Broadband Antireflective Structures for the THz Spectral Range Fabricated on High Resistive Float Zone Silicon

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Abstract—**Antireflective structures for a spectral range from 0.1-1.2 THz are applied to the surface of high resistive float zone silicon by deep reactive ion etching. Binary hexagonal and rectangular structures yield an increase in the pulse maximum of the electric field strength of about 20 percent for one structured surface.**

I. Introduction And Background

High resistive float zone (HRFZ) silicon is used as lens material in the THz spectral range to couple THz radiation out of the emitter and into the detector. The refractive index is 3.4175 for the spectral range of 0.5-4.5 THz and the power absorption coefficient is below 0.01 cm^{-1} for 0.2-1 THz and below 0.025 cm^{-1} for 0.2-2 THz[1]. The Fresnel loss of the transmitted intensity on normal incidence is about 30 percent.

Surface structures with a period smaller than the wavelength of the radiation can be used to increase the transmission[2]. An antireflective structure works as a bandpass filter: The minimum wavelength is determined by the grating period and the maximum wavelength is determined by the structural depth. For wavelengths smaller than the minimum wavelength a fraction of the intensity is diffracted into higher diffraction orders. For wavelengths larger than the maximum wavelength the structure has no effect because it is not deep enough. In an extreme case the structure works as a surface roughness.

Antireflective structures can be achieved by a continuous profile like pyramids or a step profile. A continuous profile requires positive slopes.

As an example for an antireflective pyramidal structure for the spectral range from 0.1-1.5 THz and arbitrary angle of incidence a structural period of 45 µm and a structural depth of 500 µm are required. This results in a slope of 2.57°. The fabrication of these structures requires a special adaption of the etching process. As starting point deep binary structures with a depth up to 500 µm were manufactured on 1 mm thick 4-inch HRFZ silicon wafers. For manufacturing a gas chopping method based on the so called BOSCH®-process was used, where passivation and isotropic etching cycles alternate.

As grating type the rectangular grating with equal fill factor in both directions parallel to the surface, and the hexagonal grating were chosen (see Figs. 3 and 4).

These structures work for the given spectral range as uniaxial medium with the extra-ordinary axis perpendicular to the surface[3]. At normal incidence both polarization directions experience the same refractive index and thus the structure works like a homogeneous layer with an effective index. These structures are polarization independent for normal incidence.

The refractive index required for maximum transmission is: $n_{eff} = \sqrt{n_i n_s} = 1.85$, with n_i – the refractive index of the incident medium (n_i = 1 for air) and n_s – the refractive index of the substrate material (HRFZ silicon).

With the fill factor the effective index of the structures can be adapted. For the rectangular grating the fill factor is defined as ratio of the edge-length of the pillars to the grating period. For the hexagonal grating the fill factor is defined as ratio of the diameter of the pillars to the grating period. The fill factors for the two dimensional gratings were determined with the method described in [3]. This method is based on rigorous coupled wave analysis (RCWA). Therewith, the fill factors were calculated to 0.79 for the rectangular and 0.74 for the hexagonal grating, respectively.

For both grating types a grating period of 50 µm was chosen. At normal incidence these structures work as zeroth-order diffraction grating for frequencies lower than 1.752 THz for the rectangular grating and for frequencies lower than 2.023 THz for the hexagonal grating.

The depth of the structure depends on the gradient of the refractive index. For a continuous gradient of the refractive index like a pyramidal taper or cones the depth of the structure should be about 0.2 times the largest wavelength. The spectrum of the THz pulse has its maximum amplitude around 0.4 THz (wavelength 750 µm) and the spectrum reaches from 0.1-2 THz (wavelengths 150-3000 µm). As a compromise, a structural depth of 500 µm was chosen. This structural depth provides that the structure has an antireflective effect for frequencies higher than 0.12 THz (wavelength 2500 µm), in theory.

II. Measurements And Results

The measurements were made in the collimated beam of a standard THz time domain spectroscopy setup consisting of four off-axis parabolic mirrors.

Fig. 1 shows the measured waveforms for the unstructured sample, the sample with a binary rectangular structure on one side, and the sample with a binary hexagonal structure on one side. The small oscillations in the waveforms are due to the water vapor in the air. The pulse maximum shows an increase of 21.7% for the rectangular structure and 20.2% for the hexagonal structure. Fig. 2 shows the ratio of the spectral electric field amplitude of the unstructured to the structured sample for the hexagonal and rectangular structure, respectively. Before applying the FFT the pulses were cut

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directly after the main pulse such that only the direct transmission can be compared and no modulations appear. In theory, the ratio of the electric field amplitudes at normal incidence is:

$t_{unstructured} / t_{structured} = (t_{1,u} t_{2,u}) / (t_{1,s} t_{2,s} t_{3,s}) = 0.9192$, with t – the amplitude transmission coefficient at the respective surface (see inset Fig. 1). Fig. 2 shows that the structure works almost as predicted in the range from 0.3-1 THz. Below 0.2 THz the structure is not deep enough and above 1.2 THz the structure causes diffraction into higher diffraction orders. Furthermore, the signal-to-noise ratio of the measuring signal increases strongly for frequencies above 1 THz. This is also caused by the water absorption lines in the spectrum. The deviation from the predicted value is also due to the slope of the structures, which can be observed in Figs. 3 and 4, and due to the behavior of the structure as effective medium. The theoretical curve is only valid in the quasi-static limit, i.e. for very small ratios of the grating period to the wavelength. For the high frequencies of the spectrum the grating is not in the quasi-static limit[4]. Then, the behavior of the grating can only be predicted by RCWA.

Figs. 3 and 4 show the hexagonal and rectangular structure, respectively. The etching depth of the hexagonal structure is about 500 µm, the grating period is 50.3 µm, and the diameter of the pillars is 35.7 µm. A slight slope of the pillars can be observed. After 1400 etching cycles (nearly 9h process time), the etching mask was removed. The etching depth of the rectangular structure is also about 500 µm, the grating period is about 50 µm, and the width of the pillars is 39.4 µm.

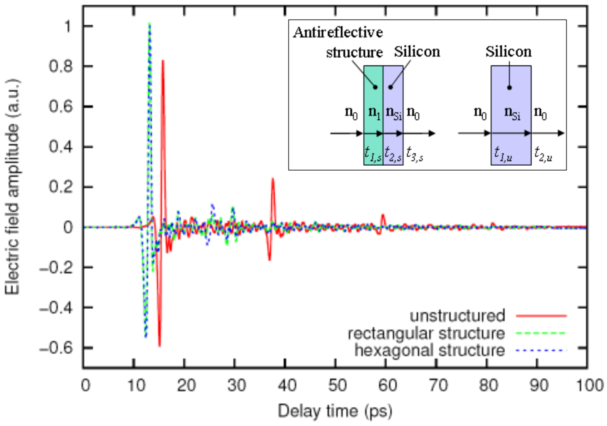

Fig. 1: Measured waveforms of the electric field strength of the unstructured sample, the sample with a binary rectangular structure and the sample with a binary hexagonal structure. The inset shows the electric field transmission coefficients for the structured and unstructured sample.

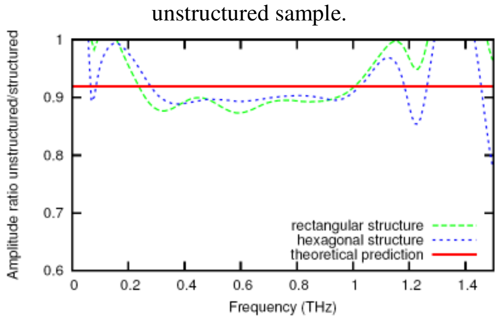

Fig. 2: Spectral analysis: Ratio of the electric field amplitudes of the unstructured and the structured sample for the rectangular and the hexagonal structure. The blue line shows the theoretical prediction for a homogeneous layer with a refractive index of n = 1.85.

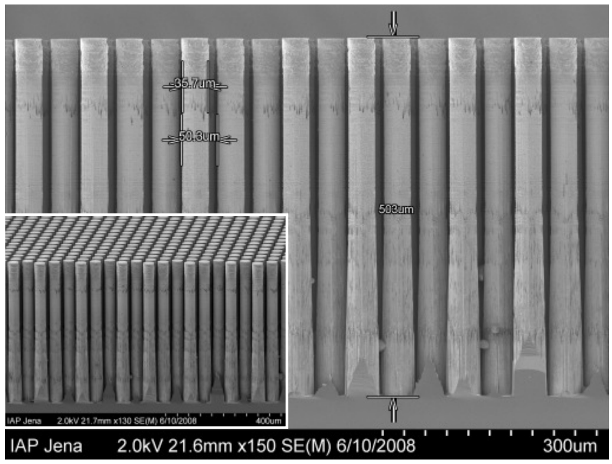

Fig. 3: Cross section view of the hexagonal structure. The depth of the structure is 503 µm, the grating period is 50.3 µm, and the diameter of the pillars is 35.7 µm. The etching mask was removed. Nearly the whole 4-inch Si-wafer consists of the shown pillars. The inset shows the structure under 15° tilt angle.

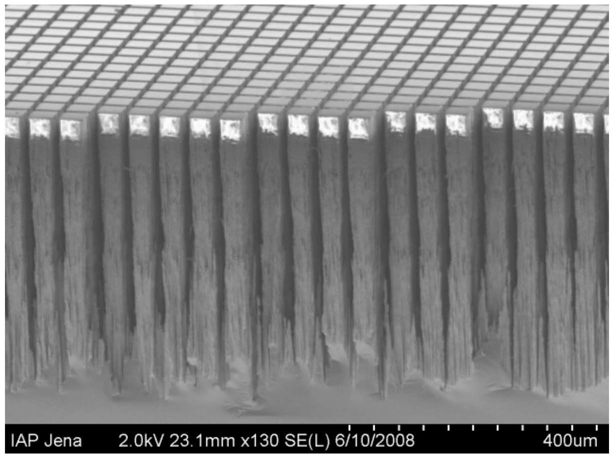

Fig. 4: SEM-image of the etched rectangular structure. Because of the (110)-orientation of the Si-wafers the cross section is not ideal.

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