

3D SIMULATIONS OF DIAMOND MICROFLUIDIC DEVICES

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Abstract

The aim of this study was to optimize the diamond microfluidic device with four microchannels. The temperature distributions in electrophoretic microchips of different geometries and different materials have been analyzed by the Coventor software. Diamond microfluidic devices are very advantageous over glass or polymer microfluidic devices; they dissipate Joule heat much more efficiently because of the highest thermal conductivity coefficient of diamond.

Keywords: diamond microfluidic devices, Coventor, Joule heating

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Introduction

Diamond reveals several extreme, very beneficial properties - the highest thermal conductivity, remarkable biocompatibility, high electrical breakdown voltage and chemical resistance against the majority of chemical solutions applied in the solid-state technology. This makes diamond thick layers the good choice for the application in microfluidic devices [1-8].

Microfluidic devices are miniaturized systems which transfer tiny quantities of samples and reagents, through a system of microchannels and microchambers made on the surface of a small plate. They are made of different materials; most often of polymers (PDMS, PMMA), glass or silicon.

These systems integrate and reduce a sample size of biochemical reactions and processes. It is a tendency to replace large, often long-lasting and expensive biological and chemical analyses, by microfluidic devices (called sometimes lab-on-a-chip or μ -TAS – micro-total-analysis-systems). A small sample size, low reagent consumption, low waste production and short time of analysis are only a few advantages of these microsystems.

Electrophoresis is a popular method of on-chip separation. It is based on the migration of biomolecules in the electric field. Electrically charged biomolecules (each of different molecular mass or different charge) have different mobilities and the separation can be achieved. In this paper we focus on microfluidic devices based on biomolecule electrophoresis on-chip.

The important issue in designing new microfluidic devices (or electrophoretic chips) is a total analysis of the processes present during the microscale chip electrophoresis. This leads to the optimal selection of the electrophoretic chip material and its optimal geometry [1-3]. The significant and undesirable phenomenon occurring during the process of electrophoresis is Joule heating [1-3,8,9]. This leads to a

temperature and gradient growth across the microfluidic channels, decreasing the quality of separation in a number of ways (sample band dispersion or peak broadening, deterioration of analysis resolution and even decomposition of thermally sensitive samples or creation of vapor bubbles in the microchannels). A proper selection of the material with a high thermal conductivity coefficient for chips and optimizing the chip geometry, as well as an efficient cooling system reduce all the above mentioned thermal effects. In our research we focused our interest on different aspects of electrophoretic chips design, with respect to minimizing an influence of Joule heating.

Numerical study

The computer modelling and simulations have been performed with commercial code – CoventorWare™ [11]. The same microchannel geometries were simulated as in the real diamond microfluidic device fabricated in the MNT-ERANET project DIAMID “Diamond Microfluidic Devices for Genomics and Proteomics” [8]. In this project the diamond microfluidic device was designed for fast electrophoretic separations of DNA and protein molecules.

The geometry was directly introduced into the CoventorWare Process Editor together with the technological steps and material parameters to generate a 3D solid model of the microfluidic device under investigation. Once the 3D model was created, the discretization of the computational domain was performed. The linear “Manhattan Bricks” elements were applied. At this stage, names were assigned to all the faces for the next step - boundary conditions definition.

Calculations were performed for stationary flow conditions. The microfluidic device consists of a plate with the system of four microchannels (FIG. 1), fluid (buffer) inside the microchannels, a support, a cap and air environment. The aim is to optimize the four channel microfluidic device and compare microfluidic devices made of diamond and glass.

The investigations were carried out for a continuous flow at the inlet, for the air flow rate 1000 mm³/s crosswise the microchannels. The current enforced between the electrodes located at the microchannel terminals was fixed at the common current density value - for the different channel cross-section areas, this common current density assumption gives four different current values: 160, 240, 400 and 800 mA. The air temperature at the inlet, as well as the temperature of the diamond chip bottom wall, were equal to 300K.

KCl 0.1 mol/dm³ buffer was applied in this model as the liquid inside the channels.

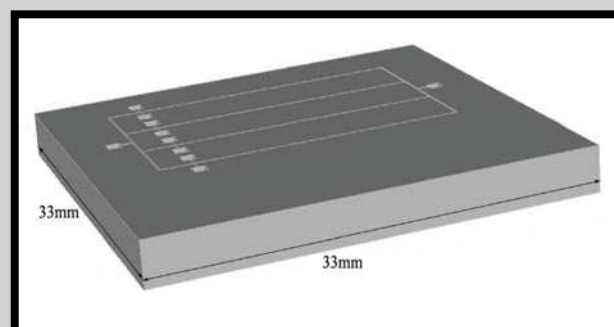


FIG. 1. Model of the chip with the system of microchannels.

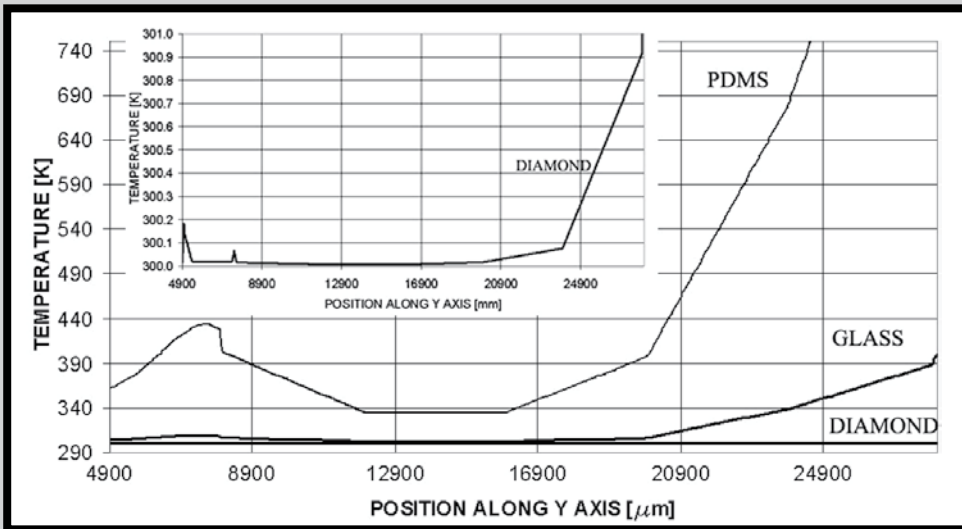


FIG. 2. Temperature profiles along the channels - simulation results for PDMS, glass and diamond chips.

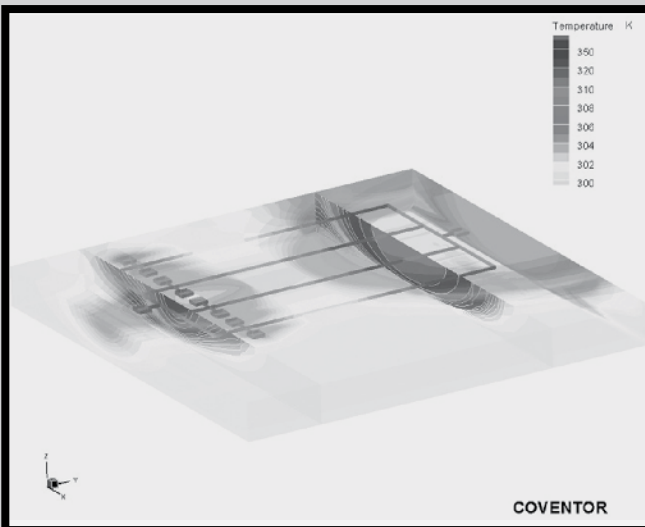


FIG. 3. Glass Microfluidic device & KCl_{0,1} mol/dm³ buffer
Channel: depth 250 μm, width 25 μm, length 23200 μm
Current 400 mA, air flow rate 1000 mm³/s along X
Air inlet, TOP & BOTTOM walls temperature fixed 300 K.

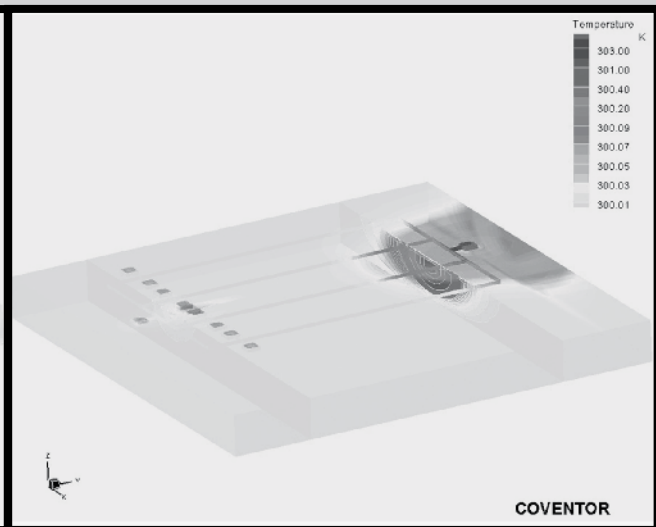


FIG. 4. Diamond microfluidic device & KCl_{0,1} mol/dm³ buffer
Channel: depth 250 μm, width 25 μm, length 23200 μm
Current 400 mA, air flow rate 1000 mm³/s along X
Air inlet, TOP & BOTTOM walls temperature fixed 300 K.

Results and discussion

For the first simulations, chips consisting of identical geometry microchannels were applied: depth 250 μm, width 25 μm and length 23200 μm. Different materials were compared: glass, polymer polydimethylsiloxane (PDMS) and diamond. The current enforced between the electrodes was 400mA, the air flow rate was 1000 mm³/s in the perpendicular direction to the microchannel length and the temperature on selected walls was equal to 300K. Significant differences between temperature profiles of the PDMS, glass and diamond chips are well visible. At the channel common inlet of the glass chip, we obtained temperatures exceeding 600K for PDMS and 320K for glass and at the channel outlet terminal even over 350K. The same chip, but made of diamond, reveals a much lower temperature increase, as was expected (FIG. 2).

FIGURES 3 and 4 show the example distributions on diamond and glass microchips with the same microchannels geometries and the same electric field applied. It is clearly seen the difference between both microchips, maximal temperature for diamond microfluidic device is 303K, for glass microfluidic device 350K.

Conclusions

On the basis of the numerical experiment and the analysis performed, it can be stated that diamond is the best material for the application of electrophoretic microchips. In comparison to glass or plastic devices, diamond offers a significant improvement to device performance parameters, it dissipates Joule heat much more efficiently what enables to apply much higher electric field during chip electrophoresis and to obtain much shorter times of separations.

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