7th VLSI Process/Device Modeling Workshop, Aug. 20-21, 1990, Kawasaki, Japan

(6-1)

Modeling Resist, EM Scattering and Topography

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Introduction

Our modeling and simulation efforts at Berkeley center on issues in the in areas of characterization of lithographic materials, studies of optical imaging and scattering, and integration of TCAD tools into a common environment. In this paper it is only possible to select a few of the recent results which illustrate the state-of-the-art and form a coherent presentation. In discussing these examples the complexity of the models, sophistication of the algorithms and the problems encountered will be emphasized.

Resist Characterization

One of the most interesting examples is the progress that has been made in modeling chemically-amplified mechanisms in deep-UV resists [Fer90a, Spe90a, Fer90b]. Since diffusion and local chemical reactions occur simultaneously during the post-exposure bake the effort to determine quantitative parameters and simulate the reaction become similar to those normally associated with modeling and simulating dopant concentrations in semiconductors. The exposure creates acid and during the bake a catalytic reaction takes place which, for example, in SNR-248 crosslinks or hardens the resist. Through FTIR measurements of peaks associated with chemical bonds the nature and kinetics of the reaction have been characterized by reaction rates with activation energies. Since the melamine cross linker has several sites and requires more than one to be activated this leads to interesting nonlinear effects which are plausible explanations for increased contrast. This material is also sensitive to electron-beam exposure and in fact it takes only about 1/3 as much energy per unit volume or 10 J/cm^3 to expose it. In comparing electron-beam and optical exposure it is interesting to note that the dissolution rate dependence on the change in infrared absorbance change is early identical as shown in Figure 1 [Tam90a].

An example of the simulation steps in using the models to predict profiles is shown in Figure 2 for a 0.3 um line/space pattern at (NA = 0.6, σ = 1) [Spe90a]. Initially the optical properties at the exposure wavelength are used to predict the local absorbed energy density and the resultant local concentration of photo produced acid throughout the resist. During the bake step this acid diffuses within the resist and appears to reduce standingwave effects. The distribution of activated melamine sites and resultant cross-linking differ somewhat from the acid distribution. During development the high contrast of the developer allows the desired feature to retain its initial thickness while developing rapidly to the substrate in unexposed areas. An SEM profile for these conditions from our microstepper are shown in Figure 3. This resist does indeed produce the very high aspect ratio feature predicted by simulation. More importantly, this feature which is 1 um high holds its shape even though it is almost three Rayleigh focal depths in length.

Lithography Simulation

While SAMPLE is being used to simulate cross sections of lines a new set of simulators is being developed for 3-D effects. To generate images of 2-D mask patterns the SPLAT program [Toh87a] based on Hopkin's transmission cross correlation formulation is used. SPLAT is also capable of simulating 2-D phase shifting masks. A new set of resist development and etching-deposition programs based on triangular elements are being written. An example of a contact hole during resist development is shown in Figure 4. Results for etching and deposition are illustrated in Figure 5.

A promising new massively parallel technique for rigorous simulation of topography issues in optical lithography has been developed and tested [Gue90a, Tad90a]. The method is equivalent to the time-domain finite-difference method used in electromagnetic scattering but exploits the parallel nature of wave propagation and the power of recent massively parallel architectures such as the Connection Machine. The convergence was found to be dominated by the physics of multiple scattering and problems 32 times as large could be solved in the same time with 32K processors as the smaller problems with 1K processors.

The suitability of this program TEMPEST for solving a large class of topography problems in alignment, metrology and projection printing has been demonstrated. Figure 6 for example shows the contours of photoactive compound concentration produced in exposure of a contact hole on a curved substrate. When a positive resist is used the specular reflection from the substrate focuses the energy back into the desired exposure area. However, when a negative resist process is used the surrounding area specularly reflects unanted light into the central unexposed area.

Common Environments for TCAD

A utility-based approach to integrated process simulation has been taken in the SIMPL-IPX program [Sch90a]. Figure 7 shows the utilities in the center providing interfaces to the user, process flow and layout to drive rigorous process simulators and analysis tools. The role of the utilities is to help with generating input scripts to processors, chain sequential use of programs together, invoke multiple processing steps and map data between data representations.

An example of some of the issues in data mapping is illustrated in Figure 8. here a trench has been etched into the substate using a mask. The data representation in the substrate must now be updated to take into account the general polygonal shape of the trench profile. The densities of vertices on the trench profile and the density of intersections with the grid may not ne compatible. Once a cut is made regriding to achieve more regular shapes near the trench may be necessary and new boundary conditions along the interfaces may need to be applied.

Utilities were developed which allow a "stitch-back" data mapping of the SIMPL profile and grid into a SUPREM-IV triangle-based mesh. An example of this interaction is presented in Figure 9 which shows the final cross section of a bipolar device with a collector plug formed using a polysilicon filled trench. Implantation and diffusion steps were simulated by SUPREM-IV while SAMPLE was used for etching and deposition.

An experiment in using direct access from within programs to a shared database is also being carried out [Won90a]. It is based on and intertool version of the profile interchange Format (PIF) which defines PIF objects and their interrelationships. A PIF toolkit gives TCAD programs such as process and device simulators access to PIF objects in an underlying database such as OCT. By using this approach process and device simulation programs can be coupled to higher level design data and tools (i.e. layout, circuit, and logic design) through the CAD Framework Initiative and an OCT/VEM/RPC implementation.

Conclusion

The trend toward higher aspect ratio topography features increases the complexity of process interactions. Rigorous process simulation is currently capable of making important contributions and relating to layout and process flow. In the future simulation will make even stronger contributions due to the rapidly decreasing computer costs and the increase in expense and lack of availability of experimental equipment.

Acknowledgment

This presentation is based on key contributions by many members of our research group. Please make direct reference to their original contributions described in the references. The work overviewed in this presentation was made possible by the Semiconductor Research Corporation (Design Sciences), Sematech and the California MICRO Program.

References

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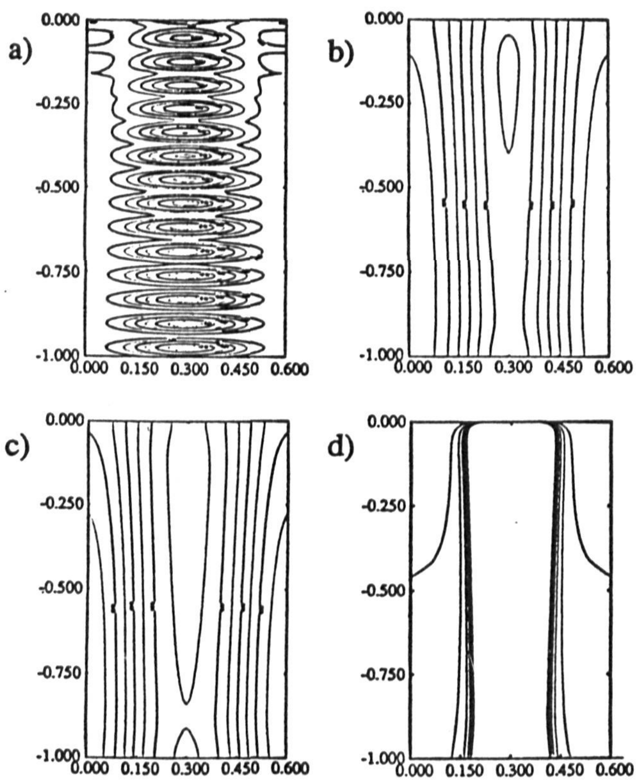

Figure 2. Simulation of o.3 um line/space profiles in 1.0 um SNR-248N a) exposure, b) diffuion of photo-generated acid, c) cross-linking, and d) development.

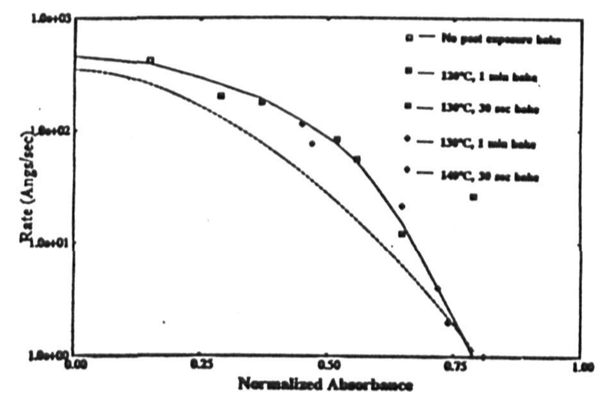

Figure 1. Dissolution rate versus IR absorbance for electron-beam and optical exposure.

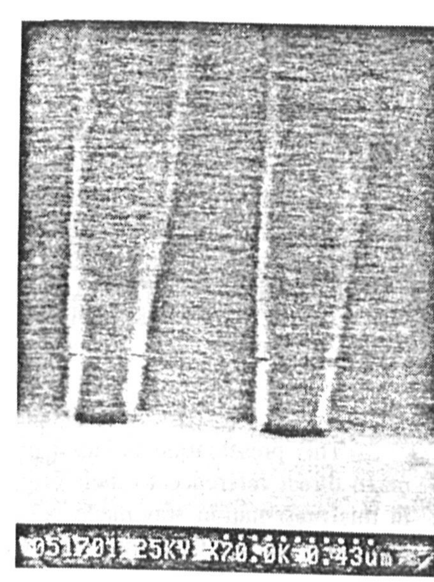

Figure 3. SEM of a SNR-248 resist profile of a 0.3 um feature.

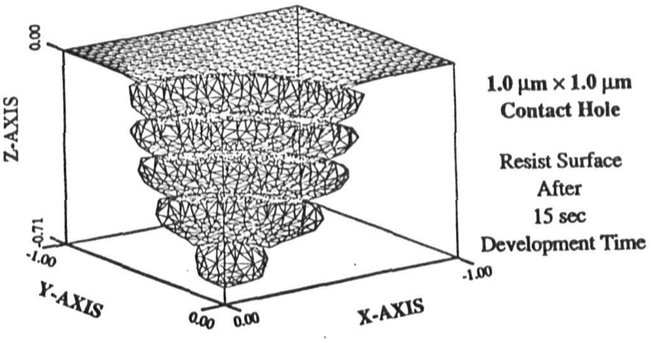

Figure 4. 3-D development of a contact hole.

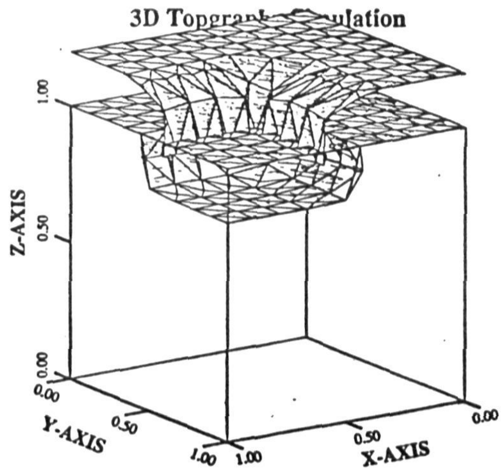

Figure 5. 3-D etching and deposition.

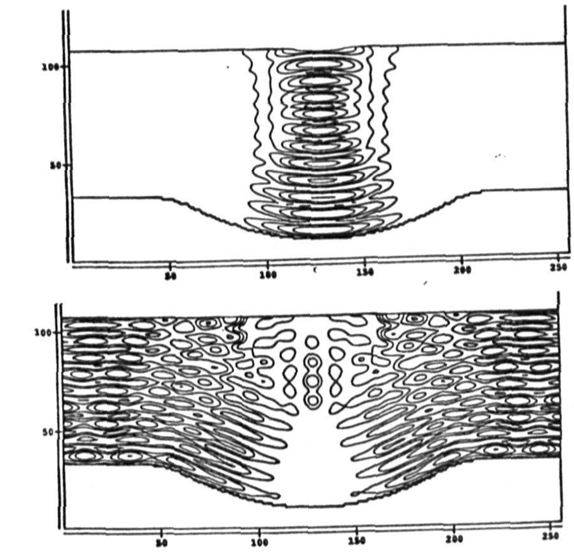

Figure 6. PAC contours for positive and negative polarity resist for a contact hole on a curved substrate.

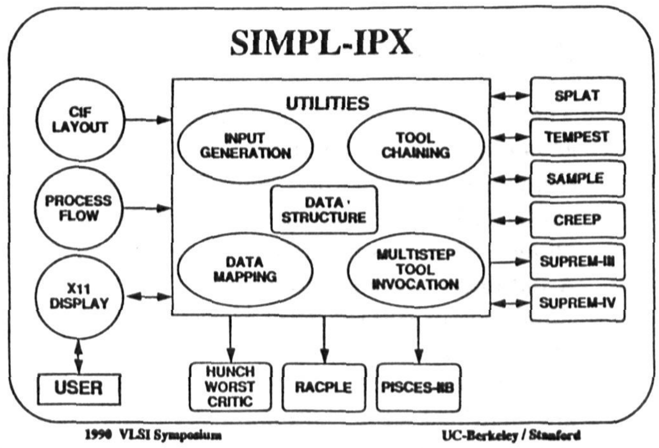

Figure 7. SIMPL-IPX Utilities

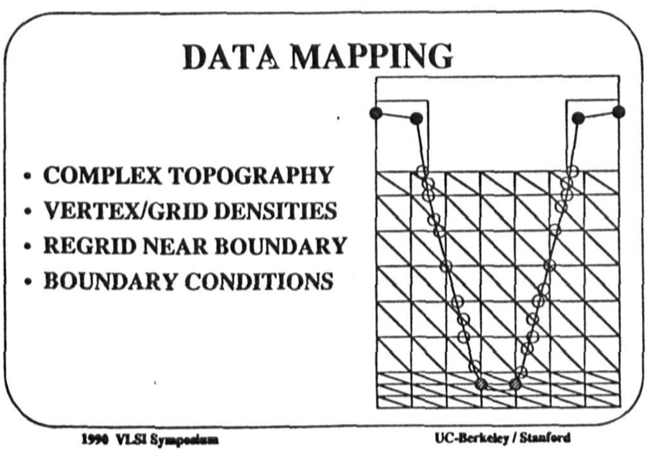

Figure 8. Data Mapping Issues

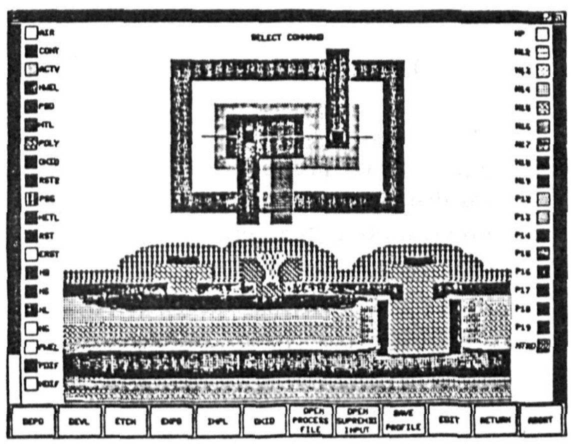

Figure 9. Bipolar Transistor with collector plug "stitch-back"