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DOI
10.1088/1742-6596/681/1/012035

Publication date
2016

Document Version
Final published version

Published in
Journal of Physics. Conference Series

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Link to publication

Citation for published version (APA):
Konakov, S. A., & Krzhizhanovskaya, V. V. (2016). 3D simulation and analytical model of chemical heating during silicon wet etching in microchannels. *Journal of Physics. Conference Series*, *681*, Article 012035. https://doi.org/10.1088/1742-6596/681/1/012035

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Journal of Physics: Conference Series **681** (2016) 012035 doi:10.1088/1742-6596/681/1/012035

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

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Abstract. We investigate chemical heating of a Silicon-on-Glass (SOG) chip during a highly exothermic reaction of silicon etching in potassium hydroxide (KOH) solution in a microchannel of 100-micron width inside a 1x1 cm SOG chip. Two modeling approaches have been developed, implemented and compared. (1) A detailed 3D model is based on unsteady Navier-Stokes equations, heat and mass transfer equations of a laminar flow of viscous incompressible fluid in microchannel, coupled to the heat transfer equation in the solid chip. 3D simulation results predicted temperature distributions for different KOH flow rates and silicon etching areas. Microchannels of a small diameter do not heat the chip due to the insufficient chemical heating of the cold fluid, whereas large-area etching (large channel diameter and/or length) leads to local overheating that may have negative effects on the device performance and durability. (2) A simplified analytical model solves a thermal balance equation describing the heating by chemical reactions inside the microchannel and energy loss by free convection of air around the chip. Analytical results compare well with the 3D simulations of a single straight microchannel, therefore the analytical model is suitable for quick estimation of process parameters. For complex microstructures, this simplified approach may be used as the first approximation.

1. Introduction in technology of etching in microchannel

Microtechnology is a rapidly developing area of research with many promising applications in semiconductor, optoelectronic, microfluidic devices, MEMS and other microsystems [1]. There are some problems and challenges in technologies, and novel methods of microfabrication should be investigated to provide a continuous progress. Microfluidics is one of the most promising parts of microtechnology. Lab-on-a-chip for DNA analysis and biomedical research, microreactors for nanoparticle synthesis and many other applications attract attention of scientists and engineers to microfluidics [2].

Microchannels for microfluidic devices are produced by etching through the mask. The groove may be of a different cross-section: circular, rectangle, trapezoidal, triangle, etc. To fabricate an enclosed microchannel, the second wafer is bonded to the grooved one. The top wafer may have a matching groove or be flat. This way, a microchannel of complex cross-section may be produced [3]. But there is a problem of misalignment while bonding the two wafers, which leads to uncontrollable changes of the cross-section shape and of hydraulic properties of the microchannel [4]. Another serious problem of this technology is the impossibility to change the channel after production. The technology applied

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in our research solves both problems. The concept of etching-in-microchannel technology is illustrated in Figure 1 by an example of producing a microstructure in silicon-on-glass (SOG) wafer.

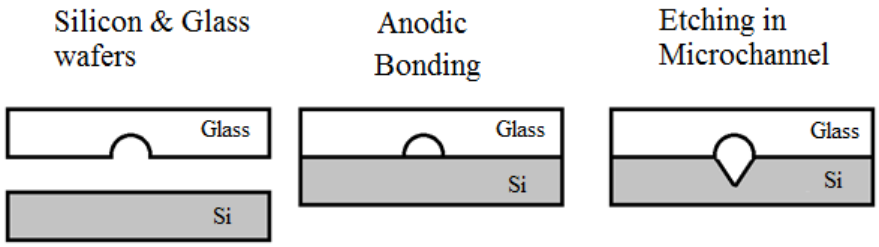

Figure 1. Scheme of etching-in-microchannel technology

The technology includes three steps. At the first, microchannel is etched in glass. At the second, silicon with (100) orientation and glass wafers are bonded together. The third step is supplying potassium hydroxide (KOH) solution into microchannel. KOH reacts with silicon, as in typical process of silicon anisotropic wet etching, and forms trapezoidal or triangle profile [5]. Edges of microchannel in glass play a role of mask for silicon wet etching and it leads to perfect alignment of microstructure. Set a time of KOH supplying into microchannel we can control geometry with high accuracy. Moreover it is possible to measure hydraulic properties of system in-situ and change them during the etching process, reaching the required parameters. Figures 2 and 3 show profiles before and after etching of silicon in microchannel by KOH solution.

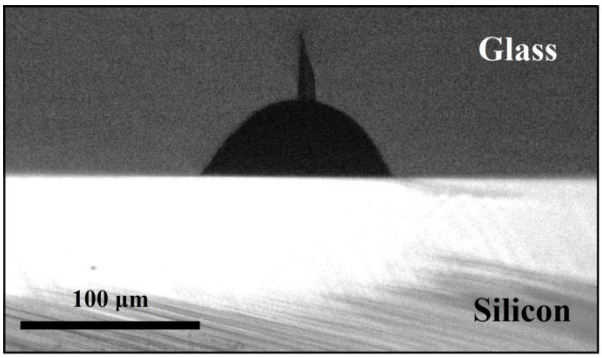

Figure 2. Microchannel in SOG ship before silicon etching

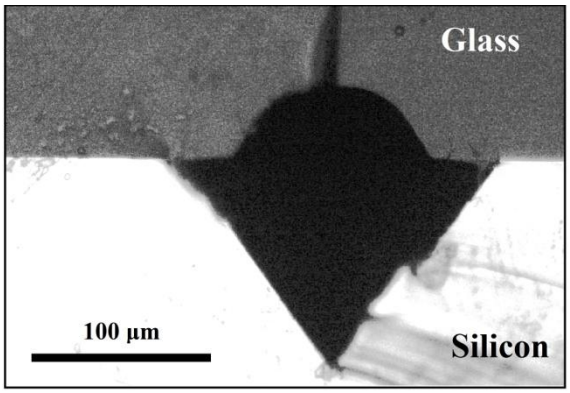

Figure 3. Microchannel in SOG ship after silicon wet etching by KOH solution

Our global goal is comprehensive investigation of technology of etching-in-microchannel. In this paper we present results of our work where problem of heat transfer during silicon etching in the microchannel was considered in detail. Figure 4 shows a scheme of SOG ship with microchannel which was investigated in the work. The chip with 10x10x1 mm dimensions consist of silicon and glass wafer. 100 µm channel have been etched in the glass before bonding of two wafers. The reaction (R1) of silicon dissolution by KOH is highly exothermal and this is a heat source leading to temperature increase.

$$Si + 2KOH + 4H_2O => K_2[Si(OH)_6] + H_2 + P_R \qquad \textbf{(R1)}$$

where P_R is heat by chemical reaction of silicon dissolution in KOH.

The chip located in air and its surfaces are cooling by free convection. In this situation we can write a govern heat balance equation (1) for the process of silicon etching in microchannel during the time when KOH solution is being supplied in it.

$$P_R+P_e+P_L=0 \quad (1)$$

where: $P_R>0$ is heat by chemical reaction; $P_e<0$ is power which heats KOH from initial temperature (T_i) to temperature at outlet ($T_{out}>T_i$); $P_L<0$ is heat loss by free convection in air with temperature T_a from top (P_{L1}) and bottom (P_{L2}) surfaces of chip. For this case we should obtain an equilibrium temperature of the chip.

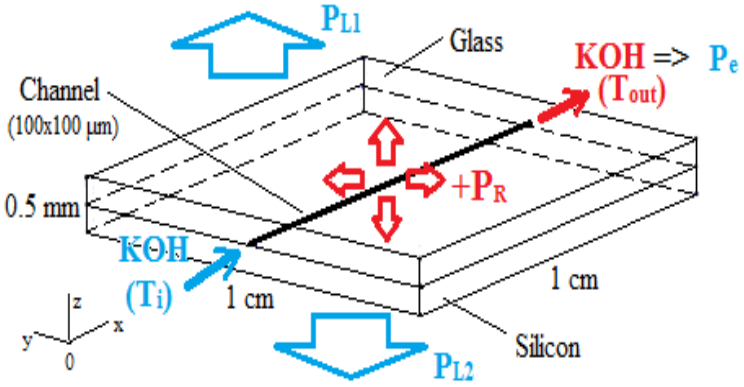

Figure 4. Scheme of SOG chip with microchannel

2. Mathematical model

2.1 Equations

We selected a continuum modeling approach to simulate a liquid flow in microchannel. Calculated Reynolds number Re=0.15 corresponds to a laminar regime. In model mass conservation law (2) and Navier-Stokes equations for a flow of KOH solution (3) describe the fluid dynamics in the channel:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho V = 0 \quad (2)$$

where ρ is density, t is time, V is velocity vector

$$\frac{\partial(\rho u_i)}{\partial t} + \nabla \cdot (\rho V u_i) = -\frac{\partial \rho_i}{\partial x_i} + \nabla \cdot (\mu \nabla u_i),\ i = x, y, z \quad (3)$$

where u_i is projection of velocity vector on i axis, μ is the kinematic viscosity

Heat transfer equation can be written as (4)

$$\frac{\partial(\rho h_o)}{\partial t} + \nabla \cdot (\rho V h_o) = \nabla \cdot (\lambda \nabla T) + \frac{\partial p}{\partial t} + P_R \quad (4)$$

where h_o is enthalpy, λ is thermal conductivity, T is temperature, p is pressure, P_R is the heat source due to chemical reactions.

2.2 Boundary conditions

For calculation of the flow in the microchannel we applied conditions of constant velocity at the inlet and outlet. The expression (5) gives us a value of the velocity.

$$U(x=0,x=10\ mm)=R/S_{ch} \quad (5)$$

Where U is flow velocity (x direction) [m/s], R is flow rate of etchant [m^3/s], S_{ch} is cross section of channel [m^2]. Velocity at the walls of microchannel was *0* [m/s]. Temperature of KOH solution was set at 300 [K] at the inlet and outlet.

Another temperature condition was applied to silicon surface in microchannel, because the etching process generates some quantities of heat. In general form this conditions expressed by (6)

$$P_R = F_{ch} \cdot P'_R \quad (6)$$

where $P_R>0$ is heat by chemical reaction of silicon dissolution in KOH [W], F_{ch} is area of Si etching [m^2], P'_R is surface heating power by Si dissolution [W/m^2]. Surface heating power can be obtained by equation (7)

$$P'_R = -\Delta H_R \cdot \rho_{Si} R_{etch}(T) / M_{si} \quad (7)$$

where ΔH_R = -247 ± 6 [kJ/mol] is enthalpy of reaction (R1) [6], ρ_{Si} is density [kg/m^3], M_{Si} is Si molar weight [kg/mol], R_{etch} is etching rate of (100) plane [m/s]. This rate is a function of temperature, described by (8)

$$R_{etch} = R_0 C_{H_2O}^4 C_{KOH}^{0.25} \exp(-E_A/K_b T) \quad (8)$$

where $R_0 = 689 \cdot 10^{-9}$ [m/s] is constant, C_{H2O}, C_{KOH} is molar concentration [mol/L], E_a = 0.595 [eV] is activation energy, $K_b = 8.617 \cdot 10^{-5}$ [eV/K] is Boltzmann constant, T is temperature [K].

Substituting expression (8) into (6) we obtain (9)

$$P_R = F_{ch} \cdot (-\Delta H_R \rho_{Si}/M_{Si}) \cdot R_0 C_{H_2O}^4 C_{KOH}^{0.25} \exp(-E_A/K_b T) \quad (9)$$

This is the boundary condition for silicon wall in microchannel in general form. Simplifying it for our case for constant concentration of KOH we can write (10).

$$P_R = F_{ch} \cdot K_e \cdot (-E_A/K_b T) \quad (10)$$

where K_e=1.233·10^{11} [W/m^2] is constant.

For boundary conditions, which applying to outer wall of the chip, we have (11)

$$P_L = P_{L1}'F_{s1} + P_{L2}'F_{s2} \quad (12)$$

where P_L' is surface heat loss by convection [W/m^2], F_s – area of chip surface [m^2]. Index 1 and 2 denote top and bottom surfaces of the chip respectively. In our model for side surfaces of the chip we consider adiabatic conditions because its area is small. To calculate P_l' we use equation (13)

$$P_l' = \alpha(T_a - T_s) \quad (13)$$

where α is heat transfer coefficient [W/m^2·K]. Expression (14) couple α and Nusslt number

$$Nu = \alpha \cdot X/\lambda_a \quad (14)$$

where Nu is Nusslt number, X is characteristic dimension of the system, λ_a is air thermal conductivity. In general form Nusslt number for free convection case can be write as (15)

$$Nu = C(Gr \cdot Pr)^n \cdot K \quad (15)$$

where Gr is Grashof number, Pr is Prandtl number, C & n are constants, K is dimensionless function. C, n and K depends from shape of cooling surface and orientation in space.

In conditions of our model Pr and Gr numbers calculated by (16, 17)

$$Pr = \nu_a \rho_a c_a/\lambda_a = 0.708 \quad (16)$$

$$Gr = g\beta\Delta T \cdot X^3/\nu_a^2 = 7.972 \cdot 10^3 \quad (17)$$

where ν_a =1.568·10^{-5} [m^2/s] is kinematic viscosity of air, ρ_a = 1.1774 [kg/m^3] is density, c_a = 1006 [J/kg·K] is air specific heat, λ_a = 0.02624 [W/m·K] is thermal conductivity, g=9.81 [m/s^2] is acceleration of gravity, β = 3.33·10^{-3} [K^{-1}] is coefficient of volumetric expansion, ΔT is temperature gradient. Composition $Pr \cdot Gr$=5.643·10^3 corresponds laminar convection [7]. Using a constants C, n and K for this case we obtain expressions (18, 19) for boundary conditions for top and bottom outer walls of chip respectively.

$$P_1 = (T_a - T_s) \cdot (\alpha_1 F_{s1}) \quad (18)$$

$$P_2 = (T_a - T_s) \cdot (\alpha_2 F_{s2}) \quad (19)$$

where α_1=12.281 [W/m^2·K], α_2= 6.14 [W/m^2·K].

2.3 Implementation

Program CFD_ACE+ used for numerical solving of equations (2, 3, 4). Finite volume method with Conjugate Gradient Squared + Precondition Solver was applied for Velocity and Enthalpy. 3D geometry model was developed for chip and microchannel. Transient simulation (until quasi stationary state) with adaptive time step was used for numerical simulation.

We simulated a process of etching in microchannel for 100 μm straight channel with constant flow rate of KOH solution R=10^{-12} [m^3/s]. Area of silicon wall was F_{ch}=10^{-6} [m^2]. Two calculations were carry out with different initial conditions: T=300 and T=380 [K]. As the approximation, to simplify a simulation, we assume a constant value of P_R = 6.17·10^{-4} [W] (that means the constant etching rate at temperature 380 [K]). In addition under the same conditions we simulate a microstructure in SOG chip with large etching surface of silicon (F_{ch}=10^{-4} [m^2]).

3. Results of numerical simulation

Figure 5 shows a flow velocity in microchannel. The maximum value is 1.9·10^{-4} [m/s]. Distribution of temperature in SOG chip is presented in figure 6. Figure 7 (A) illustrates the variation of the temperature over time for the model.

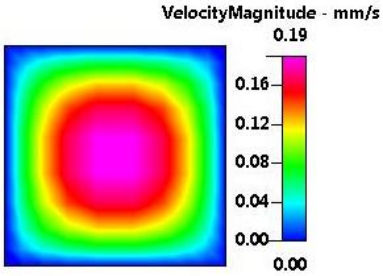

Figure 5. Velocity in microchannel (R=10^{-12} [m^3/s])

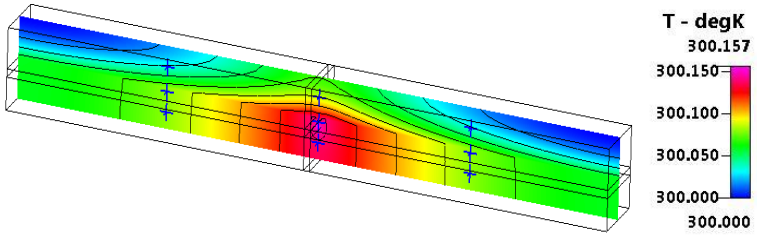

Figure 6. Temperature distribution in cross-section of chip (F_{ch}=10^{-6} [m^2], R=10^{-12} [m^3/s])

As we can see the maximum value of temperature is 300.157 [K]. It is means that insignificant heating during etching in microchannel with small area of opened silicon cannot lead to self-heating of SOG chip. So to provide a high rate of etching reaction we should supply heat to microstructure. But absence of self-heating is advantage when we need to have a low etching rate to control of microchannel geometry precision. We can see another situation for microstructure with large etching surface of silicon (F_{ch}=10^{-4} [m^2]). Figure 7 (B) shows the change in temperature over time for the case. Large etching area leads to high power of inner heating that result to significant temperature increasing. We see maximum temperature at 351.483 [K]. It shows that such microstructure can have self-heating effects during the KOH etching in microchannel. We should take into account the phenomenon when developing the technology for structures with large open surface (membranes, microfluidics filters, mixers, etc). For some devices it is possible to etch without external heating.

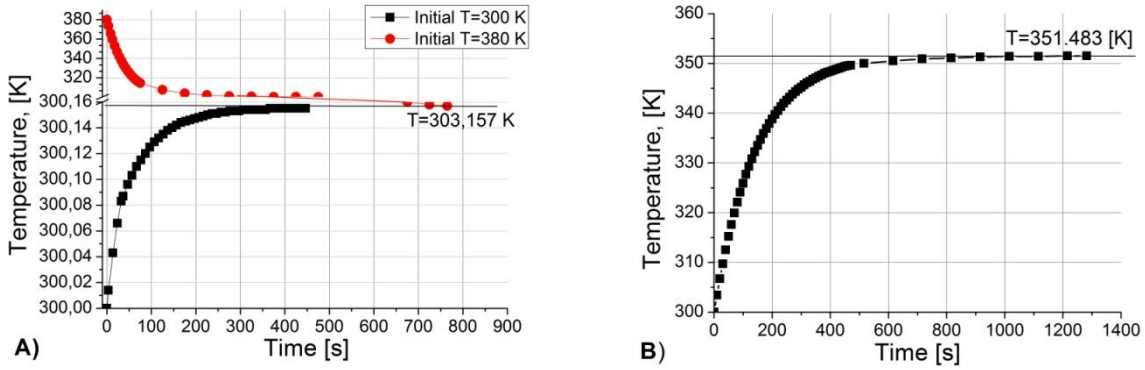

Figure 7. Maximum chip temperature change over time. (A) F_{ch}=10^{-6} [m^2], (B) F_{ch}=10^{-4} [m^2]

4. Analytical modeling

The second approach, which was used in the work, is analytical expression of equation (1). In this case we apply tree assumption: etching rate is constant; thermal conductivity of chip is infinite; temperature in the channel is equal temperature on the top and bottom surface (we denote it as T). With this assumption we can write heat balance equation (1) as (20):

$$F_{ch} \cdot \left(-\frac{\Delta H_R \rho_{Si} R_{etch}}{M_{Si}}\right) + c_e \rho_e R(T_i - T_{out}) + (T_a + T_s)(\alpha_1 F_{s1} + \alpha_2 F_{s2}) = 0 \qquad (20)$$

Express temperature from (20) we get final equation (21)

$$T = \frac{\left[F_{ch}\left(-\frac{\Delta H_R \rho_{Si} R_{etch}}{M_{Si}}\right) + c_e \rho_e R T_i + T_a(\alpha_1 F_{s1} + \alpha_2 F_{s2})\right]}{c_e \rho_e R + (\alpha_1 F_{s1} + \alpha_2 F_{s2})} \qquad (21)$$

Using (21) we can fast calculate the equilibrium temperature of the SOG chip. Figure 8 shows plots of equilibrium temperature for different etching areas and flow rates of KOH solution. In table 1 we see a compilation between numerical simulation and analytical solution. It is possible to note that even under our bold assumptions the values of temperature do not have significant differences. That means the analytical model preferably to use for fast calculations in the first approximation.

Table 1. Comparison of two models

F_{ch} [m^2]	3D Simulation	Analytical modeling
10^{-6}	ΔT=0.157 [K]	ΔT=0.335 [K]
10^{-4}	ΔT=51.483 [K]	ΔT=51.385 [K]

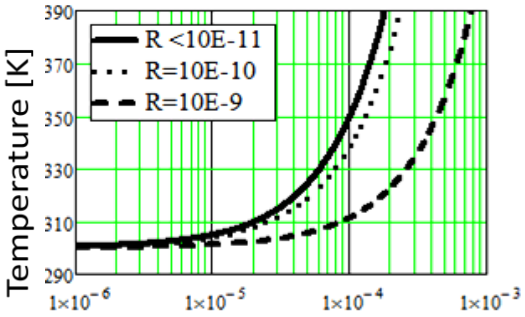

Figure 8. Equilibrium temperature of the chip. Analytical model

5. Conclusions and future plans

In the work we investigated a heat transfer problem for SOG chip during the process of etching in microchannel. Developed 3D computer model and analytical approach give the same results about equilibrium temperature of the chip. Analytical model may provide a fast estimation of temperature in the first approximation while numerical calculations allow obtain detailed information about etchant flow and temperature distribution in chip volume and their changes over time. Despite obtained results real experiments have many problems. The general issue is hydrogen generation during the etching process of silicon by KOH. Its bubbles have a strong influence on flow regime and local heat balance. Investigation of the problem requires advance multi scale 3D computer modeling, what we are planning to carry out in our further work. In spite of this the technology of etching-in-microchannel is very promising process for microfabrication of many complicated devices with unique features, such as microreactor for silicon dioxide deposition [8]. In future work we will continue our comprehensive research of the technology of etching-in-microchannel.

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