The micromixer consumes 15.6-mW power and occupies an area of only $660 \times 420 \, \mu m^2$, excluding the test pads.

ACKNOWLEDGMENTS

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field formulation or can be solved by using the recently developed weighted total-field/scattered-field (TF/SF) approach [11]. Problems (ii) and (iii) are tricky, since the resolution may require a fundamental change in the Fourier PSTD scheme. In high-contrast materials, the solution itself or its derivatives are not continuous, which makes it questionable to use Fourier series as basis functions. The common solution to problem (ii) is to use the Chebyshev polynomials and Gauss–Lobatto collocation points. This yields the multidomain PSTD algorithm [15–17], which separates the computation domain along material boundaries into smaller subdomains, each of which is a uniform medium. Then a collocation (pseudospectral) algorithm is applied in each subdomain, without being affected by the Gibbs phenomenon. To connect the neighboring subdomains, a domain-patching condition is applied to the subdomain boundaries. In addition to the multidomain PSTD approach, if the material geometry is rectangular, one can use the so-called mapped PSTD [12, 14] to reduce the singularity of the solution in a mapped space, and safely apply the Fourier PSTD algorithm. This method is shown to be accurate and efficient and only requires some minor changes to existing Fourier PSTD programs. By introducing a nonuniform grid that aligns with material boundaries as in the mapped PSTD [12], or a conformal grid as in multidomain PSTD, the small-feature problem can be accurately handled as well. However, more case studies are needed to further prove their flexibility and accuracy.

Recently, Leung and Chan suggested a combination of PSTD and FDTD method applied in different directions [5]. It was suggested that FDTD be applied to directions along which the material is highly nonhomogeneous and has fine structures and that PSTD be applied in directions along which the material property contrast is small and the structures are relatively large. In this paper, we apply this concept in 3D simulations of thin-plate problems. We use FDTD in the z direction, which is perpendicular to the thin plate surface and PSTD in the x and y directions. There are several advantages in so doing. First, normal incident waves can be introduced easily by applying the TF/SF technique in the z direction. Otherwise, if we apply PSTD in the z direction, either a scattered-field formation or the weighted TF/SF formulation will need to be used [11]. Neither of them is as efficient and simple as the TF/SF formulation in FDTD. Second, from the computation-efficiency point of view, because the vertical dimension of the computation region is very small, it is more efficient to use FDTD than PSTD in the z direction. This is because the number of numerical operations in the FFT algorithm (N log N) is less advantageous when N is small [18, 19]. Third, for thin-plate problems, thin films are usually used on the surface. This produces very fine structures in the z direction, and the dense grid of FDTD is very suitable for those fine structures. Fourth, the size of the computation region in the x and y directions is very large and the structures are relatively large in these directions. Applying PSTD in the x and y directions can save both memory and computation time [1, 12].

**2. A HYBRID PSTD-FDTD ALGORITHM**

In the hybrid PSTD-FDTD algorithm, we apply finite difference in the z direction and Fourier pseudospectral method in the x and y directions. In implementation, we simply stagger E and H grids in the z direction and use unstaggered grid in the x and y directions. Figure 1 shows the arrangement of the E and H grids in space.

In the time domain, the E and H grids are interleaved, and a leapfrog scheme is applied in time marching, the same as FDTD and Fourier PSTD. Thus, in a Cartesian coordinate, the Maxwell’s curl equations can be written as the following difference equations, after using the transformation for the H fields, $H_{\text{new}} = Z_0 H_{\text{old}}$ [20]:

\[
H^{n+1/2}_x = D_x H^{n-1/2}_x + D_y \left( \frac{\partial}{\partial x} E^n_y - \frac{\partial}{\partial z} E^n_z \right), \quad (1a)
\]
\[
H^{n+1/2}_y = D_y H^{n-1/2}_y + D_z \left( \frac{\partial}{\partial y} E^n_z - \frac{\partial}{\partial x} E^n_x \right), \quad (1b)
\]
\[
H^{n+1/2}_z = D_z H^{n-1/2}_z + D_x \left( \frac{\partial}{\partial z} E^n_x - \frac{\partial}{\partial y} E^n_y \right), \quad (1c)
\]
\[
E^{n+1}_x = C_x E^{n}_x + C_y \left( \frac{\partial}{\partial y} H^{n+1/2}_x - \frac{\partial}{\partial z} H^{n+1/2}_z \right), \quad (1d)
\]
\[
E^{n+1}_y = C_y E^{n}_y + C_z \left( \frac{\partial}{\partial z} H^{n+1/2}_y - \frac{\partial}{\partial x} H^{n+1/2}_x \right), \quad (1e)
\]
\[
E^{n+1}_z = C_z E^{n}_z + C_x \left( \frac{\partial}{\partial x} H^{n+1/2}_z - \frac{\partial}{\partial y} H^{n+1/2}_y \right). \quad (1f)
\]

In Eqs. (1a)–(1f) the constants $C_a$, $C_b$, $D_a$, and $D_b$ are defined as follows:

\[
C_a = \frac{2 \varepsilon_r \varepsilon_0 - \sigma \Delta t}{2 \varepsilon_r \varepsilon_0 + \sigma \Delta t}, \quad (2a)
\]
\[
C_b = \frac{2 \varepsilon_r \varepsilon_0 - \sigma \Delta t}{2 \varepsilon_r \varepsilon_0 + \sigma \Delta t}, \quad (2b)
\]
\[
D_a = \frac{2 \mu_r \mu_0 - \sigma^\alpha \Delta t}{2 \mu_r \mu_0 + \sigma^\alpha \Delta t}, \quad (2c)
\]
\[
D_b = \frac{-2 \mu_r \mu_0 - \sigma^\alpha \Delta t}{2 \mu_r \mu_0 + \sigma^\alpha \Delta t}. \quad (2d)
\]
We assume the $E$ grid is located at $z/H = 1/100$, $K = 0, 1, 2, \ldots$, and the $H$ grid is located at $z/H = (K + 1/2)/100$. Because the update of $E$ fields requires $H$ fields at the same $z$ location, and vice versa, we use the average value of $H$ or $E$ fields from neighboring grids in the $z$ direction. To see that, we use $E^n_{x,y,K}$ to represent the $E$-field component at $(x, y, K)z$ and $t = n\Delta t$, then $E^n_{x,y,K+1/2} = (E^n_{x,y,K+1} + E^n_{x,y,K})/2$, and $H^{n+1/2}_{x,y,K} = (H^n_{x,y,K+1/2} + H^n_{x,y,K-1/2})/2$. Now, we look at the Eq. (1a), which can be written as

\[ H^{n+1/2}_{x,y,K} = D_H \left[ H^n_{x,y,K+1/2} + \frac{\partial}{\partial y} \left( \frac{\partial}{\partial z} E^n_{x,y,K+1/2} - \frac{\partial}{\partial z} E^n_{x,y,K-1/2} \right) \right]. \]  

(3)

In Eq. (3), the spatial derivatives in the $z$ direction are carried out via central difference as follows:

\[ \frac{\partial}{\partial z} E^n_{x,y,K+1/2} = (E^n_{x,y,K+1} - E^n_{x,y,K})/\Delta z, \]  

(4)
and the derivative \( \frac{\partial}{\partial y} \) is carried out through the FFT/iFFT algorithm used in Fourier PSTD [1, 11, 13]:

\[
\frac{\partial}{\partial y} E_{z,x_0,k+1/2}^n = \frac{\partial}{\partial y} \left( E_{z,x_0,k} + E_{z,x_0,k+1} \right) / 2
\]

\[
= \text{iFFT} \left( \text{FFT}(E_{z,x_0,k} + E_{z,x_0,k+1}) / 2 \right).
\]

(5)

3. NUMERICAL RESULTS

We simulated the plane-wave normal incidence on a photo mask using the hybrid PSTD-FDTD method and the FDTD method. The mask substrate is glass and has a 100-nm-thick absorbing layer formed on its surface. The structure is shown in Figure 2, where the computation region is indicated by the dashed-line box, with dimensions \( L_x, L_y, \) and \( L_z \). The glass substrate is assumed to be semi-infinite. A polarized plane-wave soft source is launched.
towards the $+z$ direction inside the glass. The soft source is introduced by simply using the TF/SF formulation. This is consistent with the semi-infinite assumption of the substrate. The steady-state field behind the absorbing layer is the field of interest.

Second-order Liao’s absorptive boundary conditions (ABCs) are applied in the $z$ direction and periodical boundary conditions (PBCs) are assumed in the $x$ and $y$ directions. In general, if the mask patterns are not periodic in the $x$ and $y$ directions, one can simply leave enough "blank space" near the computation boundary in the $x$ and $y$ directions, without being affected by the PBC. This is because the affected regions due to the PBCs are not large when $L_z$ is very small.

As an example, we studied a small area of a photo mask, with $L_x = L_y = 2.0 \, \mu m$ and $L_z = 0.2 \, \mu m$. The mask pattern is shown in Figure 3, where the dark region corresponds to air. A normal incident plane wave, as shown in Figure 2, is polarized in the $y$ direction with amplitude of 1 and wavelength of 200 nm. The incident wave front is smoothed by a raised-cosine envelope function in order to reduce nonphysical transient effects. For the computation region, we use a grid size of $N_x = 70$, $N_y = 70$, and $N_z = 40$. As a result, $\Delta x = \Delta y = 28.57 \, nm$ and $\Delta z = 5 \, nm$. This is equivalent to 4.67 grids per minimum wavelength in the $x$ and $y$ directions and 26.67 grids per minimum wavelength in the $z$ direction. The glass/absorbing layer interface is located at $z = 25 \, nm$ and the detector plane is located at $z = 195 \, nm$. We experimented with two artificial absorbing materials. Material 1 has $\varepsilon_r = 1$, $\mu_r = 1$, $\sigma_r = 0 \, S/m$, and $\sigma = 1 \times 10^4 \, S/m$. Material 2 has $\varepsilon_r = 1$, $\mu_r = 1$, $\sigma_r = 0 \, S/m$, and $\sigma = 1 \times 10^7 \, S/m$. For the 200-nm wavelength, material 1 has a reflection coefficient $\Gamma = 0.0299$ and a skin depth $\delta = 0.53 \, \mu m$. As a result, the Gibbs phenomenon due the discontinuous material property is very small. Material 2 has $\Gamma = 0.8787$ and a very small skin depth $\delta = 4.13 \, nm$, so the solution should show a strong Gibbs phenomenon. The total fields at the detector plane, which is 70-nm behind the absorbing layer, are obtained from calculations with the aforementioned parameters, and the total $E$ fields on the detector plane are shown in Figures 4(a) and 5(a).

To verify our algorithm, we also studied the same structure with the same source using the FDTD algorithm, which also uses the same boundary conditions as the hybrid method. In comparison, the FDTD method uses a grid of $N_x = 400$, $N_y = 400$, and $N_z = 40$, with an average sampling rate of 26.67 grids per minimum wavelength in all directions. The steady state total $E$ fields are shown in Figures 4(b) and 5(b). The difference of $|E_{\text{tot}}|^2$ between these two methods are shown in Figures 6 and 7, where the “dB” for the $z$-axis is defined as $10 \log_{10}(\Delta |E_{\text{tot}}|^2)$. As can be seen in Figure 6, if the solution is smooth, that is, with little Gibbs phenomenon, PSTD is able to achieve results that are very close to those of FDTD, yet with much smaller memory usage. In this example, there is a memory saving of about 32. To compare the computation speeds, we ran simulations on a PC with 1-Gbs memory and one 1.8-GHz CPU. To conduct a fair comparison, both the FDTD and Hybrid codes were optimized and written in Matlab. In this example, the FDTD simulation ran on virtual memory and took more than 12 h to finish, while the PSTD simulation did not use virtual memory and took less than 16 min (see Table 1). To get a better idea of the computation speedup, we also ran simulations with smaller grid sizes to avoid using virtual memory in our PC. Table 2 shows that the hybrid algorithm was able to achieve a speedup larger than 13. For an analysis of the computation complexity of FDTD and PSTD, please refer to [1, 12].

### 4. DISCUSSION
In our numerical codes used in section 3, we applied the 2nd-order Liao’s ABCs [21–24] in the $z$ direction. Liao’s ABC is most effective when the boundary has a uniform propagation speed. However, in our model there are two materials on the boundaries of the computation domain. The top layers (near $z = 0$) are glass and the bottom layers (near $z = L_z$) are air. So the Liao’s ABCs are different for the bottom and top boundaries. If the same Liao’s formula is applied to both boundaries, interpolation needs to be used. In our numerical experiments, however, we found that Liao’s ABC has problems with stability and absorption if interpolation is used. To avoid using interpolation, we use multiple time steps. Specifically, we use the following formulas for the grid boundary:

$$U^{n+1}(I_b) = 2U^{n-1}(I_b) - U^{n-3}(I_b) - 2,$$  \hspace{1cm} (8)

and

$$U^{n+1}(I_b) = 2U^{n-2}(I_b) - U^{n-3}(I_b) - 2.$$  \hspace{1cm} (9)

Following the naming in [23], we call Eq. (8) a 2nd-order Liao’s T2 ABC, and Eq. (9) a 2nd-order Liao’s T3 ABC. The time step is

### TABLE 1 Summary for Computation

<table>
<thead>
<tr>
<th>Method</th>
<th>Grid Size</th>
<th>Average Sampling Rate [grid per minimum wavelength]</th>
<th>$\Delta t$ [s]</th>
<th>Number of Total Time Steps</th>
<th>Total Computation Time [min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDGD</td>
<td>$400 \times 400 \times 40$</td>
<td>26.7</td>
<td>$8.339 \times 10^{-18}$</td>
<td>360</td>
<td>760*</td>
</tr>
<tr>
<td>Hybrid</td>
<td>$70 \times 70 \times 40$</td>
<td>4.67 in $x$- and $y$-axis; 26.7 in $z$-axis</td>
<td>$8.339 \times 10^{-18}$</td>
<td>360</td>
<td>15.5</td>
</tr>
</tbody>
</table>

* running on virtual memory.

### TABLE 2 Summary for Computation

<table>
<thead>
<tr>
<th>Method</th>
<th>Grid Size</th>
<th>Average Sampling Rate [grid per minimum wavelength]</th>
<th>$\Delta t$ [s]</th>
<th>Number of Total Time Steps</th>
<th>Total Computation Time [min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDGD</td>
<td>$200 \times 200 \times 20$</td>
<td>13.33</td>
<td>$1.668 \times 10^{-17}$</td>
<td>180</td>
<td>12.58</td>
</tr>
<tr>
<td>Hybrid</td>
<td>$35 \times 35 \times 20$</td>
<td>2.33 in $x$- and $y$-axis; 13.33 in $z$-axis</td>
<td>$1.668 \times 10^{-17}$</td>
<td>180</td>
<td>0.87</td>
</tr>
</tbody>
</table>

* without using virtual memory.
fixed as $\Delta t = 0.5\Delta z/c$. Then the 2nd-order Liao’s T2 ABC is applied in the lower boundary where the material is air and the 2nd-order Liao’s T3 ABC is applied in the upper boundary where the material is glass, with a refractive index of 1.5.

The stability criterion for the hybrid algorithm is given by Eq. (7), but Liao’s ABC requires $\Delta t = 0.5\Delta z/c$. In general, if we assume $\Delta x = \Delta y$, then we can obtain the following stability criterion for using Liao’s ABC:

$$\Delta x = \Delta y \geq \frac{\pi \Delta z}{\sqrt{6}} \approx 1.283 \Delta z. \quad (10)$$

This is generally satisfied since, in the x and y directions, a lower sampling rate is usually used to take the advantage of the PSTD algorithm.

Because we use Fourier PSTD with a uniform grid in the x and y directions, the hybrid algorithm in this paper requires that the material contrast in the x and y directions is not too large. Otherwise, the severe Gibbs phenomenon will contaminate the simulation results. In our numerical experiments, we found that when skin depth of the absorbing layer is very small, in which the case Gibbs phenomenon is sure to appear, there are fairly large differences in the field values obtained via the hybrid method and those obtained via FDTD with smaller grid size (see Fig. 7). Here we propose several possible remedies for high-contrast materials and good conductors, if they are included in the computation domain: (i) If the object geometry is rectangular on the mask surface, we can use the mapped PSTD along the x and y directions to help reduce the magnitude of the Gibbs phenomenon in the mapped space [12, 14]; (ii) if the object geometry is not rectangular but can be handled with multidomain PSTD, we suggest using multidomain PSTD in the x and y directions; (iii) use regular Fourier PSTD for the x and y directions and then apply a low-pass filter to the final steady-state results contaminated by the Gibbs phenomenon. This may help restore the global exponential convergence property of the PSTD algorithm. We expect to see more progress in these areas in the near future.

5. CONCLUSION

In this paper, we have applied a hybrid PSTD-FDTD algorithm for electrically large thin-plate problems. We adopted FDTD along the vertical direction of the thin plate and PSTD along the horizontal directions. This arrangement can combine the advantages of both the FDTD and PSTD algorithms. As an example application, we studied the near-field scattering of a photo mask, and the hybrid algorithm was shown to offer large savings in memory usage and computation time, as compared with the FDTD method.

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MODELLING OF THE CMOS BURIED DOUBLE-JUNCTION PHOTODETECTOR
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ABSTRACT: In this paper, a general model of the buried double-junction (BDJ) photodetector is proposed for DC, AC, and noise analysis. In conjunction with the analytical expressions of photo-generated and dark currents, this model can be applied to all BDJ operating modes. Moreover, it can be easily extended to any multilayer PN junction device. The experimental results obtained for various devices realized using the 0.25-um CMOS technology show good agreement with the simulation.