Integrated simulation of topography evolution during plasma etching of micro- and nano-structures

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PhD Thesis abstract

The technology used for the fabrication of microelectronics devices and micro-electro-mechanical systems (MEMS) is based on the successive deposition or growth of planar layers and the subsequent transfer of the desired pattern onto these layers. Lithography and plasma or wet etching are the essential steps of this technology.

Profile control of the etched structures is necessary for the efficient operation of the corresponding microelectronics devices and MEMS. The loss of microscopic uniformity (e.g reactive ion etching lag) and deviations from the perfectly anisotropic profiles of the structures (e.g. microtrenching, sidewall bowing, roughness) are etching artifacts that make the profile control difficult. There is a need to understand the mechanisms causing these artifacts and suppress them. Besides experimental study, topography evolution simulation of the etched structures can contribute to this direction.

The goal of this work is the development of an integrated simulation framework for the topography evolution of structures etched with plasma. This framework links the bulk plasma gas phase with the profile of the etched structure and consists of:

1) A local flux calculation model. Shadowing and reemission of flux are taken into account. This model links the species fluxes in the bulk plasma gas phase with the local species fluxes inside features.

2) A surface etch model. This model includes the processes during the etching of SiO_2 and Si surface with fluorocarbon plasma. The surface model is a phenomenological model that takes into account the competitive phenomena of etching and deposition occurring during etching with fluorocarbon plasma. The model is based on site balances on the etched surface and links the species local fluxes with the local etching rate.

3) An algorithm for the topography evolution of the etched features. The level set method is implemented. The algorithm uses the local etching rate to move the topography of the etched structures.

The third component of the simulation framework, the topography evolution algorithm, is a general boundary evolution algorithm, which can be applied in several areas, such as the evolution of an interface between two fluids in fluid mechanics. The coupling of the first two models of the simulation framework [components (1) and (2)] that yields the local etching rate, defines the boundary evolution problem that the boundary evolution algorithm, namely the level set method, solves.

The main points of this work are summarized below (in the order that appear in the text):

A) The equations for the calculation of local fluxes of neutral species inside long trenches and holes with cylindrical symmetry are formulated. Several methods are used for the solution of the respective numerical problem, which is a Fredholm integral equation of the second kind. The singularity of the kernel of the integral equation is resolved. Comparative results for the local flux inside trenches and holes are presented.

B) An original surface model for the etching of SiO_2 and Si with fluorocarbon plasmas is developed.

C) An algorithm for the coupling between the local flux calculation model and the surface etch model is formulated. The central point of this coupling is the simultaneous calculation of the species local fluxes and effective sticking coefficients. The respective numerical problem is the solution of a system of nonlinear integral equations.

D) The following computational tasks included in the level set method implementation are addressed in detail and resolved: i) The solution of the level set equation, ii) the solution of the Eikonal equation, iii) the calculation of zero contour of the level set function (or generally the calculation of the contours of a function) and iv) the extension or the extrapolation of the velocity of the moving boundary away from the moving boundary. Several discretization schemes in space and time are applied for the solution of the level set equation. Some of these schemes are used for the first time in boundary evolution problems. It is ascertained that the error due to space discretization is more important than the error due to time discretization. Three different methods are used for the solution of the Eikonal equation. The fast marching method, which solves the nonlinear boundary value problem described by the Eikonal equation directly (without an iterative procedure), is the fastest. The formulated algorithm for the calculation of the zero contour of the level set function is based on the calculation of the normal vector to this contour. The respective computational task is the solution of a system of nonlinear ordinary differential equations, which is solved with explicit Runge-Kutta pairs of high orders. In all numerical tasks included in the implementation of the level set method, the need of using high order numerical schemes is investigated.

E) The simulation framework is applied in SiO_2 feature etching with fluorocarbon plasmas. The problems of microscopic uniformity loss [e.g. reactive ion etching lag (RIE lag), inverse RIE lag] are predicted and explained from first principles and without fitted parameters. Feature etching maps that link the bulk plasma gas phase with the problems of microscopic uniformity loss are constructed. The simulation framework is also applied to the multiple step, deep Si etch process (Bosch process). The level set method is used for the first time for the topography evolution simulation of the Bosch process. It is shown that the simulation framework can be used for the simulation and prediction of other problems during feature etching such as i) microtrenching and ii) surface roughness. Finally, the flexibility of the simulation framework is accentuated through its application to processes such as i) deposition and ii) photoresist development during lithography.

F) The code verification for every numerical calculation of the simulation framework is accomplished through the method of manufactured solutions.

G) The simulation framework is an important substratum, as its future user can focus on the application rather than on the numerical calculations and the simulation methods.