Analysis of Piezoresistive Effects in Silicon Structures Using Multidimensional Process and Device Simulation

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Abstract

With the view to analyzing piezoresistive effects in silicon microstructures we implemented a rigorous physically-based model in the multidimensional general purpose device simulator DESSIS^{ISE}. In this model, the dependence of the piezoresistive coefficients on temperature and doping concentration is included in a numerically tractable way. Using a commercial TCAD system (ISE), the practicability of the approach is demonstrated by performing a complete simulation sequence for realistic microdevices ranging from the layout design up to the analysis of the device operation.

1. Introduction

Mechanical distortion of silicon microstructures results in a change in the electric conductivity. In modern semiconductor technology this effect is employed in realizing smart integrated micromechanical sensors. On the other hand, piezoresistivity arises as undesired parasitic effect in silicon devices due to mechanical stress induced by thermal treatment or packaging. Up to now, a predictive numerical analysis of the performance of piezoresistive elements integrated in semiconductor microdevices was restricted to idealized structures with simplified geometry, assuming spatially uniform piezoresistive coefficients along high-symmetric crystal orientations without local dependence on the doping concentration or temperature distribution. Of course, with these quite coarse approximations a quantitative analysis of realistic devices is hardly possible. For accurate results a full multidimensional numerical simulation is required, which is based on a coupled field description of the piezoresistive effects. A reliable numerical approach is demonstrated in this work.

2. Modelling

A rigorous physically-based model [1] describing the strain-induced changes in the electric conductivity of single-crystalline silicon has been implemented in the multidimensional general purpose device simulator DESSIS^{ISE} [2]. The basic part of the model is a linear extension of the constitutive current relations for electrons and holes,

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$$\mathbf{J}_{\alpha} = -\sigma_{\alpha} \cdot \left(\mathbf{\tilde{l}} + \mathbf{\tilde{\Pi}}_{\alpha} \cdot \mathbf{\tilde{X}}\right) \cdot \mathbf{\nabla} \boldsymbol{\varphi}_{\alpha} , \quad (\alpha = \mathbf{n}, \mathbf{p})$$

where σ_{α} denotes the isotropic electric conductivity in the absence of stress, \tilde{I} the identity tensor, \tilde{X} the mechanical stress tensor, φ_{α} the quasi-Fermi potential and Π_{α} the tensor of piezoresistive coefficients which depend on the doping concentration and the temperature distribution.



The implemented model was validated with reference to experimental piezoresistive coefficients measured in diffused n- and p-type silicon layers [3]. As shown in Fig. 1 for the shear coefficient Π_{44} in p-silicon, for instance, we achieved good agreement between simulation and measurement of the test structures.

3. Simulation of integrated silicon piezoresistive sensors

The capabilities of the interfaced simulation system were demonstrated by a complete simulation sequence ranging from layout and process simulation up to piezoresistive device simulation. Two realistic microtransducer structures fabricated by means of industrial silicon IC technology were investigated. Each of them is basically a square silicon diaphragm $(10x1000x1000 \ \mu m^3)$ with integrated piezoresistors connected in a Wheatstone bridge. The first structure represents the conventional layout of a pressure sensor (Fig. 2) as proposed in [4]. The second device (Fig. 3) is an electrothermally excited microresonator with piezoresistive readout, which is used as test structure for determining thermoelastic material properties. The four piezoresistors of the Wheatstone bridge probe the thermoelastic deformations caused by a heating resistor placed at the diaphragm centre. Obviously the two structures are similar with respect to the mechanical behavior, but differ in the arrangement of the piezoresistors.





Fig. 2: Top view of a sensor structure for pressure measurement [4] (lengths in μ m).

Fig. 3: Top view of a microresonator structure with piezoresistive readout (lengths in µm).

For easy comparison of the respective sensitivities, we assumed equal technological and gcometrical parameters for both structures (namely those measured on the microresonator). The piezoresistors were fabricated using a boron implantation with subsequent drive-in diffusion. The maximum doping concentration amounts to $2x10^{18}$ cm⁻³ and is located at a depth of about 0.6 µm. In our simulations we assumed that a pressure difference $\Delta p = p_1 - p_0$ between top and bottom side of the diaphragm caused the mechanical deformation (cf. Fig. 4).





The sequence of simulation steps is shown in Fig. 5. Using the two-dimensional technology simulator DIOS^{ISE} [5] all fabrication steps of the diaphragm and the piezoresistors can be simulated, yielding their doping profile.



Fig. 5: Schematic simulation sequence and data flow.

The DIOS output mesh is adapted for the use in the piezoresistive simulation step by means of the automated grid manipulating programs MDRAW^{ISE} (2D) and OMEGA^{ISE} (3D). Multidimensional structural analysis is interfaced by projecting the resulting stress field onto the adapted grids. In order to achieve high accuracy in the calculation of the diaphragm deformation, the entire transducer structure (i.e., diaphragm and its suspension on bulk silicon) was taken into account. Also the passivation layer on top, consisting of $0.6 \ \mu m SiO_2$ and $0.3 \ \mu m Si_3N_4$, was included in the simulation domain, since it is known that the mechanical behavior can significantly be influenced by that. Fig. 6 illustrates the different areas underlying the mechanical and the electrical simulations.



Fig. 6: Embedding of the electrical simulation domains in the full diaphragm structure used in the mechanical analysis.

Lastly, with the device structure and the field of mechanical stress as input, the extended DESSIS version computed the relative change in electrical resistivity $\Delta R_i / R_0$ (i=1,...,4) for each of the piezoresistors. From this data, the output voltage of the Wheatstone bridge is determined according to [6]

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$$V_{BD}/V_{AC} = \Delta V_{BD}/V_{AC} = (-\Delta R_1 + \Delta R_2 + \Delta R_3 - \Delta R_4)/R_0$$

where R_0 is the basic reference resistance and V_{AC} denotes the supply voltage. A reasonable measure of the pressure sensitivity S can be defined as

$$S = \Delta V_{BD} / (V_{AC} \cdot \Delta p)$$

Fig. 7 displays the calculated relative change of the bridge voltage versus the applied pressure difference. For the first example (pressure sensor), a sensitivity of S = 6.1 mV / (V bar) was obtained. This value falls in a range typical of such an arrangement of piezoresistors, as it can easily be estimated from the functional dependence of the sensitivity on the diaphragm side length [6]. The sensitivity of the second structure (microresonator) was calculated to be S = 1.1 mV / (V bar), which is significantly smaller than the measured value. Presumably the difference results from a calibration problem. In experiment, the deformation of the diaphragm was caused by the thermoelastic effect as mentioned above, and not by a uniform pressure difference as simulated. Reference for the calibration was the measured elongation at the diaphragm center which, of course, is not a linear measure of the overall deformation. A comprehensive simulation of the coupled thermo-mechanical effects inside the structure, planned as future work, should provide clarity.



4. Conclusion

The presented approach constitutes a practicable method for the numerical analysis of realistic piezoresistive structures. The practicability of a full simulation sequence ranging from layout and process simulation through structural analysis up to piezoresistive device simulation has been demonstrated with reference to realistic microtransducer structures.

5. Acknowledgement

The authors are grateful to U. Krumbein, Dr. N. Strecker and Dr. A. Schenk from the Institute of Integrated Systems, ETH Zurich, for providing helpful assistance and technical support.

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