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Symmetry and the reflectivity of diffraction gratings at normal incidence

M. G. Weber and D. L. Mills
Department of Physics, University of California, Irvine, California 92717
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We present a series of numerical calculations which illustrate the role of symmetry of the profile of a diffraction grating on its reflectivity at normal incidence. Here one finds reflectivity dips (or peaks) produced by grating-induced coupling of the incident photon to surface polaritons. When the grating profile has either even or odd parity, we find one of the two reflectivity dips expected at normal incidence is absent, in agreement with recent data. In addition, we find that the peaks are caused by the vanishing of certain Fourier components of the profile function. This result agrees with analogous results obtained in the theory of atom-surface scattering.

I. INTRODUCTION

When a surface polariton propagates on a surface on which a diffraction grating has been ruled, its dispersion relation is modified, and its mean free path is limited by grating-induced radiation damping.[1] Most particularly, if the wave propagates normal to the grooves of the grating, then when the magnitude $k_\parallel$ of its wave vector parallel to the surface equals $2\pi n/a_0$, with a_0 the grating period, the grating induces small gaps ("minigaps") in the dispersion relation,[2] in a manner familiar from the theory of wave propagation in periodic media.

The grating may couple an incident photon to surface polaritons. If ω is the frequency of the photon, its angle of incidence relative to the normal is θ_I, and c is the velocity of light, then the magnitude of the component of its wave vector parallel to the surface is $k_\parallel^{(I)} = (\omega/c)\sin\theta$. If $\omega_s(k_\parallel)$ is the dispersion relation of the surface polariton on the grating, then when ω and θ are such that $\omega=\omega_s(k_\parallel^{(I)}+nG_0)$, where $G_0=2\pi/a_0$ and n is any integer, the grating induces a resonant transfer of energy from the photon to the surface polariton. At the special angles or frequencies where this condition is satisfied, one finds a pronounced dip in the reflectivity of the grating. (We shall appreciate shortly that one also finds peaks under certain conditions.) In Fig. 1, we show the surface-polariton dispersion curve in the ω-$k_\parallel$ plane; if we plot the frequency of an incident photon as a function of its wave-vector component parallel to the surface, we have a straight line with slope $c/\sin\theta$. The figure illustrates the frequencies ω_1 and ω_2 at which the incident photon couples to a surface polariton through the reciprocal-lattice vector $+2\pi/a_0$ and through $-2\pi/a_0$, respectively. In the data, one will find a sharp structure in the reflectivity at both ω_1 and at ω_2.

As the angle of incidence approaches zero, notice that point P_1 approaches $k_\parallel=+2\pi/a_0$, and the mode probed is the high-frequency partner of the pair of modes created at this special wave vector by the grating-induced minigap. Furthermore, P_2 moves to $k_\parallel=-2\pi/a_0$ and the mode probed is the low-frequency partner of the above-mentioned pair. Thus, at normal incidence, one observes a doublet in the reflectivity; the separation in frequency between the two features thus provides the value of the minigap at this particular zone boundary.

The primary motivation for the calculations reported here is the observation by Chen *et al.*[3] that on gratings studied by them under conditions where the photon couples to the surface polariton via the reciprocal-lattice vectors $\pm 4\pi/a_0$, as normal incidence is approached, the dip in reflectivity produced by the mode P_2 in Fig. 1 decreased to zero. This has led us to carry out new calculations of the reflectivity of gratings of various profiles at and near normal incidence; we find this behavior any time the grating profile has even or odd parity under reflection through the midpoint of the appropriate unit cell. The new calculations have been carried out through use of the method we used in our earlier papers.[4] In our earlier work we found that near normal incidence, for light which strikes a grating of sawtooth profile, there are small bumps (peaks) rather than dips in the reflectivity at the frequencies where the incident photon couples to surface polaritons near the gaps at $k_\parallel=\pm 4\pi/a_0$. We attributed these dips to the presence of reflection symmetry in the grating profile. We find now that this is incorrect; the sawtooth profile grating admits no even harmonics (the Fourier components in the expansion of the grating profile

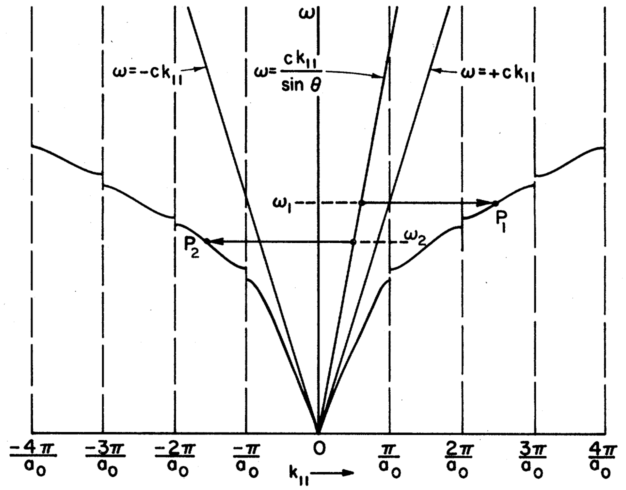

FIG. 1. A sketch of the dispersion relation for surface polaritons on a surface upon which a grating of period a_0 is ruled. We also show the curve $\omega=ck_\parallel/\sin\theta$, the frequency of a free-space photon incident on the grating at an angle θ with respect to the normal to the surface, considered as a function of its wave-vector component $k_\parallel$ parallel to the surface.

with wave vector nG_0 vanish identically when n is even), and it is this property that is responsible for the unusual shape of the reflectivity near normal incidence.

II. RESULTS AND DISCUSSION

Since the calculations reported here employ exactly the same method we used earlier,[4] we turn directly to the results with no discussion of the approach.

In order to investigate the roles of the symmetry and harmonic content of a given grating profile, we have calculated the reflectivity of a grating with a general trapezoidal profile [see Fig. 2(a)]. Thus, we can easily adjust the symmetry and even harmonic content independently by varying the profile parameters.

In the limit in which the top of the trapezoid has zero width and the bottom has the width of the grating period a, we have a sawtooth profile. If one then imposes right-left symmetry, one has a regular sawtooth. This profile is the one considered in our prior investigations of grating-induced coupling of light to polaritons, and is shown in Fig. 2(b). As mentioned previously, this grating has right-left symmetry and no even harmonics.

If we narrow the bottom of the trapezoid symmetrically to a width less than a, the profile will look like a sawtooth with the bottom clipped off. This "clipped sawtooth" still has right-left symmetry, but now has nonzero even harmonics. It is shown in Fig. 2(c). The final profile we consider here is a clipped sawtooth in which the right-left symmetry is broken by making the grating teeth lean over somewhat, as in the sawtooth on an actual sawblade. This profile has no symmetry, aside from periodicity, and is illustrated in Fig. 2(d).

Now we turn to the reflectivity of these gratings near normal incidence. In all the calculations described below, the gratings are assumed to be on silver substrates, with a height h of 300 Å, and a period of 1.1 μm. We use the dielectric constant data reported by Johnson and Christy[5] in the calculation. The reflectivity structures we are most interested in will be at or near normal incidence, and near the frequency of the $(2,-2)$ minigap. (The modes excited by the photon have wave vector $k_{\parallel}-2G_0$ and $k_{\parallel}+2G_0$, respectively, where $G_0=2\pi/a_0$.)

In Fig. 3(a), we show the reflectivity of the regular sawtooth [Fig. 2(b)] at normal incidence. We see a single feature, a peak at the frequency of the surface polariton at the Brillouin-zone boundary $\pm 4\pi/a_0$. A bit away from normal incidence at $\theta=2°$ we see a doublet, but each member is a peak rather than a dip. We remind the reader that in our earlier paper,[4] where a regular sawtooth profile grating with $a_0=8000$ Å was explored, surface-polariton-induced reflectivity maxima rather than dips were again found near normal incidence.

It is interesting to comment on the origin of these curious peaks. A study by Wolfe-Brannon and Weare[6] of the closely related problem of the scattering of helium atoms off a (periodically corrugated) crystal proves most helpful. Here an attractive well is produced outside the crystal surface by the combination of the attractive van der Waals interaction, and the strongly repulsive "hard wall" potential produced when the electron cloud of the helium atom overlaps that of the substrate atoms. This well leads to surface states that are analogous to our surface polaritons; the incoming He atom, a de Broglie wave, is coupled to the evanescent surface states by the periodic corrugation of the surface which is a consequence of its underlying atomic structure. These authors nearly always find dips in the specular reflectivity when the resonant coupling occurs, but in a small number of circumstances classified by them, maxima rather than dips appear in the calculated reflectivity. One situation where this happens is when the grating profile is such that the effective matrix element which directly couples the incident wave to the surface states vanishes, so there is no

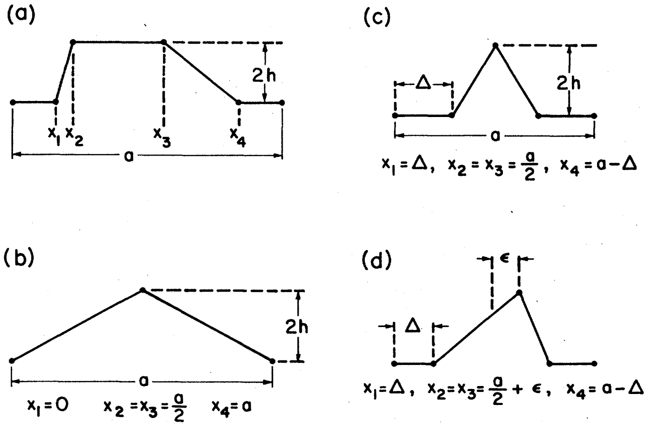

FIG. 2. We show (a) the trapezoidal grating profile considered in the paper along with a series of special cases, (b) the symmetric sawtooth profile, (c) the "clipped sawtooth," and (d) an asymmetric clipped sawtooth. The fundamental unit, repeated periodically to form the grating, has length a and it is this unit that we show in the figure.

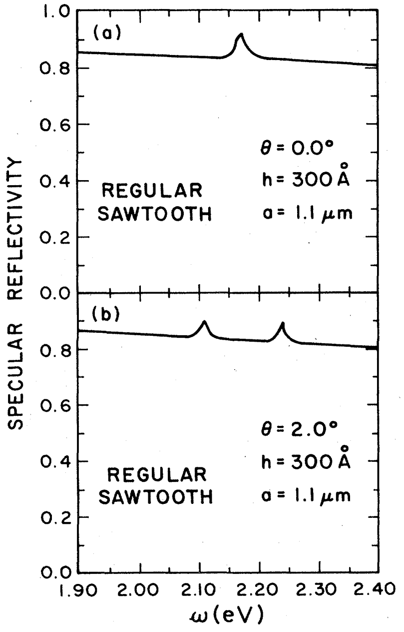

FIG. 3. The reflectivity of the regular sawtooth grating [Fig. 2(b)] (a) at normal incidence and (b) 2° off normal incidence.

feature in the reflectivity in a perturbation theoretic treatment. The regular sawtooth considered in our earlier paper and also the present note are examples of just this case; we also commented earlier there that it was the vanishing of this matrix element which led to the appearance of peaks. Coupling of the incident photon to the surface state then occurs only via higher-order processes included in our present treatment, which is not based on perturbation theory. We tested this hypothesis directly in our earlier work by exploring an asymmetric sawtooth profile, for which the relevant matrix element fails to vanish. The peaks indeed turned into dips, and we shall see similar behavior below. We stated that this particular matrix element (associated with the $4\pi/a_0$ reciprocal-lattice vector) would vanish for any grating profile of well-defined parity, a statement which is incorrect.

In Figs. 4(a) and 4(b), we show normal and near-normal incident reflectivity curves calculated for the clipped sawtooth profile in Fig. 2(c). At normal incidence, we see only a single dip, but a doublet appears 2° off normal. We have followed the evolution of the doublet, in the region $0° \leq \theta \leq 2°$. As normal incidence is approached, we find that the low-frequency member of the pair becomes progressively weaker, to have vanishing intensity at normal incidence. Very near normal incidence $(0.25° \leq \theta \leq 0.50°)$, where the intensity of the low-frequency member of the pair is still strong enough for the doublet to be resolved, we find a minigap of roughly 30 meV.

Precisely this behavior is evident in the experimental data of Chen *et al.*; the grating period used in this calculation has been chosen equal to theirs. In our calculations, the one member of the doublet disappears at normal incidence whenever the grating profile has well-defined parity. The surface polaritons right at the zone boundary $k_{\parallel} = \pm 4\pi/a_0$ are standing-wave resonances of the grating structure, a property well known for propagation on any periodic structure. Right at this value of $\mathbf{k}_{\parallel}$, the field components in the wave (that parallel to, and that normal to the surface) each have well-defined parity. If the parallel component of the field has odd parity, the normal component has even parity, and conversely. One may show that the high-frequency mode at $k_{\parallel} = 4\pi/a_0$ has a parallel component of field with odd parity, while the low-frequency member has a parallel component of field with even parity. Right at normal incidence, the incident photon field is parallel to the surface and has odd parity, so it may "mix" through the perturbation provided by the grating only with a mode of the same character. The low-frequency mode is "silent" since its parallel field component has even symmetry.

We show the influence of parity in the grating profile in Fig. 5, where for normal and near-normal incidence, we show the reflectivity calculated for the clipped asymmetric sawtooth profile [Fig. 2(d)]. We see *both* modes are active right at normal incidence as expected from the argument cited in the previous paragraph.

For a grating with a profile of well-defined parity, one may couple to both modes at $k_{\parallel} = \pm 4\pi/a_0$ by studying the reflectivity off normal incidence. In the particular example explored here, as noted by Chen *et al.*, there is an angle of incidence, off the normal, where one may couple to these modes via the reciprocal-lattice vectors $+6\pi/a_0$ and $-2\pi/a_0$. Then the field of the incident photon has no well-defined parity, and one may couple to *both* standing-wave resonances on the grating. In Fig. 6, we show the reflectivity of the regular sawtooth grating calculated for this angle of incidence. Both dips show clearly, again in accord with the data.

Our conclusion is that the study of the reflectivity of dif-

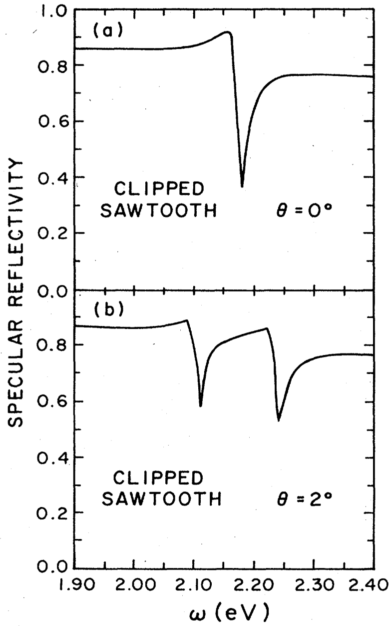

FIG. 4. The reflectivity if the clipped sawtooth grating [Fig. 2(c)] (a) at normal incidence and (b) 2° off normal incidence.

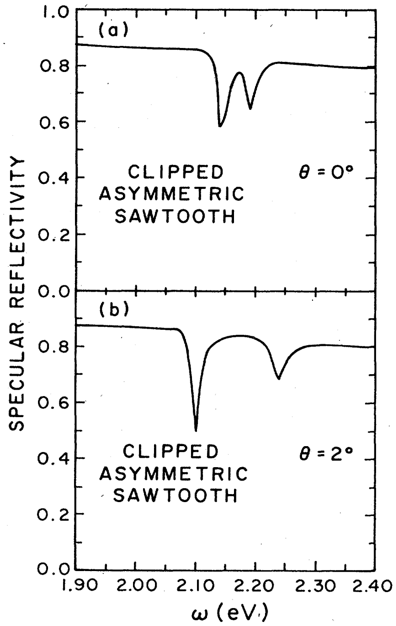

FIG. 5. The reflectivity of the asymmetric clipped sawtooth grating (a) at normal incidence and (b) 2° off normal incidence.

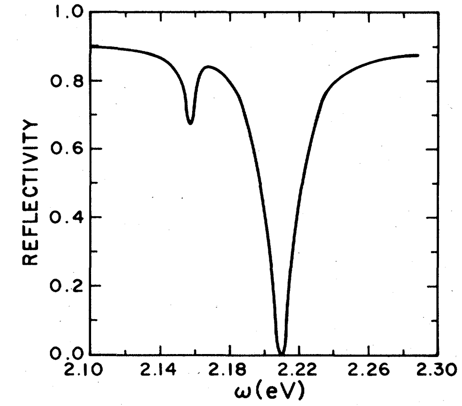

FIG. 6. The reflectivity of the clipped sawtooth grating off normal incidence, where one may couple to the surface polaritons at the $(2,-2)$ gap via the reciprocal-lattice vectors $+6\pi/a_0$ and $-2\pi/a_0$, respectively.

fraction gratings at near-normal incidence, with attention to surface-polariton-induced dips (or peaks) provides one with information of the quality of the grating profile, in that for highly symmetric profiles of well-defined parity, one of the two reflectivity dips will vanish in intensity as normal incidence is approached. Chen *et al.* observe precisely this behavior in their studies.[3]

Incidentally, in our earlier study we explored radiative damping of surface polaritons on gratings where we found vanishing radiative linewidths[1] for certain modes at the Brillouin-zone boundary. This behavior is also a manifestation of the parity argument outlined above.

ACKNOWLEDGMENTS

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[1] For explicit calculations grating-induced radiation damping, and a comparison between perturbation theoretic and exact descriptions of this phenomenon, see N. E. Glass, M. G. Weber, and D. L. Mills, Phys. Rev. B **29**, 6548 (1984). This reference also discusses the influence of the grating on the dispersion relation of the modes.

[2] Explicit expressions for the grating-induced minigaps, for arbitrary angle of propagation between the surface polariton and the grating, may be found in D. L. Mills, Phys. Rev. B **15**, 763 (1977). Note the typographical error cited in Ref. 14 of Bernardo Laks, D. L. Mills, and A. A. Maradudin, Phys. Rev. B **23**, 4965 (1981).

[3] Y. J. Chen, E. Koteles, R. J. Seymour, G. J. Sonek, and J. M. Ballantyne, Solid State Commun. **46**, 95 (1983).

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[6] K. Wolfe-Brannon and J. Weare, Phys. Rev. B **24**, 5753 (1981).