3D simulation and analytical model of chemical heating during silicon wet etching in microchannels

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Abstract.

We present simulation results of modeling silicon wet etching in microchannels. This process is applied in microsystem technology to produce self-aligned microstructures in Silicon-On-Glass (SOG) wafers used in semiconductor, optoelectronic, microfluidic devices, MEMS and other microsystems. The models developed in this work are used for designing a novel chemical heater, which can be applied in many types of devises, from microreactors to integrated microfluidic systems for biochemical analysis. Here we investigate the problem of chemical heating of a SOG chip during a highly exothermic reaction of silicon etching in potassium hydroxide (KOH) solution in a microchannel of 100-micron diameter inside a 1x1 cm SOG chip. Two modeling approaches have been developed, implemented and validated against experimental data.

First, we developed a detailed 3D model based on Navier-Stokes equations, heat and mass transfer balance equations of a laminar flow of viscous incompressible fluid in microchannel coupled to the heat transfer equation in the solid chip. Simulation results predicted temperature distributions for different KOH flow rates and silicon etching areas. Simulations show that microchannels of a small diameter do not heat the chip due to the insufficient chemical heating of the cold fluid. But large area of the etching surface (large diameter and/or length of the microchannels) lead to local overheating that may have negative effects on the device performance and durability. Simulation results were compared to experimental data for two types of microstructures: one straight channel of 100-micron diameter and array of parallel connected channels etched in silicon wafer before bonding with glass. The model correctly predicted the temperature of the chip, and therefore can be used to simulate and optimize complex microstructures.

Second, a simplified analytical model was developed as an alternative method for quick assessment of process parameters. An equation of thermal balance was solved, which included heating by chemical reactions inside the microchannel and energy loss by free convection of air around the chip at room temperature. This problem was solved analytically under the assumption of infinite thermal conductivity of chip material. An equilibrium chip temperature was obtained as a function of etching area, thus allowing fast engineering estimations at the initial stage of a device designing process. Future work includes analysis of the analytical model validity, by running additional experiments and detailed 3D/2D simulations.