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Simulation of Sputter Deposition Process by DUPSIM

M. Seifert, F. Richter†, and R. G. Spallek

Institut für Grundlagen der Elektrotechnik/Elektronik, Fakultät Elektrotechnik,
Technische Universität Dresden
Mommsenstraße 13, D-01069 Dresden, GERMANY
†Fraunhofer-Institut für Mikroelektronische Schaltungen und Systeme 2
Grenzstraße 28, D-01109 Dresden, GERMANY

Abstract

A new deposition simulator is presented that allows modeling of sputter deposition processes. Various materials as well as several types of ring shaped magnetron sources can be considered. Some applications are presented to demonstrate the possibilities of the new program. It is part of the two-dimensional process simulator DUPSIM, which is able to simulate many fabrication processes of semiconductor devices in integrated circuits. Thereby a great flexibility and ease of use is reached.

1. Introduction

During the last several years, especially two-dimensional process simulators were developed which achieved a great propagation in simulating VLSI-structures in a realistic manner [1] [2]. The modeling of deposition and etching steps, by that time probably the least developed area of IC topography simulation, became an essential part of a complete process simulation.

Because of the trend in decreasing device sizes there is an increasing need to replace simple analytic models of deposition process simulation with more far reaching solutions to investigate the typically metallization effects (see below) of submicrometre designed structures [3]. The results obtained with appropriated simulators can also be used to solve e.g. current and temperature distributions in the deposited layer [4].

This paper includes a possibility of simulating the sputter deposition process of magnetron diodes. There are no restrictions in geometry of the substrate, so every process during IC fabrication can be considered. The second part shows some applications to demonstrate the possibilities of the program by comparing calculated deposition profiles with experimentally obtained results.[8].

2. Modeling of Deposition Source

The distribution function of the oncoming vapor flux is calculated using a method described in [5] which we especially adjusted to magnetron sputtering planar diodes. Following assumptions for this model are necessary and meaningful:

1. The mean free path of atoms is large compared to the distance between target and substrate [5].
2. The sticking coefficient is assumed to be 1, i.e. there is no resputtering rate [5].
3. The direction distribution of the emitted atoms on target level is given by

$$f(\alpha) = 1/\pi \cos \alpha \tag{1}$$

4. The density of deposited layer is equal to the target material density.
5. Deposition source has a ring shaped target located parallel to the substrate (other target shapes in preparation).
6. Substrate structure is infinitely extended into the third Dimension, i.e. two-dimensional simulation.

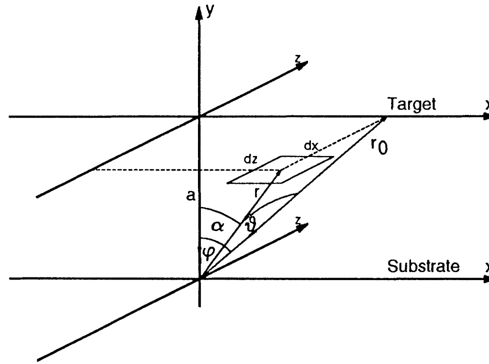

Figure 1: Main Sputter Geometry

A possibility to describe the atomic flux in the three-dimensional main geometric schema shown in (Fig. 1) is:

$$\vec{di} = dxdz\ f(\varphi, \vartheta)\ h(x, z)\ \cos\vartheta\ d\varphi d\vartheta \tag{2}$$

Here φ and ϑ represent direction α in (1) and $h(x, z)$ is given as a function modeling the target surface influenced by sputter eroding (see below).

The atomic flux density which is required to calculate the growth at a substrate point is defined as the atomic flow per an area unit (assumption 1)

$$dA = r_0 d\varphi = r^2 \cos\vartheta\ d\varphi d\vartheta \tag{3}$$

(see Fig. 1) as follows

$$\vec{dj} = \frac{dxdz\ f(\varphi, \vartheta)\ h(x, z)}{r^2} \tag{4}$$

At this point a simplification is appropriated to limit computational expenditure. Instead of flux density $\vec{dj}$ (4) the component lying in the x-y plane

$$dj_{xy} = \int \cos\vartheta\ \vec{dj} = dx \int_{-\infty}^{+\infty} \frac{f(\varphi, \vartheta)\ h(x, z)\ \cos\vartheta}{r^2}\ dz = dx\ V(\varphi) \tag{5}$$

is calculated. That means simulation is exact only on structures infinitely extended into z-direction (assumption 6). With some geometric relations (see Fig. 1) and (1) the distribution function $V(\varphi)$ finally is presentable as

$$V(\varphi) = \frac{\cos\varphi}{\pi r_0^2} \int_{-\infty}^{+\infty} \frac{h(a \tan\varphi, z)}{1 + z^2/r_0^2} \, dz \tag{6}$$

After numerical solution of this expression it is possible to calculate the layer growth as described in the following section. The process parameters at this step are the distance between target and substrate, the position of substrate towards deposition source and the measures of the used up target. If needed, a special routine hereby simulates the moving substrate on circular multi-wafer plants.

3. Numerical Model of Deposition

DUPSIM uses the wide-spread string algorithm to describe the surface of layers and their movement in case of two-dimensional simulation . The total layer thickness D is defined as follows

$$D = r \int_{x_1}^{x_2} (\vec{e}, \vec{dj}_{xz}) \tag{7}$$

where $\vec{e}$ is a unit vector located perpendicular to the wafer surface. To obtain the layer growth it is necessary to solve the expression (7) numerically for each node in both directions. In the algorithm there is involved a calculation of the limits x_1 and x_2 which are determined by the effect of shadowing. The quantified deposition rate r is determined either by the user or (as an estimation) by a special tool which includes the parameters discharge current and sputtering yield (specified by measurement).

In order to balance numerical problems such as loops, needles etc. which occurred during deposition algorithm a special interface to the layer system of DUPSIM was provided in which node management and layer handling algorithms are implemented.

4. Software Aspects

DUPSIM is a modular software system which was developed at the TU Dresden in cooperation with industrial partners. It consists of an input interpreter, several processing units [6], a graphic output package [7] and an interface to device simulation programs. The system is running on DEC-VAX computers, SUN sparc-stations and HP-Apollo workstations.

The sputter deposition program is integrated in a collection of numerical deposition models within the simulator. It is written in FORTRAN 77 in view of great portability to several computers.

5. Applications

To examine the practical possibilities of the simulator we compared simulation results with a series of deposition experiments performed on several machines. Fig. 2 shows an in z-direction infinitely extended structure with the appropriated simulation results. According to assumption 6 there is nearly exact agreement between simulation and reality to be found.

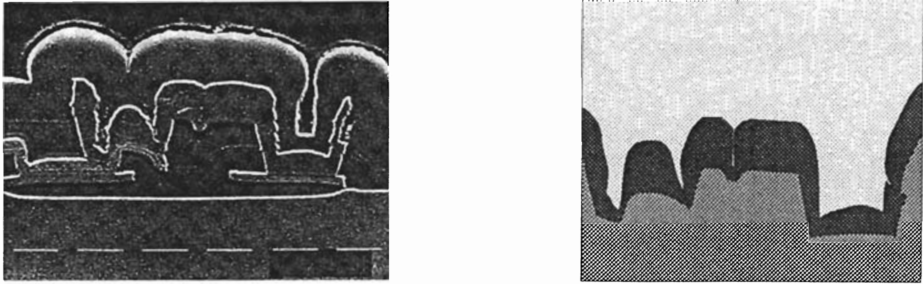

Figure 2: Infinitely Extended Structure

Figure 3: Via Contact

The above mentioned cracks e.g. appear in complicated structures like via-contacts as shown in Fig. 3.
Because of the reached agreement between calculation and experiment the effect of crack development approximately can be considered as a consequence of shadowing and directional dependence of the oncoming vapor stream in case of magnetron sputtering metallization.

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