Photoresist Process Optimization for Defects Using a Rigorous Lithography Simulator

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Abstract--Particulate contamination in photoresist is a major source of yield loss for CMOS processes. Yield loss due to such contamination is controllable by improved filtering. This paper explores the relation between particle size and line spacing for an i-line lithography process using a calibrated defect simulator.

I. INTRODUCTION

Particulate contamination is a dominant source of yield loss for IC products. The effect of contamination defects can be nonfunctional circuits, because of bridging between leads. In order to attain adequate yields, it is important to understand the interaction between the size of particles and the geometries that need to be printed. This is because, even if the lithography system can print lines of the required size, they may not yield if too many small particles or bubbles in processing materials cause bridging faults or voids. And in order to improve yield for lines of a given size, it is necessary to eliminate defects in processing materials by proper filtering or tuning of process recipes. Improved filtering is one way to eliminate or limit defects in photoresist because filtering limits the size of particles. Hence, in order to eliminate particles in processing materials, it is important to understand the filtering requirements needed for given design rules.

In this paper we study the impact of small particles on the formation of photoresist profiles in order to analyze the impact of filtering on defect levels in photoresist profiles. We show that bridging between photoresist lines depends on the size and position of a particle within the photoresist as well as the spacing between the lines. Because it is not possible to know the size of particles, but only their impact, a simulator, METROPOLE [1], that has been tuned to our i-line process, will be used. In the next section we will discuss the simulator and the tuning process. In Section 3, we show the simulation results, which indicate the impact of particles of different sizes on photoresist profiles, given different line spacings and resist thicknesses, and we conclude in Section 4.

II. CALIBRATION OF LITHOGRAPHY DEFECT SIMULATIONS

The particles have been simulated using the lithography simulator, METROPOLE, developed at Carnegie Mellon ^aDepartment of Electrical and Computer Engineering Carnegie Mellon University Pittsburgh, PA 15213-3890

University. Among the capabilities of this simulator is twodimensional modeling of i-line aerial imaging, exposure of photoresist, and development of photoresist.

The aerial image describes the light intensity that exposes the photoresist on the wafer surface. For the computation of the aerial image, vector methods, rather than scalar methods, have been used in order to attain an accurate solution of Maxwell's equations when modeling systems with high numerical aperture (NA). Numerically, the waveguide method [2] has been used. This method discretizes a structure into many thin layers in the vertical direction. And, since the structure is assumed to be periodic in the horizontal direction, the solution is discretized into spatial frequencies.

For positive photoresists, light causes a chemical reaction in the photoactive compound (PAC) in the photoresist, which creates carboxylic acid, which unlike unexposed PAC, is soluble in polar solvents. The photoactive compound also interacts with the novolak resin in such a way that the dissolution rate is enhanced when exposed and inhibited when unexposed. METROPOLE describes the rate at which this chemical conversion happens as a function of exposure energy or light intensity.

In addition to modeling the chemical conversion of the photoresist, METROPOLE models the absorption of light in the photoresist. Specifically, light is absorbed as a function of depth, reducing its intensity as it reaches the substrate. The amount of absorption is quantified not only as a function of depth into the photoresist, but also as a function of the PAC concentration of the photoresist, which changes as it is exposed to more light. Overall, positive photoresists are typically characterized by three parameters, called Dill's parameters, modeling the bleachable absorption coefficient, the nonbleachable absorption coefficient, and the kinetic rate constant [3].

Light, which exposes photoresist, not only propagates towards the substrate, but is also reflected at the interfaces of layers in the film stack. The result is standing waves. The problem of standing waves in photoresist is solved by thermal diffusion from a post-exposure bake step. The post-exposure bake step is modeled in METROPOLE by a diffusion length, quantified in terms of its standard deviation.

Finally, the simulator describes the rate at which photoresist is developed as a function of the concentration of the photoactive component. METROPOLE uses the Mack development model [4], which characterizes the develop rate by a maximum and minimum rate, PAC threshold, and selectivity. Numerically, the develop step is simulated with a string algorithm [1]. This algorithm models the develop step as a moving surface, where the local development rate is a function of the local PAC concentration.

In order to understand the impact of defects, METRO-POLE was tuned to our i-line profiles. Specifically, the aerial imaging parameters were set according to our process recipes, the resist exposure parameters, i.e., Dill's parameters, were provided by the photoresist manufacturer, and the develop rate parameters were set by optimizing the fitting of simulated profiles to observed profiles. While optimizing the develop rate parameters, we found that the maximum develop rate is primarily influenced by the time it takes for the fully exposed areas to be developed, the PAC threshold primarily influences the linewidth, once the maximum develop rate is fixed, and the selectivity seems to primarily affect the sidewall slope.

Once the nominal simulation profiles have been tuned to experimental data, experiments were run to see how various defects are likely to impact photoresist profiles. Specifically, since both 0.1 μ m and 0.2 μ m filters are common in the industry we consider the impact of highly reflective small particles of these sizes on narrow lines.

Consider for example photoresist lines with a width of 0.4 μ m and spacing of 0.4 μ m. The thickness of the photoresist is slightly over 1um. The worst case location for particles is in the spaces between photoresist lines, since particles in such locations can block or partially block exposure of the photoresist. As a result, in the presence of particles, all photoresist below the clear portion of the mask may not get developed.

Figure 1 shows a profile resulting from a 0.2 μ m particle that is centered in the exposed space between the two photoresist lines. The profile shown in Figure 1 is a cross section of the photoresist lines. The diagram outlines the physical boundary between air and photoresist, the defect, and/or the substrate after the photoresist is developed. We can see from Figure 1 that the photoresist under the particle is not fully developed and bridging can be seen between photoresist lines. Similar results are obtained for 0.1 μ m particles. Moreover, we have observed such defective photoresist patterns when inspecting wafers with a SEM (Figure 2).



Fig. 1 Simulation of a 0.2 µm particle in a 0.4 µm space between resist lines.



Fig. 2 Bridging of photoresist lines.

Obviously, the likelihood of small particles forming bridges depends on the intended spacing between the photoresist lines. Let's consider photoresist lines with a spacing of 1.0 μ m. With this larger spacing the impact of small particles is likely to be less. In fact, 0.2 μ m particles cannot cause bridging between photoresist lines for any location. However, they can result in residual resist. This is because 0.2 μ m particles block a significant amount of light. The corresponding profile is shown in Figure 3. From the figure it can be seen that a photoresist line forms under the 0.2 μ m particle. This residual photoresist has been observed when inspecting wafers for which 0.2 μ m filters were used. On the other hand, simulations of 0.1 μ m particles indicate that, although such particles also cannot cause bridging, they do not result is



Fig. 3 Simulation of a 0.2 μm particle in a 1.0 μm space between resist lines. The resulting resist profile is compared with the nominal profile.

residual photoresist under the particle. We have observed from inspecting wafers that when we moved from 0.2 μ m filters to 0.1 μ m filters, residual resist in 1.0 μ m spaces was eliminated. Because of these results, which indicate a match between observed profiles on wafers and simulated profiles, we can conclude that simulation results are reasonably accurate quantitatively.

III, RESULTS FROM SIMULATION EXPERIMENTS

Figure 4 shows how the position of a particle within the photoresist affects whether or not bridging between photoresist lines is observed. In this figure, 0.1 μ m particles were simulated. We can see from Figure 4A that a 0.1 μ m particle on the substrate has little impact, except for reflecting some light towards the photoresist under opaque sections of the mask. The result is minor thinning of the photoresist profiles. On the other hand, particles placed further from the substrate, indeed, caused more damage by partially blocking the exposure of the photoresist (Figure 4B). As a result of a 0.1 μ m particle which is centered in the exposed space between the two photoresist lines, the photoresist under the particle was not fully developed and bridging can be seen between photoresist lines.

The damage caused by a 0.1 μ m particle depends not just on its vertical location, but also on is lateral position. For example, if a particle in the top anti-reflective coating (TARC) is not perfectly centered over the space, the damage is less, i.e., there is no bridging, as shown in Figure 4C. The



Fig. 4 Simulations of 0.1 μ m particles, in positions A, B, and C, in a 0.4 μ m space between resist lines. The resulting resist profiles are compared with the nominal profile.

particle in position C only increases the critical dimension (CD) of one of the photoresist lines. In addition, there is no damage if the particle is located over the unexposed area of the resist, since there is no interference with the optical image.

Clearly, a highly reflective 0.2 μ m particle can create more damage than a 0.1 μ m particle. In Figure 5 the set of locations, where a 0.1 μ m particle can be centered and cause a



Fig. 5 Locations of 0.1 μ m and 0.2 μ m particles that can cause bridging of photoresist.



Fig. 6 The maximum particle size requirements so that bridging between photoresist lines is avoided.

short is compared with the corresponding locations for 0.2 μ m particles. As with previous simulations, the spacing between lines is 0.4 μ m. Because simulations were done in two dimensions, Figure 5 shows a worst case cross section of places where particles may be centered. The area in this cross section for 0.2 μ m particles is 73% more than that for 0.1 μ m particles. This is an estimate of the difference in the effect of 0.1 μ m particles compared with that of 0.2 μ m particles. However, this approximation of the difference in yield impact between 0.1 μ m and 0.2 μ m particles may be an underestimation, since the difference in volume in three dimensions will be larger.

Nevertheless, these simulations illustrate that 0.1 μ m filters can have a significant impact on improving yield for a line spacing of 0.4 μ m, when compared to 0.2 μ m filters. However, simulations indicate that bridging can result despite 0.1 μ m filters and improved filtration is necessary for this geometry if bridging between photoresist lines is to be avoided. Moreover, improved filtration will certainly be even more important for finer geometries. Figure 6 shows the relationship between line spacing and filtering requirements, if bridging between photoresist lines caused by small particles

is to be avoided. In other words, for a given particle size, the figure shows the minimum line spacing that can be printed without bridging. This figure also shows that modern, say 0.35 μ m, technologies have very stringent filtering requirements.

The nominal curve in Figure 6 assumes no process variations. However, fluctuations in processing conditions across a wafer and between wafers can result in some bridging for line spacings where, under nominal conditions, bridging would not occur for a given particle size. In order to study the impact of process variations, three factors were varied by 10% using a full factorial experimental design. There factors are the exposure dose, photoresist thickness, and the focal plane. It was found that the minimum line spacing that is immune to bridging for a given particle size is especially sensitive to variations in exposure and photoresist thickness, and less sensitive to the location of the focal plane. In fact, low exposure and high photoresist thickness resulted in worst case processing conditions for defects. The resulting range of line spacings that are immune to particles of a given size, in the presence of process variations, is shown in Figure 6.

IV. CONCLUSIONS

The relation between particulate contamination and line spacing requirements has been explored in this paper. It has been found that a lithography simulator, METROPOLE, can be calibrated to a submicron i-line process and can provide accurate results. In addition, the relation between particle location and the impact on photoresist profiles has been studied. Particles close to the surface of the photoresist were found to cause more damage to photoresist profiles. In addition, the interplay between line spacing requirements and filtering requirements has been explored. And, it has been shown how very tiny particles in photoresist can cause major distortions in photoresist profiles.

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