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The Effect of Surface Passivation for Sub-THz Silicon Gradient Refractive Index Lens

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Abstract — This paper describes study of impact of different passivation methods on performance of gradient refractive index (GRIN) lenses. Three different passivation layers on top of lenses are studied: PolySi, PolySi and PECVD silicon oxide (PolySi+SiO₂), and PECVD silicon oxide (SiO₂). Antenna gains and radiation patterns of fabricated lenses are measured. The study shows that passivation methods have strong impact on silicon GRIN lenses performance. A model with a low-resistivity layer on top of high-resistivity Si can explain observed effects.

Keywords — antenna, gradient index, lens, passivation, silicon, THz.

I. INTRODUCTION

Compact low-loss lenses for millimeter and submillimeter-wave beamforming are required for applications in sensing, imaging, and wireless communications [1−3]. A flat high-resistivity silicon gradient refractive index (GRIN) lenses for millimeter and submillimeter wavelengths are proposed for this purpose [4,5]. The GRIN lens is based on modulating the refractive index of the lens material. High-resistivity silicon is used as a substrate with varying sizes of round cylindrical air-filled holes in a hexagonal lattice. As the holes are much smaller than the wavelength, the perforated silicon wafer works as an effective material with refractive index modulated by the size of the holes. An inexpensive deep reactive-ion etching (DRIE) process is utilized for fabrication GRIN lenses [5,6].

The GRIN lens for a millimeter wave radiometer was developed in [7]. High-resistive silicon (HR-Si) with \( \rho > 10 \) kOhm-cm (\( \tan \delta < 6 \times 10^{-5} \) at 250 GHz) were used as lens material. However, the measured antenna gain of the fabricated lens was considerably lower than the simulated one. Impact of difference between fabricated and designed dimensions of the lens and mismatches in a measurement set up was studied but none of these effects could explain quantitatively the observed deviation of the simulated and measured gains. Nevertheless, it was possible to match simulations and experimental results with assumption that Si substrate has a very low effective resistivity of about 20−30 Ohm-cm only. It is unlikely that resistivity of Si can be changed inside of the substrate during processing. Our hypothesis is that degradation of silicon resistivity on surface of the substrate leads to observed degradation of the lens gain.

Silicon of the lens was covered by a native oxide film. It is known that oxidized HR-Si suffers from surface charge effects [8]. Charges gather close to the Si/SiO2 interface, lowering the resistivity of the silicon surface by several orders of magnitude [9]. The similar effect is observed even for case of passivation of Si surface [10]. Impact of lowering the resistivity of the silicon surface on performance of high frequency integrated circuits was studied earlier [8,9]. We can assume that the effect of charge could be even more significant for GRIN lenses because a surface area of Si raises tremendously in the case of GRIN lenses due to a porous structure and numerous etched holes of the lens which increase surface area of Si considerably. Further, the used etching method, Deep Reactive Ion Etching (DRIE), results in a rough Si surface not following the Si crystal planes, making the surface more susceptible to non-idealities. Thus, for successful use of HR-Si in GRIN lenses, one needs to minimize effect of the surface charge for example through passivation of the Si surface, especially in the etched holes.

In this work we, for the first time, study impact of different types of passivation layers on silicon surface on performance of GRIN lenses and proposing an optimal passivation method. Three different passivation layers on top of lenses are studied: PolySi, PolySi and PECVD silicon oxide (PolySi+SiO₂), and PECVD silicon oxide (SiO₂) (see descriptions on next page). These passivation layers are selected because they demonstrate the highest efficiency to suppress lowering resistivity of the silicon surface due to surface charge effects [10]. A lens without any passivation is studied for reference also.

II. LENS DESIGN

The gradient-index lens design was described in detail in [7]. The refractive index of a gradient-index lens is given by

\[
n(\rho) = \frac{n_0}{\cosh \beta \rho},
\]

where \( n_0 \) is refractive index at the center of the lens, \( \beta = 2\pi/\lambda \), \( \lambda \) is wavelength, and \( \rho \) is radial distance from the lens axis [11]. The lens is targeted for radiometer applications in which the feed antenna is placed at the focus directly on the silicon wafer or integrated on a monolithic microwave integrated circuit (MMIC). Thus, the lens consists of a solid silicon part having a perforation part on top. Starting from a chosen 675-µm thickness for the solid silicon wafer and the 3-mm diameter for the lens, the lens permittivity gradient profile was first optimized with ray-tracing principles in Zemax OpticStudio [12]. The final optimisation was done in 3D electromagnetic...
(EM) software CST Microwave Studio [13]. The lens dimensions were chosen as a compromise between size, directivity and antenna gain. The optimized lens with diameter of 3 mm has a solid silicon part with thickness of 675 μm stacked together with a perforated wafer with thickness of 1250 μm, see Fig. 1(a).

The permittivity gradient for the lens is achieved by DRIE etching different-sized holes in the silicon wafers. The hole sizes of the lens are determined from the unit-cell simulations. The holes are placed in a hexagonal grid with a 200-μm cell diameter. The hole diameters vary from 38 to 150 μm. In the perforated wafers due to variation of hole sizes, the relative permittivity \( \varepsilon_r \) varies between 3.5−11.6. The final lens geometry is shown in Fig. 1(b).

Fig. 1. Gradient-index (GRIN) lens: (a) Simulation model. Thin (2 μm) low-resistivity layers in the perforation inner walls are shown in green color in perspective view. (b) Micrograph of a manufactured lens from the front side. Passivation layers are not visible in this scale.

III. LENS MANUFACTURING

Deep reactive-ion etching is utilized for fabrication GRIN lenses. Four lenses with the same geometry were fabricated: a reference lens without passivation and three lenses with different passivation layers. The etching process results in non-uniform hole diameter with larger diameter on the side etched first. To minimize the variation of the holes diameters along the etched paths the perforated part of the lens was constructed from four thinner wafers, 313-μm thick of each. So finally, the manufactured lenses consisted of 5 different wafers stacked together.

The perforation process wafers were DSP (Double Side Polished) HR-Si (> 10 kΩ·cm) wafers. The process wafers were thinned down to the required thickness by mechanical grinding and CMP (Chemical Mechanical Polishing). Alignment marks were first dry etched on the front side of the wafers. The lithography was performed by using a Contact Mask aligner and 150-mm masks. The lens holes were defined by lithographically patterning and dry etching of 2000-nm thick silicon dioxide (SiO\(_2\)) hard mask grown by thermal oxidation. The GRIN lens holes were etched through the wafer using single-sided two-step DRIE Bosch etch process and the above-mentioned silicon dioxide layer as hard mask. The DRIE etch was stopped on the backside where a 2000-nm thick PECVD (Plasma Enhanced Chemical Vapor Deposition) layer was deposited as a stop layer.

After the DRIE etch polymers and all silicon oxide (SiO) were removed using a plasma stripper, chemical removal and 50-% HF. After the removal wafers were wet cleaned and thermal oxidized twice at 1050 °C for smoothing of etched surfaces and removal of chemical impurities.

Three different passivation layers were deposited over fabricated wafers for passivation of the surfaces of the wafers, including the surfaces of the etched holes:

1) **PolySi**
   A 900-nm thick Low Pressure Chemical Vapor Deposition (LPCVD) amorphous silicon layer deposited over the wafer.

2) **PolySi+SiO\(_2\)**
   The above-mentioned PolySi layer covered by a 1000-nm thick PECVD silicon oxide layer deposited at 300 °C.

3) **SiO\(_2\)**
   A single 1000-nm thick PECVD silicon oxide layer deposited at 300 °C.

4) **no-pass**
   A wafer without any passivation for reference.

The wafers containing the GRIN lenses were finally diced into 10-mm × 10-mm chips using mechanical sawing. The lens stack is held together using custom brass holders as is shown in Fig. 1. In future, we are planning to use wafer-level bonding technique for manufacturing lens arrays.

IV. RESULTS AND DISCUSSION

A custom WR-3 (220−325 GHz) waveguide test fixture, a spacer plate and a holder plate were designed and manufactured for RF testing of the lenses (see Fig. 2). The fixture has a flange with diameter of 40 mm. The 10-mm × 10-mm lens chips are positioned with a 1.925-mm thick spacer plate and a holder plate with 10-mm × 10-mm opening rotated by 45 degrees to hold the chip in place at its corners. The perforated part of the lens consisted of 4 stacked GRIN wafers 313-μm thick each on top of a solid 675-μm silicon wafer.

Fig. 2. WR-3 waveguide fixture for RF testing of the GRIN lens. (a) Schematics of the holder and the GRIN lens. Passivation layers are illustrated in green color (not in scale). (b) Photograph of the fixture with the lens.

\( S_{11} \)-parameter and radiation pattern of the lenses were measured. The \( S_{11} \)-parameter were measured using a vector network analyzer with an H-band (220−325 GHz) frequency extender. The radiation patterns were measured using a near-field scanner. Near-field scanner set up is described with details, for example, in [14]. Antenna gain of the lens was determined

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through three-antenna measurements using Pickett-Potter horn and open-ended waveguide as the two other antennas [15].

A. S-parameters

The simulated and measured $|S_{11}|$ of the GRIN lenses with different passivations are shown in Fig. 3. Strong standing wave phenomenon can be observed due to impedance mismatch between air-filled WR-3 and silicon body of the lens. However, a decent input matching occurs around specific frequencies such as 263 GHz and 284 GHz at which the $|S_{11}|$ is between -8 dB and -12 dB. The simulation is in accordance with the measurement and the measurement results for all passivation types are very similar which implies that $|S_{11}|$ is mainly dominated by the waveguide-silicon interface.

![Fig. 3. Simulated (s.) and measured (m.) $|S_{11}|$ of the GRIN lens with different passivations.](image)

As mentioned, the WR-3 is used for testing purposes only. Later the lens will be integrated with an on-chip antenna patterned on top of a silicon substrate. When mounted on the bottom side of the lens, the on-chip antenna is impedance matched with the silicon lens and standing-wave phenomenon seen in Fig. 3 is significantly reduced.

B. Radiation patterns

The simulated (s.) and measured (m.) maximum antenna gains as a function of frequency for different passivations are presented in Fig. 4. For the passivations PolySi and PolySi+SiO$_2$ the gain of about 10.5-12 dBi is measured around 260 GHz. For the SiO$_2$ passivation the gain is 9.7 dBi at maximum. Without any passivation (no-pass) the maximum gain is only 8.4 dBi at 265 GHz. A similar behaviour can be seen around 285 GHz. The simulation for the lens without passivation (10 kΩ cm Si resistivity) gives 13.5 dBi at 261 GHz. For all types of passivation the measured gains are considerably lower than simulated.

![Fig. 4. Simulated (s.) and measured (m.) maximum antenna gain as a function of frequency for the GRIN lens with different surface passivations. Simulations are without passivation (no-pass) and with 0.2 Ω cm, 0.5 Ω cm, 1 Ω cm surface resistivities.](image)

Simulated and measured radiation patterns for the GRIN lens with different surface passivations are presented in Fig. 5 at 263 GHz. It can be observed that the measured E-plane beam shapes and beam widths are varying for different surface passivations. The beam is the narrowest for the PolySi passivation and the widest for the lens without passivation. However, the measured H-plane patterns are very similar for all passivations and the beamwidths are almost the same. Similar behavior was observed also at other frequencies. Simulated and measured patterns have a good correspondence with the PolySi passivation (Fig. 5(a)-(b)) and for the other passivations in the H-plane. More differences can be observed in the E-plane patterns. The measured -10-dB beamwidths in E- and H-planes are summarized in Table I.
A new model is suggested to investigate a possible reason for the degradation of the antenna gain and the E-plane patterns. We use a simulation model where there are 2-μm thick conductive layers on the etched surfaces of the holes in the GRIN lens. Such layers would represent free charges in a surface layers of wafers. With the model we observed that in case of decreasing the resistivity of the surface conductor, the antenna gain is decreased, as expected (Fig. 4). The resistivity values in simulation for each passivation type were determined from the simulated corresponding maximum antenna gain matching with the measured one. The approximate matching values in simulations are: 1 Ω cm for passivations PolySi and PolySi+SiO$_2$, and 0.2 Ω cm for wafers with SiO$_2$ or no passivation. In addition, the model explains behaviour of the radiation pattern also (see Fig. 5). It should be noted that the model is representative and not supposed to be highly accurate since a real distribution of charges in silicon wafers is not known. However, the model helps to explain the characteristics of the GRIN lens when different surface passivation methods are used.

Simulation of current distribution around holes showed that the current distribution is asymmetrical. The horizontal currents cancel each other. But the E-plane oriented currents contribute in radiation together with the lens. Thus, the total net sum current is vertical (E-plane oriented) when considering all the holes symmetrically around the lens axis. The magnitude of the currents depend on the resistivity and thus the passivation type. The effect is much stronger for a surface layers with lower resistivity. Such current distribution probably explain the observed differences in the measured E-plane patterns. The beam widening can be also observed in the simulation results.

Thus, presence of lower resistivity on the surface layer of HR-Si allows to explain both degradation of the lens gains and wider E-plane radiation pattern. The results show that PolySi and PolySi+SiO$_2$ passivations are the most effective and give the best GRIN lens performance. The SiO$_2$ passivation is not as effective than the aforementioned but gives better performance than the lens without any passivation.

V. CONCLUSION

A GRIN lens antenna operating at sub-THz frequencies is developed for radiometer applications. Three different types of silicon surface passivation mechanisms were studied. The results show that the passivation has a strong impact on the performance of the GRIN lens. The polysilicon (PolySi) passivation seems a promising candidate but further studies are required for maintaining even higher resistivity for silicon wafers and ensuring an optimal performance when processing the GRIN lenses.

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