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Modeling of Integrated Lateral Capacitor Sensors

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Abstract

The behaviour of integrated silicon moisture sensors based on novel capacitor strucures has been accurately modeled. The sensors conform to a standard CMOS process with one postprocessing step, namely the deposition of thin film dielectrics. Because of the insufficiency of parallel-plate capacity estimates the electric behaviour of the sensor using a quasi-harmonic elliptic PDE for the electric potential in three dimensions has been modeled. For this purpose the finite element program SESES has been employed. The latter was specially developed by us for the study and optimisation of integrated semiconductor sensors. Variations in the sensor device geometry (interdigitated and spiral capacitors), as well as variations in the dielectric materials employed (air, polyimides, oxide, nitride) have been studied, and some general design rules have been derived. Further, the results of sensitivity as a function of the capacitor geometry, dielectric materials and their positioning and thicknesses, as well as variations of the dielectric constant in the material are presented.
Our work is applicable to all kinds of capcaitive sensors where a change in dielectric permittivity occurs.

Introduction

A simple parallel plate model does not provide a correct description of the complex capacitor geometry of the kind shown in Figs. 1 and 2, since it overestimates the true sensitivity ($S=\Delta C/C$, i.e. the relative change in capacitance) in an intolerable way. Therefore accurate 3D computations to predict exact values of S as a function of geometry factors, such as the width, spacing and height of the electrodes as well as the dielectric film thickness, are used. Interdigitated structures (Fig.1) are compared with alternative electrode configurations like the one in Fig.2, with regard to sensitivity as a function of geometry and film thickness. Permittivity gradients inside the film can easily be taken into account.

Sensor description

Standard IC technologies allow the manufacturing of capacitive sensor structures to be immersed in a suitable medium, which in the case of chemical sensors can be liquids or gases. The sensor structures considered here consist of aluminum or polysilicon electrodes on a silicon substrate, covered by a dielectric film. In most applications interdigitated microelectrodes are used similar to the one shown in Fig.1. These lateral sensors consist of two interdigitated comb-like structures. One of these electrodes is usually grounded whereas the other is maintained at a potential of typically 1V. Alternative electrode configurations like spirals (Fig.2) are simulated and compared with the interdigitated ones. Since our research is focused on moisture sensors, the dielectric films are assumed to be polyimides (PI's).

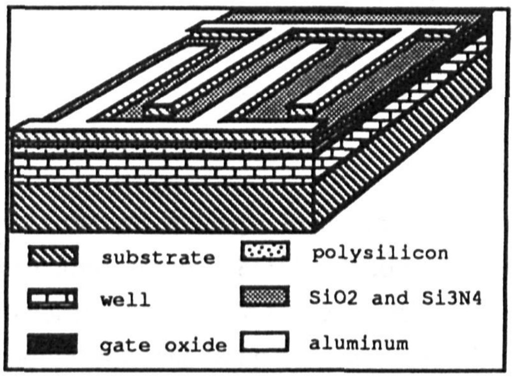

Fig.1 Schematic of interdigitated structure.

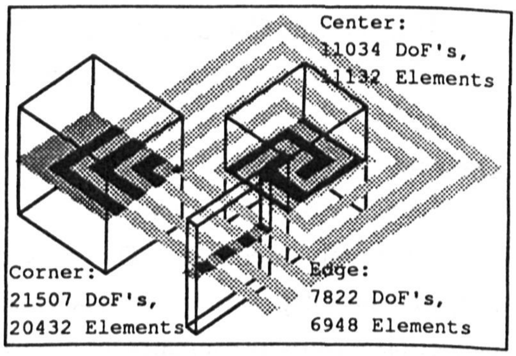

Fig.2 Schematic of spiral structure.

Properties of the polyimide

In our experiments we used a pre-imidized, planarizing and negatively photosensitive as well as humidity-sensitive polyimide (PI). The PI's photosensitivity reduces the number of post-processing steps, since standard lithography and etching techniques are not required for pattern definition. In Fig.3 a SEM photo of the spin coated PI film is shown. A detailed description of the experiments can be found in [1]. The PI has a linear uptake by weight of 5.6% at 100% RH, which is also nearly independent of temperature. Experimental investigations of humidity absorption yield relative permittivity variations between 3.2 and 4.0 corresponding to a change in relative humidity RH between 0 and 100% for frequencies up to 10 MHz. Fig.4. shows a typical hysteresis curve (2.5%) for a 4μm PI layer. The diffusion constant is large which implies response times of the order of seconds.

The PI film, as a first approximation, is thought to completely fill out the space between the electrodes and to be smooth at its surface. Quantitative estimates for the deviation from this assumption will be made below.

The Modeling problem

The electric behaviour of a capacitor with isotropic, 'simple' dielectrics can be modelled by the quasi-harmonic equation in terms of the electric potential Ψ:

$$\mathrm{div}(\varepsilon(x,y,z)\ \mathrm{grad}\ \psi) = \rho(x,y,z)$$

The electrical permittivity, $\varepsilon(x,y,z)$, is a function of the spatial coordinates, as is the space charge density, $\rho(x,y,z)$, which may occur in the dielectricum. Three types of boundary conditions occur: *Dirichlet contacts* - metalised surfaces where the electric potential is prescribed; *Floating contacts* - where the electric potential is contant (due to metallisation of the surface), but where the electric potential adjusts to a value based on the solution elsewhere in the dielectricum; *Homogenous Neumann boundaries* - symmetry planes and insulated surfaces, where the electric field is parallel to the surface. The equation system is discretised for a specific problem geometry using the finite element method [2] and the resulting system of linear equations are solved for the electric potential. Postprocessing steps involve computing the electric field and the charges on the metal contacts from the solution for the electric potential. The capacitance is determined from the charge and the applied voltage [3].

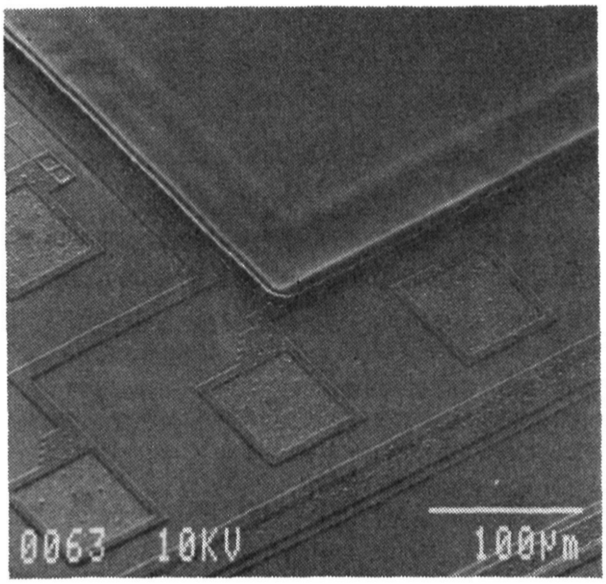

Fig.3 SEM photo of spin coated PI film.

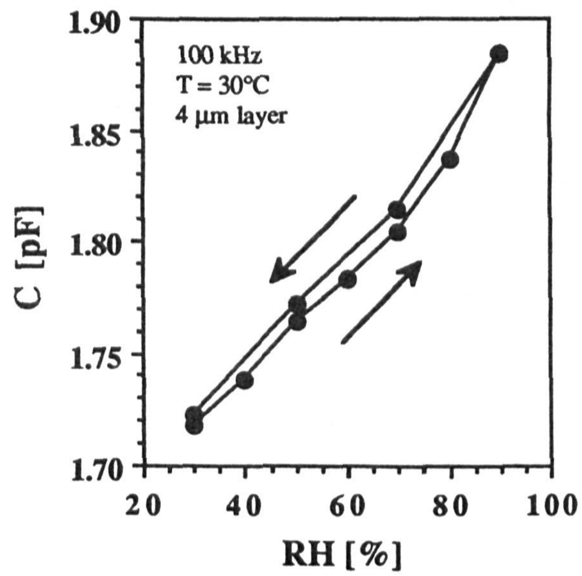

Fig.4 Hysteresis curve.

The new finite element program system SESES has been developed specifically to model problems where the geometry is strongly 'integrated-device' oriented, and the physics of interest employs not only the standard semiconductor device equations, but also some of the coupled effects that are common in sensor devices. The devices were modelled with around 5,000 - 50,000 discrete points in space, placed optimally with the mesh refinement algorithms of SESES. We also used FLOWERS, which is based on the isoparametric Finite Element Method and fulfills the same purpose as SESES, but is less geared towards device design and optimisation.

As a post-processing step, the sensitivity S was computed as:

$$S = 2*(Cwet-Cdry) / (Cwet+Cdry)$$

Dry and wet refer to simulations with 0% resp. 100% humidity.

Modeling the spiral device

The dimensions and shape of the sensor prevents a simulation with only one mesh. Details of the sensor show micro device feature sizes (~μm), whereas the whole sensor has macro overall dimensions (~0.1 mm). There are no simple symmetries as in [3], where the numerous symmetry planes allow for the reduction of the simulation to a sub-section, a method also used for the interdigitated sensor described in this paper. Hence an asymptotic study was undertaken on three regions: an edge, a corner and a center region (Fig 2). The simulation region was progressively enlarged towards the middle of the sensor, each time adding one contact. The charge densities on the contacts were compared for each simulation and found to change insignificantly, beyond a certain number of contacts (Fig. 8). The charge density on the contacts showed an interesting variation from the edge towards the center, indicating that at least five edge contacts must be treated separately; edge effects are important. For the center region, only 3.5 spirals were needed to contain the changes brought about by the irregularity there. The meshes were adaptively refined (according to the gradient of the electric potential) until the charge densities on the contacts were no longer varying as a function of the mesh size.

Once the meshes were established, the bulk of the simulations were performed. The charge on a contact was assembled from the part contributions of each simulation, by a weighted sum of the charge densities (center charge, charge per edge length and charge per corner element).

Results

Interdigitated and Spiral:

In order to optimise the sensitivity S, the dependence on geometry and film thickness are studied. Fig.5 shows that, for a particular geometry, S can be enhanced by increasing the thickness T of the film on top of the structure until a certain saturation value is reached. In the example considered, no additional improvement of S is to be expected if the film thickness T exceeds 6 μm. Since the absorption of humdity in PI is a volume effect [4], although not a homogeneous one, a further increase of T would only cause a larger diffusion-time and therefore a larger response-time of the sensor. The results for S as a function of electrode width W, electrode-electrode spacing D and electrode height H are plotted for some typical values in Fig.6. Decreasing both W and D leads to larger sensitivities (arrows 1 & 2). As expected from basic considerations, additional increase of S will be achieved by raising H (arrow 3). In the limit of lage H, the sensitivity S approaches the (ideal) parallel plate value of 22%. Two basic limitations prevent us from attempting this theoretical limit: The PI has to completely fill out the space between the electrodes and, in addition, the water has to penetrate the space between the electrodes.

The following design rules are implied from the simulations:

Rule 1: For maximum sensitivity S with a given technology, the sensor has to be designed with the smallest values for D and W that are compatible with that technology.

Rule 2: By simultaneously increasing H and W a particular value for S can be maintained. In this way we can select a value for H and D which guarantees a correct filling of the interelectrode spacing. This leads to an increased value of the resulting absolute capacitance.

We also investigated the influence of an uneven distribution of the polyimide. In the case where the polyimide fills only 30% of the space between the electrodes, the sensitivity loss is 35% (up to 50 % as the fill decreases to zero). A corresponding reduction of the absolute capacitance value (up to 25%) is observed.

As the direct contact of the aluminum electrodes with moisture causes oxidation of the aluminum, we simulated the influence of a protective passivation layer (0.5 µm Si_3N_4 and 0.5 µm SiO_2) between the top electrodes and the polyimide. S diminished by a factor of up to 90%. Therefore the passivation must be kept as thin as possible and should not fill the space between the capacitor electrodes in order to avoid too large a loss in sensitivity.

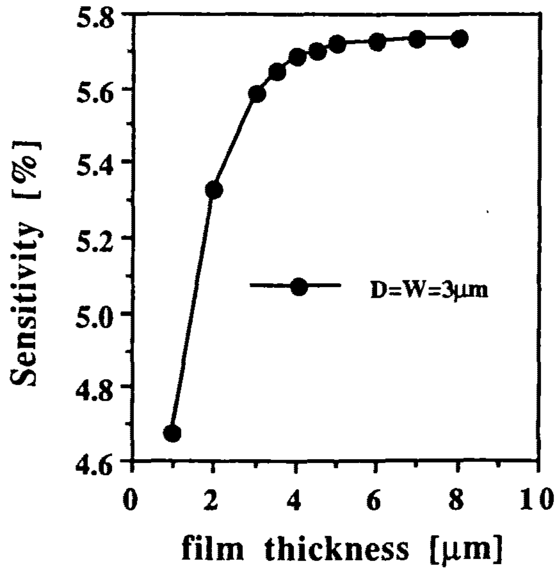

Fig.5 Sensitivity S vs film thickness T.

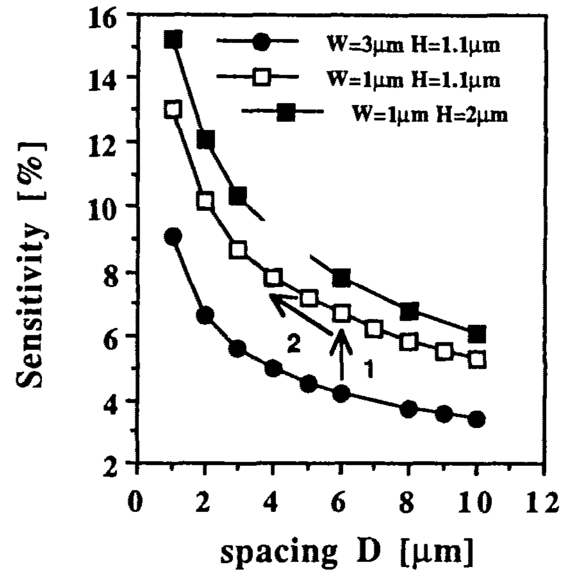

Fig.6 Sensitivity S vs electrode spacing D for the interdigitated structure.

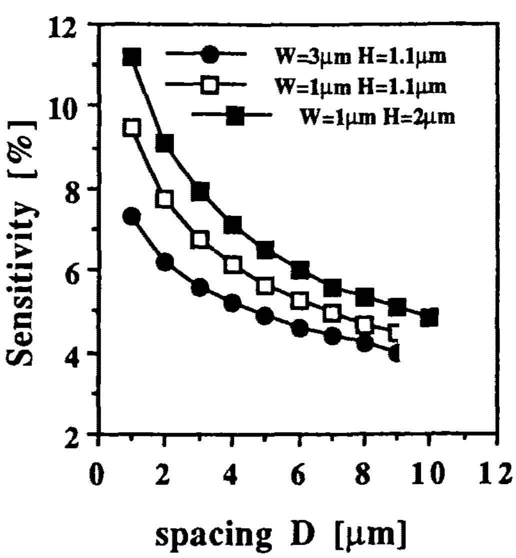

Fig.7 Sensitivity S vs electrode spacing D for the spiral structure

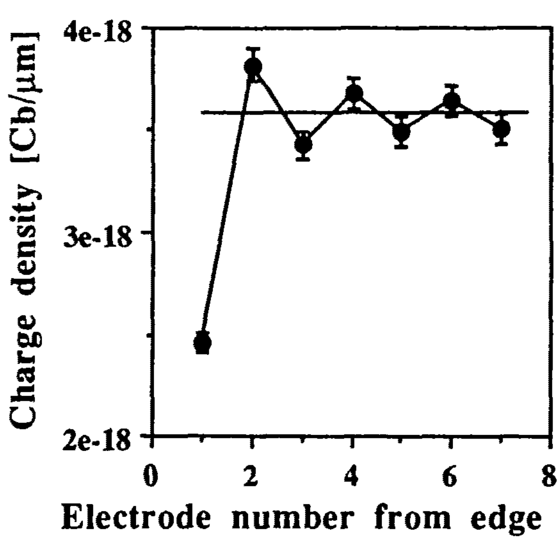

Fig.8 The edge effect for the spiral structure.

References

[1] T. Boltshauser and H. Baltes, Capacitive Humidity Sensors in SACMOS Technology with Moisture Absorbing Photosensitive Polyimide, Sensors and Actuators, A 25 - 27 (1991), 509-512.

[2] Zienkiewicz, O.C.: The Finite Element Method, London, Mc Graw-Hill 1977.

[3] L. Chandran, J.G.Korvink and H. Baltes, Three-Dimensional Modeling of Capacitive Humidity Sensors, Sensors and Actuators, A 25 - 27 (1991), 243-247.

[4] Gu Xu, C. C. Gryte, A. S. Nowick, S. Z. Li, Y. S. Pak, and S. G. Greenbaum, Dielectric Relaxation and Deuteron NMR of Water in Polyimide Films, Journal Appl. Phys., in press.