Three-Dimensional Simulation of Conventional and Collimated Sputter Deposition of Ti Layers into High Aspect Ratio Contact Holes

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***Abstract* — Three-dimensional (3D) simulations of conventional and collimated sputter deposition of titanium into contact holes with high aspect ratios have been carried out using a 3D topography simulator. In this simulation program the device surface is discretized by a set of triangles. The layer growth rate for each triangle is determined by calculating the flux of metal atoms from the gas volume at the location of the triangle. Shadowing by the device structure itself as well as by a collimator placed between substrate and target is taken into account. For a range of contact hole aspect ratios, bottom coverage resulting from conventional and collimated sputter deposition has been predicted by means of 3D simulations. The simulation results were compared to experimental data and good agreement for both conventional and collimated sputter deposition was found.**

I. INTRODUCTION

With shrinking feature sizes and increasing aspect ratios of contact holes and vias to be filled during process sequences for the fabrication of multivlevel interconnections, it becomes more and more difficult to obtain contact hole metallization. In particular, the deposition of contact and barrier layers is critical in terms of the electrical poperties of the resulting contact. Simulation tools can help to investigate the influence of the contact geometry, the deposition equipment or the process parameters on the resulting layer profile. They therefore allow the optimization of processes to achieve the desired electrical behaviour of the contact.

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In this paper, we present three-dimensional (3D) simulations of both conventional and collimated sputter deposition of titanium (Ti) which, after rapid thermal nitridation (RTN), serves as barrier layer for subsequent contact hole filling by blanket tungsten chemical vapor deposition (CVD). The electrical properties of the contacts strongly depend on the Ti bottom coverage [1]. In consequence, the prediction of the bottom coverage by means of simulation is of high interest for optimizing the process. To validate our simulator, we compared the results to measurements of step coverage of layers deposited by both conventional and collimated sputtering into contact holes of different aspect ratios [1].

II. SIMULATION METHOD

The simulator we use for predicting the profiles of sputtered layers has originally been developed for the simulation of low-pressure chemical vapor deposition (LPCVD) processes [2], [3]. The basic concept of the simulator is a triangulation of the device surface combined with a particle redistribution model to calculate the layer growth rate for each surface triangle. The parameter which has to be specified for an LPCVD process is the so-called sticking coefficient which is the probability that a reactive molecule from the gas phase reacts after striking the surface. In the case of sputtering, a sticking coefficient of the metal atoms of 1 can be assumed which means that no desorption of metal atoms from the surface occurs. In consequence, the resulting layer shape is determined only by the geometry. For the simulation of conventional sputter deposition, we assumed an isotropic velocity distribution of the sputtered metal atoms in the gas volume above the substrate. The application of the LPCVD model with a sticking coefficient of 1 then leads to the corresponding layer profile. To model collimated sputter deposition, a square grid collimator which is placed between sputter target and substrate is assumed. The surface of the

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collimator is also described by a set of triangles which automatically leads to the more directional velocity distribution of the sputtered metal atoms above the substrate. It is then possible to investigate the influence of the collimator aspect ratio on the resulting bottom coverage of the deposited layer.

An example for a triangulated collimator is shown in Fig. 1. The aspect ratio of the collimator cells is 2. The lateral extension of the collimator necessary to accurately simulate a particular equipment setup (collimator aspect ratio, ratio of collimator height to the distance between substrate and collimator) is determined according to the maximum angle to the wafer normal a particle can have after passing the collimator and arriving at the device structure. Four additional triangulated walls framing the collimator are introduced to represent complete shadowing by the collimator for angles larger than this maximum angle. The number of triangles required to represent these walls is relatively small, thus the numerical effort required to solve the model equations is reduced. The dimensions of the collimator cells (typically 1 cm) are far larger than the device feature sizes. Therefore, shadowing effects due to the collimator do not vary over a microscopic feature such as a contact hole. However, the position of the device on the wafer has an influence on the angular characteristics of the metal atoms arriving at the structure. This has been investigated by shifting the collimator with respect to the device structure. The ratio of the collimator height to the distance between the collimator and the substrate can also be varied. For the simulations presented in this paper this ratio was set to 1. As simulations have shown, varying this ratio does not significantly change bottom coverage.

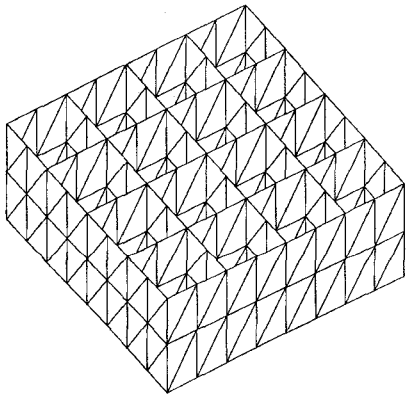

Fig. 1. Triangulated square-grid collimator. The cells of the collimator have an aspect ratio of 2.

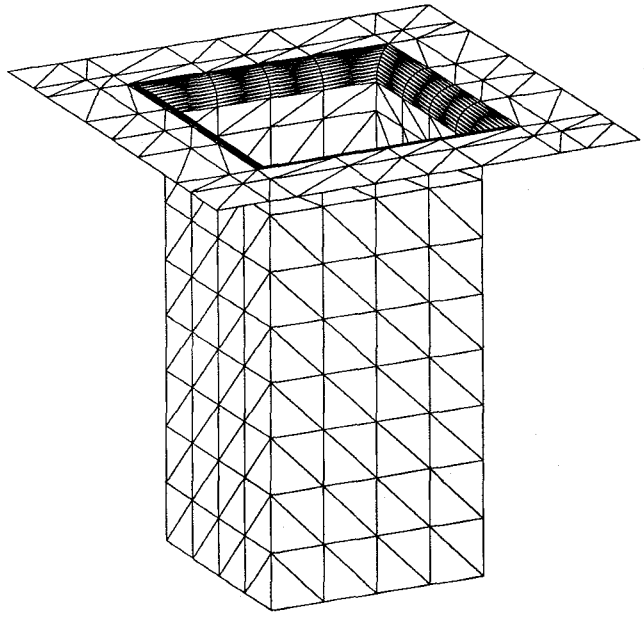

Fig. 2. Triangulation used for the discretization of a contact hole with an aspect ratio of 2.

III. SIMULATION RESULTS

We have carried out simulations of conventional and collimated sputter deposition of Ti layers with a layer thickness of 0.1 μm on the top part of the contact hole structure. A contact hole depth of 1.6 μm and different contact hole diameters were chosen. The triangulated surface of a contact hole with an aspect ratio of 2 is presented in Fig. 2. The number of triangles used is 768. Fig. 3 and Fig. 4 show the simulation results for conventional and collimated sputter deposition of a Ti barrier layer into a contact hole with a depth of 1.6 μm and a diameter of 0.6 μm. For the simulation of collimated sputter deposition, collimator cells with an aspect ratio of 2 were used. The bottom coverage is significantly improved by using a collimator whereas the sidewall coverage gets worse. Fig. 5 shows a comparison between the cross sections of the two simulations. For a range of different contact hole aspect ratios, simulations of conventional and collimated sputter deposition (collimator aspect ratio: 2) were carried out and compared to experimental data [1]. The result is shown in Fig. 6. Good agreement for both conventional and collimated deposition is achieved. The differences can be due to the experimental error when measuring the very thin layer thickness at the bottom of the contact hole.

Using simulations, it has been shown that the variations resulting from different positions of the device structure with respect to the collimator are also in this order of magnitude. The simulation results shown in Fig. 6 represent data obtained with the contact hole located exactly beneath the position where the walls of the square-grid collimator cross. Other positions result in reduced bottom coverage.

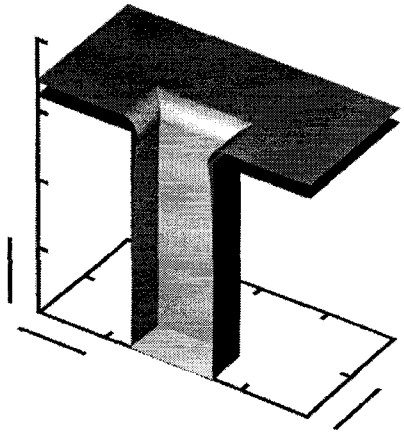

Fig. 3. 3D simulation of conventional sputter deposition of Ti. The bars represent 0.5 μm.

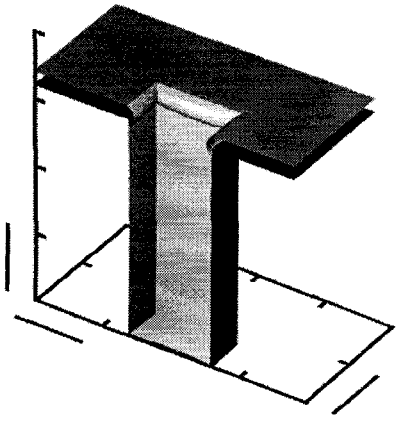

Fig. 4. 3D simulation of collimated sputter deposition of Ti. The bars represent 0.5 μm.

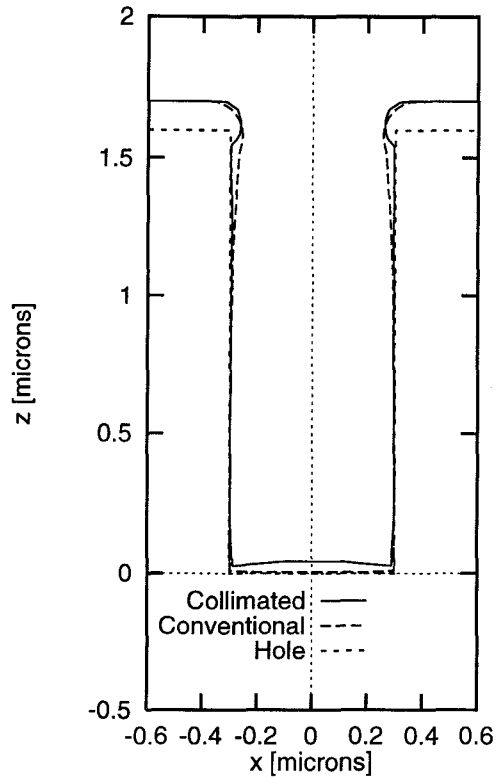

Fig. 5. Comparison between collimated and conventional sputter deposition of Ti into a contact hole.

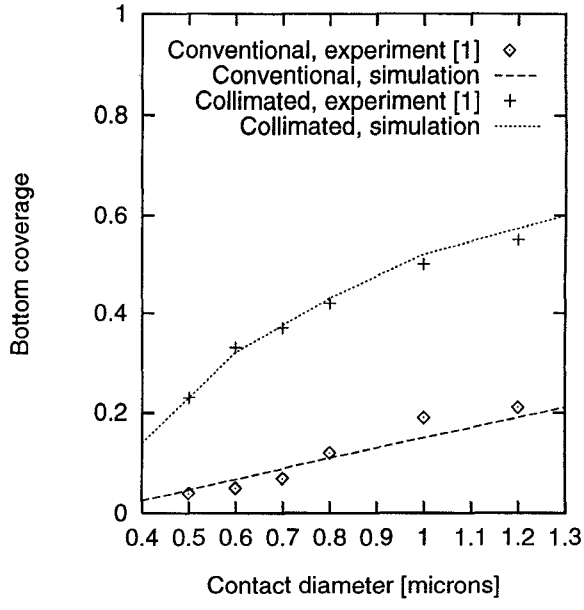

Fig. 6. Comparison between collimated and conventional sputter deposition of Ti for different contact hole diameters.

To fill the contact hole after deposition of the barrier layer, blanket tungsten CVD is used. If we assume that the tungsten is deposited by reducing tungsten hexafluoride (WF_6) by silane (SiH_4), the process can be simulated with a sticking coefficient of 0.04 [3]. The result of the simulation is presented in Fig. 7, showing both the barrier layer and the deposited tungsten. Due to its high aspect ratio, the contact hole is not completely filled with tungsten, i.e. a void remains.

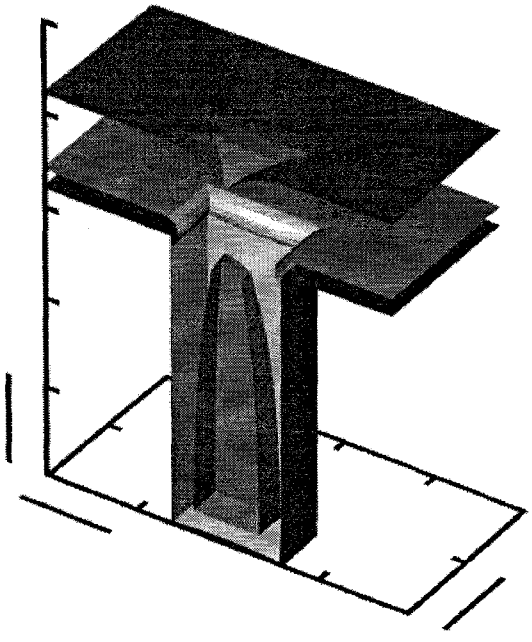

Fig. 7. Simulation of barrier layer deposition by collimated sputtering and subsequent blanket tungsten CVD into a contact hole. The bars represent 0.5 μm.

IV. CONCLUSIONS

We have presented 3D simulations of conventional and collimated sputter deposition of Ti layers into contact holes with different aspect ratios. For the model used, the only input required is the geometry of the contact hole and the collimator. There are no parameters that have to be adjusted. Good agreement between simulation and experimental data on step coverage in contact holes with different aspect ratios was obtained for conventional and collimated deposition. Thus, the simulator allows predictive simulation for other contact hole or via geometries and collimator aspect ratios to assess the capabilities of a particular sputtering process with regard to the resulting bottom coverage.

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