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Abstract: A terahertz-absorbing thin-film stack, containing a dielectric Bragg reflector and a thin chromium metal film, was fabricated on a silicon substrate for applications in bi-material terahertz (THz) sensors. The Bragg reflector is to be used for optical readout of sensor deformation under THz illumination. The THz absorption characteristics of the thin-film composite were measured using Fourier transform infrared spectroscopy. The absorption of the structure was calculated both analytically and by finite element modeling and the two approaches agreed well. Finite element modeling provides a convenient way to extract the amount of power dissipation in each layer and is used to quantify the THz absorption in the multi-layer stack. The calculation and the model were verified by experimentally characterizing the multi-layer stack in the 3-5 THz range. The measured and simulated absorption characteristics show a reasonably good agreement. It was found that the composite film absorbed about 20% of the incident THz power. The model was used to optimize the thickness of the chromium film for achieving high THz absorption and found that about 50% absorption can be achieved when film thickness is around 9 nm.

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1. Introduction

Interest in the THz spectral range for imaging applications prompted the fabrication of detectors that are sensitive in this frequency band which covers from about 100 GHz to 10 THz [1]. THz imaging has become very attractive for security applications due to its non-ionizing nature and the ability to penetrate through most textiles currently in use. The non-ionizing nature makes this radiation virtually harmless to human tissue [2]. In addition, THz radiation can be also used in medical imaging for non-invasive diagnostics [2]. Semiconductor-based THz detectors employ photoexcitation of shallow impurities which requires them to be kept at cryogenic temperatures [3]. Room temperature detection has also been achieved using either antenna coupled photodetectors [4] or microbolometers [5–7]. The advantage of using microbolometers or other thermal detectors is in their ability to detect a broad spectral range depending on the characteristics of the absorbing layer used. Originally developed for infrared wavelengths, the microbolometer detectors were used for imaging in the THz spectral range using illumination from a quantum cascade laser [6, 7]. In order to enhance the sensitivity of microbolometer detectors at THz frequencies, it is important to embed strong THz absorbing layers into microfabricated detectors. It is known that thin metal films deposited on dielectrics provide good THz absorption due to resistive losses in the film [7]. In this paper, fabrication of a multilayer stack containing a thin metal film along with a dielectric Bragg reflector for visible light (necessary for optical readout) [8,9] is described. The whole stack will ultimately be incorporated in micro-cantilever based THz detectors [9].

In addition, the THz characteristics of the stack were modeled using the analytical approach described in Ref [10], as well as by finite element modeling using COMSOL Multiphysics software.

2. Multilayer stack design and analysis

The multi-layer stack used in our model as well as our experimental measurements consisted of eleven thin films deposited on a 500 µm silicon substrate as schematically illustrated in Fig. 1. A thin (15 nm) film of chromium (Cr) was placed at the bottom of the stack, to provide the absorption in the THz band. Subsequently, five periods of SiO$_2$ and Si$_3$N$_4$ with thicknesses of 110 nm and 75 nm, respectively, were deposited using plasma enhanced chemical vapor deposition (PECVD). This particular combination of dielectric films was selected to provide good reflectance for the wavelengths in red [8] to allow optical readout of the deflection once the multistack is incorporated in micromechanical THz detectors. The THz absorption properties of the entire structure were initially calculated by evaluating the reflection and transmission coefficients using the analytical approach described in [10]. In addition, the absorption properties of the stack were modeled by finite element analysis using the COMSOL Multiphysics software package. The advantage of COMSOL, compared with the analytical approach, is that it allows us to easily determine the heat dissipation in individual layers of the stack when more than one film is absorbing radiation.

The SiO$_2$ and Si$_3$N$_4$ films in the stack were assumed to be insulators with indices of refraction of 1.46 and 2.05, respectively. The refractive indices of the Cr layer and the Si substrate were calculated using Eq. (1) [11]

$$n^\prime = n - ik,$$  \hspace{1cm} (1)

where $n$ and $k$ are the real and imaginary part of the complex refractive index respectively. The imaginary part, which governs the absorption properties had to be taken into account.
since the substrate used was doped and had some conductivity. The \( n \) and \( k \) were calculated using Eqs. (2) and 3, respectively [12],

\[
n^2 = \frac{1}{2} \left( \varepsilon_r + \sqrt{\varepsilon_r^2 + \frac{\sigma^2}{4\pi^2\varepsilon_0^2 f^2}} \right) \tag{2}
\]

\[
k^2 = \frac{1}{2} \left( -\varepsilon_r + \sqrt{\varepsilon_r^2 + \frac{\sigma^2}{4\pi^2\varepsilon_0^2 f^2}} \right) \tag{3}
\]

where \( \varepsilon_r \) is the relative dielectric constant, \( f \) is the frequency of the incoming radiation and \( \sigma \) is the conductivity of the layer. The conductivity of the silicon substrate was measured using the 4-point probing method and found to be about 10 S/m. The conductivity of Si had to be taken into account as appreciable absorption can occur in the substrate due to its relatively large thickness. The relative dielectric constant of Si was taken to be \( \varepsilon_r = 11.7 \).

![Fig. 1. Schematic of the multi-layer stack designed for high reflection in red and high absorption in the THz range.](image)

The refractive index of the Cr layer (\( n_{Cr} \)) was calculated using Eqs. (1-3) assuming the terms containing conductivity dominated the \( n \) and \( k \). Under this condition, the complex refractive index of Cr layer can be written as

\[
n_{cr}^* = (1 - i) \sqrt{\frac{\sigma}{4\pi\varepsilon_0 f}} \tag{4}
\]

The conductivity of the Cr layer was also measured using the 4-point probing method and found to be about \( 6.25 \times 10^5 \) S/m. This value is consistent with the measurements by Laman et al. [13] who showed that the conductivity of thin films is lower than that of a bulk material due to high scattering from defects playing significant role at small thicknesses. The calculated (using Ref. 7 and Eqs. (2-4) and simulated (using COMSOL) reflection and transmission coefficients of the stack in 3 to 5 THz range are shown in Fig. 2. As expected, the two approaches gave the same result, thereby validating the procedure used in COMSOL modeling.
Fig. 2. The solid and dashed lines respectively represent reflectance and transmittance modeled using COMSOL while the scatter points represent the corresponding theoretically calculated quantities.

The oscillations in the reflection and transmission spectra due to the Fabry-Perot effect associated with the 500 µm thick Si substrate. The total absorption in the stack and Si substrate can be determined by subtracting the reflection and transmission coefficients from unity. In microcantilever applications, however, where only the thin-film stack is used to absorb the THz and to optimize the sensitivity, it is important to determine the absorption in the film alone. This can be conveniently achieved in COMSOL by determining the fraction of heat dissipation in multilayer stack relative to the entire structure including the substrate as shown in Fig. 3.

Fig. 3. Plot of the ratio of the heat dissipated within the thin-film stack and the total heat dissipated within both the thin-film stack and the Si substrate.

3. Experimental measurements

The predictions from the modeling and theoretical calculations were verified experimentally. The optical characterization of the fabricated multilayer stack (see Fig. 1) was performed in
the 3-5 THz spectral band using a Fourier transform infrared spectrometer (FTIR Nexus 8700) fitted with globar source, Si beamsplitter and a pyroelectric detector. The dielectric layers in the stack were selected to provide good reflectivity in the visible band (red color in particular), for optically probing the deformation of bi-material detectors when the stack is embedded into them [9].

In order to determine the absorption in the THz band, transmission and reflection coefficients were measured by placing the structure in the sample compartment of the FTIR as illustrated in Fig. 4 (a) and (b), respectively. From Fig. 4(b), it is apparent that the reflection measurement had to be taken at off-normal incidence (30 degrees in our setup). Thus, the transmission coefficient measurement was also performed by placing the sample at 30 degrees to the incident THz beam from the spectrometer. The background used for subtraction in FTIR measurement for transmission was done without the sample in the path of the THz beam while during the reflection measurement a gold-coated mirror was placed at the location of the sample in Fig. 4(b).

![Fig. 4. (a) Schematic of the experimental configuration used for measuring the transmittance coefficient and (b) configuration used for reflection coefficient measurement. In the transmission measurement, the sample was kept at the same angle as the reflectance measurement.](image)

Solid lines in Fig. 5 show the measured transmission and reflection coefficients of the structure in the 3 to 5 THz range. The dashed lines show the corresponding simulated data indicating a reasonable match with the measurements. The oscillatory behavior observed in the measured coefficients as a function of THz frequency is primarily due to the substrate acting as a Fabry-Perot cavity. The estimated thickness of the substrate using the experimentally observed frequency of oscillations is about 507 ± 86 µm, which matches well with the nominal value of the quoted thickness of the substrate used in the experiment of 500 – 525 µm. The larger uncertainty of the estimation of the thickness using the interference fringes is due to the low resolution (1 cm⁻¹ or 14.46 GHz) of the FTIR spectrometer in the THz spectral range of interest.
The measured transmission and reflection coefficients in Fig. 5 were used to determine the absorption of the multilayer stack together with the Si substrate (summing the three coefficients yields unity) and the results are shown by the solid line in Fig. 6. It can be seen from the data that the combined absorption of the stack including the substrate in the THz band is about 30%. The measured absorption data matches reasonably well with that of the simulations. The details of the optical characteristics of the multilayer stack in the visible range will be published elsewhere.

It is worth noting that the designed film, when employed inside the detector will not include the Si substrate underneath. Since the Si substrate was doped and, therefore, conductive, the substrate itself contributed to the total absorption. In order to gain a more accurate estimate of the absorption in the multi-layer stack, the total absorption measured at each frequency was multiplied by the corresponding percentage absorption in Cr given in Fig. 3. The adjusted thin-film stack absorption is shown by the solid line of Fig. 7 while the dashed line shows the corresponding adjusted simulation values. An average absorption of
about 20% was obtained with THz incident on the stack first compared with a total absorption of the entire structure of about 30% including the Si substrate.

Fig. 7. Plots of the modeled and experimental absorptions after multiplication by scaling factors from Fig. 5.

In order to optimize the THz absorption of the stack, the absorption in the Cr layer was simulated for thicknesses ranging from 1 to 30 nm. The simulations were carried out without the substrate to better represent the application of the stack for fabricating microcantilevers. It is known that the conductivity of a thin metal film is influenced by its thickness [13] and therefore affects the absorption. This effect was incorporated into the simulation by using the measured conductivities of two Cr films (a) 15 nm (6.25 x 10^5 S/m) and (b) 30 nm (7.69 x 10^5 S/m) and assuming a linear dependence with the Cr layer thickness. Figure 8 shows the absorption of the stack, averaged over the 3-5 THz band as a function of the Cr layer thickness and it can be seen that a Cr layer having thickness of around 9 nm give the highest absorption of about 50%. The simulations carried out without the Bragg reflector on the Cr film showed no difference in absorption indicating that it did not affect the THz coupling to the Cr film. Note that there was no need for an adjustment to the absorption data as did for the data in Fig. 7 due to removal of Si substrate during the simulation.

Fig. 8. Absorption as a function of Cr layer thickness.
4. Conclusion
The THz absorption characteristics in a thin film stack containing a dielectric Bragg reflector and a metal layer was modeled and measured. A good agreement between the measurement and simulation shows that modeling can be used for determining absorption properties of thin-film structures in THz range. The model was used to optimize the metal layer thickness for obtaining high THz absorption, which is needed for use in MEMS bi-material THz sensors.

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