Surface polaritons in LO-phonon–plasmon coupled systems in semiconductors

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Surface polaritons in an LO-phonon–plasmon coupled system are studied in cylindrical and semi-infinite geometries. Characters of the dispersion relation of the surface polaritons are very different from the case of high carrier electron density and for the case of low density. With electron current the surface polaritons are destabilized in the low-density regime, while they remain stable in the high-density regime.

I. INTRODUCTION

Surface modes on the interface of a semiconductor and another dielectric (or metal) have attracted considerable interest recently. Previous studies have been carried out on the surface polaritons in association with phonons,[1] exitons,[2] plasmons,[3] and magnetoplasmons.[4] In this paper we present a theory of the surface polaritons of LO-phonon–plasmon coupled modes at the interface of a semiconductor and a dielectric. For the bulk-mode case, Mooradian and McWhorter[5] observed two branches of coupled modes of phasmons and LO phonons at various plasma densities. In n-type GaAs the electron-plasma frequency ω_e in the semiconductor becomes larger than the optical-phonon frequencies ($\omega_{\rm TO}, \omega_{\rm LO}$) when the carrier density exceeds $\sim 10^{18}$ cm^{-3}.[5] Around this value of electron concentration the interaction between plasmons and phonons is very important.

In the following sections we illustrate the transition of one type of dispersion relation to another type for the surface polaritons in an LO-phonon-plasmon coupled system. In the case of bulk modes the upper branch in the LO-phonon–plasmon dispersion relation gradually changes its phononlike character to the more and more plasmonlike character as the concentration of plasma electrons increases. In the case of surface modes (polaritons), in addition to such gradual changeover between plasmonlike and phononlike characters, there is a qualitative transition as the electron exceeds the density where $\omega_e \approx \omega_{\rm TO}$. This happens because the surface modes have a few stop bands in the ω-k plane of the dispersion relation and sometimes a specific mode is inside the stop band and is, therefore, forbidden.

We also study the properties of the dispersion relation of this LO-phonon–plasmon coupled system in the presence of current. As is well known, a current due to drifting plasma electrons causes an instability which enhances optical-phonon amplitudes. The properties of the surface polaritons excited by the current also show a drastic change with the carrier concentration. In the low-electron-density case the surface polaritons (admixture of phonons and plasmons) are made unstable by the electron current, while in the high-density case the surface polariton instability due to the current disappears.

Our approach to the present problem is the following. Basing upon the known dispersion function of the bulk system of coupled LO-phonon–plasmon in a semiconductor, we first impose boundary conditions for the semiconductor and the dielectric in a cylindrical geometry. The resultant dispersion relation for the surface modes is still valid in the limit of the infinite radius ($a \to \infty$) of the semiconductor. This corresponds to a semi-infinite flat surface. Stop bands and propagation bands of the surface polaritons are studied by a computer study of the dispersion relation. Then we study the same dispersion relation for the surface polaritons with electron current. The properties of the instability is briefly discussed. The onset of the instability and disappearance of the instability are extensively explored through the computer study. Finally we discuss the case of a small radius of the semiconductor.

II. LO-PHONON–PLASMON COUPLED SURFACE POLARITONS

To describe the dielectric properties of an LO-phonon–plasmon coupled system, we may start with the following familiar dielectric function[5]

$$\frac{\epsilon(k,\omega)}{\epsilon_\infty} = 1 - \frac{\omega_e^2}{\omega^2 - \gamma_e T_e k^2/m^*} - \frac{\Omega_p^2}{\omega^2 - \omega_{\rm TO}^2}, \qquad (1)$$

where ϵ_∞ is the optical dielectric constant of the semiconductor; m^* is the electron effective mass; γ_e is the electron-gas constant; T_e is the electron

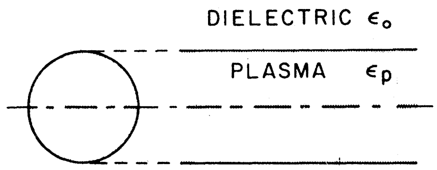

FIG. 1. Configuration of a cylindrical sample surrounded by a dielectric.

temperature; ω_{TO} is the transverse-optical phonon frequency; $\omega_e=(4\pi n_e e^2/\epsilon_\infty m^*)^{1/2}$ is the plasma frequency; $\Omega_p=[(4\pi N e^{*2}/\epsilon_\infty)(1/M_1+1/M_2)]^{1/2}$ is the ionic plasma frequency; and N, e^*, M_1, and M_2 are the ion density, ionic change, the first kind of ion mass, and the second kind of ion mass, respectively. In this section we consider the effects of a cylindrical and a semi-infinite sample geometry on the coupled modes of phonons and free-carrier plasmons. To see if the electromagnetic wave couples to the other elementary excitations through the presence of a surface, we should retain a full description of Maxwell's equations. The configuration is shown in Fig. 1. For simplicity we consider an azimuthally symmetric case.

Maxwell's equations in the cylindrical coordinate with the azimuthal number $n=0$ are

$$-\frac{\partial^2}{\partial z^2}E_\rho+\frac{\partial^2}{\partial z\partial\rho}E_z-\frac{\omega^2}{c^2}D_\rho=0\,, \qquad (2)$$

$$-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}E_z+\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial z}E_\rho-\frac{\omega^2}{c^2}D_z=0\,. \qquad (3)$$

The displacement vector $\vec{D}$ is expressed in terms of the electric field $\vec{E}$ with the dielectric function $\epsilon(\vec{k},\omega)$. We assume that ϵ does not depend on ρ. The boundary conditions are as follows: the electric field is finite at $\rho=0$ and zero at $\rho=\infty$; the electric field along z is continuous at the surface and the ρ component of the displacement is continuous across the surface. After applying these boundary conditions, we obtain the dispersion relation of the azimuthally symmetric modes in a cylindrical semiconductor plasma surrounded by a medium with a dielectric function ϵ_0 as[6]

$$\frac{\epsilon_p}{\epsilon_0}=-\frac{\beta_-}{\beta_+}\frac{K_1(\beta_+a)I_0(\beta_-a)}{K_0(\beta_+a)I_1(\beta_-a)}\,, \qquad (4)$$

where $\beta_-^2\equiv k^2-(\omega^2/c^2)\epsilon_p$, $\beta_+^2\equiv k^2-(\omega^2/c^2)\epsilon_0$, K_l, I_j are the modified Bessel functions of lth and jth order, and the wave vector k is directed along the z axis. The dispersion relation Eq. (4) is naturally a generalization of the semi-infinite case. In fact, putting the radius $a\to\infty$, we reproduce from Eq. (4) the familiar surface polariton dispersion relation[1]

$$\left(\frac{kc}{\omega}\right)^2=\frac{\epsilon_p\epsilon_0(\epsilon_p-\epsilon_0)}{(\epsilon_p+\epsilon_0)(\epsilon_p-\epsilon_0)}=\frac{\epsilon_p\epsilon_0}{\epsilon_p+\epsilon_0}\,. \qquad (5)$$

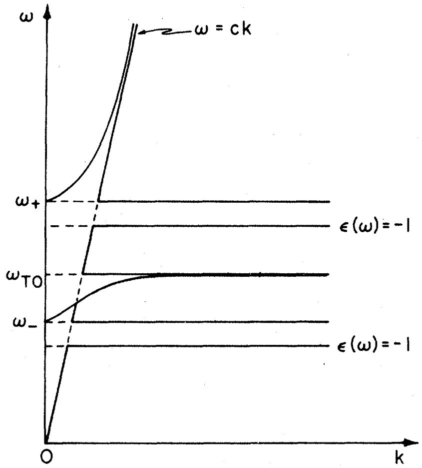

FIG. 2. Allowed areas for the surface modes (shaded areas).

Here we have used the asymptotic forms for the Bessel functions.

Among the dispersion branches generated by Eq. (5), some are entirely forbidden or partially forbidden because of the requirement that modes be localized at the surface. One can map out the forbidden (or stop) band and pass bands for the surface polaritons by requiring the following condi-

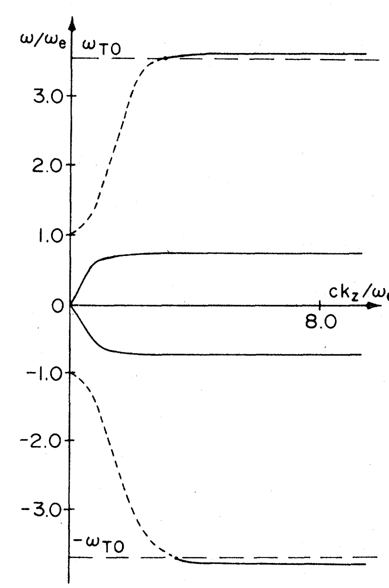

FIG. 3. Dispersion relation of the surface polaritons at the flat surface for low-plasma electron density. $\omega_{TO}/\omega_e=3.46$ and $\Omega_p/\omega_e=0.5$. The top and bottom branches are the ω_+ branches and the middle two are the ω_- branches. The surface polaritons arising from the ω_- branch are allowed throughout the entire frequency range, while the surface polaritons arising from the ω_+ branch are forbidden below ω_{TO} (dashed curve). See Fig 2.

tions:

$$\beta_+^2 \geq 0 \tag{6}$$

and

$$\beta_-^2 \geq 0 \tag{7}$$

These conditions insure that k be real, and yields from Eq. (5) the relation

$$1+\epsilon_0 - \frac{\omega_e^2}{\omega^2 - \gamma_e T_e k^2/m^*} - \frac{\Omega_p^2}{\omega^2 - \omega_{\mathrm{TO}}} < 0 \,. \tag{8}$$

The areas mapped out by Eqs. (6)–(8) are illustrated in Fig. 2. Equation (8) gives the lower pass band boundary $\omega \cong (\omega_e/\sqrt{2})(1-\Omega_p^2/\omega_{\mathrm{TO}}^2)^{1/2}$ and the upper pass band boundary $\omega^2 \cong \omega_{\mathrm{TO}}^2 + \frac{1}{2}\Omega_p^2 + \frac{1}{2}\Omega_p^2\omega_e^2/\omega_{\mathrm{TO}}^2$ for low-carrier density cases. One obtains the lower pass band boundary $\omega^2 \cong \omega_{\mathrm{TO}}^2 - \omega_{\mathrm{TO}}^2\Omega_p^2/\omega_e^2$ and the upper kind boundary $\omega^2 \cong \frac{1}{2}(\Omega_p^2 + \omega_e^2) + \omega_{\mathrm{TO}}^2\Omega_p^2/\omega_e^2$ for high-carrier density cases. (ϵ_0 was taken to be unity.)

The dispersion relation Eq. (5) with Eq. (1) has been studied numerically. Typical cases are illustrated in Figs. 3–5. Figure 3 exhibits the case where the plasma electron density is low so that $\omega_e < \omega_{\mathrm{TO}}$. The surface polaritons arising from the ω_- branch are allowed throughout the entire frequency range, while the surface polaritons arising from the ω_+ branch is forbidden below $\omega = \omega_{\mathrm{TO}}$. In this case the ω_- branch corresponds to the plasmon-dominated mode, while the ω_+ branch corresponds to the phonon-dominated polariton. Figure 5 exhibits the alternative case where the plasma electron density is high so that $\omega_e > \omega_{\mathrm{TO}}$. There is a major topological difference in this dispersion curve from that of Fig. 3. In Fig. 5 the surface polaritons arising from the ω_- branch gets cut off for larger wave vectors, while the ω_+ branch gets cut off for smaller wave vectors. (See the magnified inset in Fig. 5 for detail). In this case the upper branch is the plasmon-dominated surface polariton branch, while the lower one is phonon dominated. Note that the phonon-dominated branch does not extend to a larger wave-vector region in contrast to the case $\omega_e < \omega_{\mathrm{TO}}$. Figure 4 shows the case inbetween.

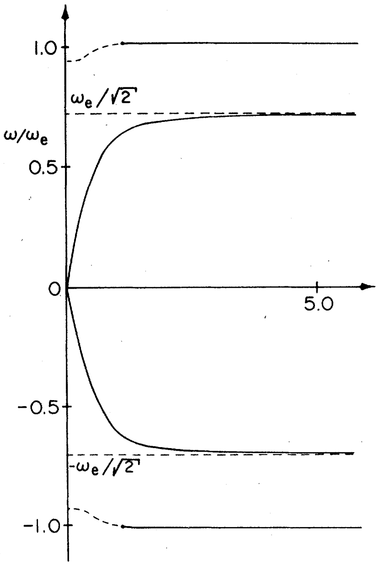

FIG. 4. Dispersion relation of the surface polaritons at the flat surface for intermediate-plasma electron density. $\omega_{\mathrm{TO}}/\omega_e = 1$ and $\Omega_p/\omega_e = 0.15$. The top and bottom branches are the ω_+ branches and the middle two are the ω_- branches.

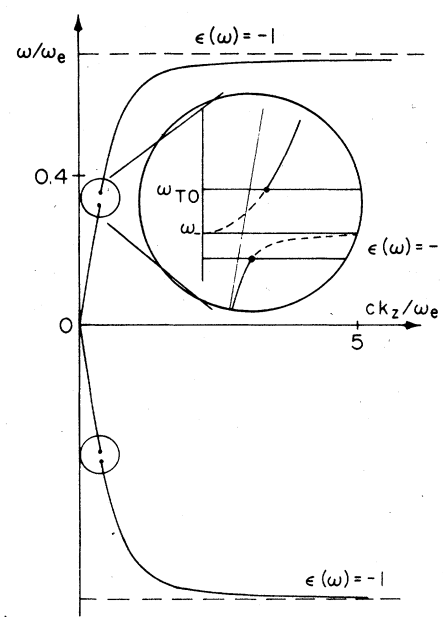

FIG. 5. Dispersion relation of the surface polaritons at the flat surface for high-plasma electron density. $\omega_{\mathrm{TO}}/\omega_e = 0.346$ and $\Omega_p/\omega_e = 0.05$. The top and bottom branches are the ω_+ branches, while the short middle branches are the ω_- branches. In contrast to Figs. 3 and 4, the surface polaritons arising from the ω_- branch are cut off for large wave vectors. The inset shows the details of this gap.

III. SURFACE-POLARITON INSTABILITIES IN THE PRESENCE OF ELECTRON CURRENT

When the plasma electrons are drifting in the semiconductor, the dielectric function becomes, instead of Eq. (1),

$$\frac{\epsilon(k,\omega)}{\epsilon_\infty} = 1 - \frac{\omega_e^2}{(\omega - k v_D)^2 - \gamma_e T_e k^2/m^*} - \frac{\Omega_p^2}{\omega^2 - \omega_{\mathrm{TO}}^2}\,, \tag{9}$$

where v_D is the drift velocity of the electrons. To have a sketch of the analytical properties of Eq.

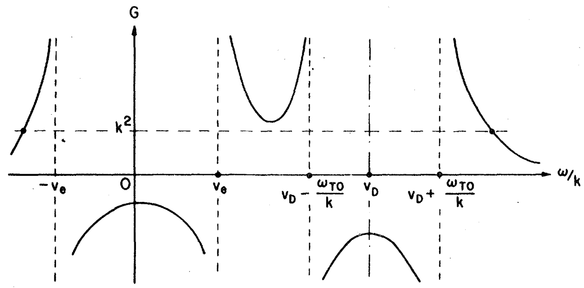

FIG. 6. Plot of the function $G(\omega/k)$. When the curve between $\omega/k = v_e$ and $\omega/k = v_D - \omega_{TO}/k$ does not cross the line $G = k^2$, a pair of complex conjugate roots (the instability) appears.

(9), we plot the graph of $G(\omega/k)$ where

$$G\left(\frac{\omega}{k}\right) = \frac{\omega_e^2}{(\omega/k)^2 - \gamma_e T_e/m^*} + \frac{\Omega_p^2}{(\omega/k - v_D)^2 - \omega_{TO}^2/k^2} . \tag{10}$$

Equation (10) is a Galilei transformed form of the last two terms (times k^2) in Eq. (9). Equation (10) and ω/k = constant are plotted in Fig. 6. If $v_e < v_D - \omega_{TO}/k$ ($v_e^2 \equiv \gamma_e T_e/m^*$), there may be a pair of complex-conjugate solutions to Eq. (9) when the curve between $\omega/k = v_e$ and $\omega/k = v_D - \omega_{TO}/k$ does not intersect the line ω/k = constant. k can be chosen $\sim\omega_{TO}/v_D$. By expansion of ω near ω_{TO} we obtain the growth rate for the instability arising from Eq. (9) as

$$\delta\omega \cong i(1/\sqrt{2})(\omega_e/\omega_{TO})^{1/2}\Omega_p , \tag{11}$$

when $|\delta\omega| \ll \omega_{TO}$ and

$$\delta\omega \cong i(\tfrac{1}{4}\sqrt{3})(\omega_e \Omega_p^2)^{1/3} , \tag{12}$$

when $|\delta\omega| \gg \omega_e$.

This instability is due to the well-known charge-bunching mechanism.[7] The instability takes place always at the crossing of the forward-propagating phonon branch and the negative-energy plasma-wave (slow phase-velocity wave) branch. Numerical results from Eq. (9) are plotted in Figs. 7 and 8. The system becomes unstable when $v_D \gtrsim 1.3 v_e$.

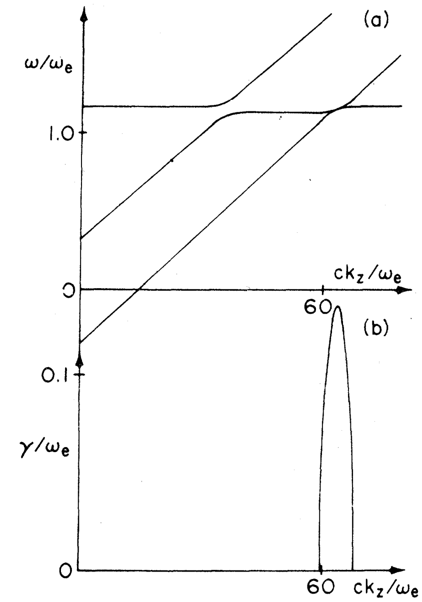

FIG. 7. Dispersion relation of the bulk modes with current. $\omega_{TO}/\omega_e = 3.46$, $\Omega_p/\omega_e = 0.5$, $v_D = 0.07c$, and $v_T = 0.01c$. The system becomes unstable when $v_D \gtrsim 1.3 v_e$ and the growth rate is a strong function of v_D/v_e: (a) the real frequency vs wave vector (the phonon branch of the negative frequency side is omitted). The top branch is phononlike and the second and the last are plasmonlike at smaller wave-vector range; (b) the growth rate vs wave vector.

Let us now consider the surface polaritons driven by the electron current. One can simply apply ϵ_p in Eq. (9) to Eqs. (4) or (5). The surface polariton dispersion relation in the semi-infinite case is

$$\frac{1}{\epsilon_0}\left(\frac{kc}{\omega}\right)^2 = \left(1 - \frac{\Omega_p^2}{\omega^2 - \omega_{TO}^2} - \frac{\omega_e^2}{(\omega - kv_D)^2 - k^2 v_e^2}\right)\left(\frac{1}{\epsilon_0} + 1 - \frac{\Omega_p^2}{\omega^2 - \omega_{TO}^2} - \frac{\omega_e^2}{(\omega - kv_D)^2 - k^2 v_e^2}\right)^{-1} . \tag{13}$$

In drawing the dispersion relation for the present system, we note from the study of the bulk modes above that the mode becomes unstable only when and where the forward phonon branch can intersect the slow wave plasma branch. As is clear from the the discussion in Sec. II, there is *no* surface polariton branch beyond $k \sim (1/\sqrt{2})\tilde{\omega}/c$, where $\tilde{\omega}$ is the root of $\epsilon(\omega) = -1$ and near $\omega = \omega_-$ when $\omega_e > \omega_{TO}$ (see Fig. 5). Therefore, there can *not* be a phonon (dominated) branch which can intersect the plasmon-dominated branch whose slope in the ω_- plane is $\sim v_D$ ($\ll c$) when $\omega_e > \omega_{TO}$. Extensive computer study of Eq. (13) has been carried out and the results are shown in Figs. 9–11.

Figure 9 is for the case where the plasma density is low and $\omega_e < \omega_{TO}$. The surface polariton can be driven unstable by the electron current in this case. The unstable wave-vector region is well localized near $k = \omega_{TO}/v_D$. Figure 10 is the case where ω_e is very close to ω_{TO} but still slightly smaller than ω_{TO}. On the other hand, Fig. 11 exhibits the case where $\omega_e > \omega_{TO}$. As we discussed, there is no crossing of the phononlike branch and the plasmonlike branch for the surface mode, and therefore no instability for the surface polaritons.

Finally let us discuss the small radius limit

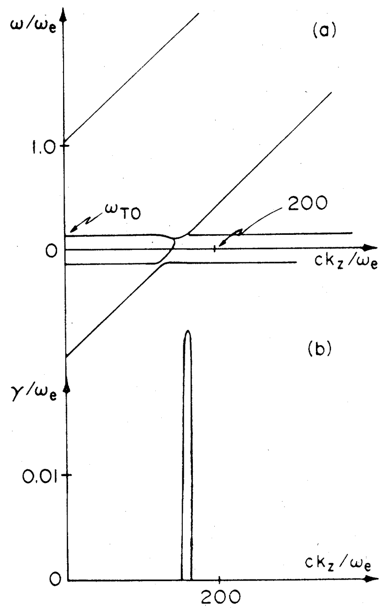

FIG. 8. Dispersion relation of the bulk modes with current. $\omega_{\mathrm{TO}}/\omega_e = 0.11$, $\Omega_p/\omega_e = 0.016$, $v_D = 0.07c$, and $v_e = 0.01c$. The instability takes place at the crossing of the optical-phonon dominated mode (ω_-) and the negative energy plasmon dominated mode (ω_+): (a) the real frequency vs wave vector. The two sloped branches are plasmonlike and the middle two branches are phononlike at lower wave-vector range: (b) the growth rate vs wave vector.

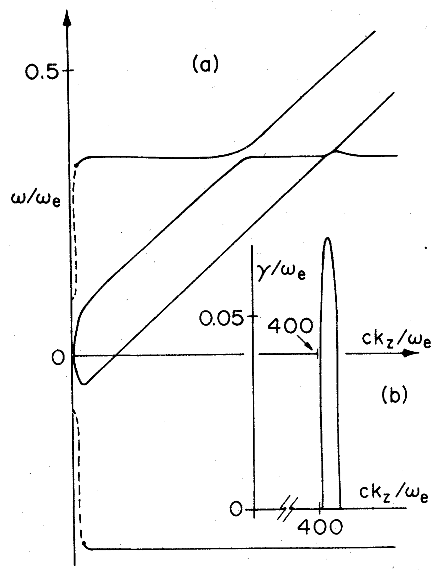

FIG. 9 Surface polariton dispersion relation in the regime of low-plasma electron density. $\omega_{\mathrm{TO}}/\omega_e = 3.46$, $\Omega_p/\omega_e = 0.5$, $v_D = 0.1c$, and $v_e = 0$. The instability occurs at the crossing of the surface phonons and the negative energy plasmons: (a) the real frequency vs wave vector. The top and bottom branches are surface phononlike and the middle two branches are surface plasmonlike at lower wave-vector range; (b) the growth rate vs wave vector.

(β_+a and β_-a are much smaller than unity). From Eq. (4) we obtain

$$\epsilon_p/\epsilon_0 \cong 2/\beta_+^2 a^2 \ln(\beta_+ a)\,, \tag{14}$$

where we utilized the small argument expansion of the Bessel functions. In order to have a localized surface mode, one should not get into the different Riemann plane at $\beta_- = 0$. Therefore, we should stay on the principal plane. Then one may set $\ln(\beta_+a) = -\Lambda$, where Λ is a very slowly varying function of ω. With this consideration, we obtain the dispersion relation from Eq. (14) as

$$1 - \frac{\omega_e^2}{(\omega - kv_D)^2 - kv_e^2} - \frac{\Omega_p^2}{\omega^2 - \omega_{\mathrm{TO}}^2} - \frac{2c^2/\Lambda}{\omega^2 - k^2c^2/\epsilon_0} = 0\,. \tag{15}$$

The dispersion relation for this small radius cylinder, Eq. (15), has been numerically studied. It turns out that the computational results are qualitatively the same as the above semi-infinite case.

In the past several years many reports of the observation of various surface polaritons by the attenuated-total-reflection (ATR) method, light scattering and low-energy-electron diffraction

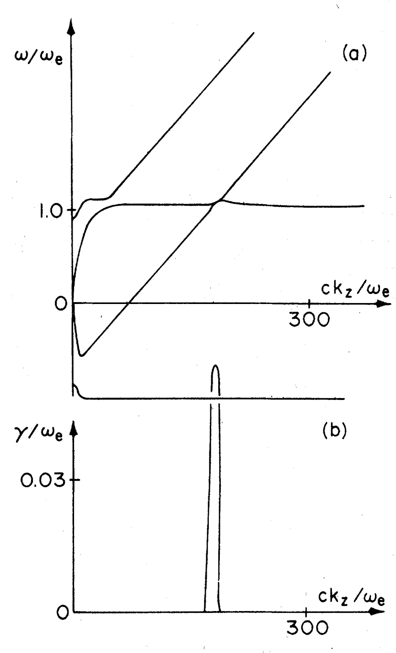

FIG. 10. Surface polariton dispersion relation in the intermediate regime. $\omega_{\mathrm{TO}}/\omega_e = 1.195$, $\Omega_p/\omega_e = 0.158$, $v_D = 0.1c$, and $v_e = 0$. (a) The real frequency vs wave vector; (b) the growth rate vs wave vector.

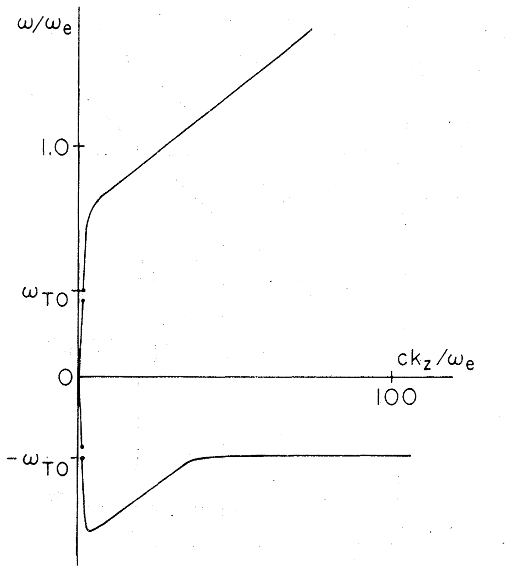

FIG. 11. Surface polariton dispersion relation in the regime of high-plasma electron density. $\omega_{TO}/\omega_e = 0.346$, $\Omega_p/\omega_e = 0.05$, $v_D = 0.1c$, and $v_e = 0$. No surface polariton instability.

(LEED) have appeared in the literature. But to the authors' knowledge no observation has been reported so far on the surface polaritons in an LO-phonon–plasmon coupled system in a doped semiconductor. One of us (S.U.) has measured the Raman spectra of a p-type GaAs film on a sapphire substrate in a near-forward scattering geometry. In this experiment the screening of the LO phonon (disappearance from the normal bulk LO-phonon position) due to free carriers was observed, but no definitive conclusion could be reached about the dispersion of the surface polaritons formed in this LO-phonon–plasmon coupled system. This is mainly due to the strong damping of the ω_+ and ω_- modes resulting from the low mobility of holes in the GaAs film. An experiment in the presence of a current will be a very exciting possibility, especially if the instabilities described above can be induced. However, choice of appropriate materials may be difficult, and moreover, since the instabilities occur away from the zone center, observation of this phenomenon by light scattering will require some ingeneous methods.

In conclusion, we have studied the properties of the dispersion relation of surface polaritons in LO-phonon–plasmon coupled system in a semiconductor. When the carrier electron density is low ($\omega_e < \omega_{TO}$), the phonon dominated surface polariton branch is forbidden below $\omega = \omega_{TO}$. With current, a surface polariton with $\omega \gtrsim \omega_{TO}$ and $k \sim \omega_{TO}/v_D$ becomes unstable. When the carrier density is high ($\omega_e > \omega_{TO}$), the phonon-dominated branch has a cutoff for larger wave vectors. There is no instability window in the surface polariton dispersion relation with current in this case.

ACKNOWLEDGMENTS

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