigma_{zz}(z,z') E_z'(z') \ .$$

Now in order to express $E_i'(z)$ and $D_i'(z)$ in terms of D_z we make use of the constitutive relations characterizing the electromagnetic response of the system: $D_i = \epsilon_{\text{ox}} E_i$ for $z<0$ (ϵ_{ox} is the dielectric constant of oxide), and

$$D_i'(z) = \sum_j \int dz' \epsilon_{ij}(z,z') E_j'(z') \quad \text{for } z>0, \tag{3.10}$$

where the dielectric tensor ϵ_{ij} is related to our conductivity tensor σ_{ij} by

$$\epsilon_{ij}(z,z') = \epsilon_{\text{sc}} \delta_{ij} \delta(z-z') + \frac{4\pi}{i\omega} \sigma_{ij}(z,z') \ . \tag{3.11}$$

Multiplying both sides of Eq. (3.10) by $F_n(z)$ and integrating over z gives

$$Z_n^{\text{ext}} = \epsilon_{\text{sc}} \sum_m (\delta_{nm} - N_{nm}) Z_m' \ , \tag{3.12}$$

where Z_n^{ext}, Z_n', and N_{nm} are defined, respectively, by

$$Z_n^{\text{ext}} = \int dz\, F_n(z) D_z(z) \ , \tag{3.13}$$

$$Z_n' = \int dz\, F_n(z) E_z'(z) \ , \tag{3.14}$$

and

$$N_{nm} = \frac{8\pi e^2 N_{\text{inv}}}{\epsilon_{\text{sc}}\hbar} \frac{\omega_{n0}}{\omega^2 - \omega_{n0}^2} L_{nm} \tag{3.15}$$

or

$$N_{nm} = \alpha_{nm} \frac{\omega_{n0}(\omega_{n0}\omega_{m0})^{1/2}}{\omega^2 - \omega_{m0}^2} \ ,$$

with L_{nm} and α_{nm} given by Eqs. (2.32) and (2.30). The continuity of D_z across $z=0$ is used to obtain Eq. (3.12). It is convenient to write Eq. (3.12) by

$$\vec{Z}^{\text{ext}} = \epsilon_{\text{sc}} (\underline{\mathbb{1}} - \underline{N}) \vec{Z}' \ , \tag{3.16}$$

that is, we can treat $\vec{Z}^{\text{ext}}$ (and $\vec{Z}$) and $\underline{N}$ as tensor quantities in the subband space. Substituting Eq. (3.16) into P_p gives

$$P_p = \text{Re} \frac{e^2}{i\hbar\epsilon_{\text{sc}}^2} N_{\text{inv}} \frac{\omega\omega_{10}(z_{10})^2 |D_z|^2}{\omega^2 - \omega_{10}^2(1+\alpha_{11}) + 2i\omega/\tau_1} \ , \tag{3.17}$$

where we have restricted ourselves to the lowest two subbands, and D_z is assumed to be homogeneous in the z direction. A phenomenological relaxation time τ_1 is introduced in the final expression of the power absorption. The resonance occurs at the frequency shifted from subband energy separation ω_{10}, and its strength is proportional to the quantity $N_{\text{inv}}\omega_{10}(z_{10})^2 |D_z|^2$, where $z_{n0} = \langle n | z | 0 \rangle$.

When we consider the case with more than one excited subband, each resonance frequency for a given intersubband transition is further modified due to couplings between different subbands. For example, for a three-subband system the power spectrum is given by[23]

$$P_p=\frac{2e^2}{\hbar\epsilon_{\rm sc}^2}N_{\rm inv}\omega^2|D_z|^2\left[\left[(\omega^2-\tilde\omega_{10}^2)(\omega^2-\tilde\omega_{20}^2)-\alpha_{12}^2\omega_{10}^2\omega_{20}^2-\frac{4\omega^2}{\tau_1\tau_2}\right]^2+4\omega^2\left[\frac{\omega^2-\tilde\omega_{20}^2}{\tau_1}+\frac{\omega^2-\tilde\omega_{10}^2}{\tau_2}\right]^2\right]^{-1}$$

$$\times\left[\frac{\omega_{10}}{\tau_1}\left[[z_{10}(\omega^2-\tilde\omega_{20}^2)+\alpha_{12}\omega_{20}\sqrt{\omega_{10}\omega_{20}}z_{20}]^2+4\omega^2\frac{(z_{10})^2}{\tau_2^2}\right]\right.$$

$$\left.+\frac{\omega_{20}}{\tau_2}\left[[z_{20}(\omega^2-\tilde\omega_{10}^2)+\alpha_{12}\omega_{10}\sqrt{\omega_{10}\omega_{20}}z_{10}]^2+4\omega^2\frac{(z_{20})^2}{\tau_1^2}\right]\right]. \quad (3.18)$$

If we ignore subband coupling [set $\alpha_{12}=0$ in Eq. (3.18)] the $0\rightarrow n$ transition occurs at the frequency $\tilde\omega_{n0}=\omega_{n0}(1+\alpha_{nn})^{1/2}$. And in the limit $\omega/\tau_n\gg1$ its strength is proportional to $\omega_{n0}(z_{n0})^2\tau_n$. However, for finite values of α_{12} and in the limit $\omega/\tau_n\gg1$, the zeros of the denominator in Eq. (3.18) occur at frequencies,

$$\Omega_\pm^2=\tfrac{1}{2}\{\tilde\omega_{10}^2+\tilde\omega_{20}^2\pm[(\tilde\omega_{20}^2-\tilde\omega_{10}^2)^2+4\alpha_{12}^2\omega_{10}^2\omega_{20}^2]^{1/2}\}\ . \quad (3.19)$$

We note that Ω_+ and Ω_- are shifted up and down, respectively, from their uncoupled resonance frequencies $\tilde\omega_{20}$ and $\tilde\omega_{10}$.

B. Si(111) inversion layers with normal valley occupancy

As is shown in the Appendix, electrons in each valley have the same effective mass for the motion normal to the surface. However, the masses in the plane depend upon an individual valley. Let us take x and y axes along $\langle 1\bar{1}0\rangle$ and $\langle 11\bar{2}\rangle$. If we sum $\sigma_{ij}^{(v)}$ over all six valleys the off-diagonal terms add up to zero and each diagonal element has an intersubband part. Keeping only the intersubband parts, we have[24]

$$\sigma_{ii}=\tfrac{1}{6}\sum_v\gamma_i^2\sigma_{zz}\ ,$$

where we have introduced σ_{zz} given by

$$\sigma_{zz}(z,z')=\frac{e^2\hbar}{2im_z^2\omega}N_{\rm inv}\times\sum_n\frac{\omega^2}{\omega_{n0}(\omega^2-\omega_{n0}^2)}F_n(z)F_n(z')\ . \quad (3.20)$$

Since $\sum_v\gamma_x^2=\sum_v\gamma_y^2$ for Si(111) layers with sixfold valley occupancy, we have $\sigma_{xx}=\sigma_{yy}$.

By employing the constitutive relation Eq. (3.10), one obtains for p-polarized incident light with homogeneous electric field in the z direction,

$$P_p={\rm Re}\frac{e^2}{i\hbar}N_{\rm inv}\left[\frac{\omega\omega_{10}(z_{10})^2|D_y|^2\left[\dfrac{m_l-m_t}{2m_l+m_t}\right]^2}{\epsilon_{\rm ox}^2(\omega^2-\omega_{\rm res1}^2+2i\omega/\tau_1)}+\frac{\omega\omega_{10}(z_{10})^2|D_z|^2}{\epsilon_{\rm sc}^2(\omega^2-\omega_{\rm res2}^2+2i\omega/\tau_1)}\right], \quad (3.21)$$

where $\omega_{\rm res1}$ and $\omega_{\rm res2}$ are given by

$$\omega_{\rm res1}=\omega_{10} \quad (3.22)$$

and

$$\omega_{\rm res2}=\omega_{10}(1+\alpha_{11})^{1/2}\ . \quad (3.23)$$

In obtaining Eq. (3.21) we have used the relation Eq. (3.16).

We recall that

$$\left[\frac{m_l-m_t}{2m_l+m_t}\right]^2=\tfrac{1}{6}\sum_v(\gamma_x)^2=\langle\gamma_x^2\rangle\ ,$$

where the angular brackets denote averaging over all occupied valleys. In Eq. (3.21) there appear two resonances at frequencies $\omega_{\rm res1}$ and $\omega_{\rm res2}$ whose strengths depend upon the y and z component of $\vec{D}$, respectively. The relative strength is given by

$$\tfrac{2}{3}\gamma_x^2\left[\frac{\epsilon_{\rm sc}}{\epsilon_{\rm ox}}\right]^2\cot^2\theta_i\ , \quad (3.24)$$

where θ_i is the angle between the direction of the incident wave propagation and the normal of the surface. For the propagation parallel to the surface ($\theta_i=\pi/2$) one would only have a single resonance at $\omega_{\rm res2}$. We note that the first resonance ($\omega_{\rm res1}$) appears at ω_{10}, the subband energy separation.[24]

For s polarization we obtain

$$P_s={\rm Re}\frac{e^2}{i\hbar\epsilon_{\rm ox}^2}N_{\rm inv}\left[\frac{m_l-m_t}{2m_l+m_t}\right]^2\times\frac{\omega\omega_{10}(z_{10})^2|D_x|^2}{\omega^2-\omega_{\rm res1}^2+2i\omega/\tau_1}\ , \quad (3.25)$$

where $\omega_{\text{res}1}$ is given by Eq. (3.22). In obtaining this result we have made use of the fact that $\sum_v (\alpha_{xz})^2 \neq 0$. Here we note that the components D_y in p polarization and D_x in s polarization have the same effect in the result for the power absorbed, which is understandable from symmetry considerations. In the p-polarized spectrum, the relative strength of the two resonances can be diversified by varying the angle of incidence of the incoming electromagnetic wave. The strength can also be dependent upon the thickness of the oxide layer and of the metallic gate in the metal-oxide-semiconductor structure, because these parameters together with boundary conditions determine the values of the components of $\vec{D}$ at the surface of the space-charge layer.

C. Si(111) inversion layers with twofold valley occupancy

In Si(111) layers with twofold valley occupancy[18] there can exist two different kinds of occupied valley pairs due to the unequal two-dimensional effective masses in the plane parallel to the surface. If we take x and y axes along $\langle 1\bar{1}0 \rangle$ and $\langle 11\bar{2} \rangle$, the two valleys along the y axis have the inverse effective mass given by

$$\underline{\alpha} = m \begin{bmatrix} m_t^{-1} & 0 & 0 \\ 0 & \frac{1}{3}(m_t^{-1} + 2/m_l) & -\frac{\sqrt{2}}{3}(m_t^{-1} - m_l^{-1}) \\ 0 & -\frac{\sqrt{2}}{3}(m_t^{-1} - m_l^{-1}) & \frac{1}{3}\left[\frac{2}{m_t} + m_l^{-1}\right] \end{bmatrix} . \tag{3.26}$$

On the other hand, those for the remaining two pairs of valleys can be written as

$$\underline{\alpha} = \frac{m}{2} \begin{bmatrix} m_t^{-1} + m_l^{-1} & \pm\frac{1}{\sqrt{3}}(m_t^{-1} - m_l^{-1}) & \mp\frac{\sqrt{2}}{\sqrt{3}}(m_t^{-1} - m_l^{-1}) \\ \pm\frac{1}{\sqrt{3}}(m_t^{-1} - m_l^{-1}) & \frac{1}{3}(5/m_t + m_l^{-1}) & \frac{\sqrt{2}}{3}(m_t^{-1} + m_l^{-1}) \\ \mp\frac{\sqrt{2}}{\sqrt{3}}(m_t^{-1} - m_l^{-1}) & \frac{\sqrt{2}}{3}(m_t^{-1} - m_l^{-1}) & \frac{2}{3}(2/m_t + m_l^{-1}) \end{bmatrix} . \tag{3.27}$$

The derivations of Eqs. (3.26) and (3.27) are given briefly in the Appendix.

The components of the conductivity tensor with nonzero intersubband terms are related to each other as follows:

$$\sigma_{ij} = \gamma_i \gamma_j \sigma_{zz} , \tag{3.28}$$

where σ_{zz} is given by

$$\sigma_{zz} = \frac{e^2 \hbar}{2i m_z^2 \omega} N_{\text{inv}} \sum_n \frac{\omega^2}{\omega_{n0}(\omega^2 - \omega_{n0}^2)} F_n(z) F_n(z') . \tag{3.29}$$

Let us first consider the pair of valleys with the effective mass described in Eq. (3.26). The components σ_{xy}, σ_{xz}, σ_{yx}, and σ_{zx} vanish for these valleys. Under p-polarized incident light the absorption spectrum becomes

$$P_p = \text{Re} \frac{e^2}{i\hbar \epsilon_{\text{sc}}^2} N_{\text{inv}} \frac{\omega \omega_{10} (z_{10})^2}{\omega^2 - \omega_{\text{res}}^2 + 2i\omega/\tau_1} \times \left| D_z + \gamma_y \frac{\epsilon_{\text{sc}}}{\epsilon_{\text{ox}}} D_y \right|^2 , \tag{3.30}$$

where

$$\gamma_y^2 = 2 \left[\frac{m_l - m_t}{2m_l + m_t} \right]^2 . \tag{3.31}$$

The resonance occurs at the frequency given by Eq. (3.23). We note that strength of the resonance depends upon the angle of incidence of the polarizing field. In obtaining Eq. (3.30) we have used the relation

$$\vec{Z}' + \frac{\gamma_y}{\epsilon_{\text{ox}}} \vec{Y}^{\text{ext}} = \frac{1}{\epsilon_{\text{sc}}} (\underline{1} - \underline{N})^{-1} \left[\vec{Z}^{\text{ext}} + \frac{\epsilon_{\text{sc}} \gamma_y}{\epsilon_{\text{ox}}} \vec{Y}^{\text{ext}} \right] , \tag{3.32}$$

where $\vec{Y}^{\text{ext}}$ is defined in the same way as was done for $\vec{Z}^{\text{ext}}$ with the replacement of D_z with D_y in Eq. (3.13). There is no intersubband transition with s-polarized radiation in this case.

Now, let us consider the other pair of valleys tilted with respect to $\langle 11\bar{2} \rangle$ or $\langle 1\bar{1}0 \rangle$. The occupancy of these pairs of valleys leads us to resonance absorption with both polarizations. The effective masses for these valleys are described in Eq. (3.27). In this case motions in x, y, and z directions are coupled to one another. With p-polarized incident radiation one obtains the absorption spectrum in the form of Eq. (3.30), where the values of γ_x and γ_y are, respectively,

$$\gamma_x = \left[\frac{3}{2}\right]^{1/2} \left[\frac{m_l - m_t}{2m_l + m_t}\right]$$

and (3.33)

$$\gamma_y = \frac{1}{\sqrt{2}} \left[\frac{m_t - m_l}{2m_l + m_t}\right] .$$

The resonance occurs at the frequency given by Eq. (3.23). The coupling of the motions in x and y directions and that in the z direction shifts the resonance frequency from ω_{10} to ω_{res}. The strength again depends upon both D_z and D_y.

With s-polarized light the absorption spectrum becomes

$$P_s = \text{Re} \frac{e^2}{i\hbar\epsilon_{\text{sc}}^2} N_{\text{inv}} \frac{\omega\omega_{10}(z_{10})^2 \, | D_x |^2 \gamma_x^2}{\omega^2 - \omega_{\text{res}}^2 + 2i\omega/\tau_1} , \tag{3.34}$$

where, in this situation, the resonance frequency is the same as that of p polarization. However, we see that its strength is reduced by the amount γ_x^2. In obtaining this result we have used the relation

$$\frac{\gamma_x}{\epsilon_{\text{ox}}} \underline{N} \vec{X}^{\text{ext}} = (\underline{1} - \underline{N}) \vec{Z}' \tag{3.35}$$

or

$$\vec{Z}' + \frac{\gamma_x}{\epsilon_{\text{ox}}} \vec{X}^{\text{ext}} = (\underline{1} - \underline{N})^{-1} \frac{\gamma_x}{\epsilon_{\text{ox}}} \vec{X}^{\text{ext}} , \tag{3.36}$$

where $\vec{X}^{\text{ext}}$ is defined by Eq. (3.13) with the replacement of D_z by D_x. We note that resonances occur at the same frequency for both polarizations in Si(111) inversion layers with twofold valley occupancy, but their strength of resonance depends upon the configurations of the valleys.

D. Si(110) inversion layers with normal valley occupancy

Now we consider the case in which only the four valleys with the larger value of m_z are equally occupied. We take x and y axes along $\langle 1\bar{1}0 \rangle$ and $\langle 001 \rangle$, respectively, so that four occupied valleys are projected onto the x axis and the other two valleys onto the y axis. The total conductivity tensor is diagonal and only the xx and zz components have intersubband parts since the motion in the y direction is not coupled with those in the x and z directions,

$$\sigma_{xx} = \gamma_x^2 \sigma_{zz} , \tag{3.37}$$

where

$$\sigma_{zz} = \frac{e^2\hbar}{2im_z^2\omega} N_{\text{inv}} \sum_n \frac{\omega^2}{\omega_{n0}(\omega^2 - \omega_{n0}^2)} F_n(z) F_n(z') . \tag{3.38}$$

By substituting the last two equations into Eq. (2.21) and employing the constitutive relation Eq. (3.10), one obtains the absorption spectra in the form

$$P_p = \text{Re} \frac{e^2}{i\hbar\epsilon_{\text{sc}}^2} N_{\text{inv}} \frac{\omega\omega_{10}(z_{10})^2 \, | D_z |^2}{\omega^2 - \omega_{\text{res}1}^2 + 2i\omega/\tau_1} \tag{3.39}$$

for p polarization, and

$$P_s = \text{Re} \frac{e^2}{i\hbar\epsilon_{\text{ox}}^2} N_{\text{inv}} \frac{\omega\omega_{10}(z_{10})^2 \, | D_x |^2}{\omega^2 - \omega_{\text{res}2}^2 + 2i\omega/\tau_1} \left[\frac{m_l - m_t}{m_t + m_l}\right]^2 \tag{3.40}$$

for s polarization. The resonance frequencies are given, respectively, by

$$\omega_{\text{res}1} = \omega_{10}(1 + \alpha_{11})^{1/2} \tag{3.41}$$

and

$$\omega_{\text{res}2} = \omega_{10} . \tag{3.42}$$

The D_y component in p polarization does not contribute to intersubband transitions. In obtaining Eqs. (3.39) we have used Eq. (3.16). We note that γ_x^2 is just equal to

$$\left[\frac{m_l - m_t}{m_l + m_t}\right]^2 .$$

The resonance strength with s polarization is reduced by this factor relative to that with p polarization if we assume $| D_z |^2 = | D_x |^2$.

With the polarization of

$$\vec{D} = (D_x, 0, D_z) \exp[i\omega t - i(q_x x + q_z z)]$$

the resonance would occur at both frequencies $\omega_{\text{res}1}$ and $\omega_{\text{res}2}$, the relative strengths depending upon the angle of incidence of the light. There would be no resonance if we take the polarization

$$D = (0, D_y, 0) \exp[i\omega t - i(q_x x + q_z z)] .$$

E. Si(110) inversion layers with twofold valley occupancy

Let us take the coordinates in the same way as those in the preceding subsection; x axis along $\langle 1\bar{1}0 \rangle$ and y axis along $\langle 001 \rangle$. The inverse effective masses are described by

$$\underline{\alpha}=\frac{m}{2}\begin{bmatrix} m_t^{-1}+m_l^{-1} & 0 & \pm(m_t^{-1}-m_l^{-1}) \\ 0 & 2/m_t & 0 \\ \pm(m_t^{-1}-m_l^{-1}) & & m_t^{-1}+m_l^{-1} \end{bmatrix}, \tag{3.43}$$

and the intersubband part in the conductivity tensor can be written by

$$\sigma_{ij}=\frac{e^2\hbar}{2im_z^2\omega}N_{\text{inv}}\gamma_i\gamma_j \times\sum_n \frac{\omega^2}{\omega_{n0}(\omega^2-\omega_{n0}^2)}F_n(z)F_n(z')\ , \tag{3.44}$$

where $i,j=x,z$.

The p-polarized incident light leads to the absorption spectrum given by Eq. (3.39) with the resonance frequency of Eq. (3.41). The finite intersubband part in σ_{xz} gives the shifts in the resonance frequency from ω_{10} to ω_{res}.

On the other hand, with the s-polarized incident light we use the relations

$$(\underline{1}-\underline{N})\vec{Z}'=\frac{\gamma_x}{\epsilon_{\text{ox}}}\underline{N}\vec{X}^{\text{ext}} \tag{3.45}$$

to obtain the power absorption

$$P_s=\text{Re}\frac{e^2}{i\hbar\epsilon_{\text{ox}}^2}N_{\text{inv}}\frac{\omega\omega_{10}(z_{10})^2\,|D_x|^2}{\omega^2-\omega_{\text{res}}^2+2i\omega/\tau_1}\gamma_x^2\ , \tag{3.46}$$

where the resonance frequency is also given by Eq. (3.41). We note that, in this case, both p and s polarizations give similar resonance absorption; the resonance frequencies are equal to each other but the strength of the s-polarized one is reduced by the same factor γ_x^2. Since σ_{xz} has a finite intersubband part, the x and z motions are coupled to give a shift in the resonance frequency from corresponding subband separation. The D_y component in p-polarized incident light has no contribution to the intersubband transitions in this case since σ_{yy} has no intersubband part.

IV. EFFECT OF FINAL-STATE INTERACTION

In the preceding section we have explored the polarization dependence of intersubband absorption spectra within the framework of self-consistent field approximation. One of the results is that resonance frequency depends upon the polarization of incident light. This resonance screening effect is caused by the screening of incident light by the inversion-layer electrons. In the presence of an external electromagnetic field, in addition to this change in Hartree potential, the exchange-correlation part of the potential is also modified due to the local change in density which is really a vertex correction or a correction due to exciton-like final-state interaction.

In this section we introduce an effective conductivity to investigate the effect of the final-state interaction on intersubband absorption spectra. The effective conductivity could be obtained perturbatively by adding to the perturbing Hamiltonian the contribution due to the change in the exchange-correlation potential:

$$H_1=-\frac{e}{2mc}(\vec{p}\cdot\underline{\alpha}\cdot\vec{A}+\vec{A}\cdot\underline{\alpha}\cdot\vec{p})-e\phi_{\text{xc}}\ , \tag{4.1}$$

where the last term on the right-hand side is given by Eq. (2.7).

We can write the effective change in surface electron concentration by

$$\delta n(z')=\delta n_H(z')+\delta n_{\text{xc}}(z')\ , \tag{4.2}$$

where $\delta n_H(z')$ is the change in the absence of ϕ_{xc} (Ref. 17) and the additional term in Eq. (4.2) is defined by

$$\delta n_{\text{xc}}(z')=n_v n_\sigma \sum_{nn'k}\frac{f^0(E_{n'}(k+q))-f^0(E_n(k))}{E_{n'n}(k+q,k)-\hbar\omega}\zeta_n(z')\zeta_{n'}(z')\int dz\,\zeta_n(z)\zeta_{n'}(z)\frac{\delta v_{\text{xc}}}{\delta n}\delta n\ . \tag{4.3}$$

In the long-wavelength limit $\delta n(z')$ reduces to

$$\delta n(z')=\delta n_H(z')+\frac{2N_{\text{inv}}}{\hbar}\sum_n\frac{\omega_{n0}}{\omega^2-\omega_{n0}^2}\zeta_n(z')\zeta_0(z')V_n\ , \tag{4.4}$$

where V_n is defined by

$$V_n=\int_0^\infty dz\,\zeta_n(z)\zeta_0(z)\frac{\delta v_{\text{xc}}}{\delta n}\delta n(z)\ . \tag{4.5}$$

We multiply $\delta n(z')$ with

$$\frac{\delta v_{\text{xc}}}{\delta n}\zeta_m(z')\zeta_0(z')$$

and integrate it over z' to obtain

$$\vec{V}^{H}=(\underline{\mathbb{1}}-\underline{B})\vec{V}\ . \tag{4.6}$$

Here we have introduced V_n^H and B_{nm}, defined by

$$V_n^H=\int_0^\infty dz\frac{\delta v_{xc}}{\delta n}\zeta_n(z)\zeta_0(z)\delta n_H(z) \tag{4.7}$$

and

$$B_{nm}=\frac{2N_{\text{inv}}}{\hbar}\frac{\omega_{m0}}{\omega^2-\omega_{m0}^2}T_{nm}\ . \tag{4.8}$$

The quantity T_{nm} is given by Eq. (2.16).

Now one can evaluate the overall induced current in the system by introducing the modification in the density matrix due to ϕ_{xc}:

$$\vec{j}_{\text{ind}}(z)=\vec{j}_H(z)+\vec{j}_{xc}(z)\ , \tag{4.9}$$

where $\vec{j}_H(z)$ is the current density in the absence of ϕ_{xc} in the perturbing Hamiltonian and $\vec{j}_{xc}(z)$ is given by

$$\vec{j}_{xc}(z)=i\frac{e}{m}N_{\text{inv}}\underline{\alpha}\cdot\hat{z}\sum_n\frac{\omega}{\omega^2-\omega_{n0}^2}F_n(z)V_n\ . \tag{4.10}$$

We can write Eq. (4.10) in terms of the self-consistent field $\vec{E}'$,

$$\vec{j}_{xc}(z)=\int_0^\infty dz'\,\underline{\sigma}^{xc}(z,z')\cdot\vec{E}'(z')\ , \tag{4.11}$$

where

$$\sigma_{ij}^{xc}(z,z')=\langle\gamma_i\gamma_j\rangle\sigma_{zz}^{xc}(z,z')\ . \tag{4.12}$$

If we consider only the lowest three subbands, we find

$$\begin{aligned}\sigma_{zz}^{xc}(z,z')=\frac{e^2\hbar}{2im_z^2}N_{\text{inv}}\omega\{[\omega^2-\omega_{10}^2(1-\beta_{11})][\omega^2-\omega_{20}^2(1-\beta_{22})]-\beta_{12}^2\omega_{10}^2\omega_{20}^2\}^{-1}\\ \times(\{[\omega^2-\omega_{20}^2(1-\beta_{22})]\beta_{11}\omega_{10}-\beta_{12}^2\omega_{10}\omega_{20}^2\}F_1(z)F_1(z')(\omega^2-\omega_{10}^2)^{-1}\\ +\{[\omega^2-\omega_{10}^2(1-\beta_{11})]\beta_{22}\omega_{20}-\beta_{12}^2\omega_{20}\omega_{10}^2\}F_2(z)F_2(z')(\omega^2-\omega_{20}^2)^{-1}\\ +\beta_{12}\sqrt{\omega_{10}\omega_{20}}[F_1(z)F_2(z')+F_2(z)F_1(z')])\ .\end{aligned} \tag{4.13}$$

The effective conductivity $\underline{\sigma}^{\text{eff}}(z,z')$ is the sum of $\underline{\sigma}^{xc}(z,z')$ and $\underline{\sigma}^{H}(z,z')$ of Eq. (3.1). If we neglect subband coupling [set $\beta_{12}=0$ in Eq. (4.13)] the effective conductivity $\underline{\sigma}^{\text{eff}}(z,z')$ becomes

$$\sigma_{ij}^{\text{eff}}(z,z')=\langle\gamma_i\gamma_j\rangle\sigma_{zz}^{\text{eff}}(z,z')\ , \tag{4.14}$$

where

$$\sigma_{zz}^{\text{eff}}(z,z')=\frac{e^2\hbar}{2im_z^2}N_{\text{inv}}\omega\sum_n\frac{F_n(z)F_n(z')}{\omega_{n0}[\omega^2-\omega_{n0}^2(1-\beta_{nn})+2i\omega/\tau_n]}\ . \tag{4.15}$$

By employing the effective conductivity Eq. (4.15) in the calculation of absorption spectra we observe that each resonance frequency is shifted from that obtained in the preceding section to a reduced frequency,

$$\tilde{\omega}_{\text{res}}=(\omega_{\text{res}}^2-\beta_{nn}\omega_{n0}^2)^{1/2}\ . \tag{4.16}$$

For example, in Si(110) or Si(111) surface inversion layers with normal valley occupancy of four or six intersubband resonances occur at

$$\omega_{10}(1+\alpha_{11}-\beta_{11})^{1/2}\ \text{for } p \text{ polarization} \tag{4.17}$$

and

$$\omega_{10}(1-\beta_{11})^{1/2}\ \text{for } s \text{ polarization}\ . \tag{4.18}$$

However, for the system with twofold valley occupancy the resonance frequency is equal to $\omega_{10}(1+\alpha_{11}-\beta_{11})^{1/2}$ for both polarizations.

V. RESULTS AND CONCLUSIONS

The electronic properties of semiconducting space-charge layers with tilted ellipsoidal energy surfaces are studied in this paper. In evaluating the quasiparticle energy of low-lying subbands in Si(111) surface inversion layers we have employed a method of energy-functional perturbation theory.[18] Variational wave functions are used as the basis functions in the calculation of the many-body effects. Only the lowest-order contribution to the self-energy correction is included, and the plasmon-pole approximation is used to describe the screened electron-electron interaction. There are several advantages in our formalism. We have employed basis functions which are simple but more reliable than conventional variational wave functions due to relatively small perturbation corrections associated with the difference between the full electron-electron interaction and the single-particle approximation to it.

Recently, Cole and McCombe[25,26] have reported the observation of intersubband resonances on n-type Si(111) and Si(110) surface inversion layers. They have used the technique of far-infrared Fourier transform spectroscopy,[27] with which one can obtain the intersubband absorption spectra as a function of frequencies of incident light at any desired surface electron concentration. They observed distinct differences in resonance absorption for samples with different valley occupancies. The resonance frequencies for samples with p and s polarizations were very close to each other (shift is approximately 1 meV). The resonance with s polarization was observed at a reduced intensity compared to that with p polarization. The resonance frequencies for samples with normal valley occupancy are observed at frequencies much lower [approximately $8\sim10$ meV for a Si(111) sample] than those with twofold valley occupancy. However, their observations for normal valley occupancies appear to lie below subband separation within Hartree approximation. Because exchange-correlation effects should lead to an increase in the subband separation, there is a discrepancy between experiment and theory, the cause of which remains undetermined.[28]

In general, the resonance frequency is known to be shifted from the differences in the eigenvalues of the Schrödinger equation for the system, i.e., subband energy separation including the self-energy correction due to the many-particle effects. Both the effect of the depolarization of the system and the effect of the final-state interactions are included in this work and the results are the following: The magnitude of the shift in resonance frequency is shown to depend upon the characteristics of the system, such as the shape of the constant-energy surface, and upon the properties of the probe, such as the polarization of the incident light.

We have applied a linear-response theory of quasi-two-dimensional systems with arbitrarily tilted ellipsoidal energy surfaces to study intersubband resonance absorption and its relation to collective modes of the system. From the fact that the condition for resonance absorption is the same as the condition for collective modes of the system, we understand the resonances observed in far-infrared optical studies of semiconducting space-charge layers to be associated with the intersubband collective modes of the system. The polarization dependence of absorption spectra for the intersubband transitions is examined explicitly for a system with isotropic constant-energy surfaces, and for Si(111) and Si(110) surface inversion layers, respectively.

For a system with isotropic effective mass we have resonance absorption only with p-polarized incident light, and its strength is proportional to the dipole matrix element. For Si(111) or Si(110) inversion layers with normal sixfold or fourfold valley occupancy the conductivity tensor is diagonal and, hence the motions in different directions are not coupled to one another. However, each diagonal element σ_{ii}, except σ_{yy} for Si(110), has a finite intersubband part, which leads to intersubband transitions in these samples. Hence for these cases with normal valley occupancies we have observed that both p- and s-polarized incident light can induce intersubband transitions. Our calculation demonstrates that former resonance occurs at the frequency shifted from the corresponding quasiparticle energy difference due to both the depolarization effect and the final-state interaction; however, the latter one is affected only through the final-state interaction. For Si(111) and Si(110) layers with reduced valley occupancy, both resonance frequencies are shifted away from the corresponding quasiparticle energies due to coupling of motions in x (or y) and z directions. The intersubband transition energies are shown in Figs. 1 and 2 as a function of the surface electron density. The enhancement in the resonance

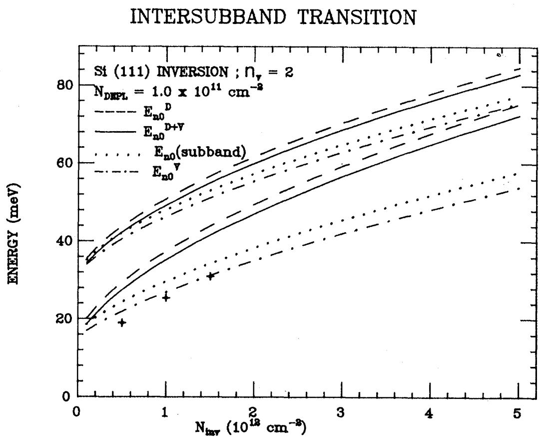

FIG. 1. Intersubband (0↔1 and 0↔2) transition energy in Si(111) surface inversion layers with $n_v=2$ as a function of inversion-layer electron concentration in the energy-functional perturbation method. Some of the experimental results are also indicated by the pluses (Ref. 25). The solid line represents the transition energy including both effects of the depolarization and the final-state interactions. The dotted lines show the quasiparticle energy separations (E_{n0}). The dashed and the dot-dashed curves correspond to $E_{n0}(1+\alpha_{nn})^{1/2}$ and $E_{n0}(1-\beta_{nn})^{1/2}$, respectively.

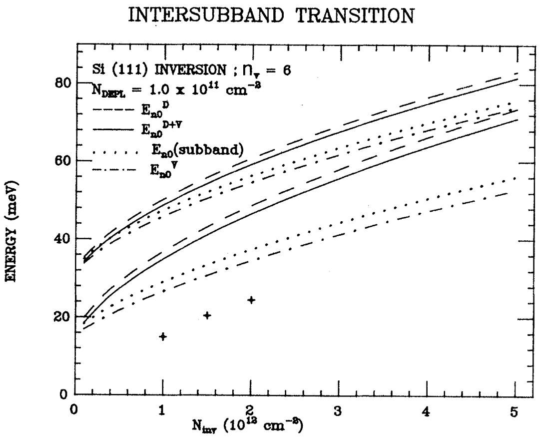

FIG. 2. Intersubband (0↔1 and 0↔2) transition energy in Si(111) surface inversion layers with $n_v=6$ as a function of inversion-layer electron concentration in the energy-functional perturbation method. Some of the experimental results are also indicated by the pluses (Ref. 25). The solid line represents the transition energy including both effects of the depolarization and the final-state interactions. The dotted lines show the quasiparticle energy separations (E_{n0}). The dashed and the dot-dashed curves correspond to $E_{n0}(1+\alpha_{nn})^{1/2}$ and $E_{n0}(1-\beta_{nn})^{1/2}$, respectively.

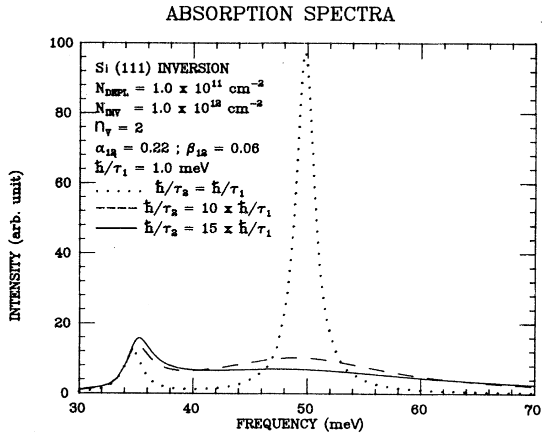

FIG. 3. Absorption spectra for intersubband transitions in Si(111) surface inversion layers with $n_v=2$. These are the results with $N_{\text{inv}}=10^{12}/\text{cm}^2$ and $N_{\text{depl}}=10^{11}/\text{cm}^2$. The coupling between the first-excited and the second-excited subbands is taken into account in the calculation; the parameters α_{12} and β_{12} are related to the degree of coupling between those two excited subbands [cf. Eq. (2.30)]. The dotted, the dashed, and the solid curves correspond to the absorption spectra with different sets of the relaxation times.

frequency for the system with reduced valley occupancy is in agreement with experiment. However, our agreement is only qualitative because the subband separations are certainly overestimated through the use of approximate variational wave functions for excited subbands. We have displayed some of the absorption spectra for Si(111) surface inversion layers with twofold valley occupancy in Figs. 3 and 4 for several different values of relaxation time. The coupling between the excited subbands shifts the resonance frequencies apart but the amount of the shift is relatively small in this case. As one increases the linewidth of the first excited subband relative to the higher ones the corresponding absorption peak becomes weaker. The dependence of the absorption spectra upon the angle of incidence of the perturbing electromagnetic wave is shown in Fig. 5 for Si(111) layers with the normal sixfold valley occupancy.

In general, the resonance strength for p-polarized light depends strongly upon the angle of incidence of the incoming light and the thickness of the oxide layer and of the gate electrode. In addition, we have also shown that the resonance strength for s-polarized light is reduced relative to that for p-polarized light in a system with given valley occupancy, as observed in experiment.[25] The decrease in the absorption strength for s-polarized light is related to the tilt angle of the system relative to the principal axes of the occupied valleys.

Finally, we have demonstrated that our calculation is in qualitative agreement with observations by Cole and McCombe.[25] It would be useful to demonstrate experimentally that intersubband resonance

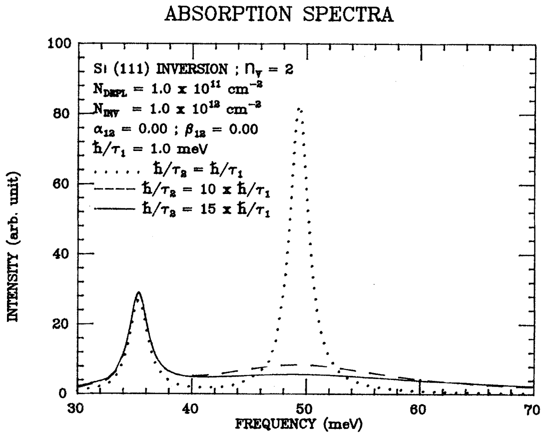

FIG. 4. Absorption spectra for intersubband transitions in Si(111) surface inversion layers with $n_v=2$. These are the results with $N_{\text{inv}}=10^{12}/\text{cm}^2$ and $N_{\text{depl}}=10^{11}/\text{cm}^2$. The coupling between the excited subbands is neglected in the calculation; the parameters α_{12} and β_{12} are related to the degree of coupling between the first-excited and the second-excited subbands. The dotted, the dashed, and the solid curves correspond to the absorption spectra with different sets of the relaxation times.

strength depends upon the thickness of the oxide layer and of the gate electrode, and the angle of incidence of the infrared light as predicted in this paper. The behavior of the resonances as a function of these parameters should be a useful tool in identifying which resonances are being observed. The analysis presented here, together with further experiments of the kind performed by Cole and McCombe should help to clear up the puzzle of the valley degeneracy on Si (111) and (110) surfaces.

ACKNOWLEDGMENT

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APPENDIX: EFFECTIVE-MASS TENSORS IN TILTED SILICON INVERSION LAYERS

Let us consider the effective masses in silicon inversion layers tilted by angle θ from (110) to (111) around $\langle\bar{1}10\rangle$. The surfaces with high symmetry Si (001), (110), and (111) correspond to $\theta=\pi/2$, $\theta=0$, and $\theta=\cos^{-1}(\frac{2}{3})^{1/2}$, respectively. Inverse effective-mass tensors in each tilted layer are given, for a given valley v, by

$$\underline{\alpha}^{(v)}(\theta)=\underline{R}(\theta)\underline{\alpha}^{(v)}\left[\frac{\pi}{2}\right]\underline{R}^{-1}(\theta)\ , \qquad \text{(A1)}$$

where $\underline{R}(\theta)$ and $\underline{R}^{-1}(\theta)$ are the rotations

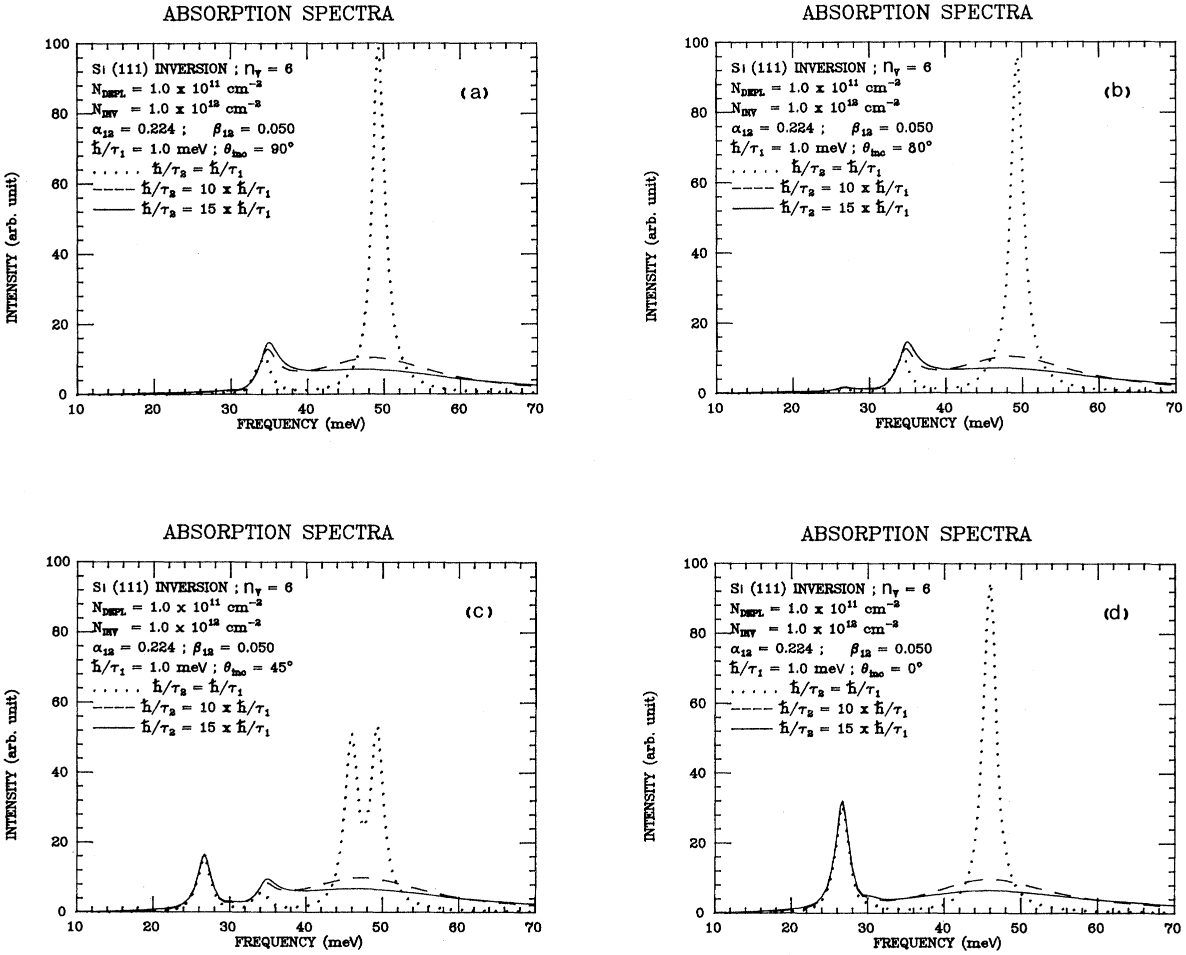

FIG. 5. Absorption spectra for intersubband transitions in Si(111) surface inversion layers with $n_v=6$. These are the results with $N_{\text{inv}}=10^{12}/\text{cm}^2$ and $N_{\text{depl}}=10^{11}/\text{cm}^2$. The coupling between the first-excited and the second-excited subbands is taken into account in the calculation; the parameters α_{12} and β_{12} are related to the degree of coupling between those two excited subbands [cf. Eq. (2.30)]. The angle of incidence is (a) 90°, (b) 80°, (c) 45°, and (d) 0°. The dotted, the dashed, and the solid curves correspond to the absorption spectra with different sets of the relaxation times.

$$\underline{R}(\theta)=\begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}}\sin\theta & -\frac{1}{\sqrt{2}}\sin\theta & \cos\theta \\ \frac{1}{\sqrt{2}}\cos\theta & \frac{1}{\sqrt{2}}\cos\theta & \sin\theta \end{bmatrix}, \qquad \text{(A2)}$$

$$\underline{R}^{-1}(\theta)=\begin{bmatrix} -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\sin\theta & \frac{1}{\sqrt{2}}\cos\theta \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\sin\theta & \frac{1}{\sqrt{2}}\cos\theta \\ 0 & \cos\theta & \sin\theta \end{bmatrix}, \qquad \text{(A3)}$$

and $\underline{\alpha}^{(v)}(\pi/2)$ is

$$\underline{\alpha}^{(v)}\left[\frac{\pi}{2}\right]=m\begin{bmatrix} \frac{1}{m_1^{(v)}} & 0 & 0 \\ 0 & \frac{1}{m_2^{(v)}} & 0 \\ 0 & 0 & \frac{1}{m_3^{(v)}} \end{bmatrix}. \qquad \text{(A4)}$$

Here $m_1^{(v)}$, $m_2^{(v)}$, and $m_3^{(v)}$ are the transverse or the longitudinal principal effective masses for an electron in a bulk silicon depending upon each valley,

$$\underline{\alpha}^{(a,b)}\left[\frac{\pi}{2}\right]=m\begin{bmatrix} m_t^{-1} & 0 & 0 \\ 0 & m_l^{-1} & 0 \\ 0 & 0 & m_t^{-1} \end{bmatrix}, \qquad \text{(A5)}$$

$$\underline{\alpha}^{(c,d)}\left[\frac{\pi}{2}\right]=m\begin{bmatrix} m_l^{-1} & 0 & 0 \\ 0 & m_t^{-1} & 0 \\ 0 & 0 & m_t^{-1} \end{bmatrix}, \qquad \text{(A6)}$$

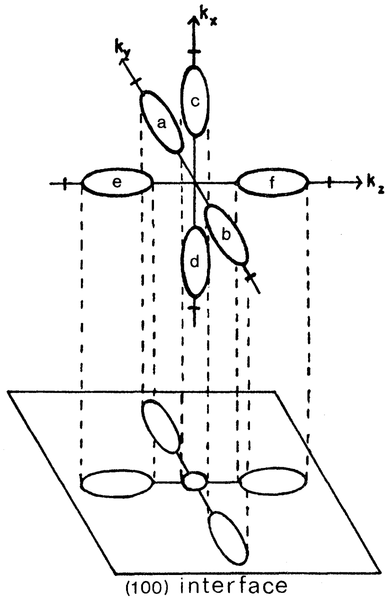

FIG. 6. Schematic representation for the constant-energy surfaces near the conduction-band minima in bulk silicon. The constant-energy surfaces are ellipsoids of revolution about the ⟨100⟩ axes. For the (100) surface orientation those valleys along k_x are equivalent and have the largest effective mass normal to the surface so as to be occupied by the electrons.

$$\underline{\alpha}^{(e,f)}\left[\frac{\pi}{2}\right]=m\begin{bmatrix} m_t^{-1} & 0 & 0 \\ 0 & m_t^{-1} & 0 \\ 0 & 0 & m_l^{-1} \end{bmatrix}. \qquad \text{(A7)}$$

In Eqs. (A5)–(A7), *a*, *b*, *c*, *d*, *e*, and *f* denote, respectively, each valley in Fig. 6.

Here let us show the results for electrons in the lowest valleys in Si (001), (110), and (111), respectively. For Si(001) it is the same as that in Eq. (A7). For Si(110),

$$\underline{\alpha}^{(ab,cd)}=\frac{m}{2}\begin{bmatrix} m_t^{-1}+m_l^{-1} & 0 & \pm(m_t^{-1}-m_l^{-1}) \\ 0 & \frac{2}{m_t} & 0 \\ \pm(m_t^{-1}-m_l^{-1}) & 0 & m_t^{-1}+m_l^{-1} \end{bmatrix}. \qquad \text{(A8)}$$

For Si(111),

$$\alpha^{(ab,cd)}=\frac{m}{2}\begin{bmatrix} m_t^{-1}+m_l^{-1} & \pm\frac{1}{\sqrt{3}}(m_t^{-1}-m_l^{-1}) & \mp\left[\frac{2}{3}\right]^{1/2}(m_t^{-1}-m_l^{-1}) \\ \pm\frac{1}{\sqrt{3}}(m_t^{-1}-m_l^{-1}) & \frac{1}{3}\left[\frac{5}{m_t}+m_l^{-1}\right] & \frac{\sqrt{2}}{3}(m_t^{-1}-m_l^{-1}) \\ \mp\left[\frac{2}{3}\right]^{1/2}(m_t^{-1}-m_l^{-1}) & \frac{\sqrt{2}}{3}(m_t^{-1}-m_l^{-1}) & \frac{2}{3}\left[\frac{2}{m_t}+m_l^{-1}\right] \end{bmatrix} \qquad \text{(A9)}$$

and

$$\alpha^{(e,f)}=m\begin{bmatrix} m_t^{-1} & 0 & 0 \\ 0 & \frac{1}{3}\left[m_t^{-1}+\frac{2}{m_l}\right] & -\frac{\sqrt{2}}{3}(m_t^{-1}-m_l^{-1}) \\ 0 & -\frac{\sqrt{2}}{3}(m_t^{-1}-m_l^{-1}) & \frac{1}{3}\left[\frac{2}{m_t}+m_l^{-1}\right] \end{bmatrix} . \tag{A10}$$

The principal inverse effective masses for electrons in a surface channel are, respectively,

$$\alpha_1,\alpha_2=\tfrac{1}{2}(\beta_{xx}+\beta_{yy}) \pm\tfrac{1}{2}[(\beta_{xx}-\beta_{yy})^2+4\beta_{xy}^2]^{1/2} \tag{A11}$$

and

$$\alpha_3=\alpha_{zz} . \tag{A12}$$

The β_{ij} are defined by

$$\beta_{ij}=\alpha_{ij}-\frac{\alpha_{zi}\alpha_{jz}}{\alpha_{zz}} , \tag{A13}$$

where i and j are x, y, or z.

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