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Finite-Difference Time-Domain Modeling of Periodic and Disordered Surface Gratings in AlInSb Light Emitting Diodes With Metallic Back-Reflectors

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Abstract—Two-dimensional finite-difference time-domain modeling is undertaken to study the optical behaviour of midinfrared AlInSb light-emitting diode devices with close metallic back reflectors. The location of the source and mirror is investigated in detail and optimised for peak emission at \( \lambda_0 = 4 \) \( \mu \)m. A periodic surface grating is added and it is found that greater than 98% of the light at a specific wavelength may be extracted for specific grating parameters, an enhancement of \( \sim 20 \)-fold. A novel type of grating termed disordered-periodic is then studied and is shown to have a much broader spectral response with more than 50% of the power extracted across a broad wavelength range.

Index Terms—Finite-difference time-domain modeling, integrated optoelectronics, light-emitting diodes.

I. INTRODUCTION

The optical extraction efficiency of conventional light-emitting diodes is fundamentally limited by the discontinuity in refractive index between the bulk dielectric in which the light is generated and the surrounding medium into which the light is emitted. In a typical semiconductor light-emitting diode (LED) structure the difference in refractive index at the interface between the device and the surrounding medium \( \Delta n \sim 2.5-3 \) results in a large amount of the generated optical power being trapped within the device. This is chiefly due to total internal reflection (TIR) which imposes an approximate limit of \( \sim \eta_T = 1/(n(n - 1)^2) \) on the extraction efficiency of the device [1]. Moreover, for light incident within the escape cone at the dielectric interface formed by TIR further Fresnel reflection will occur. In combination these effects lead to extraction efficiencies of the order of \( \sim \eta_T = 1/(n(n - 1)^2) \) [2].

Many methods have been proposed to overcome this fundamental limitation, including adding a metallic rear reflector to the substrate side of the device [3], employing non rectangular parallelepiped chip geometries [4], [5], resonant-cavity devices [6], [7], lens immersion [8], surface patterning [9], surface roughening [10], [11], and two-dimensional surface relief diffraction gratings [12]–[15].

This study investigates the use of metallic back reflectors in conjunction with periodic and disordered surface gratings. It has long been understood that rough surfaces enable higher extraction efficiencies due to path randomisation within the bulk semiconductor. However this understanding relies on the presence of a back recycling mirror to give rays multiple escape chances at the surface. In a previous study the effect of periodic and disordered periodic surface gratings without a back mirror was examined [16]; it was found that the introduction of disorder did not automatically lead to lower extraction efficiencies, implying that a back mirror is not always necessarily for increased extraction efficiency with randomised surfaces. In this study the effect of adding a back mirror is investigated together with both periodic and disordered periodic surface gratings. Although a full 3-D model was used in our previous work this study is carried out in 2-D to simplify the understanding of the effects and increase the lateral dimensions of the simulation significantly to approach the true dimensions of a LED element. This allows a larger range of grating parameters to be simulated. The reduced run-times also allow multiple realisations of disordered surfaces to be simulated from which average behaviour can be calculated. The phenomena are investigated in detail using the 2-D Finite-Difference Time-Domain (FDTD) simulation method using the freely available MEEP software package [17]. The simulations are run in parallel on a High-Performance Cluster to afford increased simulation throughput. The physical structure and parameters of the model are based on an AlInSb LED operating in the midinfrared and are described in detail in [18].

In the following section the FDTD model is described together with the process for measuring the enhancement in optical output power afforded by the mirror and the surface grating. In further sections the optimum location of the rear mirror is investigated via FDTD simulations and validated with scalar theory. The role of both perfectly periodic and disordered-periodic gratings is then investigated in detail.

II. FDTD MODEL

The FDTD method has been chosen to model the behaviour of the various structures [19]; it has the advantage of directly solving Maxwell’s curl equations in the time-domain and as such presents a simple theoretical structure whilst allowing the
broadband response of complex arbitrary geometries to be simulated. The accuracy of the model and size of domain is limited only by the available computing resources. The limitations are reduced by using parallel FDTD, which allows the computational burden to be shared by many processors. The result is reduced run-times for larger structures.

The model used in these simulations is illustrated in Fig. 1 and consists of several components, each of which may be “switched off”. The simulation space is 50 × 17 μm in size and has three principal layers: the cover (or air) layer with \(n_{\text{cover}} = 1\), the bulk layer (representing AlInSb) containing the emitting active layer with \(n_{\text{bulk}} = 3.96\) and the substrate layer to represent the rear mirror. Each layer may be switched on or off with the default background refractive index being that of the bulk layer. The space is uniformly meshed with a resolution of at least \(\lambda_i/15\) in all materials, where \(\lambda_i = \lambda_0/n_i\).

A single point source, excited with a Gaussian modulated sinusoid with a centre emitting wavelength of \(\lambda_0 = 4 \, \mu m\), is placed in the centre of the active layer at a distance \(d_{\text{ss}} = 1.03 \, \mu m\) from the surface to represent an emitter in the centre of the active layer [18]. The simulation space is surrounded by perfectly matched layers (PMLs) to minimise reflections at the boundaries. In order to assess the energy flow within the simulation, virtual surfaces, or flux lines, are placed within the simulation. These monitor the total power flow out of each layer by accumulating the normal component of the Poynting vector \(\mathbf{S}\). These monitor the total power flow out of each layer. The simulation space is 50 μm in size and has three principal layers: the cover (or air) layer with \(n_{\text{cover}} = 1\), the bulk layer (representing AlInSb) containing the emitting active layer with \(n_{\text{bulk}} = 3.96\) and the substrate layer to represent the rear mirror. Each layer may be switched on or off with the default background refractive index being that of the bulk layer. The space is uniformly meshed with a resolution of at least \(\lambda_i/15\) in all materials, where \(\lambda_i = \lambda_0/n_i\).

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for one wavelength will not be optimum for another. However, for clarity, in this study the LED is treated as an ideal quantum well device and a single emitter is used, with multiple sources to be treated in further studies.

It is assumed, in this case, that the unmodified internal field $E_{in}$ emission pattern is isotropic. The presence of the cavity serves to alter the emission pattern of the source due to the influence of the cavity modes. This is illustrated in Fig. 3, where the introduction of a back reflector forms modes of emission within the cavity. Of course these patterns and effects are considered at a single wavelength. Across the full spectral emission of the LED the effects may be different and the cavity will serve to promote emission at a resonant wavelength and produce sharper spectral emission. Although not studied in this paper it must be noted that a change in the internal emission pattern may translate into an alteration in the far-field radiation pattern, deviating from the Lambertian emitter of Fig. 3(a). The cavity factor, $C_i$, is periodic with $\phi$ and its peaks occur with a metal mirror ($r_2 = -1$) at cavity lengths of

$$L = \frac{m_c \lambda_0}{4 n_{\text{bulk}}}, \quad (5)$$

where $m_c$ is any odd integer number. The spacing between optimum cavity lengths is in terms of the internal wavelength $\lambda_i$ then

$$\Delta L = \frac{\lambda_0}{2n_{\text{bulk}}} = \lambda_i/2. \quad (6)$$

An approximate measure of extraction efficiency at a certain $L$ and $d_{ss}$ is then to determine the normalised proportion of $\zeta \times C$ that falls within the escape cone of the source

$$\eta_{\text{ext}} = \int_0^{\phi_c} \frac{\zeta \times C d\theta}{\int_0^{\phi} \zeta \times C d\theta} \quad (7)$$

where $\phi_c$ is the critical angle at the device surface. This extraction efficiency is compared with data from the numerical FDTD simulations described in the next section.

**B. Simulations of Metal Mirror Position**

Simulations are performed for a range of source-mirror positions $d_{ss} = 0.57-6.57 \, \mu m$ with $\Delta d_{ss} = 0.1 \, \mu m$ with a single $E_c$ excitation. In the model, the distance from the source to the semiconductor-air interface remains fixed at $d_{ss} = 1.03 \, \mu m$ to represent an emitter in the centre of the active region [18]. This distance determines whether the antinode and cavity factors vary in phase or out of phase for the wavelength under consideration. The output power will therefore be optimum for that wavelength at which the antinode and cavity factors vary in phase. The value of $d_{ss}$ should then be an integer multiple of $\Delta L$ in the case of a metal mirror. In the wavelength range of interest $d_{ss} = 1.03 \, \mu m$ is optimum for $\lambda_0 = 4.08 \, \mu m$.

The data for both the simulated and analytical normalised power flows are plotted in Fig. 4(a)–(c) for wavelengths of $\lambda_0 = 3.5 \, \mu m$, $\lambda_0 = 4.0 \, \mu m$ and $\lambda_0 = 5.0 \, \mu m$ for a range of $d_{ss} = 0 - 6.58 \, \mu m$. The data show that the simulated results follow the theory well, with the maximum normalised output intensities being seen for $\lambda_0 \approx 4.0 \, \mu m$. The results show that for a well chosen localised source-mirror position the extracted power may be $>60\%$ of the total power at $\lambda_0 = 4.0 \, \mu m$, an enhancement of greater than fifteen-fold over a simulation without a mirror in which only $4\%$ of the power is extracted. The optimum mirror positions for $\lambda_0 = 4.0 \, \mu m$ occur at

$$d_{ss} \approx \frac{m_{m} \lambda_0}{4 n_{\text{bulk}}} \quad (8)$$

where $m_{m}$ is any integer. (As the wavelength is close to $4.08 \, \mu m$ this matches (4) closely.) At this wavelength both the antinode and cavity factors are varying in phase as $d_{ss}$ increases. The data also show that a close mirror is desirable—as $d_{ss}$ increases the peak output power decreases. This is due to the presence of both maxima and minima (4 and 0) in the antinode factor across the angular range within the escape cone. Also the larger the cavity, the more modes it will support and less energy will appear within the escape cone. For a single source at $\lambda_0 = 4.0 \, \mu m$, or well localised set of sources, a metal mirror should therefore lie at a small as possible integer multiple of a quarter wavelength from the source.
The data for $\lambda_0 = 3.5\,\mu m$ and $\lambda_0 = 5.0\,\mu m$ also show periodic variation. However, the magnitudes of the normalised peak intensities are not as large. This is due to the antenna and cavity factors varying with a non-zero phase difference; the fixed das is not optimal for these wavelengths. As both factors have the same tangential components of the incident and transmitted wavevectors, this leads to Snell’s law and a condition for transmission for an air interface

$$k_0\sin\theta_1 \leq k_0 \quad (9)$$

On the introduction of a surface grating an additional set of scattered tangential wavevectors, $Q$, is generated which serve to enable super-critical angular transmission and alter the transmission condition (9) to

$$|k_0\sin\theta_1 - Q| \leq k_0 \quad (10)$$

The set of scattered wavevectors are defined as: $Q = Nk_0 = N2\pi/\lambda$. Unfortunately, the equations tell us nothing about the relative magnitude of these scattered waves only the range of incident angles and periods for which their wavevectors satisfy (10).

By adding the rear metal mirror strong waveguiding will occur in the bulk layer. It is clear from the results in the previous section that a rear mirror position can be chosen for a particular wavelength such that either nearly all of the light is trapped within the bulk layer as guided modes, or most of the light escapes and less is trapped. These correspond to the zeros and peaks in Fig. 4(a)–(c). It is to be expected therefore that these effects will provide further constraint on the grating parameters that give enhanced transmission through the surface and a more complex behaviour will be observed. By using a simple ‘bouncing ray’ approach [25] the number of modes together due to the cavity, but they do not destroy it in these two cases. For the optimum output case the multiple sources reduce the peak output by 37%, while for the worst output case the output power is increased by a factor of 6. However, there is still a significant difference in output between the two cases due to the retention of the cavity factor. Thus, it is found that the mirror position remains important in spite of a diffuse set of sources, but much of the variation is reduced.

IV. REGULAR SURFACE GRATING

The presence of a surface grating goes some way to overcoming the total internal reflection problem that is present when extracting light from a medium of high refractive index into a medium of low refractive index [12], [15]. This is achieved by coupling energy that is trapped in the guided modes of the high index layer into radiation modes of the air layer. The analysis of regular surface gratings may be treated with methods such as rigorous coupled wave theory, coupled mode theory [21], effective source current or volume current methods [22], [23]. In this paper we use the FDTD method to analyse these structures; the method is equally applicable for the case of regular surface gratings as for arbitrarily disordered gratings.

As outlined in a previous study [16], by using the theoretical approach outlined in [23], [24] we may estimate the grating periods which may result in enhanced output power by solving for the transmission condition at the dielectric boundary. At a smooth dielectric boundary between two media with refractive indexes $n_1$ and $n_2$ conservation of momentum requires that the tangential components of the incident and transmitted wavevectors are equal: $k_{||1} = k_{||2}$, where $k_{||1,2} = k_0\sin\theta_{1,2}$, $k_0 = 2\pi/\lambda_0$ and $\theta_1$ and $\theta_2$ are the incident and transmitted wave angles. This leads to Snell’s law and a condition for transmission for an air interface

$$k_0\sin\theta_1 \leq k_0 \quad (9)$$

As alluded to above, the response in the presence of a distributed set of sources will move away from the ideal case of a single source. Two simulations for two metal mirror positions, which provide both peak and trough responses at $\lambda_0 = 4.0\,\mu m$ for a single source, are executed to illustrate the effect of multiple sources. The mirror positions are $d_{ss} = 1.77\,\mu m$ and $d_{ss} = 2.07\,\mu m$, which give $P_{\text{air}} = 0.601$ and $P_{\text{air}} = 0.007$ respectively (see Fig. 4(a)). These same simulations are performed 100 times for different realisations of 1000 multiple sources. Each source has a uniformly random location in the notional active region ($50 \times 1\,\mu m$) and also a uniformly random start time and phase. It is found that for $d_{ss} = 1.77\,\mu m$ the normalised output power becomes $P_{\text{air}} = 0.377$ and for $d_{ss} = 2.07\,\mu m$, $P_{\text{air}} = 0.043$. The multiple sources reduce the extreme variation
with their bouncing angle relative to the surface normal, \( \alpha \), and effective index, \( n_{\text{eff}} \), may be calculated by solving the guided mode guidance condition. A perfect metal mirror introduces a constant phase shift \( \varphi_{\text{ph}} = \pi \) while the bulk-air interface introduces a variable phase shift upon total internal reflection of \( \varphi_{\text{ir}} = 0 - \pi \). For example, at \( \lambda_0 = 4 \mu m \) for a bulk layer thickness of \( d_{\text{bulk}} = d_{\text{air}} + d_{\text{ss}} = 1.79 \mu m \) there are 3 guided modes (Transverse Electric (TE)) which may propagate in the guiding layer, each of which may be scattered by its own range of grating wavevectors \( Nk_q \) and grating periods \( \Lambda \) (see Table I).

### Table I

<table>
<thead>
<tr>
<th>Mode</th>
<th>Mode Angle, ( \theta )</th>
<th>Effective Mode Index, ( n_{\text{eff}} )</th>
<th>Range of Grating Periods, ( \Lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>TE_0</td>
<td>74°</td>
<td>3.82</td>
<td>( 0.21 \lambda_0 \leq \Lambda \leq 0.37 \lambda_0 )</td>
</tr>
<tr>
<td>TE_1</td>
<td>59°</td>
<td>3.39</td>
<td>( 0.26 \lambda_0 \leq \Lambda \leq 0.52 \lambda_0 )</td>
</tr>
<tr>
<td>TE_2</td>
<td>40°</td>
<td>2.55</td>
<td>( 0.38 \lambda_0 \leq \Lambda \leq 1.56 \lambda_0 )</td>
</tr>
</tbody>
</table>

![Fig. 5](image-url) Grating parameters: period \( \Lambda \), width \( w \), depth \( d \), and random offset \( s \).

The onset of grating effects is dependent on the wavelength under consideration and is determined from the theory to be \( \Lambda \approx \lambda_0/5 \). At \( \lambda_0 = 3.5 \mu m \) some increases in output power which are dependent on period are seen from \( \Lambda > 0.5 \mu m \) but the effects begin in earnest around \( \Lambda > 0.7 \mu m \) as predicted by the theory. At \( \lambda_0 = 4.0 \mu m \) and \( \lambda_0 = 5.0 \mu m \) the effects begin at approximately \( \Lambda > 0.85 \mu m \) and \( \Lambda > 1.1 \mu m \) with some scattering seen at smaller periods. Above \( \Lambda > 1.0 \mu m \), the qualitative response from the grating is similar at all wavelengths with peaks in output seen at the same grating period intervals. These areas offer enhancement at all three wavelengths which from (10) implies that enhancement is seen for either a changing incident angle \( (\theta_1) \) and constant output angle \( (\theta_2) \) or constant incident angle and changing output angle. However the grating period band that exhibits the peak power varies from wavelength to wavelength. For example at \( \lambda_0 = 3.5 \mu m \) the peak enhancement is seen at the \( \Lambda = 2.8-3.0 \mu m \) band, while at \( \lambda_0 = 5.0 \mu m \) the band showing peak enhancement is \( \Lambda = 3.25-3.5 \mu m \). Further analysis of the far-field response should reveal the behaviour in terms of incident and output angles, but as stated above this work is primarily concerned with enhancements in total power output rather than the radiation pattern. It is clear that the response of the grating to a point source is non-trivial and contains effects based on incident angle, output angle, incident wavelength, grating period and grating order. Further refinements of the model to extract this information are planned.

If we examine the normalised spectral response at grating realisations that exhibit peaks in output power we may assess the wavelength selectivity of the grating in these areas. The data is plotted in Fig. 6(d) together with the data for a flat surface. The flat surface displays a uniform spectral response. At the three gratings with peak output intensities, Fig. 6(d) (i)-(iii), there is a degree of wavelength selectivity with the peaks having a full-width half-maximum (FWHM) of \( \Delta \lambda > 500 \text{ nm} \). In general the data show that in a device without a rear mirror, and hence no guiding layer, a grating may provide good enhancement over a flat surface with a maximum increase of \( \sim 9 \) seen at \( \lambda_0 = 5.0 \mu m \) for \( d = 0.9 \mu m \) and \( \Lambda = 3.3 \mu m \). However in the parameter range simulated it is still the case that a large amount (greater than 50%) of the energy will be lost downwards through the bulk layer due to total internal reflection at the surface.

2) **Surface Grating With Rear Metallic Mirror:** Upon the introduction of the perfect metal back mirror the role of the grating becomes more complicated and more “dynamic”. Three mirror positions are simulated: \( d_{\text{ss}} = 0.76, 1.77 \text{ and } 2.07 \mu m \) to represent three different points of interest on the output response of Fig. 4(b). The normalised vertical output power through the
parameters for each wavelength due to the wavelength selectivity of the grating and cavity combination. It should also be noted that these optimal grating parameters occur at both those wavelengths for which the source-mirror position is optimal for output (e.g., $\lambda_0 \approx 4.0 \, \mu m$ for $d_{ss} = 0.76$ or 1.77 $\mu m$) and at the wavelengths where it is non-optimal (e.g., $\lambda_0 \approx 3.5 \, \mu m$ at all three grating depths simulated). Thus, there are gratings that extract almost all the energy at both $\lambda_0 = 3.5 \, \mu m$ and $\lambda_0 = 5.0 \, \mu m$ for $d_{ss} = 0.76 \, \mu m$, where the rear mirror and flat surface alone achieve extraction efficiencies of merely 3.5% and 4.5%; the grating enables a greater than 26-fold and 22-fold enhancement over a flat surface-mirror combination in these cases.

Two modes of grating behaviour are apparent from the data. The grating response depends on whether the source-mirror location is set for “peak output” or “peak guiding”. At $\lambda_0 = 4.0 \, \mu m$ and $d_{ss} = 0.76$ and 1.77 $\mu m$ for example (Fig. 7(d) and (e)) the behaviour displays features similar (but not identical) to that seen in the simulations without a rear mirror. In these cases the mirror position is set for maximum output power through the surface and so the guided energy is minimised; it is no surprise therefore that the behaviour shares features to simulations in which no guiding is present. However, these mirror positions do not totally eliminate guiding and so extra features are seen in which it is apparent that the guided energy is being coupled out by the grating. At $d_{ss} = 2.07 \, \mu m$, where the mirror position ensures peak guiding, this “peak output” behaviour is not apparent, reinforcing the above interpretation. Instead, for “peak guiding” cases a different behaviour is seen in which peak output contours follow an upward diagonal response in several distinct lines (seen in Fig. 7(a, f, g) and i most clearly). These distinct lines correspond to the outcoupling of different modes of the system. Taking one example at $d_{ss} = 0.76 \, \mu m$ at $\lambda_0 = 5.0 \, \mu m$ (Fig. 7(g)) there are 3 calculated guided modes (see Section IV). The resultant grating period range that satisfies the transmission condition for the first mode with grating order $N = 1$ is: $1.1 \, \mu m < \Lambda < 1.95 \, \mu m$; and for $N = 2$: $2.2 \, \mu m < \Lambda < 3.9 \, \mu m$. These ranges delineate areas of enhancement in the grating response with the diagonal peak contours displaying the optimum parameters for the outcoupling of guided modes.

However the grating parameters which allow these optimum extraction efficiencies are in general quite narrow: for example for $d_{ss} = 0.76 \, \mu m$ at $\lambda_0 = 4.0 \, \mu m$ (Fig. 7(d)) an optimum grating occurs for a period $\Lambda = 1.45 \, \mu m$ and depth $d = 0.6 \, \mu m$ giving $P_{air} = 0.98$. A difference of ±50 nm in the grating period means a minimum reduction in normalised output intensity of $\Delta P_{air,mn} = 0.3$ (from $P_{air} = 0.98$ to 0.68 at $\Lambda = 1.5 \, \mu m$) and a maximum reduction of $\Delta P_{air,mn} = 0.8$ (from $P_{air} = 0.98$ to 0.50 at $\Lambda = 1.4 \, \mu m$). There are, however, locations which afford more flexibility in grating parameters however: for example for deep gratings ($d > 0.8 \, \mu m$) at $d_{ss} = 0.76 \, \mu m$ for $\lambda_0 = 5 \, \mu m$ and for $\Lambda \approx 2.0-2.2 \, \mu m$ and $d = 0.5-0.8 \, \mu m$ at at $d_{ss} = 0.76 \, \mu m$ for $\lambda_0 = 3.5 \, \mu m$.

The spectral responses of some grating configurations which exhibit maxima at the chosen wavelengths are shown in Fig. 8 for the three mirror positions. They illustrate both the optimal maxima in the normalised output intensity and the wavelength selectivity of the maxima. It is immediately to be noticed that an optimum grating realisation at one wavelength may also be

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**Fig. 6. Normalised output power through surface $P_{air}$ for surface grating without rear metal reflector: (a) at $\lambda_0 = 3.5 \, \mu m$; (b) at $\lambda_0 = 4.0 \, \mu m$; (c) at $\lambda_0 = 5.0 \, \mu m$. (d) Normalised spectral power for a flat surface and (i) $d = 0.7 \, \mu m$, $\Lambda = 3.0 \, \mu m$; (ii) $d = 0.9 \, \mu m$, $\Lambda = 1.05 \, \mu m$; (iii) $d = 0.7 \, \mu m$, $\Lambda = 3.3 \, \mu m$.**
Fig. 7. Normalised vertical output power through surface $P_{ov}$ for surface grating with rear metal reflector at three wavelengths and three mirror distances: (a)–(c) at $\lambda_0 = 3.5 \, \mu m$ for $d_{ss} = 0.76, 1.77$ and $2.07 \, \mu m$; (d)–(f) at $\lambda_0 = 4.0 \, \mu m$ for $d_{ss} = 0.76, 1.77$ and $2.07 \, \mu m$; (g)–(i) at $\lambda_0 = 5.0 \, \mu m$ for $d_{ss} = 0.76, 1.77$ and $2.07 \, \mu m$. 
optimum at another but not at the wavelengths in between (e.g.,
\(\lambda_0 \approx 3.8 \mu m\) and \(\lambda_0 \approx 5.0 \mu m\) in Fig. 8(b)(iii)). It is no
surprise given that a grating at one wavelength is a higher order
grating at a smaller wavelength and so on for decreasing wave-
length and increasing order. The broadest simplest peak occurs
around the longer wavelength of \(\lambda_0 \approx 5.0 \mu m\) in Fig. 8(b)(iii); at
other wavelengths the peaks are more complicated and in
general less broad in wavelength. For example in Fig. 8(a)(i)
the peak around \(\lambda_0 \approx 3.5 \mu m\) has a full-width half-maximum
(FWHM) of \(\sim 100\) nm and is part of a complex spectral re-
sponse, whereas in Fig. 8(b)(iii) the peak at \(\lambda_0 \approx 5.0 \mu m\) has a
FWHM of \(\sim 500\) nm and no significant sub-peaks. This may be
due to there being fewer guided modes (3 as compared to 4) at
\(\lambda_0 = 5.0 \mu m\) and so the grating is enhancement is clearer; the
peak around \(\lambda_0 = 4.0 \mu m\) (in Fig. 8(b)(ii)) is also broader but
not as simple.

The spectral responses are very sensitive to wavelength be-
cause of the wavelength selectivity of both the cavity formed
by the metal mirror and surface and the surface grating. The
behaviour is complex and requires that the grating and mirror
position be matched exactly to the desired output wavelength.
However, by undertaking this optimisation it is possible, with
an ideal back reflector, to extract almost all of the energy at a
certain wavelength for a given emitter position.

3) Lossy Metallic Mirrors: At optical wavelengths metals
become lossy and so the reflectivity deviates from the idealised
case of \(R = 1\) and the phase shifts on reflection \(\phi \neq \pi\). The
effect of lossy metals may be included in FDTD over a narrow
bandwidth by equating the parameters of the frequency domain
Drude model of metals with a Lorentzian harmonic represen-
tation of material polarisation in the time domain [27], [28].
Using this process a thick lossy gold mirror is placed beneath
the source in place of the perfect metal. Due to the absorbing metal,
the normalisation procedure used before is not appropriate as
the location of the flux plane in the gold layer would not ac-
count for the losses incurred in the mirror and so the total power
value would be incorrect. Instead, an enhancement factor \(G\) is
defined as the ratio of the vertical output power through the top
flux line to the vertical output power in a reference simulation
with a flat surface and no rear mirror.

Three sets of simulations are undertaken with a lossy gold
mirror with dispersive parameters determined using the method
set out in Skinner et al. [27]. In brief, this method recognizes
the similarity between the Drude model of complex permittivity
in metals and the summed Lorentzian polarisabilities used in
MEEP. By using readily available frequency domain data (for
example from Luxpop [29]) this may be transferred to equiva-
 lent (but narrow band) parameters for the time domain polaris-
ability in MEEP.

The mirror is placed in three different locations from the
source: \(d_{ss} = 0.76, 1.77,\) and \(2.07 \mu m\). The results for a sur-
face grating with varying surface parameters are compared to
those obtained for a perfect metallic mirrors. The data show
that, as to be expected, the lossy mirror has a detrimental ef-
fect on the output powers seen in each case. For example, for
the data at \(d_{ss} = 2.07 \mu m\), a perfect metal mirror displays an
area of enhanced output of \(G = 34.0\) with grating parameters of
\(d = 0: 5 \mu m\) and \(\Lambda = 2.15 \mu m\). In the lossy case, the en-
hancement for the same grating parameters becomes \(G = 22.1\), a
significant fall factor 0.65. This result shows that the presence of
a lossy mirror can significantly affect the output power achiev-
able with a rear metallic mirror. As this effect will be exacer-
bated with increased “bounces”, the mirror should be placed for
peak output, or the grating designed to extract the energy with
minimum “extraction length”.

4) Disordered Periodic Grating: It has been observed that
introducing roughness to the surface of a dielectric material,
in conjunction with a rear reflecting layer, produces enhanced
output powers into free space [11], [26]. In this section a peri-
odic surface pattern, such as those investigated above, is “ran-
donised” with varying degrees of disorder to reproduce a rough
surface. An initially periodic grating composed of surface fea-
tures as illustrated in Fig. 5 is disordered by applying normally
distributed random offsets to each element. A single offset to
a surface feature, \(s\), is shown in Fig. 5; in ensemble the off-
sets have a standard deviation \(\sigma\) and a mean of zero. Thus, in-
creased “randomness” is achieved by increasing the standard de-
viation of the offset statistics. Overlaps into neighbouring cells
is allowed. It should be noted that the grating now contains an
ensemble of grating periods, and consequently an ensemble of
grating wavevectors [23], but due to the zero mean of the random

Fig. 8. Normalised spectral response of vertical output power through surface
\(P_{\text{surf}}\) for flat surface and optimal surface gratings with rear metal reflector at
three wavelengths and \(d_{ss} = 0.76 \mu m\): (a) flat surface response and (i) optimal
grating at \(\lambda_0 = 3.5 \mu m\) (\(\Lambda = 2.75 \mu m\) and \(d = 0.55 \mu m\)); (b) optimal gratings
at (ii) \(\lambda_0 = 4.0 \mu m\) (\(\Lambda = 2.85 \mu m\) and \(d = 0.6 \mu m\)) and (iii) \(\lambda_0 = 5.0 \mu m\)
(\(\Lambda = 1.15 \mu m\) and \(d = 0.85 \mu m\)).
offsets the mean period of the grating remains that of the initial periodic grating \( \langle \Lambda \rangle = \Lambda \).

Randomised gratings are investigated for a mirror position of \( d_{ss} = 1.76 \mu m \) and for two grating depths \( d = 0.4 \mu m \) and \( d = 0.85 \mu m \). Ten different realisations of a random grating are investigated for a given randomness \( \sigma \). In order to get the general response of the randomised grating the arithmetic mean of the output powers, \( \langle P_{ar} \rangle \), from the ten realisations is taken. The data for random gratings from \( \sigma = 0 \)–0.4 are shown in Fig. 9.

The data show that by adding disorder the behaviour of the surface grating is changed to become much more uniform across variations in period. Also the enhancements offered by the grating are apparent from much lower periods than for a periodic grating. The effect is most clearly seen at \( \lambda_0 = 3.5 \mu m \) (Fig. 9(a) and 9(b)). The mirror position ensures that the energy is in a “peak guiding” condition as described above (cf. Fig. 9(a)) and the periodic grating \( (\sigma_s = 0) \) does not begin to have an effect until \( \Lambda \geq 0.7 \mu m \) (as predicted by the theory). Above this period the output power experiences large peaks and troughs dependent on the grating period. As a small amount of disorder \( (\sigma_s = 0.1 \mu m) \) is introduced to the grating the magnitude of these variations is reduced, but they remain in large part. As the disorder is increased these variations begin
wavelengths for a grating depth of $d = 0.85 \, \mu m$ is possible. By examining some spectral responses taken from these data it is possible to confirm this. Fig. 10 shows the normalised spectral response data for two grating configurations: (a) $\Lambda = 1.0 \, \mu m$, $d = 0.4 \, \mu m$ and (b) $\Lambda = 1.6 \, \mu m$, $d = 0.85 \, \mu m$. For each configuration three spectral responses are shown: a flat surface reference response, a perfectly periodic grating response and a response of a disordered grating with the same mean period. The data show that at both depths the disordered response displays a considerably broader spectral response (particularly in Fig. 10b) than the perfectly periodic case and does not suffer as much from the large troughs due to the wavelength selectivity of the grating and cavity. This flatter response comes at the cost of peak power out with the disordered gratings not reaching the levels of the periodic gratings. However the data show that by tailoring the roughness it is possible to achieve a broadband spectral response which still offers considerable enhancements over a flat surface and translates the advantages afforded by the cavity to a larger wavelength range. The data also show that the disorder ought to also reduce the constraints on the source positions within the cavity as the disordered gratings show much the same response in output power at the three wavelengths considered, regardless of whether the source-mirror distance and cavity length result in a “peak output” or “peak guiding” response.

V. Conclusion

This study has investigated in detail the effects of a rear perfect back reflector, perfectly periodic surface gratings and disordered periodic surface gratings. It has been shown that a rear metal mirror in conjunction with a periodic surface grating may result in optimum extraction efficiency where more than 98% of the energy at a certain wavelength may be extracted. This behaviour is heavily dependent on specific grating parameters and mirror positions and is inherently narrowband in its spectral response. By adding disorder to the surface grating it is shown that the spectral response may be made to be much broader whilst maintaining a reasonable normalised output power ($P_{\text{air}} > 0.5$). Further investigation is underway to study these effects in more detail and refinements of the model are planned to include optical losses and real metals as well as multiple sources to represent a spontaneous emission more accurately.

REFERENCES
