Mound defect modeling in yield forecasts

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Mound Defect Modeling in Yield Forecasts
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Abstract—Although the majority of defects found in manu-
facturing lines have predominantly two-dimensional effects, there 
are many situations in which 2-D defect models do not suffice, e.g.,
tall layer bulks, residual resist flakes, and extraneous materials 
embedded in the IC. In this paper a more general model based on 
mound defects is presented. Both catastrophic and soft effects of 
mound defects are investigated. The defect model is based on the 
geometrical properties that result from the interaction between IC 
and defect size in two coordinate spaces: $x$-$y$ and $z$. The approach
to model catastrophic effects is a natural extension to the concept 
of critical areas, namely, the extraction of critical volumes. The 
simplicity of the extraction method makes it suitable for inclusion in 
common layout editing tools. Through the course of this work, 
hints to the origins of mound defects will be given, conditions to 
capture critical volumes will be developed, realistic layout results 
will be shown, and a yield model taking into account these new 
kind of defects will be presented.

I. INTRODUCTION

In spite of the stringent contamination control in modern 
manufacturing lines, IC’s are still affected by random 
contaminant phenomena causing defects. Some sources of 
these phenomena are particles lost due to equipment wear out, dust, 
and impurities of the chemicals used in the semiconductor process [1]. As technological processes advance more 
and more into submicron resolution features, the IC's 

dimensional plane is of importance, e.g., the one parallel to 
the surface of the wafer. Furthermore, to quantify the “size” 
of defects, the radius of the circle, or the diameter of the 
square modeling it are accounted for. However, despite the 
majority of defects are in fact two-dimensional in nature there 
are many situations in which 2-D models do not suffice, e.g.,
tall layer bulks disrupting the continuity of subsequent layers, 
abrupt surface topologies, extraneous materials embedded in 
the IC [12]. In the course of this presentation this last kind of 
defects is referred to as mound defects.

As early as 1969, Yaniwaga published a study on mound 
defects [13]. His experimental work revealed that epitaxial 
mounds had catastrophic effects on contact lithography printing. 
Among the defects that he reported are microcracks, 
definition of emulsion photomask layers, accumulation of 
defects around a mound, and propagation effects through sev-
eral layers. With the improvement of lithography processing 
equipment these kinds of defects were possible to ignore. 
However, in contemporary state-of-the-art VLSI technologies 
where resolution features are pushed towards the equipment’s 
feature reproduction limits the effect of these defects can no 
longer be overlooked. In multilevel metallization advanced 
technologies, the depth of field of lithographic equipment is 
not good enough to compensate for small bulks, rises, or 
pressions on the wafer. That is, the beam cannot focus 
in the wafer to make sufficiently fine lines. Planarization of 
the metal and dielectric layers becomes essential for these 
technologies. Moreover, investigations on multilevel intercon-
nects have shown that the existence of abrupt mounds impairs 
semiconductor yield. Several research studies have already 
been pointing out three-dimensional defect models to address 
the previously mentioned experimental results [14]-[16].

The effects of mound defects can be classified as single-
layer or as multilayer. Single-layer effects result in primitive 
fauxts such as bridged and broken patterns. The common 
denominator of these faults is that they take place in the same 
layer where the defect occurs. On the other hand, multilayer 
effects result in faults from the interaction between defect and 
several layers. For instance, an isolated spot of polysilicon on 
top of a diffusion area causes a parasitic transistor fault, or, 
a missing thick oxide between a poly-metal crossing induces a 
short circuit fault. Fortunately, the electrical effect of spot 
defects on actual circuit designs can be predicted through a 
“critical area” analysis. Roughly speaking, a critical area is 
the place where the center of a defect must lie to introduce a 
fault [7], [8].

A common feature in state-of-the-art research on defect 
modeling is that the defect models employed are two-
dimensional [8]-[11]. Typically, spot defects have been 
modeled as squared or round objects in which only a two-
dimensional plane is of importance, e.g., the one parallel to 
the surface of the wafer. Furthermore, to quantify the “size” of 
the defect, the radius of the circle, or the diameter of the 
square modeling it are accounted for. However, despite the 
majority of defects are in fact two-dimensional in nature there 
are many situations in which 2-D models do not suffice, e.g.,
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been pointing out three-dimensional defect models to address 
the previously mentioned experimental results [14]-[16].

The effects of mound defects can be classified as direct 
and indirect. Indirect effects deal with lithography printing 
problems while direct effects address the damage introduced 
by mound defects to the silicon layer structure of the IC. 
In this paper a model for mound defects is introduced and 
the conditions under which such mound defects become cat-
astrophic are derived. In Section II a brief investigation of 
indirect effects is presented. Section III presents geometrical 
conditions to compute critical volumes in order to qualify
and quantify the catastrophic effect of mound defects. This work, in particular, is an extension to the well known work on critical areas [7]. Lastly, yield formulae are derived taking into account the presence of mound defects to evaluate their effect in yield forecasts.

II. INDIRECT EFFECTS

The effect of mound defects is manifested indirectly on the lithographic resolution of resist imaged patterns. In other words, a mound defect can result just in linewidth changes rather than in layout topology changes. As device dimensions go into submicron ranges, resist flakes and other contaminant objects will impair the minimum attainable resolution features. To see how this is possible consider the set-up presented in Fig. 1 illustrating a “projection printing” optical lithography technique. Based on this arrangement it can be shown how the system is defocused through the presence of a mound defect. That is, as the system defocuses, the optical image coming from the mask degrades resulting in a blurred image on the resist layer. Practical optical systems are much more complex but the basic properties of refractive imaging are contained in this set-up. Let the mask be at an object distance D from the lens, and let the resist layer be at a focal distance D’ also from the lens. Because the lens is of limited size, only those rays leaving the mask within certain solid angle can pass and consequently be imaged. In practice, this limit is imposed by the aperture or diaphragm of the system. The numerical aperture (N.A.) relates the size of this stop to the image distance, and is given by N.A. = 2r/D’, where r is the radius of the aperture and D’ is the distance from the center of lens to the resist layer. As it was mentioned earlier, if the location of the layer to be printed varies from the ideal focal plane, a perceptible degradation might take place. The amount of defocusing that can be tolerated is called depth of focus and can conveniently be expressed in terms of the Rayleigh depth d = λ/2(N.A.)2 where λ is wavelength of the source light. Let the height of the mound defect be δ. In the presence of this defect, proper patterning will occur if the focal plane is now changed to D’ − δ. In other words, a defocus equal to the magnitude of the defect has to be tolerated. In common practice the maximum tolerated defocus is limited by the technology and the equipment. Mound defects higher than this depth of focus will create blurred images. Preventive actions such as IBM’s chemical–mechanical polishing of the wafer might be taken at this point in order to suppress mound defects [17]. However, not all the fabs possess this capability and also the expenses incurred in this extra step might rise very sharply.

Simulated and experimental results have been presented in the technical literature for fixed pattern heights and several defocus ranges [18]. These results demonstrate that the linewidth increases and that the pattern thickness decreases according to the severity of the defocus. Here, we examine the case of variable pattern height and zero defocus. This will allow us to illustrate the integrity of the imaged pattern. The set-up presumes a defect-free situation based on a fixed resist thickness of 1 μm. The effect of the mound defect was simulated by increasing the resist thickness by 0.5× and 1× while keeping the focal plane fixed at its original position. The simulation is carried out with SAMPLE [19] running on a grating of three patterns of 1 μm width and 3 μm long, each. Table I presents the parameters used during the simulation.

To further simplify the analysis, incoherent imaging of an equal line and space grating is considered. The grating is imaged with diffraction limited optics at wavelength 0.4358 μm and variable numerical aperture N.A. Imaging is simulated near the resolution limit using a numerical aperture equal to 0.28, and with a great margin using a numerical aperture equal to 0.56. The latter case takes into account defocus due to the presence of the mound defect. The results of both simulations are shown in Fig. 2. It can be seen that for mound defects of 1 μm height the linewidth of the original patterns varied almost 50% at each side when imaging is near the resolution limit. The effect of mound defects of this magnitude is actually catastrophic since the empty spaces among patterns almost disappeared. Notice that under the simulated optical environment a defect of 0.5 μm can perfectly be tolerated. In the case of N.A. equal to 0.56 the patterns are perfectly imaged. Although the simulation presented here is a conservative extreme case, the same behavior can be expected for more aggressive resolution features, especially for multilevel interconnect technologies.

III. DIRECT EFFECTS

In modeling mound defects one has to consider that they are actually extraneous “objects” embedded in the IC. These objects can cause perturbations which are more detrimental to the IC and relatively harder to perceive than the ones coming from 2-D spot defects. Unlike the theory of 2-D spot defects where defects are classified as belonging to some layer, mound defects do not. Mound defects can be particles of dust, resist

![Fig. 1. Indirect effects of mound defects. (a) Projection lithography. (b) Projection lithography with a mound defect.](image-url)
flakes, scum, as well as extra pieces of material. It is due to this fact that their electrical properties can be classified simply as conducting and insulating. Thus, defects of a conducting type can cause breaks in insulating layers, say, $L_2$ and consequently shorts between any conducting layers insulated by $L_2$. On the other hand, defects of an insulating type can cause breaks in both conducting and insulating layers, yet their effect may not be noticeable in insulating layers. Notice that conducting defects on conducting layers and insulating defects on insulating layers are actually meaningless. A special effect arises from having mound defects in a stack of layers. Namely, the effect of the mound is accumulated from the bottom most to the top most layer of the stack.

It has been shown that modeling defects as squares proved to be a simple and efficient technique [8]. As mound defects are three-dimensional objects, right rectangular prism models will be used in this presentation. A right rectangular prism is a geometrical object defined by a finite set of plane rectangles such that every edge of the rectangle is shared by exactly one other rectangle and no other subset of rectangles has the same property.

During the course of this work, it will be assumed that the defect is orthogonal to the surface of the IC. Mound defects will be modeled with two degrees of freedom in the Euclidean space $E^3$. One degree of freedom will be used for the defect’s plane parallel to the IC surface, e.g., the plane constituted by the set of points $(x, y) \in E^3$. The second one will be used for the planes parallel to the IC surface, e.g., the set of points $(x, z) \in E^3$. Furthermore, assume that the modeling of conventional 2-D spot defects is restricted to the plane constituted by the points $(x, y) \in E^3$. As an illustration, Fig. 3 shows the coordinate space of reference.

It is said that a mound defect is catastrophic if its height, $\delta$, is greater than the thickness of the pattern where it is embedded. Additionally, a “tolerance value,” $\xi$, will be used to account for the effect of manufacturing fluctuations on the topography of the IC, e.g., in additive technological processes $\xi$ can be used to model the maximum allowed layer lifting arising from its interaction with a mound defect, refer to Fig. 4 for a set-up.

To evaluate the magnitude of the damage that the defect can cause on the IC let us formulate the concept of critical volume. A critical volume is defined as the three-dimensional space where the centroid of the mound defect must lie to cause a primitive failure. This concept is an extension to the well known “critical area” [7].

A. Critical Volumes for Bridges

Consider two distinct conducting patterns $L_1$ and $L_3$ separated by an insulating pattern $L_2$. Let their length be $l$, their width $w$, and their height $h_1$, $h_3$, and $h_2$, respectively. Let also $\xi_i$, $i = \{1, 2, 3\}$, be the tolerance value of each pattern. Assume now that a mound defect originates in layer $L_1$ and that its height is $\delta_2 = h_1 + h_2 + \xi_1 + \xi_2$. Furthermore, assume that the mound is embedded through the three layers as shown in Fig. 5 causing a bridge between $L_1$ and $L_3$. Observe that the bridge is present even if the defect’s center is located half the defect size away from the patterns contour and that the defect needs only to bisect $L_2$ to create the bridge. Then, the critical volume for this defect is computed as

$$V_{ZY} = |\delta_z - (h_2 + \xi_2 + h_1 + \xi_1)|_{\text{height}} \times \left[ \frac{l}{2} + \frac{w}{\text{width}} \left( \frac{l}{2} + \frac{h_2}{2} \right) \right] \text{length}$$

which reduces to

$$V_{ZY} = |\delta_z - (h_2 + \xi_2 + h_1 + \xi_1)|_{\text{height}} \times |\delta_z + w|_{\text{width}} \left( \frac{l}{2} + \frac{h_2}{2} \right) \text{length}.$$  

The term $|\delta_z - (h_2 + \xi_2 + h_1 + \xi_1)|_{\text{height}}$ corresponds to the critical region in the $Z$ direction; the remaining terms correspond to the critical regions in the $X$ and $Y$ directions. Notice that this conducting mound is meaningless in $L_2$ since it is an insulating layer.

The previous results can be abstracted to the general case of a stack with $n$ patterns. Without loss of generality assume that conducting and insulating layers are alternating. Then, the critical volume for a bridge between layer $L_k$ and layer $L_{n-1}$
is computed as

\[
V_{ZY} = \left[ \delta_z - \left( \sum_{i=k}^{m-1} h_i + \zeta_i \right) \right]_{\text{height}} \times [\delta_x + w]_{\text{width}} [l + \delta_y]_{\text{length}}. \tag{2}
\]

The upper bound of the summation assumes that the mound only needs to bisect layer \( L_n \) to create the bridge.

**B. Critical Volumes for Cuts**

A necessary and sufficient condition to assert that a pattern has been broken by a mound defect is if the breaking process creates two disconnected sections of the same pattern. This is achieved when either two of the three dimensions of the defect are greater than the corresponding dimensions of the pattern. For instance, when the defect's height is greater than the pattern's thickness and when the defect's length or width is greater than the pattern's length or width, respectively. This simple condition ensures that the pattern is broken in both vertical and horizontal directions.

Consider now the pattern set-up shown in Fig. 6. Let us assume that the defect's height is \( \delta_z > h_z \) and that its width is \( \delta_x > w \). Based on the above stated condition, notice that a break occurs when the defect's center is located only half the
Defect Sensitivities

A software prototype was implemented based on the concepts explained in Sections III-A and III-B. The critical area extractor LASER [8] was modified to include three-dimensional effects. To give the reader an insight on the critical volumes, the layout shown in Fig. 7 is analyzed for mound defects originating in the polysilicon layer; critical volumes will be highlighted in black. Let the thickness of polysilicon, thick-oxide and metal be 1 μm each. Fig. 8(a) shows an aerial view of the layout: (a) Overall view. (b) Close-up view of the critical volume. (c) Close-up view of the critical volume from a different angle.

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of the effect of insulating mound defects of 5 μm of height and width on polysilicon-metal crossings. Fig. 8(b) displays the aerial view for conducting mound defects.

To quantify the catastrophic effect of mound defects it is necessary to have a figure of merit. The layout defect sensitivity can be used as such, and in this case it is interpreted as the ratio of the total critical region to the total region of the layout. This region can be an area or a volume. The defect sensitivity for bridges of polysilicon and metal are displayed in Figs. 9(a) and 9(b), respectively, and the ones for polysilicon-metal bridging and breaking crossings in Fig. 9(c) and 9(d), respectively. Observe that the number of overlaps between both polysilicon and metal masks is small. Therefore, in the case of bridges, the critical height and width is less than for nonoverlapped patterns. To infer this quantitatively recall that in the case of overlaps, the critical height is given as the difference of the defect’s height and the sum of the thicknesses of the layers involved in the overlaps, whereas for nonoverlaps the critical height is obtained simply as the difference of the defect’s height and the layer’s thickness. Similarly, recall that in the case of overlaps the critical width is obtained by adding the defect size to the pattern’s width, whereas in the case of single-layer patterns the width is computed by taking the difference of the defect’s width and the space between adjacent patterns. If both pattern’s width and space are comparable in magnitude, we have a difference factor of approximately 2× the pattern’s width. This can be a dominating factor while computing sensitivities and it is the trend observed in Fig. 9.

IV. YIELD FORECAST

Rather than considering indistinguishable spot and mound defects, in this analysis a distinction between them is emphasized. That is, the yield formulas to be developed will consider their effects separately. This is necessary because the effect of mound defects is cumulative from layer to layer while the spot defect’s effect is not. In other words, the yield of layer \(L_j\) is dependent on the yield of layer \(L_{j-1}\) and so on in the presence of mound defects. For simplicity a Poisson yield model will be adopted to demonstrate the impact on yield losses.

Consider now an IC of area \(A\) and concentrate for a moment on layer \(L_j\). Let the defect density of this layer be \(D_j = D_j^{(2)} + D_j^{(3)}\) where \(D_j^{(2)}\) is the defect density of two-dimensional defects and \(D_j^{(3)}\) the corresponding to mound defects. Then, the yield of layer \(L_j\) can be expressed as

\[
Y_j = \exp(-AD_j). \tag{5}
\]

Since only a fraction of the total number of defects is catastrophic, the layout defect-probability kernel must be taken into account. This probability associates distinct defect sizes with their corresponding layout defect sensitivities. Moreover, since we are dealing with distinguishable defects, the corresponding defect-probability kernels must also be different. In fact, the cumulative effect of mound defects is reflected on the defect-probability that is formed from layer to layer. Then reformulating (5) we have

\[
Y_j = \exp\left(-A\left(\Theta_j^{(2)} D_j^{(2)} + \Theta_j^{(3)} D_j^{(3)}\right)\right) \tag{6}
\]

where \(\Theta_j^{(2)}\) and \(\Theta_j^{(3)}\) are the defect-probability kernels due to spot and mound defects, respectively. Since the direct effect of mound defects is on the layer where it originates and the layers on top of it, \(\Theta_j^{(3)} D_j^{(3)}\) can be expanded to

\[
\Theta_j^{(3)} D_j^{(3)} = \sum_{i=1}^{j} \sum_{k=1}^{i} \Theta_{ik}^{(3)} D_i^{(3)} \quad \forall j = 1, 2, 3, \ldots N_{\text{layer}} \tag{7}
\]

where \(\Theta_{ik}^{(2)}\) is the mound defect-probability for defects originating in layer \(L_i\) and having effect through layer \(L_k\). \(\Theta^{(3)}\) can be seen as an upper triangular matrix with each nonzero element taking care of the cumulative effect, from layer to layer, of mound defects. Introducing (7) into (6) yields

\[
Y_j = \exp(-A(\Theta_j^{(2)} D_j^{(2)} + \sum_{i=1}^{j} \sum_{k=1}^{i} \Theta_{ik}^{(3)} D_i^{(3)})) \tag{8a}
\]

which reduces to

\[
Y_j = \exp(-A(\Theta_j^{(2)} D_j^{(2)}) \prod_{i=1}^{j} \prod_{k=1}^{i} \exp\left(-A\Theta_{ik}^{(3)} D_i^{(3)}\right) \tag{8b}
\]
Fig. 9. Mound defect sensitivity. (a) Single-layer polysilicon bridges. (b) Single-layer metal bridges.

This last expression is a clear extension to the Poisson model that takes into account different classes of defect mechanisms and their cumulative effects. Let us investigate now these cumulative effects on yield forecasts. Fig. 10 presents simulation results plotting the marginal yield of a layer due to both spot and mound defects. For the simulation, nine layers below the current one were assumed and the following mound defect probability matrix was adopted:

\[
\Theta_{ik} = \begin{bmatrix}
10^{-1} & 10^{-2} & 10^{-3} & 10^{-4} & 10^{-5} & \ldots & 10^{-10} \\
0 & 10^{-1} & 10^{-2} & 10^{-3} & \ldots & 10^{-9} \\
0 & 0 & 10^{-1} & 10^{-2} & \ldots & 10^{-8} \\
0 & 0 & 0 & 10^{-1} & \ldots & 10^{-7} \\
0 & 0 & 0 & 0 & 10^{-1} & \ldots & 10^{-6} \\
0 & 0 & 0 & 0 & 0 & \ldots & 10^{-5} \\
0 & 0 & 0 & 0 & 0 & 0 & 10^{-4} \\
0 & 0 & 0 & 0 & 0 & 0 & 10^{-3} \\
0 & 0 & 0 & 0 & 0 & 0 & 10^{-2} \\
0 & 0 & 0 & 0 & 0 & 0 & 10^{-1}
\end{bmatrix}
\]
This matrix implies that defects far away from the current layer have little or negligible effect. This is of course to be expected in any manufacturing line with strict particle contamination control. Spot defect density-area products of $10^5$ greater than the corresponding for mound defects were used for ten consecutive area values as a vehicle of comparison. In particular, a mound defect density of $0.1$ and a spot defect density of $1$, both normalized to unit area, were used. The simulation results of Fig. 10(a) show, as it is expected, that yield decreases with the presence of mound defects. Notice from Fig. 10(b) that the decrease is logarithmic as the number of layers increases and that the error is accumulated from layer to layer.

Although the simulations are presented for particular sets of defect sensitivity area products, the trends are general enough to be applied readily to actual products if the defect-size probability density function of mound defects is known. More advanced yield formulae can be used, yet, the scope of this presentation is to provide a systematic method for introducing the effect of mound defects in yield computations.

V. CONCLUSION

In the research hereby presented the modeling of mound defects is addressed using a three-dimensional Euclidean space. Unlike spot defects that can be collectively treated even without knowing their exact nature, mound defects require special attention to model indirect and direct effects. Indirect effects are concerned with linewidth resolutions while direct effects deal with the cumulative consequences that mound
defects have from layer to layer. Let us end this presentation with a couple of remarks. Notice that catastrophic defects in a 2-D Euclidean space are not necessarily catastrophic in the corresponding 3-D Euclidean space. However, every catastrophic defect in the 3-D space is also catastrophic in a 2-D space. Furthermore, it could also be seen that 2-D shorts map onto 3-D shorts but not all 2-D breaks map on the corresponding 3-D space. Yield simulations for single layers show that forecast errors increase with number of layers underneath the layer in question.

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Jose Pineda de Gyvez received the degree in Electronic Systems Engineering from the Technological Institute of Monterrey, Mexico, major in computer engineering, the M.Sc. degree from the National Institute of Astrophysics Optics, and Electronics, Mexico, and the Ph.D. degree from the Eindhoven University of Technology, The Netherlands, in 1982, 1984, and 1991 respectively.

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