RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 32, NUMBER 6 15 SEPTEMBER 1985

Inelastic electron scattering by collective charge-density excitations at the surface of a semiconductor superlattice

Pawel Hawrylak, Ji-Wei Wu, and J. J. Quinn
Brown University, Providence, Rhode Island 02912
(Received 10 May 1985)

Using linear response theory and the diagonal approximation, we calculate exactly and analytically surface response of a semi-infinite semiconductor superlattice to an electron moving in the vacuum. This response determines the scattering process. The electron-energy-loss spectrum due to surface intrasubband and intersubband plasmons is predicted for the first time.

Collective charge-density excitations of a semi-infinite semiconductor superlattice have been studied recently.[1–3] Intrasubband and intersubband surface modes have been found. These modes can exist only for a wavelength smaller than a critical value λ^*. They can be studied by the inelastic Raman scattering and electron-energy-loss spectroscopy[4] (EELS), but have not yet been observed experimentally. Recent calculations of Raman intensities[2,5] indicate possible difficulties in the ability to resolve surface modes from the bulk spectrum. Therefore, in this Rapid Communication we investigate the inelastic scattering of electrons from the surface of the semiconductor superlattice.

The semiclassical approach of Schaich[6] and of Camley and Mills[7] is used. This is well justified by the long-range nature of the scattering process and low-energy losses (10–100 meV). However, we do not model the superlattice by layers of materials with *a priori* given local dielectric function.[7] We treat the external electron as a perturbation and, within diagonal approximation, calculate exactly and analytically linear charge-density response of the superlattice and the scattering probability.

The model system under consideration consists of a semi-infinite array of quantum wells of thickness L, with centers separated by distance a. It is embedded in a semiconductor with a background dielectric constant ϵ, which occupies the half space $z>0$. An insulator (vacuum) occupies the space $z<0$. The single-particle electronic states are assumed to be of the form

$$\exp(i\mathbf{k}\cdot\mathbf{x})\xi_n(z-la-\delta) \ ,$$

where n is the subband index, $\mathbf{k}$ is the momentum in the plane prependicular to the z axis, and the integer l denotes the quantum well centered at $z=la+\delta$ $(\delta \geqslant L/2)$. Single-particle energies are simply $E_{nk}=E_n+\hbar^2k^2/2m$, where E_n is the subband energy, so the minibands are flat and electrons are localized in "quantum wells."

The classical trajectory of the scattering electron is given by $\mathbf{r}(t)=(\mathbf{x}(t),z(t))$, and its velocity by $\mathbf{v}=(\mathbf{v}_{\parallel},v_{\perp})$. The potential in the vacuum $\phi_<(z<0)=\phi_<(\mathbf{q},\omega,z)\times\exp(i\mathbf{q}\cdot\mathbf{x}-i\omega t)$ is written as

$$\phi_<(z)=A\left[\cos\left[(\omega-\mathbf{q}\cdot\mathbf{v}_{\parallel})\frac{z}{v_\perp}\right]+Re^{+qz}\right] \ . \tag{1}$$

The first part is the potential due to the moving electron in the vacuum and $R\exp(qz)$ is the induced potential, i.e., the response of the superlattice to an external charge. The amplitude A is given by

$$A=\frac{8\pi e v_\perp}{v_\perp^2q^2+(\omega-\mathbf{q}\cdot\mathbf{v}_{\parallel})^2} \ .$$

The probability $P(q,\omega)\,d^2\mathbf{q}\,d\omega$ that the electron is inelastically scattered into the range of energy losses between $\hbar\omega$ and $\hbar(\omega+d\omega)$, and into the range of momentum losses parallel to the surface between $\hbar\mathbf{q}$ and $\hbar(\mathbf{q}+d\mathbf{q})$, is given by[6,7]

$$P(\mathbf{q},\omega)=\frac{4e^2v_\perp^2q}{\hbar\pi^2}\frac{\mathrm{Im}[-R(q,\omega)]}{[q^2v_\perp^2+(\omega-\mathbf{q}\cdot\mathbf{v})^2]^2} \ . \tag{2}$$

$P(\mathbf{q},\omega)$ completely specifies the kinematics of the electron at the detector. Total information about the system is in the response function $R(q,\omega)$.

In order to calculate $R(q,\omega)$ we must calculate total potential in the superlattice $\phi_>(q,\omega,z)$. Then the continuity of the total potential $\phi_<(0)=\phi_>(0)$ determines R. We decompose $\phi_>(z)$ into the sum of external potential $\phi_>^{\mathrm{ext}}(z)$ and induced potential $\delta\phi_>(z)$. The external potential, including the effect of image charge is simply given by $\phi_>^{\mathrm{ext}}(z)=A\exp(-qz)/(\epsilon+1)$. The induced potential is related to the induced charge density by Poisson's equation, which in its integral form gives $(z,z'>0)$

$$\delta\phi_>(z)=\int dz'\,G(z,z')\delta n(z') \ . \tag{3}$$

The Green's function $G(z,z')$, including effects of the image charges is given by[3,8]

$$G(z,z')=V_q(e^{-q|z-z'|}+\alpha e^{-q(z+z')}) \ , \tag{4}$$

with $V_q=2\pi e^2/\epsilon q$ and $\alpha=(\epsilon-1)/(\epsilon+1)$. The induced density is related to the total potential by the use of standard perturbation theory.[3,9] To simplify the algebra we assume that only the lowest subband is occupied and that there is no mixing of different intersubband excitations (diagonal approximation[9]). Then the induced potential on the surface $(z=0)$ is simply related to the total potential in the *entire* superlattice.

$$\delta\phi_>(0)=(1+\alpha)e^{-\delta q}\sum_{n,l}S_nV_q\chi_n^0\phi_{n0}(l)e^{-qla} \ , \tag{5}$$

where

$$\phi_{n0}(l)=\int dz\,\phi_>(z)\psi_n(z-la-\delta) \ ,$$

$$S_n=\int dz\,e^{-qz}\psi_n(z),\quad \psi_n(z)=\xi_n(z)\xi_0(z) \ ,$$

and $\chi_n^0(q,\omega)$ is the layer-independent polarizability of the noninteracting system.[3,9] Clearly, the induced potential at the surface depends on the total potential, with the values close to the surface contributing most.

We define the dielectric matrix[3] $\epsilon(l,l';n)$ as

$$\epsilon(l,l';n)=\delta_{l,l'}-\chi_n^0 V_{n,n}(l,l') \ , \tag{6}$$

with

$$V_{n,n}(l,l')=\int dz \int dz' \psi_n(z-la-\delta) \times G(z,z')\psi_n(z'-l'a-\delta) \ . \tag{7}$$

Then the total potential is related to the external potential by the inverse dielectric matrix $\epsilon^{-1}(l,l',n)$:

$$\phi_{n0}(l)=\sum_{l'}\epsilon^{-1}(l,l';n)\phi_{n0}^{\mathrm{ext}}(l') \ . \tag{8}$$

When we define the effective inverse dielectric function $1/\epsilon_n$ for the inelastic electron scattering as

$$\frac{1}{\epsilon_n}=\sum_{l,l'}\epsilon^{-1}(l,l')e^{-qla}e^{-ql'a} \ , \tag{9}$$

we arrive at the final expression for the response of the superlattice on the surface

$$R=\sum_n \frac{1+\alpha}{1+\epsilon}e^{-2\delta q}S_n^2 V_q \chi_n^0 \frac{1}{\epsilon_n}+\frac{1}{\epsilon+1}-1 \ . \tag{10}$$

The first term is proportional to the density of electrons. It is simply the sum of all possible processes by which an electron can lose energy to the collective excitations of the superlattice. The second term is due to the background semiconductor, and it mixes with electronic excitations. The effective inverse dielectric function is calculated by inverting the dielectric matrix for a finite system of N layers[5] and at the end taking $N\rightarrow\infty$ limit. In doing so the transformation introduced by Jain and Allen[2] is used. We give here only the final result

$$\frac{1}{\epsilon_n}=\left[1+\frac{\chi_n^0 V_q G_{-n}\sinh(qa)(1+e^{\beta}e^{qa})}{\gamma(1-e^{\beta}e^{qa})(b^2-1)^{1/2}}\right] \Big/ \gamma(1-e^{-2qa})+\frac{\chi_n^0 V_q(e^{\beta}A-2B+Ce^{-\beta})}{\gamma^2 2(e^{\beta}-e^{-qa})(b^2-1)}\frac{1}{Q} \ . \tag{11}$$

All new symbols appearing in Eq. (11) are defined below:

$$\gamma=1-\chi_n^0 V_q(V_{-n}-G_{-n}) \ , \tag{12.1}$$

$$b=\cosh(qa)-\chi_n^0 V_q G_{-n}\sinh(qa)/\gamma \ , \tag{12.2}$$

$$e^{\beta}=b+(b^2-1)^{1/2} \ , \tag{12.3}$$

$$(a_0,b_0,c_0)=G_{-n}(1,\cosh(qa),1)+G_{+n}(e^{qa},e^{qa},1) \ , \tag{12.4}$$

$$H=\frac{e^{-\beta}(b^2-1)^{-1/2}-e^{-qa}\sinh^{-1}(qa)}{2\sinh(qa)G_{-n}} \ , \tag{12.5}$$

$$G=\frac{(b^2-1)^{-1/2}-\sinh(qa)^{-1}}{2\sinh(qa)G_{-n}} \ , \tag{12.6}$$

$$Q=1-G(a_0+c_0)+2b_0H+(H^2-G^2)(b_0^2-a_0c_0) \ , \tag{12.7}$$

$$(A,B,C)=(b_0^2-a_0c_0)(G,H,G)+(a_0,b_0,c_0) \ , \tag{12.8}$$

$$V_{\pm n}=\int\int dz\, dz'\, \psi_n(z)e^{-q|z\pm z'|}\psi_n(z') \ . \tag{12.9}$$

The matrix elements G_{+n} are defined by a similar expression, except for the replacement of $|z\pm z'|$ by $(z\pm z')$. Here e^{β} is defined such that $|e^{\beta}|>1$, if not the replacement $\sqrt{b^2-1}$ by $-\sqrt{b^2-1}$ is understood everywhere.

We identify the first term as the bulk contribution. By this we mean the answer one obtains if in Eq. (9) one approximates the inverse dielectric function by the expression appropriate for the infinite, translationally invariant system. The second term is the surface correction. It diverges when $Q(q,\omega)=0$, which gives dispersion of surface modes. In this case $\mathrm{Re}\beta>0$ and β plays the role of the decay length. Bulk modes are given by $|b|<1$. The dispersion relation of bulk and surface modes are obtained in a standard way,[1-3] and are shown in Fig. 1. Parameter values are $L=200$ Å, $a=404$ Å, $m=0.068m_e$, $n=4.2\times10^{11}$ cm^{-2}, and $E_{10}=21.7$ meV, corresponding to the n-type GaAs-Al$_x$Ga$_{1-x}$As sample studied by Pinczuk *et al.*[10] Long-wavelength limits of the polarizability $\chi_n^0(q,\omega)$ have been used and matrix elements have been approximated by the infinite well expressions.[3] The coupling to optical phonons is included by in-

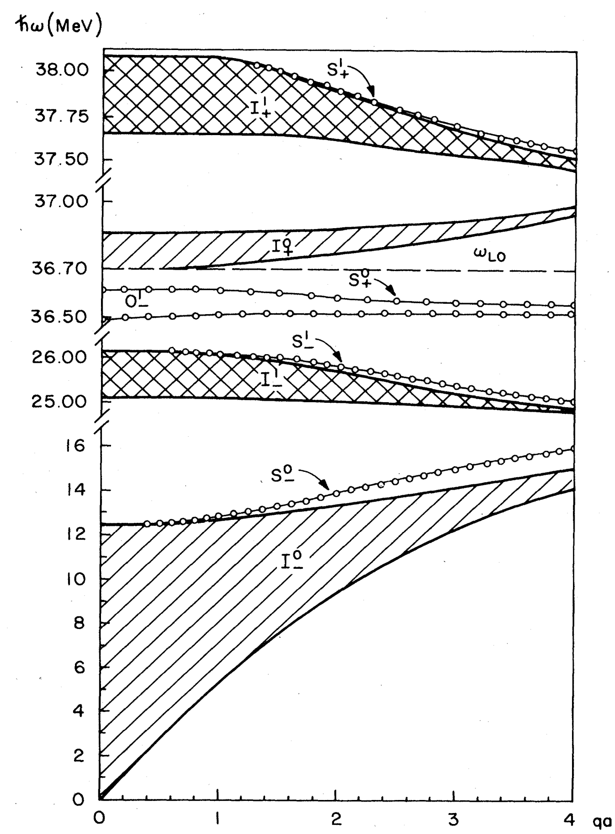

FIG. 1. Dispersion relation ω vs q for bulk (shaded area) and surface (broken line) intrasubband ($m=0$) and intersubband ($m=1$) modes. The values of parameters are as follows: $n=4.2\times10^{11}$ cm^{-2}, $a=404$ Å, $L=200$ Å, $2\delta=L$, $m=0.068m_e$, $\epsilon_\infty=11.1$, $\hbar\omega_{\mathrm{LO}}=36.7$ meV, $\hbar\omega_{\mathrm{TO}}=33.6$ meV, and $E_{10}=21.7$ eV. Bulk (surface) modes are denoted by $I_{+,-}^m$ ($S_{+,-}^m$); O^m are new surface modes associated with intersubband transitions. For better visibility different energy scales are used.

troducing the frequency-dependent dielectric function

$$\epsilon(\omega) = \epsilon_\infty(\omega^2 - \omega_{LO}^2)/(\omega^2 - \omega_{TO}^2)$$

with $\epsilon_\infty = 11.1$, $\hbar\omega_{LO} = 36.7$ meV and $\hbar\omega_{TO} = 33.6$ meV as the background dielectric constant. This results in coupled plasmon-optical phonon modes.

We now turn to the scattering probability $P(\mathbf{q},\omega)$. Figure 2 shows $P(\mathbf{q},\omega)$ (normalized to the intrasubband surface mode value) along the line $q = (k_i \sin\theta_i)\, \hbar\omega/2E_i$, where k_i, E_i, and θ_i are the incident wave vector, energy, and angle of 10-eV electrons specularly scattering at $\theta_i = 55°$ from the surface. Here only lowest-energy excitations are shown with energy below the optical phonon energy $\hbar\omega_{LO}$, while full discussion is deferred to future publication.[11] The low-energy peak at 13.1 meV corresponds to the intrasubband surface plasmon S_-^0 and the higher-energy peak at 25.6 meV to the intersubband surface plasmon S_-^1. The difference in intensity is mainly due to the kinematic factor which enhances energy losses at low frequencies. The width of the peaks is controlled by the finite mobility of electrons and finite phonon lifetime (here $\gamma_e = \gamma_{ph} = 0.3$ meV). The broadening due to the bulk excitations is indicated, along with frequencies of the bulk plasmon band edges ($\hbar\omega_{max}, \hbar\omega_{min}$). Complete calculation of EELS would average $P(\mathbf{q},\omega)$ over the experimental angle and energy resolution functions, but surface modes are clearly well resolved.

In conclusion, we find that EELS should prove useful in the observation of surface collective modes in semiconductor superlattices. Simple, analytical, and exact results presented here will allow for clear and elegant interpretation of experimental results.

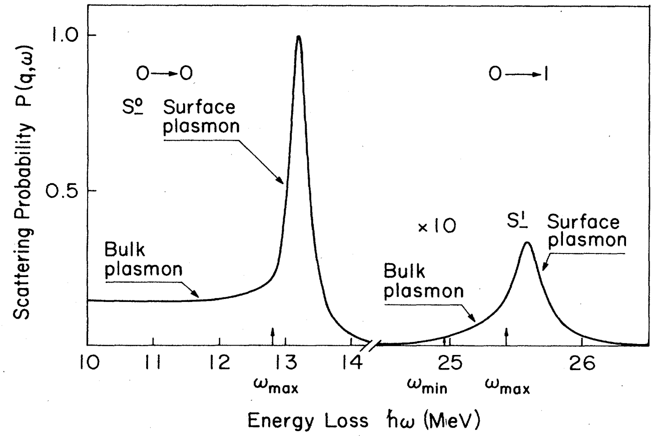

FIG. 2. Scattering probability $P(\mathbf{q},\omega)$ (normalized to the S_-^0 surface plasmon value) for intrasubband (0-0) and intersubband (0-1) surface plasmons as a function of energy loss for 10-eV electrons specularly scattering from the surface at the angle of incidence $\theta_i = 55°$ along the $q = (k_i \sin\theta_i)\hbar\omega/2E_i$ line. All other parameters as in Fig. 1 (see text).

Financial support of the U.S. Army Research Office, Durham, is acknowledged.

[1] G. F. Giuliani and J. J. Quinn, Phys. Rev. Lett. **51**, 919 (1983).
[2] J. K. Jain and P. B. Allen, Phys. Rev. Lett. **54**, 947 (1985).
[3] P. Hawrylak, J. W. Wu, and J. J. Quinn, Phys. Rev. B **31**, 7855 (1985).
[4] For a review, see H. Ibach and D. L. Mills, *Electron Energy Loss Spectroscopy and Surface Vibrations* (Academic, San Francisco, 1982).
[5] P. Hawrylak, J. W. Wu, and J. J. Quinn (unpublished).
[6] W. L. Schaich, Phys. Rev. B **24**, 686 (1981).
[7] R. E. Camley and D. L. Mills, Phys. Rev. B **29**, 1695 (1984).
[8] D. L. Dahl and L. J. Sham, Phys. Rev. B **16**, 651 (1977).
[9] A. C. Tselis and J. J. Quinn, Phys. Rev. B **29**, 3318 (1984).
[10] A. Pinczuk, J. M. Worlock, H. L. Stormer, R. Dingle, W. Wiegmann, and A. C. Gossard, Solid State Commun. **36**, 43 (1980).
[11] P. Hawrylak, J. W. Wu, and J. J. Quinn (unpublished).