Liquid Crystal Orientation on Patterns Etched in Silicon-on-Insulator

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ABSTRACT

Liquid Crystals have many applications in photonics, but often the geometrical properties of the photonic structures give problems for controlling the alignment of the liquid crystal. We demonstrate the effect on the orientation of a nematic liquid crystal by structures etched in Silicon-on-Insulator (SOI) wafers, produced by photolithography. We characterize the alignment effect of several patterns, including configurations that allow multiple stable director orientations. Also, the influence of a surface treatment (like deposition of a monolayer on the structured surface) is discussed.

Keywords: Liquid Crystal Alignment, Liquid Crystal Cladding, Integrated Photonics, Silicon-on-Insulator

1. INTRODUCTION

Liquid crystals (LCs) have many potential applications in photonics because of their enormous electro-optical properties[1]. For example in planar integrated optics, the use of LCs can lead to very compact electrically reconfigurable components. By switching the liquid crystal electrically, the director (the local orientation of the liquid crystal molecules) changes and hence – via the birefringent property of LC –the refractive index profile of the component.

These devices have two extreme states. In the presence of a high electric field, the director is everywhere parallel to field. A careful design of the electrodes that generate the field can make that the liquid crystal molecules are almost parallel in the whole liquid crystal layer. This normally gives optimal behavior.

Without electric field, the director is determined by the surface in which it is confined. A key problem that arises when using liquid crystals in photonic components is the effect of the geometry of the photonic component on the director field. Indeed the liquid crystal layer is not one-dimensional between parallel plates as it is in display technology, but it is confined in two-dimensional or even three-dimensional geometry. For example, it can be inside a small channel (e.g. a waveguides with a core of liquid crystal), inside cylindrical cavities (e.g. in 2D-photonic crystals), it can be along a ridge waveguide or it can surround a ring resonator. These complex geometries give a non-homogenous director in the absence of the electrical field: it may vary on a scale that is comparable to the typical size of the features of the confinement.

This inhomogeneity gives suboptimal behavior: the effect on the refractive index profile (determined by director orientation relative to the electrical component of the optical field) is different for all points in the LC-layer. The effect will be reduced or even completely annihilated. The problem is the worse if an important fraction of the light in the liquid crystal is close to the surfaces or to sharp features, which is often the case. Because the light has to be both in the liquid crystal and in at least one other material (that defines the optical confinement and optical functionality), surfaces are always involved. When regions with a very large contribution for the electrical effect coincide with regions of large direction variations, the device becomes extremely sensible for small inaccuracies in design or fabrication. This may happen quite often: for example, ridge waveguide edges typically have a relative high value for the non-principal component of the electric field, while they also induce a large director tension.

Redesigning the component in a way that the liquid crystal forms a nice homogeneous layer is mostly impossible. However, small variations in geometry are allowed, and so are surface treatments. Also, in the regions where there is no light intensity (e.g. between waveguides), we can introduce artificial structures with a strong preferential direction that will determine the dominant director orientation. Reducing the effect of the optically important part can be done by avoiding strong preferential directions that are not parallel to this dominant orientation, by using flat or slightly curved surfaces if possible.

When determining the influence of a photonic component geometry on the alignment of liquid crystal, not only the geometry but also the details of the fabrication process play an important role. Small variations in a surface, for example due to an etch process, can have a significant influence on the orientation of the liquid crystal director: they may for instance introduce preferential orientation. Moreover, the sharpest features – which have often a large dependency of the fabrication process – have the most important influence on the alignment.

As a consequence, a first step in introducing liquid crystals in integrated optics, is to make a detailed characterization of the alignment properties of the particular technology one wants to use. For this purpose, we present here we have investigated in a systematical way the alignment of nematic liquid crystals on patterns etched in silicon-on-insulator (SOI).

SOI is a highly promising material system for making integrated optical components: it has the advantages of being a silicon-based technology and the high contrasts allow for small components. It is however mainly restricted to passive components. The use of liquid crystals opens a world of new electro-optical and even opto-optical (nonlinear) functionalities. The basic idea is to replace the cladding materials (air or silica) partly by nematic liquid crystal. The huge birefringence of recent liquid crystals again will lead to small designs and highly integratable components.

The patterns in the SOI that we will discuss were fabricated by deep-UV photolithography. This technique does not give the finest structures but it has the potential to become the standard for photonic SOI components because it allows for mass production.

This paper is structured as follows: in the next section we will give an introduction in the principles of liquid crystal alignments. In section 3 we describe the cell structure and experimental setup. Next we describe the results for several patterns. We first discuss in a systematic way for 2D-rectangular gratings in section 4. Later we discuss in section 5 the alignment effect for more complex patterns like patterns that have multiple preferential directions and we show the conclusions that can be drawn based on the experimental results.

2. LIQUID CRYSTAL ALIGNMENT IN COMPLEX GEOMETRIES

Nematic liquid crystals consist of long-shaped organic molecules that tend to align parallel to each other[2]. The unit vector in the common direction is called the *director*. For all other aspects, the material behaves like a normal liquid: the molecules can move with respect to each other and will fill the space in which they are confined in the same way as a liquid, including effects of gravity and capillary forces.

Because the molecules align parallel, there is an internal preferential direction and on a macroscopic scale the material becomes anisotropic, which is normally considered as a crystal property – hence the name liquid crystal. This anisotropy is used in two ways for the electro-optic effect of liquid crystal: the static dielectric anisotropy will make that the director tends to be parallel to the electric field, but while rotating, also the axes of the optical anisotropy rotate and thus the optical properties of the material change – at least when one is working with polarized light.

Because the aligning forces are rather weak, the liquid crystal molecules are not always perfectly parallel, and on a macroscopic scale the director may vary. The result is an optical material where the optical axes is only defined locally, and can be different for each point in space.

The tensions that are created this way give an increase of internal energy of the material. This energy can be calculated as a function of the material parameters and the type and magnitude of the director variation.

When a liquid crystal contacts to another material (in most cases a solid), the liquid crystal molecules that are close to the surface feel inter-molecular forces with the molecules on the other side of the surface, in addition to the aligning force of the surrounding liquid crystal molecules. The LC molecules will reorient themselves in a way dependent on the material parameters and the state of the surface. For example, silicon tends to align the molecules parallel to the surface. This is called *planar anchoring*. If, on the contrary, molecules are preferentially orthogonal to the surface, the anchoring

is said to be *homeotropic*. When the alignment differs from the preferential direction, a surface energy can be associated with the difference.

If the liquid crystal is confined between several surfaces, it will try to minimize the total internal energy, i.e. the sum of the surface and bulk energies. For complex geometries, one often finds multiple stable minima. For optical applications this means one can create structures with the same geometry but with different optical properties.

3. TEST SETUP

For fabricating our test samples, we started with an SOI wafer: this consists of a silicon substrate, with on top a 1µm thick layer of silica. On top of this there is again a silicon layer with thickness of 220 nm. The latter consists of monocrystalline silicon because the complete structure is the result of a bonding process in which the top silicon was part of the substrate of the second layer.

In this system the patterns were defined by deep-UV photolithography. The smallest features we could define this way have a width between 150 and 200 nm. Two etch masks were used: one to define patterns with a depth of about 70 nm (so the top surface is still silicon), and a second with a depth of 220 nm that just frees the silica surface.

For confining the liquid crystal, we made a cavity between the SOI sample on one side and on the other side a glass substrate. In fact, this glass substrate was also a layered stack: on the glass there was a thin ITO layer for applying electric fields, and on top of that there was another flat layer of a material with known liquid crystal aligning properties. We will discuss the type and the effect of this layer further in this paper.

The two substrates were bond together with glue in which a set of glass microspheres was mixed. The diameter of the spheres (chosen to be 1.6µm) fixes the width of the cavity. The glue mixture was deposited only on the border of the sample, so that in the centre of the device the pattern in the silicon remained free to the air. The resulting structure is shown in Figure 1.

Finally, the liquid crystal was inserted into the cavity. This is done while both the sample and the liquid crystal are heated above 80° degrees. At this temperature, the liquid crystal material acts as a normal isotropic liquid (it has no internal preferential orientation), the viscosity is decreased and it easily fills the cavity by capillary forces. We used the liquid crystal E7, which is a commonly used nematic with a birefringence of $\Delta n = 0.2$ in the visible range.
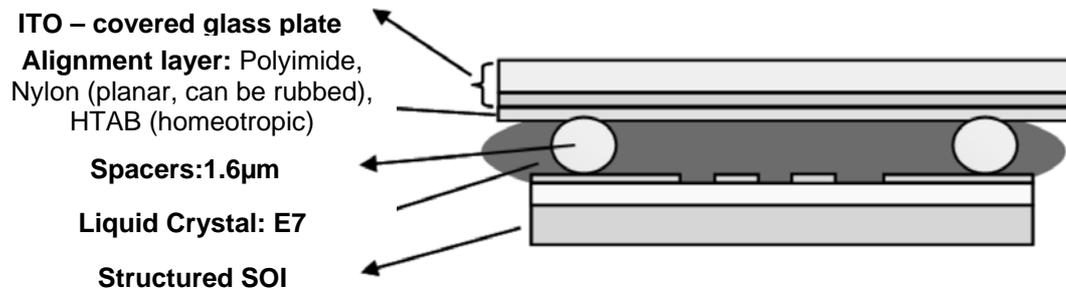
Figure **1**: Cell structure

After the insertion of the liquid crystal the cell is cooled down very slowly. The goal of this annealing process is to reach a liquid crystal alignment state that has a low internal energy. Fast cooling or inserting in the liquid crystal at low temperature can lead to defects (for example local discontinuities in the director orientation). However, even a slow cooling does not guarantee that a unique alignment is found, if there exists multiple stable alignment states with no or very little energy difference. In this case, heating the cell and cooling down again can lead to a different alignment. We will give examples of this effect later.

In order to see the liquid crystal orientation in the cells, they where placed under microscope "between crossed polarizers". This means that the sample is illuminated by polarized light, while the reflected light passes through a polarizer orthogonal to the polarization of the incident light. Therefore, only light that has obtained a polarization change is being measured. This can be because incident light is not aligned along the principle axes of the liquid crystal (the axes related to the director); the birefringence will then lead to a polarization conversion. Also, the diffraction of the silicon pattern itself may be polarization dependent. The latter effect occurs even without the presence of liquid crystal but was in our experiments negligible compared to the effect of the liquid crystal alignment.

For our purposes, we looked to the liquid crystal alignment with a vertical setup in reflection: the illumination is done from the top, the silicon surfaces reflect it. Therefore, the light passes the liquid crystal layer twice and the polarization conversion is doubled.

4. RECTANGULAR PATTERNS

In order to determine accurately the alignment behavior of liquid crystal on LC we tested real photonic structures (waveguides, ring resonators, photonic crystals) as well as non-photonic structures, mainly gratings. We will restrict this paper to these gratings because they give results that are easy to interpret. The pitches range from few 100s of nanometers up to 50 µm.

1. A simple one dimensional grating

It is well known that a one-dimensional grating made in a material that gives a homogeneous, horizontal director orientation parallel to the grating. It is easy to verify that this configuration is the only one that has no internal elastic tensions and where the surface energies are minimal everywhere. However, this is only true just above the silicon surface. In the bulk of the liquid crystal layer the director is also influenced by the top alignment layer (see figure 1).
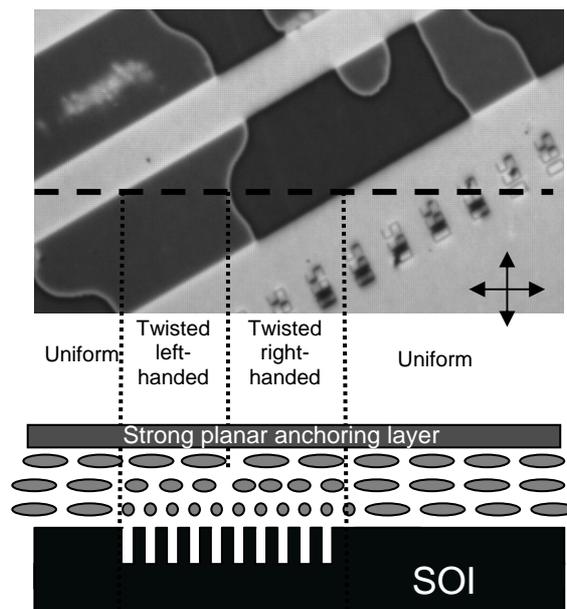
Figure **2**: visualization of the liquid crystal alignment effect of a grating etched in silicon-on-insulator

An example of the aligning properties of etched silicon grating is shown in figure 2. It shows the resulting view for a simple one-dimensional grating. The polarizers where chosen be along horizontal and vertical axes of the picture (like the cross in the down right corner of the picture).

The alignment layer on top of the liquid crystal was chosen to be a strong planar anchoring with alignment direction orthogonal to the grating. Above the plane silicon (the brightest regions in the figure), the liquid crystal forms a homogeneous layer: the LC molecules are parallel to the upper alignment direction everywhere. Above the grating (the dark stripes), the lower liquid crystal is parallel to the grating while the upper molecules are parallel. In between, there is a twist that can be either left or right-handed, which gives the two types of domains in figure 2.

The situation of figure 2 occurs because the two twisted regions are energetically completely equivalent. When the angle between grating and polarizers is a multiple of 45°, there is no visible difference between them. When the top alignment layer is not completely orthogonal to the grating, the two twist types will have a different elastic energy and the one with the smallest twist (lowest energy) will dominate. An error of 5° will already give homogeneous alignment above the grating regions.

The same experiment for different grating pitches showed good alignment for pitches between 400nm and 10μm. Larger pitches will give areas of homogeneous alignment (like above the planar silicon), while smaller pitches have too many defects due to the fabrication.

Besides changing the geometrical parameters, we also changed the chemical parameters of the silicon surface by covering it with a surfactant. For example, we dip coated the SOI samples in a solution of hexa-decyl-trimethyl-ammonium bromide (HTAB). This surfactant, which is in a very small layer between the silicon (or oxide) and the liquid crystal, is known to have homeotropic anchoring. This means the simple solution of alignment along the grating is not longer valid: there is even no component along the direction. The overall anchoring of the grating is homeotropic but there is locally (between the ridges) a strong deviation to the horizontal direction orthogonal to the grating. This can be made visible by using a homeotropic top alignment layer: the dominant vertically aligned liquid crystal will not give any polarization conversion but the deviation gives a small effect. Also, when using an planar alignment layer with preferential direction parallel to the grating, we again can see a split up in two regions. This is however, a more complex configuration because is mixed with the variation from vertical to horizontal position above the ridges.

2. Influence of the top alignment layer

Before moving to 2-dimensional gratings, we want to draw attention on the influence of the alignment layer on the glass plate. As mentioned in the previous subsection, the difference between homeotropic or planar anchoring (the latter with or without preferential orientation in the plane) can be exploited to visualize different alignment effects. We always used strong anchoring materials, i.e. that the penalty energy for having a deviation from the anchoring direction is always high compared to any other energy (be it elastic or electric) in the bulk of the liquid crystal layer.
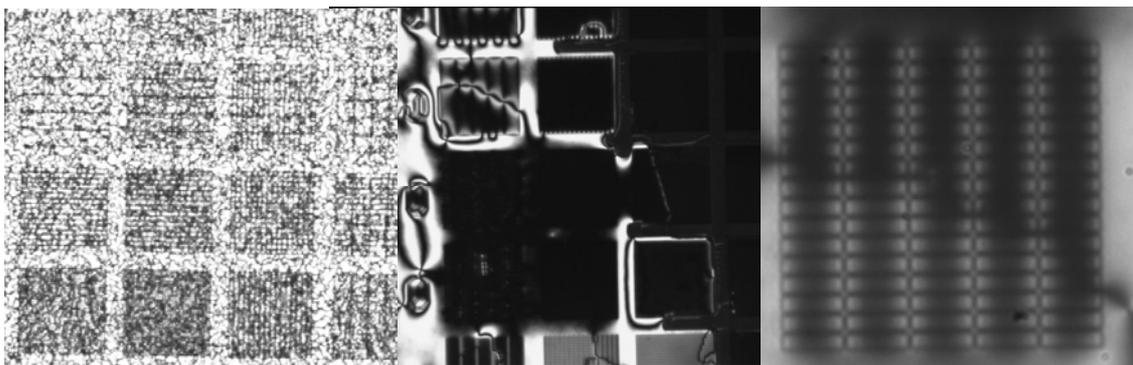
Figure 3: view on 2-dimensional gratings with a planar alignment on the glass side without preferential orientation. Left: Nylon-6, Middle: polyimide PI-2610. Right: close up of a PI-2610 pixel

However, even those strong anchoring materials can have different behaviors. Figure 3 shows a view on two similar test samples where the glass side has planar alignment on the glass side without a preferential orientation. On a polyimide

(PI-2610) sample, one can see there is a strong alignment effect of the gratings on the liquid crystal layer. On a nylon-6 alignment layer, there seems to be no or little effect although there is a similar silicon pattern on the bottom.

The clue of this effect can be found in the way the polymer layer align the liquid crystal. Although there is no preferential orientation in a plane parallel to the surface, for most materials this does not mean the molecules can rotate in that plane. The direction in which the LC molecules are fixed to the surface is determined either at the first contact or in the cooling process. The first case leads to a situation like the left-hand side of Figure 3. In the second case, the orientation of the molecules at the surface has time to adapt to the minimal energy configuration forced by the grating on the other side.

We remark that silicon and silicon oxide themselves behave similar to the polyimide: it adapts the preferential orientations to the minimal energy state. However small deviations are possible and one can see small deviations from the dominant alignment on a plane silicon surface under certain circumstances.

One can say the silicon alignment is stronger then the PI-2610 but weaker than the nylon, but of course this has to be seen in the temperature context and does not say anything about the strength of the silicon pattern. Therefore, we will have a look at the 2D-grating structures.

3. Two-dimensional gratings

We made a set of gratings by simple etching rectangular holes in the silicon. We varied both pitches through the whole range of 400nm-50µm and this for all possible combinations. This means the aspect ratio varies between 1 and 125. Examples are given in figure 3. Each pixel is a different 50µm x 50µm grating. The fill factor is chosen to be about 80%.

We will restrict the discussion to situations with a top alignment layer with no in-plane preferential orientation. This can be either homeotropic alignment or the polyimide-like planar alignment described in the previous subsection: the results are very similar. We also used alignment layers with strong anisotropic planar alignment but they did not lead to more conclusions about the alignment of the silicon patterns.

The gratings with a high aspect ratio behave very much like very much like the one-dimensional gratings described in the first part of this section. It is however interesting to look at the liquid crystal behavior at the places where the channels end. In fact they can be seen as artificial defects in a normal 1D-grating. Checking for imperfections in a nicely aligned liquid crystal layer is rather easy because when the alignment is parallel to the polarizer, the pixel is completely black and the imperfections light up.
For pitches larger than 1.5µm, we found is a clear disturbance of the ideal alignment at the defects. For smaller pitches then 800nm, the alignment is not disturbed, even while the defect barriers themselves – with width up to few micrometers – were clearly visible in a non-polarized microscope setup. This is an important conclusion for the photonic applications: it shows that a simple etched grating (with a reasonable pitch) can do the alignment for liquid crystal on a waveguide orthogonal to the grating.

On the gratings with squares (aspect ratio 1) between 3µm down to 800 nm the liquid crystal aligns along the diagonal of the structure. This is a more or less predictable result: the planar liquid crystal configuration in a square is known and the average is always along one of the diagonals. For larger pitches there is again no homogeneous alignment, although we still could observe a dominant diagonal alignment inside the squares. Of course, there are two diagonals, so this is another example of a situation were there are two equivalent stable solutions. We remark that even for the very big square, the choice of the diagonal is strongly correlated between several individual squares. This is because in this case the elastic energy in the liquid crystal layer above the borders minimal. Indeed, we observed that by reducing the liquid crystal layer thickness, this correlation was broken.

For squares with smaller pitches, the alignment is along the grating direction (i.e. along the sides of the squares). The fact that there is a pitch dependent difference may be related to the ratio between the pitch and the cell height, but in our case it is more probable due to the fabrication process: for small structures the photolithography will round the edges of the squares, so that it become more cylindrically shaped structures. Liquid crystal alignment in cylinders is more

complex[3]: there are at least six types of solutions, depending on the exact dimensions and even the type of liquid crystal (the elastic constants). In this case, a so-called planar polar configuration Moreover, because the holes here where undeep and there is a thick liquid crystal layer above the pattern, there will be a strong correlation for the exact position of the two "poles" (where the liquid crystal is orthogonal to the cylinder wall): they will attract. Finally, this gives a dominant alignment along a grating direction.

When the aspect ratio of the rectangles is not too high, there may be an alignment that is not the grating directions nor along their diagonals. This effect was only present for the large pitches (>800nm). For smaller pitches the liquid crystal always aligns along the principal axes of the grating. We only found one situation where this gave a homogeneous: 800nm x 1500nm. For larger pitches there was no homogeneous alignment, but a typical alignment pattern within one unit cell.

In the right-hand picture of Figure 3, the pitches were 3µm and 10µm. Although this is clearly a situation where the alignment is not homogeneous, some interesting effects are visualized in this sample. For example, one can see the dominant horizontal alignment: the black region in the middle. The pitch is too large so there is a strong influence of the vertical defect lines. The average alignment is not perfectly horizontal: it is also possible to see a big boundary wall. On the cells above this line, the liquid crystal is, on average, tilted in a slightly different direction as the cells below.

We found very little influence of the etch depth. A possible reason for this is that the top edges of an etched pattern are the most important factor in the alignment effect of this kind of structures[4]. Even the undeeply etched (70 nm) stripe can align the liquid crystal on the flat silicon surface for several micrometers. In fact, this distance is more related to the cell thickness and could be higher if we had taken thicker cells.

5. MULTISTABLE PATTERNS

In order to obtain more insight in the aligning functionality of the silicon geometry, we produced some more complex patterns. Their common property is that they not a single dominant direction. A lot of such patterns are described in litterature[5]. In fact they are similar to the squares described in the previous section.

Figure 4 shows an example of such a pattern. On the left hand side the microscopic pattern is displayed. It has a three-fold symmetry. On the right side, one can see the structure covered with liquid crystal in crossed polarizer setup. The top layer has no preferential alignment, which gives three equivalent alignment states.

The conditions for obtaining the large domains in the 50µm x 50 µm pixel of Figure 4 are critical: when the cooling process after the filling with liquid crystal is too fast, the domains will be much smaller. And when the cell is too thick, only one big domain will form. Therefore, these structures are very useful for optimizing the fabrication process of SOI components covered with liquid crystal.
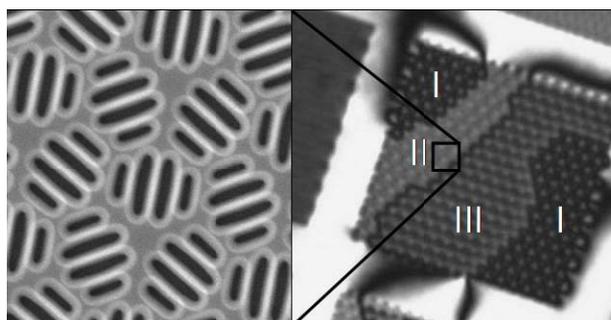
Figure 4: SEM view (left) and view with crossed polarizers (right) of a tri-stable structure in SOI. The size of a unit cell is about 1.6µm
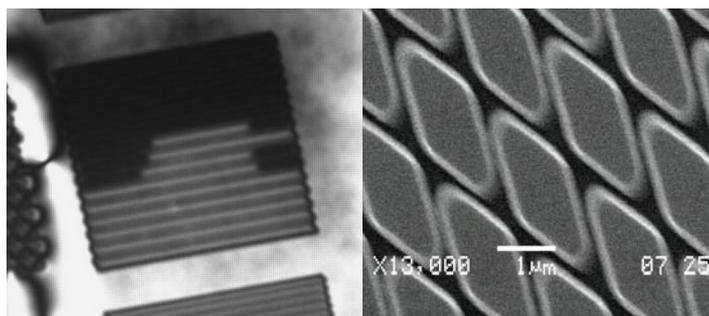
Figure 5: Rhombus based multistable pattern (right: SEM view, left: crossed polarizers)

Figure 5 shows the SEM view and liquid crystal alignment on a structure made of rhombuses. It has two stable states; both are depicted in the figure. Unlike the gratings with the squares, the two states are not orthogonal to each other – this makes it easier for the liquid crystal for moving from one state to another. The polarizers are aligned along the alignment of the upper half, so that part is completely black. As one can see, it has a nice homogeneous alignment. The stripes in the bottom half are due to the variations in the thickness of the liquid crystal layer and the difference in reflection between silicon oxide and silicon: the alignment itself is as homogenous as in the other half of the pixel. The deep-UV technology did not allow the angle between these directions to less then 30° (unless we would end up with an unacceptable vertical pitch), but up this to border we could find a homogeneous alignment along the edge directions of the rhombuses.

The possibility for creating multistable orientations may be important for photonic applications. After all, the use of liquid crystal is restricted to slow applications, like fine tuning a channel or reconfigure an optical connection. This means the component does not has to be electrically connected all the time if the liquid crystal remains in the correct stable alignment state. By applying the correct field (which should be horizontal in our examples), one can switch the component from one state to another once it is has to be reconfigured.

6. CONCLUSION

We examined the alignment of liquid crystal on patterns etched in silicon-on-insulator, fabricated with deep UV photolithography. We found that a textured silicon surface has a strong influence on the alignment of a liquid crystal layer on top of it and that this influence can extend laterally up to several times the etch depth. We discussed the parameters that are important for this effect, like surface treatments and the influence of defects. We also demonstrated that it is possible to fabricate surfaces that allow multiple stable alignments with this technology.

ACKNOWLEDGEMENTS

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