Accurate Modeling of Ti/TiN Thin Film Sputter Deposition Processes

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Abstract

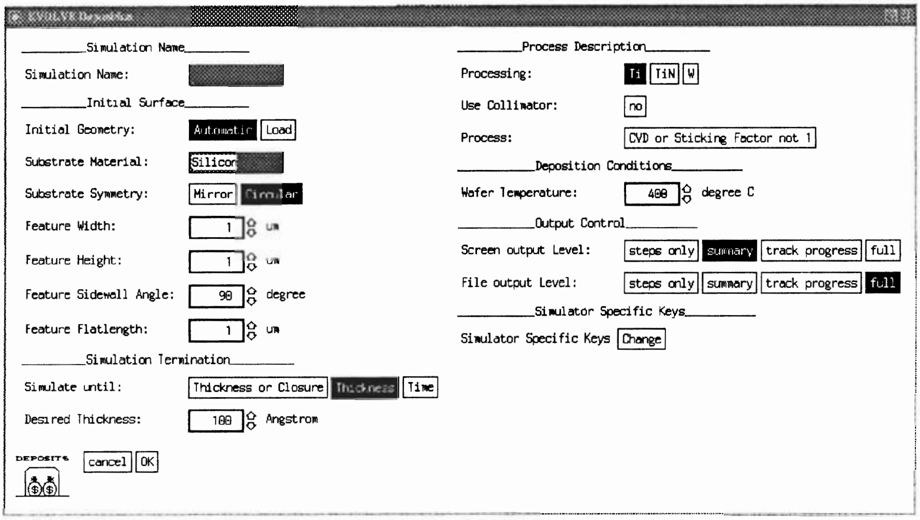
An accurate and user friendly tool for the simulation of Ti/TiN sputter deposition processes has been developed. Simulations have been compared to SEM measurements, which exhibit excellent agreement for both, the collimated as well as the uncollimated case. A final test showed that this simulator is capable of predicting the deposited film on the collimator sidewalls.

1. Introduction

With the growing number of metallization levels, thin film applications have become the main focus point for technologists. One of the most prominent techniques is the sputter deposition of Ti and TiN. With this method very thin layers of metallization can be produced. But, as device features shrink step coverage and film conformality become increasingly difficult. Currently, two methods are used to solve this problem: First, the deposition can be performed at high substrate temperatures; this technique is mostly applied to Al depositions. Second, a collimator can be used to decrease the spread of the incoming particle flux. In this work we focus on the effect of collimation.

A collimator is used when a temperature increase either does not improve the step coverage or is forbidden because of the impact on other properties of the device (such as concentration profiles or previous metallization levels). The collimator improves the bottom coverage of trenches or vias by removing particles with a high incoming incident angle (*beaming effect*) from the incoming particle flux [1]. However, those filtered particles are deposited on the collimator side-walls leading to a shrinking of the cell opening size. Thus, with increasing collimator lifetime, the total number of particles reaching the wafer surface decreases significantly and the beaming effect is enhanced.

For the simulations we used EVOLVE 4.0 [2] from Arizona State University, which was calibrated to the specific equipment used at National Semiconductor Corporation (M2000 from Varian). In parallel a graphical user interface (GUI) based on the VISTA-framework [3] from TU Vienna was developed.



Simulation Name

Simulation Name:

Initial Surface

Initial Geometry: [✓ Automatic] Load

Substrate Material: Silicon

Substrate Symmetry: Mirror [✓ Circular]

Feature Width: 1 um

Feature Height: 1 um

Feature Sidewall Angle: 90 degree

Feature Flatlength: 1 um

Simulation Termination

Simulate until: Thickness or Closure [✓ Thickness] Time

Desired Thickness: 100 Angstrom

Process Description

Processing: [✓ Ti] TiN W

Use Collimator: no

Process: CVD or Sticking Factor not 1

Deposition Conditions

Wafer Temperature: 400 degree C

Output Control

Screen output Level: steps only [✓ summary] track progress full

File output Level: steps only summary track progress [✓ full]

Simulator Specific Keys

Simulator Specific Keys Change

Figure 1: Graphical user interface for EVOLVE, based on VISTA.

2. Calibration of EVOLVE

For the calibration three vias with different aspect ratios were used at two different deposition temperatures for the collimated case as well as for the uncollimated case. These twelve experiments were conducted for both, Ti and TiN. It was found that for uncollimated deposition the main influencing factor were the sticking coefficients. They were determined to be 0.7 and 0.8 for Ti and TiN, respectively. Other factors such as temperature (250° - 400° C), gas flow rates (Ar 20 - 80 sccm, N_2 75 - 120) and the chamber pressure (0.02 - 20 mTorr) showed no impact on deposition rates in the given ranges. The deposition power was held constant (12 kW for Ti and 20 kW for TiN). For simulation purposes the incoming particle flux distribution was approximated by a generalized cosine function.

In the case of collimated deposition the same sticking factors were applied. But the assumption of a cosine distribution for the incoming particle flux can not be sustained. This distribution depends on the collimator lifetime, because of the increasing beaming effect. Thus, the collimator lifetime becomes the key factor for collimated deposition processes. To take this fact into account the deposited film thickness on the collimator sidewalls was computed using EVOLVE. A comparison at 491 kWh showed very good agreement: The simulated thickness was 1.4 mm, which was assumed to be constant along the collimator sidewall. The measurements showed values between 1.5 mm (at the entrance of the collimator) to 1.2 mm (at the exit of the collimator).

In our experiments we used a collimator with hexagonal cells. The ratio of the cell width to the cell height was 1:1. The information about the total thickness of the collimator cell's sidewall together with the geometrical information of the collimator was then used by a Monte Carlo based simulator [4] to determine the incoming particle flux on the wafer surface. The computed flux distribution was fed into EVOLVE.

3. The Graphical User Interface

EVOLVE was integrated into VISTA for two main reasons: First, a convenient GUI (see Fig. 1), which takes care of the automatic and correct generation of the required input file, could be developed easily, based on the capabilities of the framework. Second, in this environment time-consuming and tedious tasks such as the determination of the dependence of growth rates on the collimator lifetime could be performed conveniently by executing several runs in parallel on different workstations. In the future it can also be used to substitute other less accurate deposition simulations.

The development of the GUI was necessary, because the input format of EVOLVE is too complicated and the interdependences are too complex for the every-day usage of this simulator. Additionally, the interdependencies of the different parameters are crucial, but hard to obeye. All of the above is now taken care of by the GUI. The user selects the type of process to be simulated (e.g. Ti deposition) and the GUI will only allow the input of the appropriate parameters, automatically. Thus the user is reliefed from the tedious task of generating an input deck and can concentrate on the real, physical parameters.

4. Results

In Fig. 2 and Fig. 3 simulation results and comparisons to actual experiments are presented. Fig. 2 shows the result of a 1000 Å Ti deposition step without collimation in a 1.0 μm wide and 1.5 μm deep via. The input geometry was scanned in directly from the SEM photograph shown in the right half of the figure. Perfect agreement could be obtained.

In Fig. 3 results of a collimated TiN deposition are presented. The initial geometry was a 0.8 μm wide and 1.5 μm deep via on which 500 Å of TiN were deposited. As there is a notable difference in the deposition rate on the sidewall of the via compared to the deposition rate on the flat surface, the *kink* is formed. This kink is very important for the real process, because it can lead to a lack of film coverage at certain points. Thus, it's accurate modeling becomes a crucial issue for the simulation. Further investigations showed, that the formation and the appearance of the kink

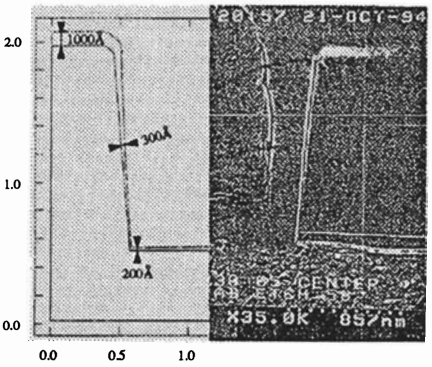


Figure 2: Uncollimated sputter deposition of Ti in a via.

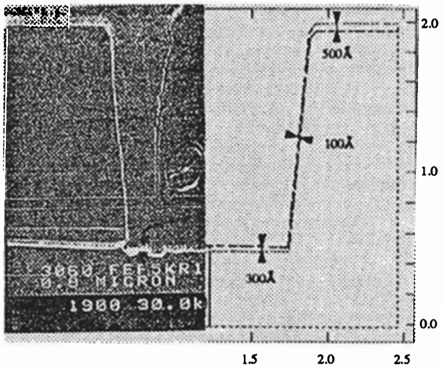


Figure 3: Collimated sputter deposition of TiN in a via.

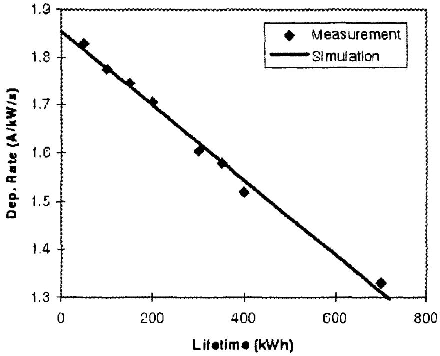


Figure 4: Deposition rate as a function of collimator lifetime for Ti.

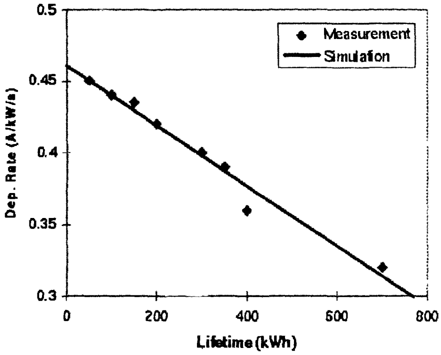


Figure 5: Deposition rate as a function of collimator lifetime for TiN.

strongly depend on the collimator lifetime: With increasing lifetime the kink becomes larger, which can be attributed to the growing beaming effect.

Fig. 4 and Fig. 5 show the deposition rates for Ti and TiN, respectively, as a function of the collimator lifetime. The correct prediction of this dependency is critical for process engineers: When the deposition rate falls below a certain limit the film conformality can not be guaranteed anymore; voids can occur in the deposited film. Thus, the collimator needs to be changed.

5. Conclusion

We have calibrated EVOLVE for sputter Ti and TiN processes. The only parameter that had to be calibrated was the sticking factor. For collimated deposition processes the dependence of the growth rates on the collimator lifetime can be predicted for both, Ti and TiN. The deposited film thickness on the collimator side-walls could be modeled correctly.

To allow easy input definition via a GUI and parallel execution EVOLVE was integrated in VISTA. Excellent agreement with measurements was found, and the kink formation for collimated TiN depositions - crucial for this process - can be predicted accurately.

References

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