Method for Film Thickness Calculation and Resist Profile Design in Thin Film Patterning via Lift-off Process*

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Recently, manufacturing of flat panel displays has been required to achieve high cost-performance and to concern about environmental issues. For these reasons, application of the lift-off process in place of the etching process to electrode patterning in manufacturing of plasma display panels was considered. To resolve problems in conventional lift-off process caused by inappropriate resist profiles, the inversely-tapered resist profile with interstice was proposed, and its fundamental feasibility was experimentally proved. However, even if this resist profile is employed, the problems in the lift-off process still occur when its dimensions are inappropriately given. Therefore, proper design of that resist profile is important. Generally, design of the profile is achieved by iteration of two processes: one is calculation of thickness distribution of the formed electrode pattern, and the other is optimization of dimensions of the profile. It is required that the calculation process is carried out with small computational load and supplies useful information for the optimization process. For this reason, a calculation method which meets the requirements and a design method based on this new method were proposed. However, this calculation method considers only two-dimensional behavior of depositing material in a cross sectional plane. This paper describes enhancement of the calculation method by taking three-dimensional behavior of depositing material into consideration, and reports better consistency between calculation results by the proposed method and experimental results.

Key Words: Film thickness distribution, Deposition, Resist profile design, Thin-film, Lift-off process, Plasma display panels

1. Introduction

In the flat panel display (FPD) field, there has been recently a strong need for achievement of high cost-performance manufacturing. In addition, as with other electronics fields, the FPD field is required to concern about environmental issues. For these reasons, a research was carried out to apply the lift-off process in place of the etching process to electrode patterning in manufacturing of plasma display panels (PDPs). In the lift-off process, inappropriate resist profiles cause covering of deposited material on resist patterns which brings about serious problems in PDP manufacture. In that research, the inversely-tapered resist profile with interstice was proposed and its feasibility was experimentally proved. However, it was also reported that, even if this proposed profile is employed, improper dimensions of the profile still cause the same problems. Therefore, the inversely-tapered resist profile with interstice should also be designed properly.

Design process of the resist profile pattern consists of iterations of the following two processes. One is calculation of thickness distribution of an electrode pattern formed in a given resist pattern profile. The other is optimization of dimensions of the resist pattern profile based on the calculation result. It is desired that the calculation process is operated with small computational load in a short time. Furthermore, it is also desired that the calculated result is given in a mathematical form to efficiently operate the optimization process by taking advantage of the mathematical information or employing a mathematical optimization framework. That research1) provided a film thickness calculation method which meets the above requirements and then a design method of the resist profile using this calculation method. In addition, an identification method of a process parameter in the calculation method and an enhanced design method considering optimization of multiple design variables were also given2). In that calculation method, depositing material is regarded as a particle with infinitesimal radius, and it is assumed that each of the particles approaches a substrate in accordance with a Gaussian-like angular distribution. By considering the range of angles with which a particle can arrive at each point on the substrate in the resist pattern, film thickness at each of the points can be calculated. However, this method considers two-dimensional (2D) behavior of depositing material in a cross-sectional plane of the resist pattern, and hence does not cover behavior of other depositing material in outside of the plane.

This paper enhances this 2D calculation method by taking three-dimensional (3D) behavior of depositing material into consideration, and provides a design method of the resist profile based on this 3D method. This paper is organized as follows: Section 2 reviews the new film electrode patterning method via the lift-off process using the inversely-tapered resist profile with...
interstice, and describes the necessity of proper resist profile design and film thickness calculation for the design. Section 3 refers to the method for thickness distribution calculation of deposited electrode material with small computational load proposed in the previous work, and then describes enhancement of this method by taking 3D behavior of depositing material into consideration. In Section 4, this 3D method is applied to the design method of the resist profile given in the previous work, and Section 5 presents conclusions.

2. New Lift-Off Process for PDP Manufacture

In PDP manufacture, patterned electrode is required to be resistant to oxidation and corrosion, since heat-treatment is executed in a post-process for transparent dielectric layer formation. Although it is general to employ the etching process for film electrode patterning, meeting this requirement results in high cost. To satisfy this requirement with low cost, it is effective to employ the lift-off process in place of the current etching process (Fig. 1). However, as shown in Fig. 2, a covering of deposition material on resist patterns causes some problems in the lift-off process: turning-up of the edge of patterned electrode, resist residue, difficulty in resist removal, and so on. Furthermore, in PDP manufacture, the former two problems affect seriously the post process for dielectric layer formation. For these problems, the new lift-off process using the inversely-tapered resist profile with interstice (Fig. 3) was proposed. Although its feasibility was experimentally proved, it was also shown that the same problems still occur if dimensions of the profile are wrongly given. Therefore, the resist profile needs to be designed properly.

The inversely-tapered resist profile with interstice can be modelled as shown in Fig. 4, where \( H \) is the thickness of the resist; \( a \) and \( b' \) are halves of resist pattern widths at the top and bottom of the inversely-tapered part, respectively; \( h \) and \( w \) are the height and depth of the interstice; \( T(x) \) stands for the thickness of the formed electrode pattern at the position \( x \); \( l \) is the length from the entrance of the interstice (\( x = \pm b' \)) to the edge of the patterned electrode.

Although the dimensions \( H, a, b', h, w \) need to be determined, the former three dimensions \( H, a, b' \) are determined mainly by other reasons than those of the lift-off process; \( H \) is determined by line-up and choice of dry film resist, and this process is performed mainly from the cost point of view; One of \( a \) and \( b' \) is determined by specification of the electrode pattern; The other can be regarded as a design variable, but from the viewpoint of dominance to the problem of a covering of deposition material on resist sidewalls, this dimension is less dominant than the rest of the above five dimensions. For this reason, in this paper, this dimension is also regarded as a given one (The case where one of \( a \) and \( b' \) is regarded as a design variable was discussed in the reference 2). Therefore, \( H, a \) and \( b' \) are regarded as given parameters, and only \( h \) and \( w \) are considered as design variables. Excessively small \( w \) or \( h \), and excessively large \( h \) result in partial coverage of the electrode pattern on the resist sidewall, and then cause turning-up of the electrodes. Excessively large \( h \) also results in large \( l \), which means low pattern accuracy. Therefore, proper design of \( h \) and \( w \) is necessary.

Design process of the resist profile consists of iteration of the following two processes. One is the calculation process of the thickness distribution of an electrode pattern formed in the resist profile with the given three parameters and the two design variables which values are temporarily determined. The other is the optimization process of the temporarily given resist profile based on the calculation result. As stated in the previous section, the calculation process should be operated with small
computational load in a short time, and the calculated result is desired to be given in a mathematical form. In the semiconductor field, there have been proposed a lot of deposition simulation methods taking a string approach, a ballistic approach, a cellular automaton approach, a Monte Carlo approach, etc. It is natural to apply them to the calculation process. However, these methods generally require large computing power and long computation time, since behavior of all deposition material is necessary to be simulated. In particular, when these methods are applied to the deposition process in PDP manufacture, this computational problem becomes more serious since pattern scale is much larger than that in the semiconductor field. In addition, thickness distribution obtained by these methods is numerical and therefore it is not useful enough for the optimization process. Thus, existing deposition simulation methods do not meet the above requirements from the viewpoint of resist profile design. Hence, we proposed a calculation method which satisfies those requirements. In the next section, this calculation method is described and then enhancement of the method is given.

3. Calculation Method of Thickness Distribution of Electrode Pattern

This section describes the thickness calculation method in our previous work which meets the requirements of calculation with small computational load and of supplying useful information for the optimization process. Then, the method is enhanced by considering 3D behavior of depositing material, and its effectiveness is shown by some case studies.

3.1 Calculation Method Based on 2D Model

The following assumptions are introduced concerning to deposition phenomena:

Assumption 1
The deposition is achieved dominantly by the process (called the F process in this paper) in which depositing particles with infinitesimal diameter reach the substrate directly. Deposing particles make perfectly inelastic collisions at the surface of the substrate.

Assumption 2
At an arbitrary point on the surface of a horizontal plane, the quantity of the incoming particles in a unit time depends on their incoming angle \( \theta \). The angular distribution is described as the following distribution function \( p(\theta) \) based on the Gaussian-like function \( q(\theta) \) with standard deviation \( \sigma \) (Fig. 5):

\[
p(\theta) = \begin{cases} \frac{1}{Q} (q(\theta) - q(0)), & \theta \in [0, \pi] \\ 0, & \text{otherwise} \end{cases}
\]

\[
q(\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{1}{2\sigma^2} (\theta - \frac{\pi}{2})^2 \right)
\]

\[
Q = \int_q^\pi (q(\tau) - q(0)) d\tau = \text{erf}\left( \frac{\pi}{2\sqrt{2}\sigma} \right) - q(0)
\]

\[
erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt.
\]

As shown in Fig. 6, the incoming angle \( \theta \) with which a particle reach the point in the resist pattern \( (x, 0) \) is in the range from \( \theta_u(x) \) to \( \theta_d(x) \). Since particles reach the point with the possibility \( p(\theta) \), the amount of the particles which reach the point in a unit time, \( f(x) \), is given by the followings:

\[
f(x) = \int_{\theta_d(x)}^{\theta_u(x)} p(\theta) d\theta
\]

\[
= \frac{1}{2Q} \left[ \text{erf} \left( \frac{\theta_u(x) - \frac{\pi}{2}}{\sqrt{2}\sigma} \right) - \text{erf} \left( \frac{\theta_d(x) - \frac{\pi}{2}}{\sqrt{2}\sigma} \right) \right] - \frac{q(0)}{Q} \left[ \theta_u(x) - \theta_d(x) \right]
\]

\[
= \left\{ \begin{array}{ll}
\tan^{-1} \frac{H}{a-x}, & x \in [-c, a] \\
\frac{\pi}{2} - \tan^{-1} \frac{H}{x-a}, & x \in (a, b] \\
\frac{\pi}{2} - \tan^{-1} \frac{h}{x-b}, & x \in (b, c] \\
0, & \text{otherwise}
\end{array} \right.
\]
where \( b \) is the position of the point at which the extended line of the taper and the substrate intersect, and is given by \( b = (Hb' - ha) / (H - h) \). If the specified film thickness, denoted by \( T \), is small enough, the whole thickness distribution obtained after deposition \( T(x) \) can be approximated by a scalar multiple of the thickness distribution with deposition in a unit time \( f(x) \):
\[
T(x) = \alpha \cdot f(x), \quad \alpha \geq 0,
\]
and the scalar \( \alpha \) is given by
\[
\alpha = \frac{T}{f(0)}.
\]
Therefore, the whole thickness distribution is calculated by the following approximation:
\[
T(x) = \frac{T}{f(0)} f(x).
\]
This can be easily calculated, since the error function can be efficiently calculated numerically by using approximation formulae. In addition, as described in Section 4, the thickness of only some points need to be calculated for the design of the resist profile. Therefore this is achieved with small computational load.

The length from the edge of the interstice to the edge of the electrode pattern is also required to be calculated for the resist profile design. This is given as follows by geometrical relationships:
\[
l_p = c - b = \frac{(a + b)h}{H - h},
\]
where \( c = (Hb' + ha) / (H - h) \) is the position of the most inward point in the interstice at which depositing particles can directly arrive.

Equation (11) describes the length when only the deposition process stated in Assumption 1 (F process) is considered. This assumption is considered to be valid when applied to the deposition method in which materials are deposited with relatively low energy (for instance, the electron beam deposition (EBD) method). However, the dominance of the F process stated in Assumption 1 would be invalid if applied to the deposition methods where materials are deposited with high energy such as the electron-beam plasma deposition (EBPD) method, the sputter deposition, etc. This in particular is serious for calculating the length from the edge of the interstice to the edge of the electrode pattern. Therefore, for the calculation of the length, we consider another extreme process, which we call G process, where depositing particles reach the substrate after perfectly elastic collision at the resist sidewall (Fig. 7). By considering this G process, the length from the edge of the interstice to the edge of the electrode pattern, \( l_o \), is geometrically given as follows:
\[
l_o = \max \left\{ l_p, \frac{h(H - h)(H - h) + (H - h) + (H - h)}{H^2}, \frac{(H - h)(H - h) + (H - h) + (H - h)}{H^2} \right\}
\]
By the equations (11) and (12), the length from the edge of the interstice to the edge of the electrode pattern is given as follows:
\[
l = \begin{cases} l_p, & \text{for the deposition where depositing material has low energy} \\ l_o, & \text{for the deposition where depositing material has high energy} \end{cases}
\]

**Remark 1**

In the previous paper in which this method was proposed, the G process was also considered when the thickness distribution with deposition in a unit time was derived. As a result, the total thickness distribution in a unit time was given as the weighted sum of each distribution in a unit time by the F and G processes. However, in the case study in that paper, in which experiment was carried out by using EBPD method, the value of the weighting constant for the G process was much smaller than that for the F process. This implicitly indicates that, concerning to calculation...
of thickness distribution, the G process can be ignored. Therefore, in this paper, only the F process has been considered in calculation of thickness distribution. Note that, as described in section 3.3, concerning to the length from the edge of the interstice to the edge of the electrode pattern, the G process is required to be considered when the film material is deposited with high energy.

3.2 Extension of 2D Calculation Method to 3D Model

The 2D model considers behavior of depositing particles in the \( zx \)-plane, and does not take deposition particles coming from outside of the plane into consideration. In this subsection, the 2D model is enhanced by considering 3D behavior of all depositing particles.

Let consider the resist line pattern having the inversely-tapered profile with interstice as shown in Fig. 8, and assume that Assumption 2 holds in any plane which is vertical to the substrate (Fig. 9). As shown in Fig. 10, let us focus on an arbitrary point in the \( xy \)-plane \( P(x, y, 0) \). We define the \( x' \) and \( z' \)-axes which pass through \( P \) and are parallel to the \( x \) and \( z \)-axes respectively. These preparations enable us to define the plane \( S(x, y, \phi) \) by rotating the \( z'x' \)-plane around the \( z' \)-axis with angle \( \phi \in (-\pi/2, \pi/2) \). Figure 11 describes the geometrical relationship between the resist profile and depositing particles in \( S(x, y, \phi) \), where

\[
\theta_\alpha(x, \phi) := \begin{cases} 
\tan^{-1} \frac{H \cos \phi}{a - x}, & x \in [-c, a) \\
\frac{\pi}{2}, & x = a \\
\pi - \tan^{-1} \frac{H \cos \phi}{x - a}, & x \in (a, b] \\
\pi - \tan^{-1} \frac{b \cos \phi}{x - b'}, & x \in (b, c] \\
0, & \text{otherwise}
\end{cases}
\]

(14)

\[
\theta_\beta(x, \phi) := \begin{cases} 
\tan^{-1} \frac{b \cos \phi}{-b' - x}, & x \in [-c, -b) \\
\frac{\pi}{2}, & x = -b \\
\tan^{-1} \frac{H \cos \phi}{-a - x}, & x \in (-b, -a) \\
\pi - \tan^{-1} \frac{H \cos \phi}{x + a}, & x \in (-a, c] \\
0, & \text{otherwise}
\end{cases}
\]

(15)

Note that these relationships are independent of the \( y \)-coordinate value of \( P \), since the considered resist profile is uniform with \( y \). This results in uniformity of the thickness distribution with respect to \( y \). Therefore, without loss of generality, we focus on thickness distribution in the \( zx \)-plane and then on \( P(x, 0, 0) \). The quantity of deposited particles on \( P(x, 0, 0) \) in \( S(x, 0, \phi) \) in a unit time, denoted by \( d(x, \phi) \), is given by

\[
d(x, \phi) = \int_{\theta_\alpha(x, \phi)}^{\theta_\beta(x, \phi)} p(\theta) d\theta.
\]

(16)

Therefore, the quantity of whole depositing particles onto \( P \) in a unit time \( D(x) \) is given as follows:

\[
D(x) = \int_{-\pi/2}^{\pi/2} d(x, \phi) d\phi = \int_{-\pi/2}^{\pi/2} p(\theta) d\theta d\phi
\]

(17)

By the same argument in the 2D model, if the specified film thickness \( \bar{T} \) is small enough, the whole thickness distribution is calculated by the following equation:

\[
T(x) = \frac{\bar{T}}{D(0)} D(x).
\]

(18)

As stated in the previous subsection, for the design of the resist profile, the length from the edge of the interstice to the edge of the electrode pattern is required to be calculated. In \( S(x, 0, \phi) \), the \( v \)-coordinate value of the most inward point in the interstice where a depositing particle in this plane can reach directly is given by geometrical relationships as \( (c-x)/\cos \phi \), where \( c \) is defined as same as in the 2D model (11). Therefore, the \( x \)-coordinate value of the most inward point in the interstice in \( zx \)-
plane where a depositing particle can reach directly from the direction of the angle \( \phi \), is obtained by moving \( P(x, 0, 0) \) in the direction of \( +x \) to the point at which the following equation is satisfied:

\[
x = y - (\tan \phi)x = \frac{(b-a)x - Hb}{-\tan \phi}.
\]  

(19)

This means, the \( x \)-coordinate of the most inward point in the interstice in the \( \text{zx} \)-plane where a depositing particle can reach directly, is determined without relation to \( \phi \) as follows:

\[
x = c.
\]  

(20)

Therefore, the length from the edge of the interstice to the edge of the electrode pattern based on the \( F \) process, denoted by \( l_F \), is same as that by the 2D model given by (11).

As also stated previously, depending on utilized deposition method, the assumed dominance of the \( F \) process is invalid for consideration of the length from the edge of the interstice to the edge of the electrode pattern. Therefore, the \( G \) process is considered again, where depositing particles reach the substrate via perfectly elastic collision at the resist sidewall. From this assumption, it is derived that particles flying in the plane \( S(\tau, -\tan(\phi)(x-\tau), -\phi) \) make the collisions at the point on the left resist sidewall in \( S(x, 0, \phi) \) which \( x \)-coordinate value is \( \tau \in [-b', -a] \) and then fly in \( S(x, 0, \phi) \), because the segment of intersection between \( S(x_c, 0, \phi) \) and the inversely-tapered part of the left resist sidewall is described by

\[
x = y - (\tan \phi)x_c = \frac{(b-a)x - Hb}{-\tan \phi}.
\]  

(21)

\( S(x, 0, \phi) \) and \( S(\tau, -(\tan \phi)(x-\tau), -\phi) \) can be matched by rotating one of them around the axis which is parallel to the \( z \)-axis and passes the point \( (\tau, -\tan \phi)(x-\tau), 0) \) on the \( xy \)-plane. The discussion about the most inward point in the interstice where depositing particle can reach does not require considering behavior of the particles in the direction perpendicular to \( S(x, 0, \phi) \). Therefore, it is allowed that we consider only 2D elastic collisions in \( S(x, 0, \phi) \) in the same way as taken in the 2D model.

As a result, by geometrical relationships in this plane, the \( v \)-coordinate value of the most inward point in the interstice where a depositing particle can reach by the \( G \) process is given as

\[
\begin{align*}
\frac{1}{\cos \phi} & \left[(b-a)[Hb + (H+b)a] \cos \phi \right] \\
& \leq H^2[(H-b) \cos \phi] \left[(b-a)[Hb + (H+b)a] \cos \phi \right].
\end{align*}
\]  

(22)

Therefore, the \( x \)-coordinate value of the most inward point in the interstice in \( \text{zx} \)-plane where a depositing particle can reach through the \( G \) process from the direction of the angle \( \phi \), is obtained by moving \( P(x, 0, 0) \) in the direction of \( +x \) to the point at which the value of (22) is equal to 0, and desribed as follows:

\[
C(\phi) = \begin{cases} 
\frac{1}{\cos \phi} & \text{if } (22) \leq 0 \\
\phi & \text{otherwise}
\end{cases}
\]  

(23)

Therefore, the length from the edge of the interstice to the edge of the electrode pattern based on the \( G \) process is given as follows:

\[
l_G = \max_{\phi \in [-\frac{\pi}{2}, \frac{\pi}{2}]} (C(\phi) - b').
\]  

(24)
Since $B(\phi)$ takes the maximum value at $\phi = 0$, (25) is reformulated as (12) which is derived in the 2D model. Hence, equations (11), (12) and (13), which give the length from the edge of the interstice to the edge of the electrode pattern in the 2D model, also hold in this 3D model.

### 3.3 Evaluation of Proposed Model

For evaluation of the proposed calculation method, calculated results were compared with experimental results. Figure 12 shows the experimental result by electron beam deposition (EBD) of chromium and copper to the thickness of 200nm and 800nm onto the resist-patterned substrate with the inversely-tapered profile with interstice which dimensions are $200 \mu m$ and $800 \mu m$ onto the resist-patterned substrate with the deposition (EBD) of chromium and copper to the thickness of 50nm, 100nm, 2.5\,\mu m, and 100nm onto the resist-patterned substrate with the profile of $H=32.8[\mu m]$, $h=5.7[\mu m]$, $a=12.3[\mu m]$, and $b'=14.1[\mu m]$. By finding the value of $a$ by which equations (10) and (18) simulate the experimental result well – in particular the thickness at the entrance of the interstice and overall similarity, $a=5.5 \times 10^{-2}$ and $a=7.6 \times 10^{-2}$ were obtained for the 2D and 3D models, respectively. Figure 13 shows the results by each of the calculation models and also the observed experimental result. The calculated results also show good consistency with the experimental result, and the result by the 3D model shows better consistency with the experimental result than the result by the 2D model as can be seen in Fig. 13(b). Althogh there are still a little inconsistency, from the viewpoint of application of this calculation method to resist profile design, these are considered to be satisfying results, since the value of $T(b')$, which is most important for the design as described in the next subsection, is calculated with adequate accuracy ($0.081 \mu m$ and $0.074 \mu m$ by the 2D and 3D models, and $0.08 \mu m$ by the experiment). The length from the edge of the interstice to the edge of the electrode pattern was calculated for this case, though there are no difference between the 3D and 2D models about this quantity. Since the electron beam deposition method was applied to this experiment, equation (11) was employed. The calculated and observed results were $1.575 \mu m$ and $1.1 \mu m$, respectively. Considering errors in observation and variations in the resist profile formation in actual manufacturing, this can be regarded as a satisfying result.

Figure 14 shows the experimental result by electron beam plasma deposition (EBPD) of chromium-oxide, chromium, copper, and chromium to the thickness of 50nm, 100nm, 2.5\,\mu m, and 100nm onto the resist-patterned substrate with the profile of $H=32.8[\mu m]$, $h=5.7[\mu m]$, $a=12.3[\mu m]$, and $b'=14.1[\mu m]$, which was reported previously. Thickness calculation by the 2D and 3D models were also carried out for this case. The best value of $a$ was obtained as $a=7.0 \times 10^{-2}$ to the 2D model and $a=1.13 \times 10^{-3}$ to the 3D model, respectively, by heuristic search. As shown in Fig. 15, both of the calculated results simulate the experimental result well, and the result by the 3D model simulates better than that by the 2D model. The length from the edge of the interstice to the edge of the electrode pattern was also calculated. In this case, equations (12) was employed, since depositing material has higher energy in EBPD than in EBD. The result was $9.244 \mu m$, and the observed length was $9.0 \mu m$, which means a satisfying result considering errors in observation. The length equation (11) gave $5.553 \mu m$, which justifies employment of the $G$ process.

These calculations were carried out with a generic personal computer (Intel Pentium D Processor 915 (2.80GHz, dual-core); 512MB memory). Each calculation of the thickness distribution were completed in a few minutes, and the thickness at a specified position was obtained instantly, since the calculation requires at most numerical integration of a function of just one variable even in the 3D model. This shows the adequacy of the proposed calculation method for the iterative process of the resist profile design.

**Remark 2**

In the early stage of the electron device research area, Blech proposed a deposition simulation method for step coverage prediction, and the method was enhanced to accomodate a moving substrate. In this method, an angular distribution of flux of depositing materials is derived from the following two assumptions: one is that the mean free path of depositing materials is larger than the source-to-substrate distance, and the other is that the flux of depositing materials is proportional to the area which the materials pass through. This distribution gives film build-up in a unit time in the horizontal direction and the vertical direction at each point on a substrate. This film build-up is calculated for every point given by division of the substrate and this calculation is iterated for every time step. The concept of this method is similar to the concept of the method
proposed in this paper. However, the first assumption is usually unrealistic to be applied to actual deposition. In addition, as with other conventional simulation methods, this method also requires heuristic operation in optimization of design variables. From these points of view, we propose the new method described in this section.

**Remark 3**

Each model proposed in this section can be easily enhanced to accommodate to the case where the substrate is set on a deposition device at a tilt, though there may be almost no need to consider such case from the industrial point of view. See Appendix A for detailed description.

**4. Profile Design Based on 3D Calculation model**

The 3D calculation method given in the previous section has been proved to be usable to the iterative design process. In this section, this 3D model is applied to the resist profile design method which was proposed previously.

Requirements for the profile design are described as follows:

A) To assure high pattern accuracy.

B) To avoid partial coverage of the resist sidewall by the electrode pattern.

These requirements are sufficiently described as the following conditions:

A') To minimize the height of the interstice $h$.

B') To keep enough value of $h$ and $w$ such that the resist sidewall is not covered by the electrode pattern.

These requirements are defined as the mathematical programming problem finding minimal $h$ and $w$ which satisfy $T(\pm b',h)<h$ and $l(h)<w$ (Since $T(x)$ and $l$ in Section 3 are dependent on $h$ which is now a design parameter, they are re-described as $T(x,h)$ and $l(h)$). Since $w$ is independent of $T(x,h)$, this quantity can be given independently from $h$ as long as $l(h)<w$ is satisfied. Therefore, the design problem can be divided into two processes: one is the optimization process of $h$, and the other is the decision process of $w$. The former is the optimization process of just one variable. Based on the above description given in the previous work, the following simple iterative method based on the bisection method can be proposed using the 3D calculation method.

**Method**

Step 1 Assign an adequately large value to the initial value of height of the interstice $h$, so that $h>T(\pm b',h)>0$ holds. Set $h_0$ as 0 and also the counter $i$ as 1. Let $tol_1$ be a constant for minimization accuracy, and $tol_2$ be a constant for margin.

Step 2 Calculate $T(\pm b',h)$ by equation (18). If $h>T(\pm b',h)>tol_1$, then go to Step 3; otherwise, go to Step 4.

Step 3 Define $h_{i+1}=h_i+|h_i-h_1|/2$, and go to Step 5.

Step 4 If $h>T(\pm b',h)\in[0,tol_1]$, go to Step 6, else define $h_{i+1}=h_i$ and go to Step 5.

Step 5 Increment $i:=i+1$, and go back to Step 2.

Step 6 Define $h:=h_i$. Calculate $l(h)$ by (13) considering utilized deposition method, and define $w:=l(h)+tol_1$. Then stop.

This set of steps gives the optimal value of $h$ and $w$ with the accuracy of $tol_1$ and $tol_2$, respectively.

This method was applied to the condition with $H=24.6[\mu m]$, $a=12.1[\mu m]$, $b'=14.0[\mu m]$, and $T=1.0[\mu m]$. By setting $h_0=T$, $tol_1=0.1$, $tol_2=0.1$ and $\sigma=7.6 \times 10^{-2}$ for the 3D model, $h=0.125[\mu m]$ and $w=0.314[\mu m]$ are obtained after 4 iterations.
with a few seconds by the generic computer described in Section 3.3. Although the number of iterations was just 4 in this case, generally speaking, the number can increase depending on design problem and given initial values, and therefore the small computational load in this case shows a great potential of the proposed methods.

Figure 16 shows the resist profile obtained by this method and prospective film thickness distribution calculated by the 3D model. Since $T(\pm b', h) = 0.074[\mu m]$ and then $h-T(\pm b', h)$ is quite small, $l$ is just $0.214[\mu m]$, which means good pattern accuracy. Strict validation of this design method requires experimental evaluations. Unfortunately, this is currently infeasible and will be considered in a future work, since formation methodology for the inversely-tapered resist profile with interstice has not been established enough. However, considering the promising results concerning to prediction of film thickness distribution described in Section 3, this design result can be regarded as a credible one.

5. Conclusion

This paper has discussed the design problem of the inversely-tapered resist profile with interstice, toward practical application of the lift-off process to electrode pattern formation in PDP manufacture. The design problem requires thickness distribution of the formed electrode pattern to be given in a mathematical form and calculated with small computational power. This paper has enhanced the previously proposed calculation method which meets these requirements by considering 3D behavior of depositing material. It has been proved that the proposed method gives practically better calculation result than the previous 2D model. This 3D calculation method has been applied to the design method of the resist profile which was proposed by using the 2D model. It has been shown that, by using the design method, proper dimensions of the resist profile can be obtained with very small computational load, since the calculation method requires numerical integration of a function of just one variable even if the 3D model is employed.

As with the 2D method, the proposed 3D calculation method gives results with mathematical information. This feature of the calculation method has not been exploited, since the design problem considered in this paper has involved the optimization of just one variable and the simple bisection method was useful enough. However, the detailed resist profile design which involves the taper angles, deposition conditions, etc., will involve multi variable optimizations. The feature of the calculation method has a strong advantage in such detailed design.

For further academic contributions for realization of thin film patterning via the new lift-off process in industry, the following issues are required to be taken into consideration in future works:

1. Development of a sophisticated formation method of the inversely-tapered resist profile with interstice, and strict validation of the proposed resist profile design method.
2. Thorough validation of the proposed calculation method including detailed analysis of deposition phenomena.
3. Enhancement of the resist profile design method towards integrated design method of resist profile and deposition process.

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Appendix

The 2D and 3D models can be easily enhanced to accommodate the case where the substrate is set on a deposition device with tilt angle, though this may be rarely required. Let the substrate be set on deposition device at a tilt of $\psi_t$ as shown in Fig. A1. In this case, thickness distribution of the formed electrode pattern based on the 2D model can be obtained by just substituting $\theta_s(x)-\psi_t$ and $\theta_d(x)-\psi_t$ into $\theta_s(x)$ and $\theta_d(x)$ in equation (5).

The same concept can be applied to the 3D model. Let the substrate be set on deposition device in the orientation where the $x'y'z'$-coordinate system of the substrate coincide with the coordinate system obtained by rotating the $X'Y'Z'$-coordinate system of the deposition device with yaw $\psi_y$, pitch $\psi_p$ and then roll $\psi_r$ (Fig. A2). Since the angular distribution of quantity of depositing material $p(\theta)$ is constant to $\phi$ in Fig. 9, $\psi_t$ can be set to 0 without loss of generality. By introducing coordinate transformation matrices for these rotations, the relationship between the angle which a vector in $S(x, 0, \phi)$ makes to the $v$-coordinate, $\theta$, and the angle which the vector makes to the plane of deposition device, $\theta_s$, is obtained as

$$
\theta_s = \text{sgn}(-\cos \theta \sin \psi_v + \sin \theta \sin \psi_v \cos \psi_y) \cos \theta + \cos \theta \sin \psi_v \sin \psi_y \sin \psi_v \\
\cos \theta \sin \theta \sin \psi_v \cos \psi_y \\
\cos \theta \sin \theta \sin \psi_v \sin \psi_y \cos \psi_y + \sin \theta \sin \psi_v \sin \psi_y \sin \psi_y
$$

(A1)
Hence, the quantity of depositing particles reaching the point \( P(x, 0, 0) \) in Fig. 10 in a unit time, \( D(x) \), can be described as

\[
D(x) = \int_{x_{\min}}^{x_{\max}} \int_{\psi_{\min}}^{\psi_{\max}} \rho(\theta) d\theta d\varphi,
\]

and then thickness distribution can be calculated by equations (18) and (A2). Unlike the case described in Section 3.2, where both \( \psi_1 \) and \( \psi_2 \) are 0, the equation (A2) which is given in double integral form cannot be expanded to single integral unfortunately. Therefore, double numerical integration is necessary for calculation of thickness distribution, and this involves larger computational load than (18). However, thickness calculation of just one position, which is required for resist profile design, takes only a few minutes. Considering this fact and the feature that useful information for optimization can be obtained, this method still has certain advantage even in this case.

For evaluation of these models, a deposition experiment was carried out. A resist patterned substrate with the inversely-tapered profile with interstice, which dimensions were \( H=23.4\[\mu m] \), \( h=0.68\[\mu m] \), \( a=12.8\[\mu m] \), and \( b'=14.8\[\mu m] \), was set on a deposition device at a tilt of 0.069rad. Onto this substrate, chromium-oxide, chromium, copper and chromium were deposited to the thickness of 50nm, 100nm, 3\[\mu m] \), and 100nm by electron beam plasma deposition. Figure A3(a) shows this experimental result, and Fig. A3(b) describes calculated results by the 2D model with \( \sigma=3.5 \times 10^{-2} \) and \( \psi_1=0[\text{rad}] \), \( \psi_2=0.067[\text{rad}] \). Considering errors of the tilt angle when setting the substrate, these results can be regarded as successful one, that is, the proposed models can simulate the experimental result well enough even when the substrate is set on a deposition device with a tilt.

**References**


