Dispersion of surface plasmons in inhomogeneous media

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We show that recent claims for the existence of an extra branch in the surface plasmon dispersion for an inhomogeneous medium are based on the use of a series solution of the wave equation that does not converge for the parameters of the "extra branch." This solution is nevertheless useful for obtaining a dispersion relation for the usual branch that is valid for larger differences between surface and bulk dielectric functions than had been treated previously.

In a recent paper[1] (hereafter referred to as I) it was pointed out that the claim of Guidotti, Rice, and Lemberg[2] (to be referred to as GRL) to have demonstrated the existence of an extra branch of the surface-plasmon dispersion for a medium with an accumulation or depletion layer is not justified. The statements of neither Refs. 1 nor 2 were complete, however. Now that the details of the GRL calculations have been published (hereafter referred to as II),[3] it is possible to make a more complete argument, and also to use their solution to obtain a dispersion relation valid over a much greater range of inhomogeneity than that derived in I.

In both I and II the situation studied was that of a medium with dielectric function ϵ varying below the surface ($z=0$) according to

$$\epsilon = \epsilon_b + \Delta\epsilon\, e^{z/d}, \tag{1}$$

d being a constant, in contact with a medium with dielectric function ϵ_2, independent of coordinates and frequency. Equation (1) assumes a local relation between $\vec{D}$ and $\vec{E}$. A local relation (although different in detail) was also used by Cunningham *et al.*[4] in studying dispersion of surface plasmons in inhomogeneous media. Discussing its validity at length, they point out that the local approximation is questionable only in the region where carrier concentration or electric field varies rapidly with z over a distance comparable to the screening length. Certainly in a region where ϵ goes through 0, resulting in the electric field becoming infinite,[4] the validity of the local approximation is doubtful. The difficulty arises, however, from the use of a real ϵ and can be avoided by the use of complex ϵ, with both real and imaginary parts satisfying (1). Then in a region where the real part of ϵ, ϵ_R goes through 0, the imaginary part of ϵ, ϵ_I dominates the behavior. In practical cases, ϵ_I is both slowly varying with z and large enough so that the electric field rises but little (certainly less than an order of magnitude) in the region where $\epsilon_R \to 0$.[5] Since complex ϵ was used by GRL in obtaining the solution and the dispersion relation in II, their use of the local approximation should not be a source of significant error in their calculated dispersion.

Following a procedure similar to (although not identical with) that in II, we simplify the wave equation for the (only) magnetic field component H_y in the conducting medium by assuming a solution in the form

$$H_y = e^{p_0 z} F(e^{z/d}) e^{i(k_x x - \omega t)}, \tag{2}$$

where

$$p_0 = (k_x^2 - \epsilon_b \omega^2/c^2)^{1/2}, \tag{3}$$

representing the reciprocal of the plasmon decay length if the medium were homogeneous. With the substitution

$$y = -(\Delta\epsilon/\epsilon_b) e^{z/d}, \tag{4}$$

one obtains from the wave equation the differential equation for F:

$$y(y-1)\frac{d^2F}{dy^2}+[2p_0dy-(2p_0d+1)]\frac{dF}{dy}-\left(p_0d+\epsilon_b d^2\frac{\omega^2}{c^2}(y-1)\right)F=0. \quad (5)$$

Solutions to this may be obtained, as in II, by expanding around the singular point at $y=0(z=-\infty)$, in the form

$$F=a_0y^r\sum_{n=0}^{\infty}\alpha_n y^n, \quad (6)$$

a_0 being an arbitrary constant. Of the two values of r found to satisfy (5), 0 and $-2p_0d$, the latter is discarded because it leads to a solution not finite at $z=-\infty$. For $r=0$, one finds[3]

$$\alpha_1=-(\beta-q)/(2\beta+1),$$

$$\alpha_2=-\frac{\beta^2-q^2}{2(2\beta+1)(2\beta+2)}-\frac{q}{2(2\beta+2)},$$

$$\alpha_3=-\frac{(2+3\beta+q)}{2\times3(2\beta+2)(2\beta+3)}\left(\frac{\beta^2-q^2}{2\beta+1}+q\right)+\frac{q(\beta-q)}{3(2\beta+1)(2\beta+3)}, \quad (7a)$$

$$\alpha_4=-\frac{(6+5\beta+q)(2+3\beta+q)}{2\times3\times4(2\beta+2)(2\beta+3)(2\beta+4)}\times\left(\frac{\beta^2-q^2}{2\beta+1}+q\right)+\frac{(6+5\beta+q)(\beta-q)q}{3\times4(2\beta+1)(2\beta+3)(2\beta+4)}+\frac{q}{2\times4(2\beta+2)(2\beta+4)}\left(\frac{\beta^2-q^2}{2\beta+1}+q\right),$$

where

$$\beta\equiv p_0d, \quad q\equiv\epsilon_b\omega^2d^2/c^2. \quad (7b)$$

Before deriving the dispersion relation, GRL simplified the solution (6), (7a), (7b) by dropping all terms higher than linear in y, p_0d, and $\epsilon_b d^2\omega^2/c^2$. (Note that the restriction $p_0d\ll1$ is not necessary and thus the validity of their approximate solution and dispersion relation is not limited to small k_x, as they state.) The solution they obtain is then

$$H_y=a_0e^{p_0z}\left(1+\frac{\Delta\epsilon}{\epsilon_b}\frac{\beta-q}{2\beta+1}e^{z/d}\right)e^{i(k_xx-\omega t)}. \quad (8)$$

This is precisely the solution, to terms linear in $\Delta\epsilon/\epsilon_b$, obtained by expanding the Bessel function in the solution (11) of I for d small enough so that $\beta\simeq2\Delta\epsilon/\epsilon_b$. As noted in I, the dispersion relation GRL obtained using (8) is also essentially the same as that obtained in I for the limit of small d, differing only by a term of the order of $(\Delta\epsilon/\epsilon_b)^2$. Thus, there is essentially no disagreement between the calculations of I and II for the usual surface-plasmon branch and small $\Delta\epsilon/\epsilon_b$.

In the numerical evaluation of the dispersion, in both I and II, ϵ_I was assumed to be zero (corresponding to ∞ scattering time) and ϵ was taken as

$$\epsilon=\epsilon_\infty(1-\omega_p^2/\omega^2). \quad (9)$$

This is the usual procedure in dispersion calculations when damping is not expected to be large. Consistent with our earlier discussion, it should not lead to serious error where $\Delta\epsilon/\epsilon_b$ is small, and ϵ therefore slowly varying, throughout, as is the case for the usual surface-plasmon branch. The extra branch found by GRL, however, lies in a narrow frequency range between the plasma frequency ω_{pb} for the bulk carrier concentration and the plasma frequency ω_{ps} for the surface carrier concentration. Thus, in the frequency range of the extra branch, for an accumulation layer, where $\omega_{ps}>\omega_{pb}$, the surface value of ϵ, ϵ_s, will be less than 0 and $\epsilon_b>0$, while for a depletion layer $\epsilon_s>0$ and $\epsilon_b<0$. In both cases ϵ goes through 0 somewhere inside the sample. Thus the existence of the extra branch found by GRL is open to question because of their use of a local approximation with ϵ real and going through 0. Note, however, that use of a local approximation in such a case, although it does not give the correct electric fields in the neighborhood of $\epsilon=0$, may still yield the correct dispersion. This was demonstrated by Cunningham, Maradudin, and Wallis for one particular case. Also, the dispersion they calculated for other cases in which ϵ went through 0 seemed quite reasonable, certainly showing no extra branches. The more serious objection to the extra branch stems from the fact that, when ϵ_b and ϵ_s have opposite signs, the value of y at the surface, given by $(\epsilon_b-\epsilon_s)/\epsilon_b$ according to (1) and (4), is greater than unity. As can be seen by extending (7a), the series (6) does not converge for $y>1$. Thus the solution (8) can hardly be considered to represent the correct solution at $z=0$ for the frequency range of the extra branch. In fact, (8) and the resulting dispersion relation can only be considered valid when $|\Delta\epsilon/\epsilon_b|\ll1$, and thus the theory of GRL is essentially identical to that of I for the case of small d.

Although (6), plus (7), is not a valid solution for $|\Delta\epsilon/\epsilon_b|>1$, it does represent a useful solution so long as $|\Delta\epsilon/\epsilon_b|<1$. By matching, at $z=0$, H_y and E_x obtained from (6), (7), (4), and (2) with exponentially decaying H_y and E_x for a homogeneous medium above $z=0$, we obtain the dispersion relation

$$\frac{p_2}{\epsilon_2} = -\frac{p_0}{\epsilon_s}\left[1 - \frac{1}{p_0 d}\left(\frac{\Delta\epsilon}{\epsilon_b}\right)\left(\frac{dF/dy}{F}\right)_{z=0}\right] \quad (10)$$

$$= -\frac{p_0}{\epsilon_s}\left[1 - \frac{1}{p_0 d}\left(\frac{\Delta\epsilon}{\epsilon_b}\right) \times \frac{\alpha_1 - 2\alpha_2(\Delta\epsilon/\epsilon_b) + 3\alpha_3(\Delta\epsilon/\epsilon_b)^2 + \cdots}{1 - \alpha_1(\Delta\epsilon/\epsilon_b) + \alpha_2(\Delta\epsilon/\epsilon_b)^2 + \cdots}\right], \quad (11)$$

where

$$p_2 = (k_x^2 - \epsilon_2\omega^2/c^2)^{1/2}. \quad (12)$$

It is apparent that in the limit that $\Delta\epsilon/\epsilon_b$ vanishes, ϵ_s becomes identical with ϵ_b, and we recover from (11) the dispersion relation for a homogeneous conductor. To terms linear in $\Delta\epsilon/\epsilon_b$, (11), with α_1 taken from (7a), (7b), is identical with the dispersion relation (15) of I, valid for small $\Delta\epsilon/\epsilon_b$. (Note that ϵ_2 was taken as unity in I.) In the limit $p_0 d \rightarrow \infty$, the α's approach constant values independent of $p_0 d$, as can be seen in (7a) and (7b), and the series F and dF/dy still converge provided $|\Delta\epsilon/\epsilon_b|$ is not greater than unity. The $p_0 d$ in the denominator then makes the second term in braces vanish and the dispersion relation becomes

$$(p_2/\epsilon_2) = -(p_0/\epsilon_s), \quad k_x \rightarrow \infty . \quad (13)$$

This allows us to generalize the result obtained in I, that the limiting value of ω is given by $\epsilon_s = -\epsilon_2$, to arbitrary magnitude of $\Delta\epsilon/\epsilon_b$, provided $|\Delta\epsilon/\epsilon_b| < 1$.

The form (11), with the α's given by (7a) and (7b), should be useful for calculation of plasmon dispersion in semiconductors with accumulation or depletion layers. When $|\Delta\epsilon/\epsilon_b|$ is close to unity, so that the real part of ϵ becomes very small, it will be necessary, consistent with the above discussion, to use complex ϵ in numerical evaluation of the dispersion.

Note added in proof. Since the time this comment was written, C. Kao and myself have solved the wave equation for the case where the real part of ϵ goes through 0 in the sample. The dispersion we obtain is quite different from that described by Guidotti and Rice in the following comment. Our work appears in Phys. Rev. B 14, 2464 (1976).

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[1]E. M. Conwell, Phys. Rev. B 11, 1508 (1975). This paper will be referred to as I.

[2]D. Guidotti, S. A. Rice, and H. L. Lemberg, Solid State Commun. 15, 113 (1974).

[3]S. A. Rice, D. Guidotti, H. L. Lemberg, W. C. Murphy, and A. N. Bloch, in *Advances in Chemical Physics*, edited by I. Prigogine and S. A. Rice (Wiley, New York, 1974), Vol. XXVII. This paper will be referred to as II.

[4]S. L. Cunningham, A. A. Maradudin, and R. F. Wallis, Phys. Rev. B 10, 3342 (1974).

[5]E. M. Conwell and C. C. Kao (unpublished).