Determination of surface-polariton minigaps on grating structures: A comparison between constant-frequency and constant-angle scans

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(Received 28 April 1986)

When surface polaritons propagate on a diffraction grating, their interaction with the periodic structure induces gaps in frequency in the dispersion relation. The dispersion curves near the gaps have been explored by two experimental methods: One may probe the reflectivity as a function of angle of incidence θ, with radiation of fixed frequency ω, or one may measure the reflectivity as a function of frequency, with angle of incidence fixed. In either case, resonant coupling to the incident photon produces narrow dips in the reflectivity. Information on the dispersion curve is extracted by following the position of the dip as a function of ω when θ is scanned, or its variation with θ when ω is scanned. In the minigap region, a theoretical study shows the first method can yield unphysical results, while those from the second method provide dispersion curves in good accord with theory.

When a surface polariton propagates on a surface upon which a diffraction grating is ruled, its dispersion relation is modified. In particular, when the magnitude $k_\parallel$ of its wave vector equals $n\pi/a_0$, with n an integer and a_0 the grating period, the grating induces frequency gaps in the dispersion relation.[1] These are called minigaps.

One can study the surface-polariton dispersion relation experimentally by measuring the position of dips in the reflectivity produced by grating-induced coupling of the incident photon to surface polaritons. This may be done in two ways. One may employ radiation of a fixed frequency ω and measure the reflectivity $R(\omega,\theta)$ as a function of the angle of incidence θ, noting the grating allows coupling of the photon to surface polaritons of wave vector $(\omega/c)\sin\theta+2\pi n/a_0$. It is assumed that a dip occurs when this coupling is phase matched so the wave vectors of surface polaritons of frequency ω may be inferred from the values of θ where dips occur. On the other hand, we may fix θ and scan the frequency ω. These are two different methods of probing the function $R(\omega,\theta)$ which may be viewed as defining a surface in a coordinate system with axes labeled by ω, θ, and R. We note that an earlier discussion of the attenuated-total-reflection (ATR) method of measuring surface-polariton curves shows that these two methods produce different results, particularly in spectral regions where there is strong dispersion.[2]

We have explored this question for the case where the dispersion relation of surface polaritons on a grating is measured by the two different methods outlined above, and we also find they yield distinctly different results near grating-induced minigaps. When the reflectivity is scanned as a function of frequency with θ fixed from the position of the reflectivity dips as a function of θ, one constructs a dispersion curve in excellent accord with that which emerges from theoretical treatments.[1] On the other hand, scanning θ with ω fixed produces features hard to interpret, in the vicinity of the minigaps. The "dispersion curve" constructed by the experimentalist in this case bears little relation to that envisioned in theoretical treatments. A saddle point in the reflectivity surface is responsible for the difficulty, as we shall see.

In our calculation of the reflectivity surface $R(\omega,\theta)$, we have used the (exact) extinction-theorem method. Since this has been described elsewhere, and, in fact, forms the basis for our earlier calculations,[3] we omit discussion of the technique. Figure 1 shows the reflectivity surface $R(\omega,\theta)$ of a silver diffraction grating with a 1.1-μm period and a sawtooth profile with 300-Å height (it is 600 Å from the bottom of the trough to the tip of the sawtooth). The two sets of lines on the figure are lines of constant ω and lines of constant θ.

One can see a saddle-shaped region in the center of the figure. If one traces the reflectivity through the saddle point along the ω direction (constant-θ frequency scan), one obtains the curve in Fig. 2(a). For this choice of θ, one is probing surface polaritons at the zone boundary, and the separation between the two minima is the grating-induced minigap. For this example, its magnitude agrees well with that calculated from the theoretical dispersion relation.[1] However, if one traces the reflectivity

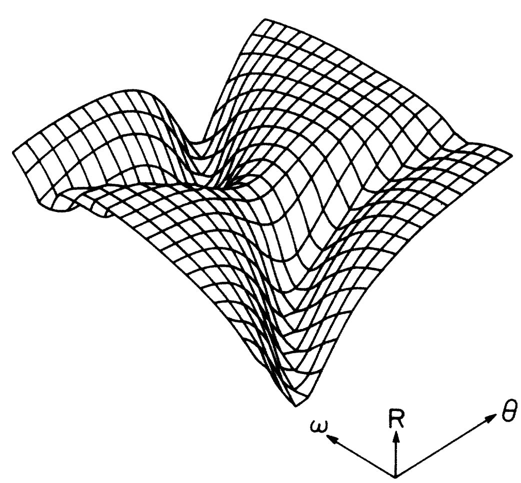

FIG. 1. The reflectivity surface $R(\omega,\theta)$ for the model grating described in the text, with constant frequency (ω) and constant angle of incidence (θ) lines superimposed on the surface.

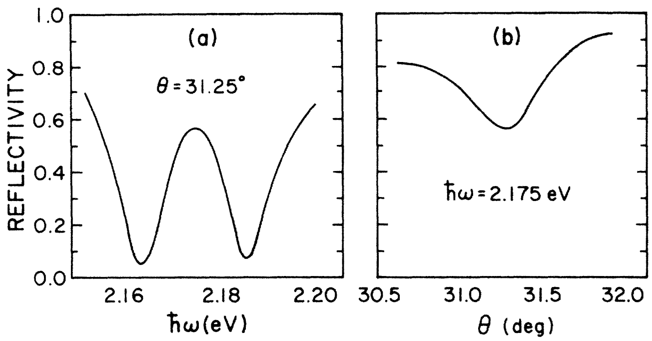

FIG. 2. (a) The reflectivity as a function of frequency, with angle of incidence fixed so the minigap portion of the reflectivity contour is explored. (b) The reflectivity as a function of angle of incidence, with the frequency fixed in the middle of the minigap.

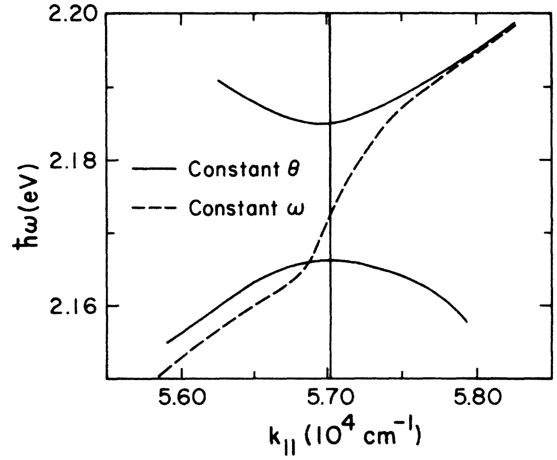

FIG. 3. The dispersion curves deduced from the constant-θ scan with frequency varied (solid line), and with θ varied and frequency held fixed (dashed line).

through the saddle point along the θ direction (constant-ω θ scan), one finds a *single* dip, as displayed in Fig. 2(b).

These two results seem contradictory. The constant-ω scan in Fig. 2(b) would lead the experimentalist to believe that a single surface polariton is excited at the saddle point, but Fig. 2(a) shows a reflectivity *maximum* here, with a surface-polariton-induced dip on either side. Near the minigap, the two measurement techniques give very different results.

If we convert the dip trajectories in each case to dispersion curves, the two methods give different results, with that provided by the constant-ω θ scan rather unphysical. The two dispersion curves are displayed in Fig. 3 for the example considered.

Quite clearly, the information provided by the constant-ω θ scan is difficult to interpret. The dispersion curve does not possess the proper reflection symmetry about the line $k_{\parallel}=\pi/a_0$, the first-Brillouin-zone boundary of the grating reciprocal lattice. There is no gap in frequency as expected from general considerations of wave propagation on periodic structures. Indeed, in the scan shown in Fig. 2(b), the problem is that one is not probing the "troughs" in Fig. (1) clearly associated with surface polaritons, but a topological feature of the reflectivity surface unrelated to these modes. Farther from the minigap region the constant ω scan sweeps one through only one of the surface-polariton troughs for our example, so this kinematical constraint allows one to probe only one branch. It should be stressed that the single dip moves smoothly and monotonically in position as one scans θ for various fixed frequencies, as one can see from Fig. (1).

These calculations were motivated by experiments of Szentirmay and collaborators[4] who extracted the surface-polariton curves on a tunnel junction structure upon which a diffraction grating had been ruled. These authors used θ scans at fixed frequency. In the minigap region, they find evidence for a gap in *wave vector* (not frequency) in the dispersion curve they deduce from their data.

We have not encountered an example of such behavior in our calculations, though we do see quite explicitly that the use of θ scans with frequency held fixed can lead to misleading results near the minigap region. The saddle point which leads to the single reflectivity minimum displayed in Fig. 2(b) may not be present for gratings with profile different than that explored here, or for more complex structures such as multilayer tunnel junctions. If, for example, the saddle point in Fig. (1) were replaced by a maximum that is rather broad in a constant-ω scan with θ varied, then to the experimentalist the reflectivity dip probed in the measurement would disappear at a wave vector near the zone boundary, very much like that observed in Ref. 4.

Our conclusion is that near the minigap region, the reflectivity surface should be measured with θ held fixed and the frequency scanned, if dispersion curves are desired which can be compared with calculations such as those presented in Ref. 1. The minigap displayed in Fig. 2(a) is in excellent quantitative accord with these calculations, as remarked earlier. Accurate measurements in this geometry have been reported, with a dye laser as the exciting source.[5]

One of us (D.L.M.) enjoyed stimulating discussions of this problem with N. Kroo and Zs. Szentirmay.

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