THREE-DIMENSIONAL MODELS AND ALGORITHMS FOR WAFER TOPOGRAPHY EVALUATION

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Accurate simulation of topography processes increasingly requires three-dimensional models and algorithms for wafer topography evaluation. In this paper a new fundamental method for general three-dimensional surface advancement is presented and coupled with physical process models for etching and deposition.

The algorithm for surface movement is based on morphological operations derived from image processing which provide a well defined method for altering a given image with respect to some predetermined geometric shape known as *structuring element* [1]. The basic idea behind the surface evolution algorithm is to consider the simulation geometry as a black and white image and to relate the spatial dimensions of the structuring element at a surface point to a precalculated etch or deposition rate [2]. The material is represented using an array of square or cubic cells, where each cell is characterized as etched or unetched. Additionally, a material identifier is defined for each cell, therefore material boundaries need not be explicitly described. To advance the surface a position dependent structuring element is applied for the exposed cells as shown in Fig. 1. Depending on the simulated process either material cells are removed or added which are located within the structuring element. Usually, for anisotropic three-dimensional surface advancement structuring elements are ellipsoids, for isotropic movement of surface points structuring elements are spheres. The material surface is finally described by the exposed sides of material cells that are in contact with vacuum cells.

To determine the rate contributions of incoming particles both in etching and deposition the simulator must be capable to calculate the resulting particle flux incident at a surface point. Therefore the region above the wafer is divided into several patches, and the incident flux is then integrated over those patches of the "sky" which are visible from the surface point as shown in Fig. 2. To determine if a patch is visible from a point on the surface a shadow test has to be performed along a given direction which is within the cellular material structure simply the matter of following a discretized line of cells from the surface cell to the boundary of the simulation area. If any cell on this line is a material cell, then the surface cell is shadowed. As a basic concept for modeling etching processes we consider a linear combination of isotropic and anisotropic reactions of directly and indirectly incident particles to calculate the resulting velocity vector of a surface point. The isotropic reaction is mainly a chemical reaction affected by a reactive gas, in which the reactive particles have short mean free paths and move randomly. The etch rate has no orientation or flux dependencies and is described as a constant. The anisotropic reaction is a physical or chemical reaction, where the particles have long mean free paths compared to the device dimensions and angular particle fluxes must be considered. Rate contributions from directly incident ions, directly incident neutral particles, and from reflected particles are taken into account to calculate the resulting etch rate of a surface point. Deposition modeling is based on the original work of Blech who developed a model for describing two-dimensional profiles of evaporated thin films over steps [3]. This model is directly applicable to three-dimensional simulation. The growth vector of a surface point can be calculated by considering the angular flux distribution of incoming particles at a surface point. Different assumptions on the flux distribution function result in evaporation or sputter deposition processes.

Fig. 3 shows chemical etching caused by reactive neutrals leading to a poor anisotropy of the etched trench. The flux distribution of incoming neutral particles is described by a hypercosine function. High anisotropy is achieved if reactive sputter etching is applied as shown in Fig. 4, where etching due to physical momentum transfer predominates the surface reaction. The flux distribution of incident ions is described by a Gaussian distribution with a very narrow standard deviation. Fig. 5 shows the typical barreling phenomenon in reactive ion etching due to high energetic ions that increase the etch rate where they hit the surface (mainly at the bottom of the trench) and due to reactive neutral particles which also attack the sidewalls. The picture also shows the well known aperture effect (etch rate decreasing due to limited delivery of ions and radicals) resulting in a deeper trench where the mask size opening is larger. Patterning and metallization of a contact hole are shown in Fig. 6. Subsequently, isotropic and directional etching followed sputter deposition with a cosine based flux distribution was simulated to study the step coverage of the contact hole metallization.

REFERENCES

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[2] E. Strasser et al., IEICE Transactions on Electronics, Vol. E77-C, pp. 92-97, 1994.
[3] I.A. Blech, Thin Solid Films, Vol. 6, pp. 113-118, 1970.

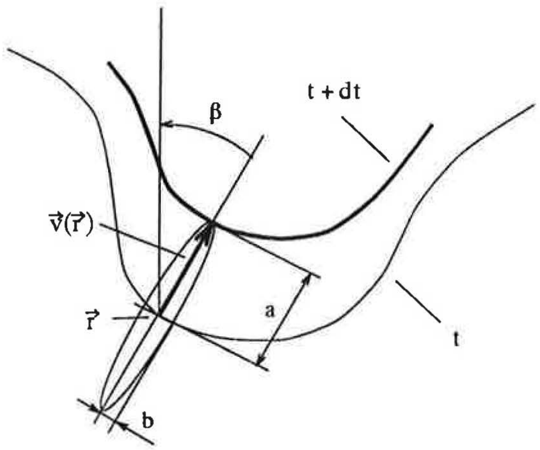

Figure 1: The structuring element for surface advancement.

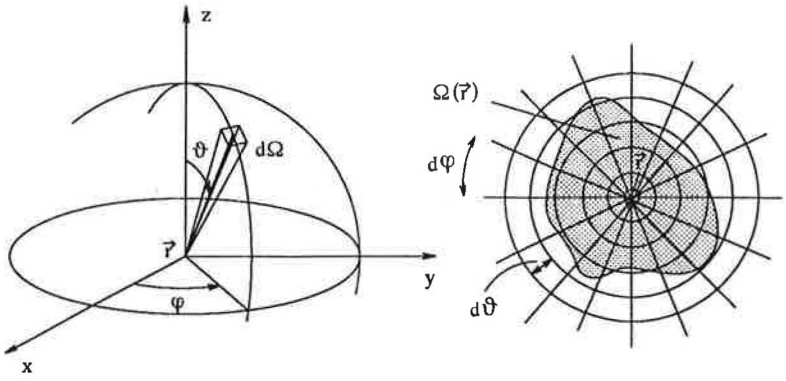

Figure 2: Efficient visibility calculation.

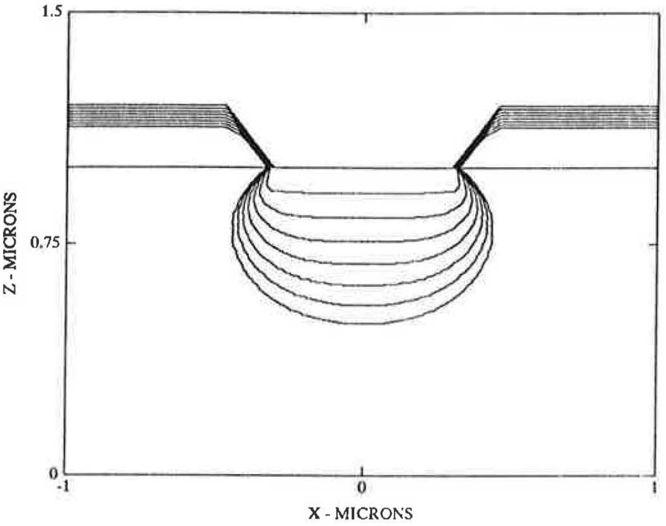

Figure 3: Chemical etching caused by reactive neutrals.

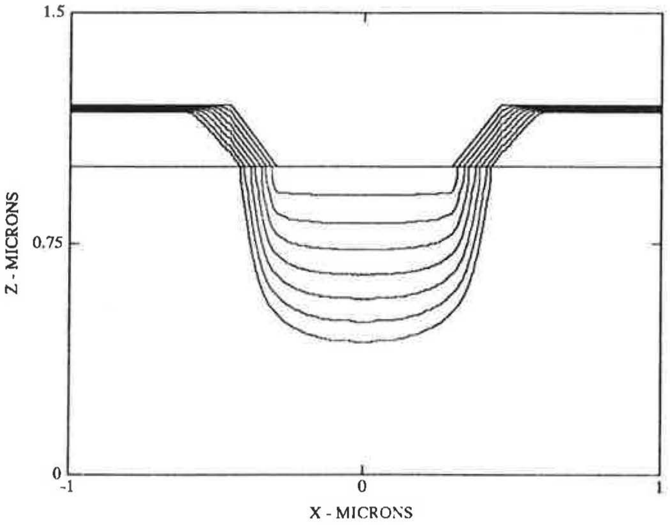

Figure 4: Reactive sputter etching.

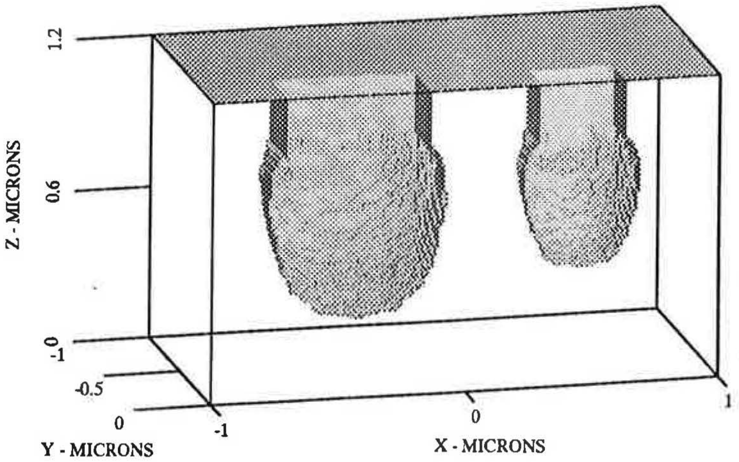

Figure 5: Reactive ion etching.

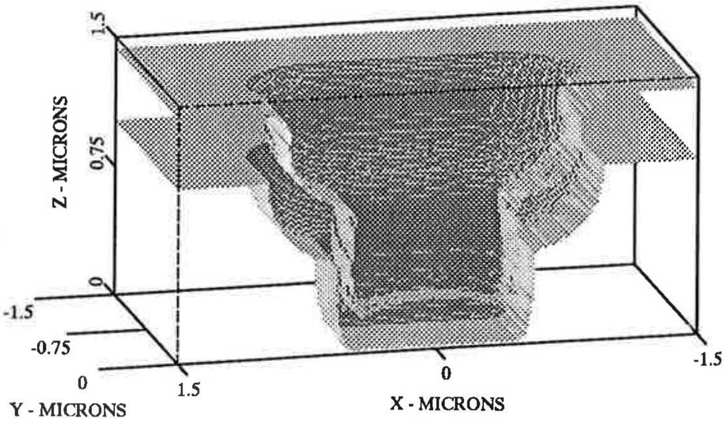

Figure 6: Patterning and metallization of a contact hole.