

# Broad band infrared spectroscopy of grooved silicon

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## ABSTRACT

Grooved silicon (gr-Si) structures with a period of few micrometers, which were formed by anisotropic etching of (110) Si wafers, have been investigated by means of broad band infrared (IR) and submillimeter transmission spectroscopy. In the spectral region of 50-1000  $\mu\text{m}$  the results are well explained by an effective medium model, which predicts a strong birefringence with a difference between refractive indices for ordinary and extraordinary beams to be about 0.73-0.77. The IR transmission of gr-Si in the range from 1 to 30  $\mu\text{m}$  is strongly influenced by light scattering. The experimental results measured in the region 1-5  $\mu\text{m}$  can be understood in the terms of the geometric optics.

**Keywords:** IR spectroscopy, anisotropic silicon structure, effective medium model

## 1. INTRODUCTION

Gr-Si structures are usually formed by anisotropic etching of (110)-oriented c-Si wafers in alkaline solution<sup>1,2</sup>. Since gr-Si consists of Si layers alternating with empty regions (grooves) with typical thickness of about several micrometers there is a periodicity in the refractive index and a one dimensional photonic band gap (PBG) appears in the spectral range of the order of the grooves period<sup>3</sup>. The PBG appears in gr-Si when the incident light falls along the direction normal to Si layers or grooves. If the incident light shines in the direction along Si layers and grooves the optical properties of gr-Si are strongly anisotropic<sup>4</sup>. In terms of effective optical media this material is a uniaxial birefringent crystal with an optical axis perpendicular to the grooves<sup>5</sup>. The birefringence found in gr-Si is several times stronger than that known for other types Si-based micro- and nanostructures such as porous Si<sup>6</sup> and Si/SiO<sub>2</sub> superlattices<sup>7</sup>. However the reported birefringence strength (the maximal difference between the refractive indices for ordinary and extraordinary waves) in gr-Si was nearly two times larger than it should be accordingly to the conventional effective media model (EMM)<sup>4</sup>. In the present work we have investigated the optical transmittance in several samples of gr-Si in the wide spectral range from 1 to 1000  $\mu\text{m}$  in order to explore the possibilities of the unusually strong birefringence of these structures and to formulate an adequate model to explain this property.

## 2. EXPERIMENTAL

Gr-Si structures were prepared on substrates of (110) c-Si wafer with specific resistivity of 20-100 Ohm-cm. The anisotropic chemical etching was performed in 44% aqueous solution of KOH at 70<sup>0</sup> C for 4 hours. A photolithography process was used to form the patterns and a thermal oxide of 0.8-0.9  $\mu\text{m}$  thick served as a mask during the etching (see for details<sup>2,3</sup>). A part of the microscopical optical image of the top of our sample is shown in Figure 1 (a) where black and white regions are grooves and non-etched Si parts, respectively. Si stripes, which are tilted to the grooves and periodical with a period of 200  $\mu\text{m}$ , serve as hardness ribs. Samples parameters are listed in Table 1. The thicknesses of gr-Si layer and substrate (see Fig.1b) are  $l = 30 \mu\text{m}$  and  $L = 170 \mu\text{m}$ , correspondingly.

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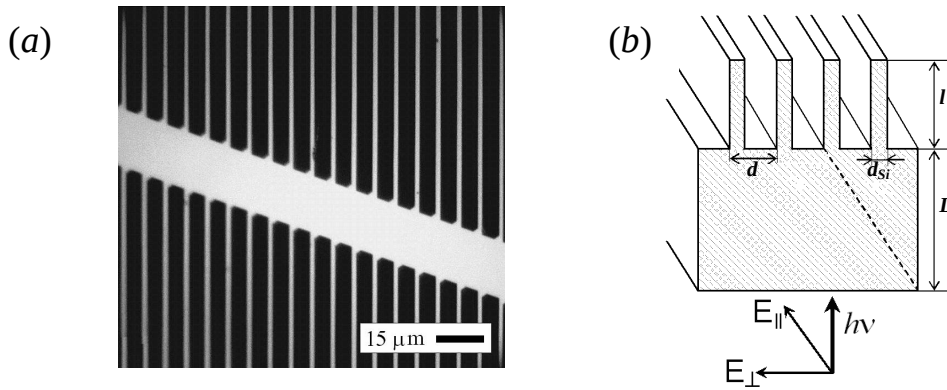


Figure 1: (a) Top view of a sample of gr-Si; (b) sketch of the sample cross section and geometry of the optical transmission experiment, where  $d$  and  $d_{Si}$  are the groove period and thickness of Si walls, respectively.

Fig. 1b represents a sketch of the sample cross section as well as the direction of incident radiation and used orientations of its electric field. Optical transmission measurements were done at normal incidence for light polarized along and perpendicular to the grooves. For comparison the optical transmittance of the substrate was measured. A Bruker FTIR spectrometer was used for the measurements in the range from 1 to 500  $\mu\text{m}$  (wave numbers  $\nu=10000\text{-}20\text{ cm}^{-1}$ ). A sub-millimeter (sub-mm) spectroscopy setup was employed for the spectral range of 500-1000  $\mu\text{m}$  ( $\nu=20\text{-}10\text{ cm}^{-1}$ ). The measurements were carried out in air or in vacuum at room temperature.

Table 1. Structure parameters of the samples and their refractive indices calculated in the framework of EMM, where  $n_{\parallel}$  and  $n_{\perp}$  are those for the light polarized along and perpendicular to grooves.

| Sample | $d\ (\mu\text{m})$ | $d_{Si}\ (\mu\text{m})$ | $n_{\parallel} = \sqrt{\epsilon_{\parallel}}$ | $n_{\perp} = \sqrt{\epsilon_{\perp}}$ | $\Delta n = n_{\parallel} - n_{\perp}$ |
|--------|--------------------|-------------------------|-----------------------------------------------|---------------------------------------|----------------------------------------|
| 1      | 4                  | 1.0                     | 1.91                                          | 1.14                                  | 0.77                                   |
| 2      | 7                  | 1.6                     | 1.85                                          | 1.12                                  | 0.73                                   |

### 3. EFFECTIVE MEDIUM MODEL

Before presenting the experimental data it is useful to underline the main prediction of EMM for the gr-Si structures investigated. First of all, the grooved layer can be considered as a homogeneous effective medium for the electromagnetic radiation with wavelength  $\lambda \gg d, d_{Si}$ . This allows us to calculate the effective dielectric function by using the following formula:

$$\epsilon_{\parallel} = f_1 \epsilon_1 + f_2 \epsilon_2, \quad \epsilon_{\perp} = \frac{\epsilon_1 \epsilon_2}{f_1 \epsilon_2 + f_2 \epsilon_1}, \quad (1)$$

where  $\epsilon_{\parallel}$  and  $\epsilon_{\perp}$  are the principal components of the effective dielectric function  $\epsilon$ , when the electric field vector is parallel and perpendicular to the grooves, respectively;  $\epsilon_1 = 11.7$  and  $\epsilon_2 = 1$  are the dielectric functions of Si layers and grooves, respectively;  $f_1 = d_{Si}/d$  and  $f_2 = 1 - f_1$  are the corresponding filling factors. The effective refractive indices of gr-Si, i.e.  $n_{\parallel}$  and  $n_{\perp}$ , as well as the birefringence value of  $\Delta n = n_{\parallel} - n_{\perp}$  are listed in Table 1.

#### 4. EXPERIMENTAL RESULTS AND DISCUSSION

Figure 2 shows typical polarisation-resolved transmittance spectra of a gr-Si sample measured in the broad spectral range. The transmittance is modulated by oscillations, which are caused by interference in the gr-Si layer and substrate. A decrease of the mean transmittance with decreasing wavelength is obviously related to scattering of the IR radiation. An abrupt drop of the transmittance at  $1\text{ }\mu\text{m}$  can be attributed to band gap absorption in c-Si walls and substrate.

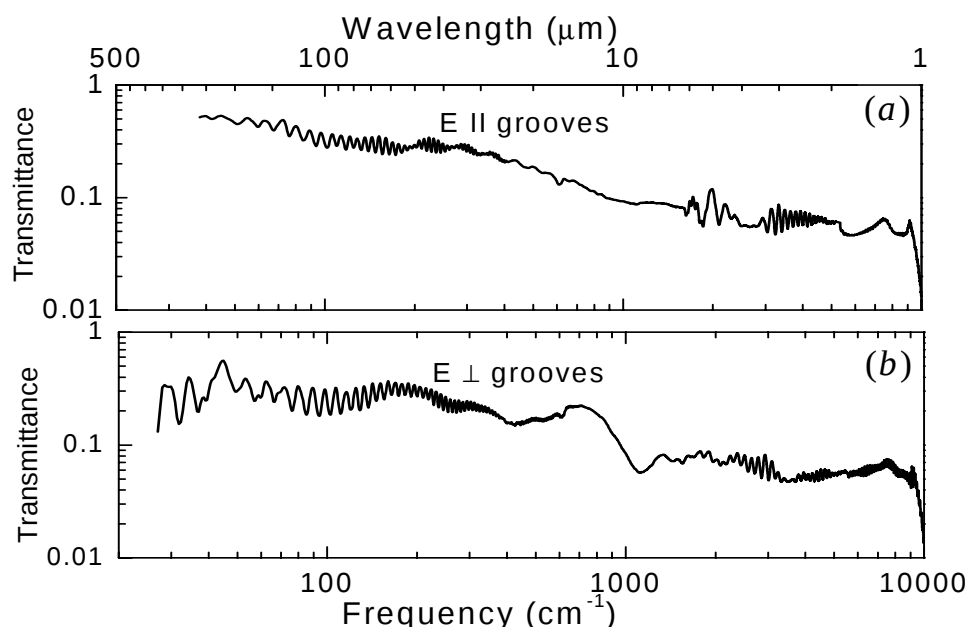


Figure 2: Transmittance spectra of a gr-Si sample detected for light polarized along (a) perpendicular and (b) to the grooves.

As one can see from Fig. 2 there is a distinction between the interference fringes for different polarization directions, this is caused by anisotropy of the effective dielectric function of gr-Si. This anisotropy is discussed below in more detail, starting from the low frequency region.

The transmission coefficient and phase shift of gr-Si detected in the sub-mm spectral range for different polarization directions are shown in Figure 3. The data for the substrate, which is not polarization dependent, is also plotted. The transmission of gr-Si is larger in comparison with the substrate (see Fig 3a) because of the Fresnel's factor related to the phase shift of sub-mm radiation in the grooved layer, which acts as a homogeneous effective medium in this spectral range. For gr-Si both the transmission and phase shift are sensitive to the polarization direction of sub-mm radiation. Note, the transmission coefficient of the substrate does not depend on polarization due to an isotropic cubic lattice of c-Si.

Fitting of the experimental data have been performed by considering the investigated structure as a two layer system (grooved layer of thickness  $l$  on c-Si substrate of thickness  $L$ ). The multiple interference and interference in each layer cause a phase shift of gr-Si, which generates an interference pattern in transmittance spectra of samples. We omit the exact expressions used for fitting due to their complexity (see Ref.<sup>5</sup> for details). By using real  $\epsilon'$  and imaginary  $\epsilon''$  parts of the effective dielectric function as fitting parameters the experimental transmittance spectra were simulated: the interference pattern gives us the real part of the dielectric function  $\epsilon'$  whilst the absolute value of the transmittance gives us the imaginary part of dielectric function  $\epsilon''$ . This fact allows us to analyze these two functions independently.

It has been found that the transmittance of gr-Si in the sub-mm spectral range is dependent on the free carrier density. Our experiments with the samples excited by laser irradiation at 0.532  $\mu\text{m}$  showed a decrease of the transmission coefficient for sub-mm radiation polarized along grooves, while the transmission coefficient for the perpendicular polarization was not significantly changed. These results indicate a possibility to create optically pumped modulators and switches based on gr-Si.

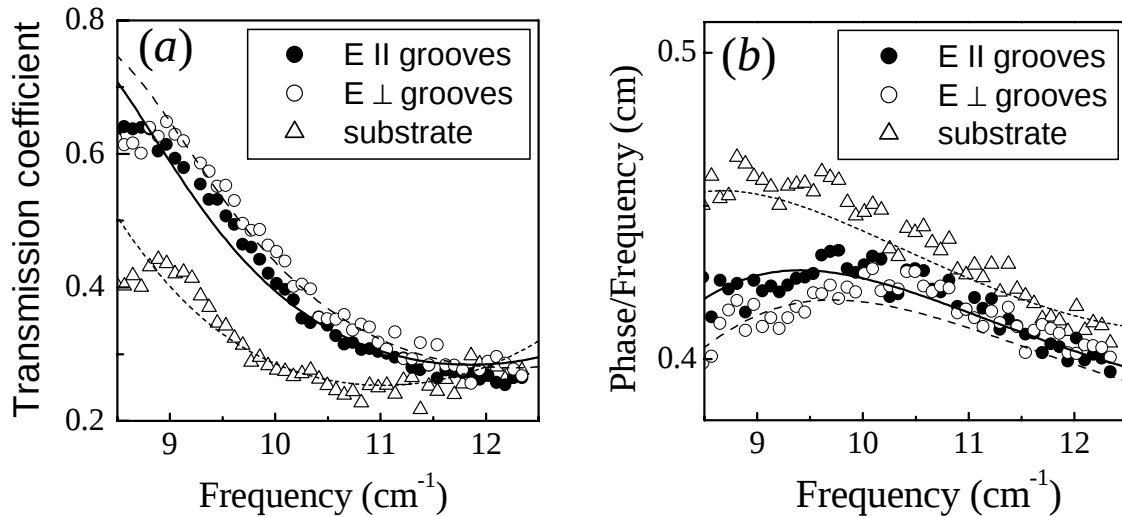


Figure 3: Spectra of the transmission coefficient (a) and phase shift divided on frequency (b) for the gr-Si with  $d = 7 \mu\text{m}$  as well as for the substrate. Points and lines are experimental data and EMM fits, respectively.

Far-IR spectra of the transmission coefficient of a gr-Si measured for different polarization directions are shown in Figure 4. The transmission coefficient is spectrally modulated because of interference in the substrate as well in the gr-Si layer. On the one hand, the smaller period of the fringes is not dependent on the polarization direction and it is obviously related to the interference in the substrate:  $\Delta\nu_0 = (2L \cdot n_{\text{Si}})^{-1}$ , where  $n_{\text{Si}} = 3.4$  is the refractive index of c-Si. On the other hand, the larger period oscillations correspond to interference in the gr-Si layer:

$$\Delta\nu_{\parallel} \approx (2l \cdot n_{\parallel})^{-1} \text{ and } \Delta\nu_{\perp} \approx (2l \cdot n_{\perp})^{-1}. \quad (4)$$

As we say, in the whole far-IR range the experimental data can be explained as a result of interference in a two-layered system of gr-Si/substrate. The real part,  $\epsilon'$ , of the effective dielectric function is significantly larger than the imaginary one,  $\epsilon''$ , in agreement with the low doping level of the samples. Therefore the transmittance is mainly determined by  $\epsilon'$ . The non-monotonic dependence of both  $\epsilon'$  and  $\epsilon''$  at lower frequencies can be attributed to the scattering of IR radiation on the hardness ribs of the samples. Additionally, the scattering effect is stronger for light whose wavelength is closer to the groove period, e.g. for the sample with  $d = 7 \mu\text{m}$  in the higher frequency region. This effect is probably responsible for the normal dispersion of  $\epsilon'$  visible in Fig. 4 (a).

Spectra of the refractive indices of gr-Si obtained from the corresponding spectra of  $\epsilon'$  and  $\epsilon''$  are plotted in Figure 6. In the range of 100-300  $\text{cm}^{-1}$  the refractive indices are close to those predicted by EMM and given in Table 1. The difference between the refractive indices obtained by fitting the transmittance spectra and the values calculated by using Eq.(1) can be explained by an artificial dispersion of gr-Si, which is related to the scattering phenomenon. In the lower

frequency range the scattering is caused by interaction of the IR light with the hardness ribs as is discussed above for  $\epsilon'$  and  $\epsilon''$ .

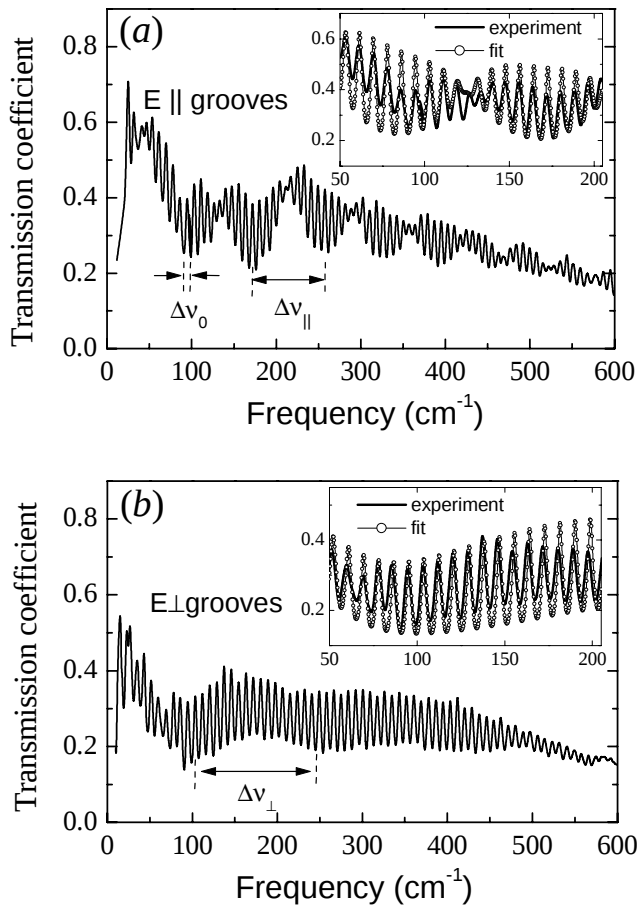


Figure 4: Transmission spectra of the sample with  $d = 7 \mu\text{m}$  measured for the IR radiation polarization along (a) and perpendicular (b) to the grooves. Insets show selected parts of the spectra and their fits, assuming the dispersion of the effective dielectric function.

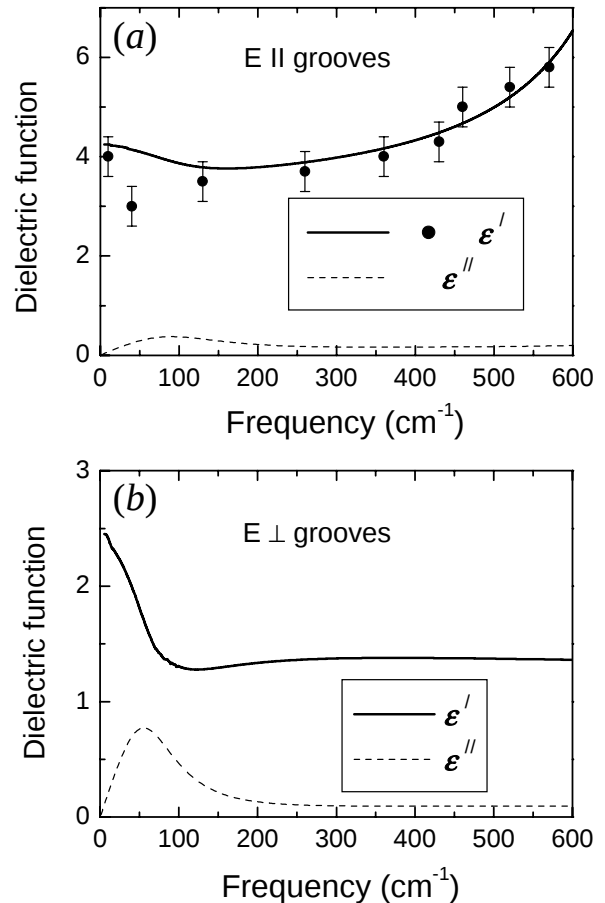


Figure 5: Dielectric function spectra of the samples with  $d = 7 \mu\text{m}$  (a) and  $d = 4 \mu\text{m}$  (b) obtained from the fits of the corresponding transmission spectra. Points in panel (a) are obtained from the interference fringes period accordingly to Eq. (4).

Transmittance spectra of the samples in the middle IR range are plotted in Fig. 7. The absolute value of the transmittance is pretty low due to the scattering. The period of interference fringes  $\Delta\nu$  observed for both samples does not significantly depend on the polarization of IR radiation. The transmittance oscillations are a result of the interference between the beams passed through the grooves and the beams transmitted via the Si walls (see inset of Fig. 7). In fact,  $\Delta\nu \approx [l \cdot (n_{\text{Si}} - 1)]^{-1}$ .

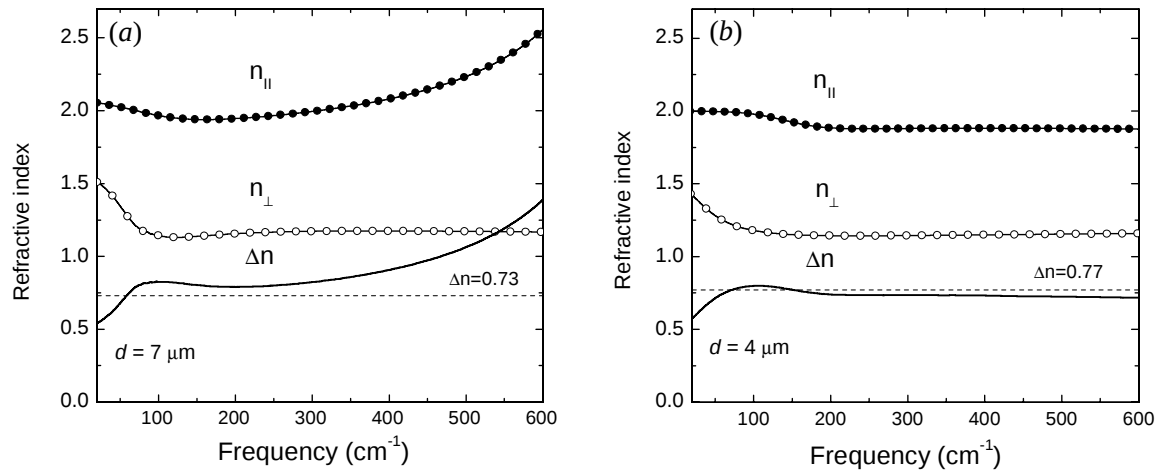


Figure 6: Refractive indices of gr-Si with  $d = 7 \mu\text{m}$  (a) and  $d = 4 \mu\text{m}$  (b) obtained from the fits of the transmission spectra. Dashed lines represent the birefringence values calculated accordingly to Eq. (1).

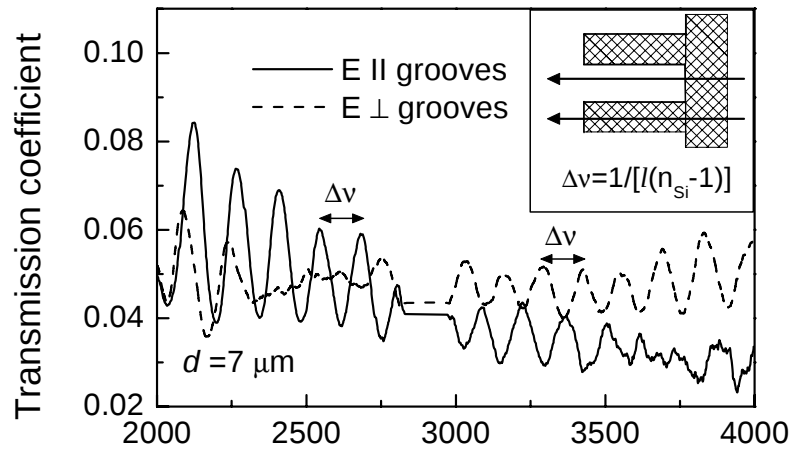


Figure 7: Transmittance spectra of gr-Si with  $d = 7 \mu\text{m}$  in the middle IR range. Inset shows a sketch of the gr-Si structure as well as beam propagation in accordance with the geometrical optics approximation.

## 5. CONCLUSIONS

The anisotropy of the transmittance of gr-Si in the IR and sub-mm spectral range is well explained by using a set of models, which consider the interference of light in gr-Si. The calculations based on EMM agree with the experimental data in the spectral range where the light wavelength is much larger than the dimensions of the inhomogeneities of the material. In general the scattering of light can result in an artificial dispersion of the effective dielectric function and then an unusually strong birefringence can appear.

## ACKNOWLEDGMENTS

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