Accurate determination of terahertz optical constants by vector network analyzer of Fabry-Perot response

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We present a method based on a Fabry-Perot model to efficiently and accurately estimate optical constants of wafer samples in transmission-only measurements performed by Vector Network Analyzer(VNA). The method is demonstrated on two separate wafer samples: one of silicon and the other of polymethlmethacrylate (PMMA). The results show that the method can not only accurately and simply acquire optical constants over a broad frequency domain, but also overcome limitations of calculation for dispersive and lossy materials, to which existing methods are susceptible as based upon VNA-driven quasi-optical transmissometers and THz Time-Domain Spectrometry.

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The broad versatility and advantages of terahertz (THz) methods have been demonstrated in: label-free sensing of DNA binding [1]; spectrometry [2]; and imaging [3]. In exploiting such advantages, THz time-domain spectrometric (TDS) system has been rapidly developed in both transmission and reflection modes to investigate and characterise materials [4–7]. However the application of THz-TDS particularly, has been widely limited by many factors. Its complexity in practical implementation makes it highly prone to misalignment errors. Maintenance of mechanical alignment is therefore essential. But with advances in microelectronics, microwave-based sources are encroaching into the THz spectral domain and this has enabled vector network analyzer (VNA) to assist in the metrology of optical constants [8, 9]. Compared with laser-enabled TDS, the VNA is more compact, easier to operate, and offers superior coherent source performance with less frequency drift and amplitude variation. Moreover, the VNA has higher frequency-resolution (MHz or even KHz) compared with that of TDS (tens GHz). This is significant when characterising metamaterials, for example, which may be designed to have narrow resonance phenomena [10].

Existing VNA-based methods for estimating the dielectric response of materials via S-parameter analysis, proceeds by manifold complicated procedures, as exemplified by Hasar et al [11] and Williams et al [12]. Hasar proposed a simple procedure for permittivity determination of low-loss materials using transmission-only measurements [13]. However the procedure for estimating permittivity, using Newton's algorithm, requires a very restricted initial guess. This is not suitable for dispersive materials. In addition the procedure can be only used under circumstances where the sample fills the waveguide cross-section. Yang et al [14] have subsequently, successfully characterized the permittivity of samples in the millimetre wave band using VNA-driven quasi-optics. Their method calculates the real part of refractive index n, only at frequencies where extrema in transmission occur. A general dispersive analysis follows by interpolation between extrema. Estimation of the extinction coefficient, k, has to be worked out from flanking nearest-neighbor transmission values under the assumption of the material being low loss. This method therefore lacks generality, where it is suited to determination of optical constants of low loss material at discrete frequencies. A method for continuous frequency dispersive analysis is very therefore much preferred.

In this paper a Fabry-Perot transfer function is used to not only establish an initial value of n, but also couple-solved its experimental and theoretical ones with Levenberg-Marquardt (LM) algorithm. By this method, the frequency-dependent optical constants can be accurately determined from the data sampled by the VNA in transmission-only measurements. This method effi-

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ciently works in the case of dispersive materials.

In a quasi-optical transmissometer driven by VNA, a sample with more parallel and less roughness surfaces on both sides is required to assure the accurate thickness of sample because of large beam size (50mm), in which the Fabry-Perot (FP) effect is induced. While the FP effect in the TDS system can be deliberately avoided by selecting a proper time-window to gate out multiple reflections, it is an unavoidable effect in a quasi-optical transmissometer. The schematic of Fig. 1 depicts the sequential propagation of the principle THz signal and the multiple internal reflection events within a plane-parallel slab. The order of each multiple reflection is offset for clarity. For true normal incidence of the principle beam, all orders will overlie each other. Considering two parallel reflecting surfaces, separated by a distance L in Fig. 1, the three parts labeled 1, 2,and 3, present the three regions: air, sample and air. Corresponding refractive indices are respectively 1, $\widetilde{n}_2$, and 1, $E_{THz}(\omega)$is the electric field of incident THz wave; $E_{tm}(\omega)$ the m^{th} transmitted field, and $E_{rm}(\omega)$ is the m^{th} reflected field. Applying appropriate Fresnel formula, the ratio of the total emergent THz field to the incident field can be written,

$$\dot{H} = \frac{\sum_{m=0}^{\infty} E_{tm}}{E_{THz}} = \frac{(1-R)exp(-i\omega(\tilde{n}_2-1)L/c)}{1-Rexp(-i\omega\tilde{n}_2 L/c)} \qquad (1)$$

where $R = (\frac{\tilde{n}_2-1}{\tilde{n}_2+1})^2$; c is the light speed in vacuum. Eq. (1) completely describes the propagation process of the THz field in the sample. The unknown parameter $\tilde{n}_2 = n - ik$ is to be resolved and remaining optical constants are derived from $\widetilde{n}_2$. Thus the analysis for s polarization is described; p polarization follows a similar analysis. To get the unknown $\widetilde{n}_2$, the experimental

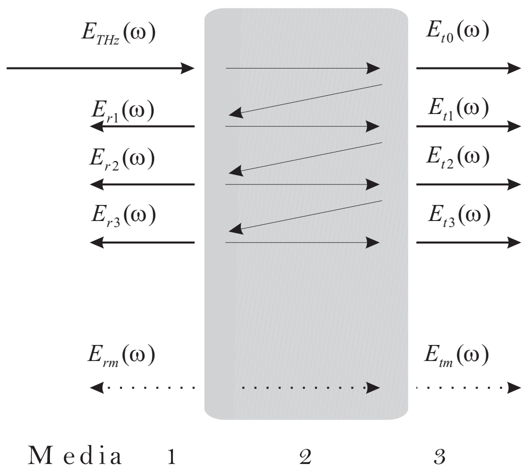

Fig. 1. Sketch of terahertz wave propagation in the wafer performed by VNA.

transfer function $\dot{H}_{exp}$ and the theoretical $\dot{H}_{theor}$ are jointly-resolved. Being complex quantities, the experimental and theoretical transfer functions, will introduce equivalent pairs of equation. Here the complex quantities are resolved via equation of moduli and arguments. The Levenberg-Marquardt (LM) algorithm, a blend of Gradient descent and Gauss-Newton iteration [15, 16], is adopted to resolve the equations in this work, As a non-linear least squares minimization algorithm, its function to be minimized is in the following form:

$$f(x) = \frac{1}{2}\sum_{j=1}^{m} r_j^2(x) \qquad (2)$$

where $x = (x_1, x_2, ..., x_n)$ is a vector , the r_j are as residuals and it is assumed that $m \geq n$. f can be rewritten as $f(x) = \frac{1}{2} \parallel r(x) \parallel^2$, and it derivatives using the Jacobian matrix $J(x)$. As the residuals here are non-linear, we have

$$\nabla f(x) = \sum_{j=1}^{m} r_j(x)\nabla r_j(x) = J(x)^T r(x) \qquad (3)$$

$$\nabla^2 f(x) = J(x)^T + \sum_{j=1}^{m} r_j(x)\nabla^2 r_j(x) \qquad (4)$$

The second term in Eq.(4) can be ignored because of small residuals. To solve the equation $\nabla f(x) = 0$, the gradient of f is expanded by using of a Taylor series around the current state x_0, one obtains

$$\nabla f(x) = \nabla f(x_0) + (x - x_0)^T \nabla^2 f(x_0) + ht \qquad (5)$$

where ht is higher order terms of $(x - x_0)$. Assuming f to be quadratic around x_0, the higher order terms are neglected. To Solve for the minimum x by setting the left hand side of Eq.(5) to 0, the update rule is

$$x_{i+1} = x_i - (\nabla^2 f(x))^{-1}\nabla f(x_i) \qquad (6)$$

Adding the gradient descent into Eq.(6), the update becomes

$$x_{i+1} = x_i - (H + \lambda I)^{-1}\nabla f(x_i) \qquad (7)$$

where H is the Hessian matrix evaluated at x_i. λ is the flexible scaling factor. Our iterations update as directed by the rule above, by which experimental and theoretical FP Transfer functions are couple-resolved.

Seed values to initiate the non-linear algorithm begin by taking modulus of Eq.(1), thus

$$\frac{I_T}{I_0} = \frac{1}{1 + F\sin^2\delta} \qquad (8)$$

where $F = \frac{4R'}{(1-R')^2}$ is analogous to the coefficient of Finesse in optics; $R' = (\frac{n-1}{n+1})^2$,and δ is the item of $2\omega nL/c$

with multiple of 2π. From Eq.(8), we see that the transmitted intensity is a periodic function of δ varying between extremes, so that

$$(I_T)_{max} = I_0, \delta = p\pi, p \quad an \quad integer \tag{9}$$

$$(I_T)_{min} = \frac{I_0}{1+F}, \delta = (p+\frac{1}{2}\pi) \tag{10}$$

In this paper, the same quasi-optical transmissometer is used as described by Yang et al [14]. The quasi-optical circuit was driven by a HP N5244A VNA. Fig. 2 shows the experimental curves measured by the VNA for a 1.98 mm thick silicon wafer sample. Included curves are the transmitted amplitude and phase difference. In this experiment, the measurement frequency is from 0.22 to 0.3 THz in steps of 17.5 MHz. The oscillations in Fig. 2 in the amplitude and phase traces are due to FP processes. Randomly selecting the peak transmittance and its nearest neighbor trough in Fig. 2, and substituting into Eq.(9)and Eq.(10) yields $R' = 0.30$, corresponding initial value $n = 3.46$. The initial value of k can be either determined from $(1-R')$, or just set to zero. Meanwhile, with the above rough initial values, n and k are worked out simultaneously.

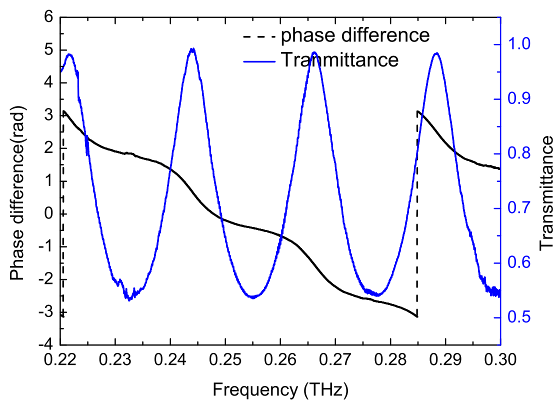

Fig. 2. The measured transmittance and phase difference of the silicon wafer.

The real part of the refractive index for a silicon wafer is presented in Fig. 3. The values obtained via the VNA with the proposed method are plotted using a continuous line, and those obtained from the VNA via the method of Yang et al are marked with solid squares. those obtained by TDS are marked with open circles. The mean value of n in this frequency domain is 3.417(5). The drift of measured transmission amplitude is ±0.001 dB, which dominates errors in this method. One may think that the interpolation algorithm of Yang et al is an acceptable way to accurately estimate spectral permittivity, but when there is only one oscillation in the transmitted amplitude over the spectral domain, the method is compromised. The same silicon wafer is also measured by a typical THz TDS system [17], its refractive index values are marked with hollow circles in the same figure. Compared with the results obtained from TDS, the results from the transmissometer have high spectral resolution and reduced fluctuation. The algorithm for determination of complex optical constants by TDS is an approximate method, in which only the first order reflection is used while other higher ones are ignored by selecting a proper time-window. Furthermore, a simple approximation expression is used for determining n and k from TDS measurements [18, 19]. It is impossible to experimentally cover all existing FP effects in TDS by scanning the delay to infinity as well. Therefore, the presented method works well to get the optical constants of samples over the working spectral domain.

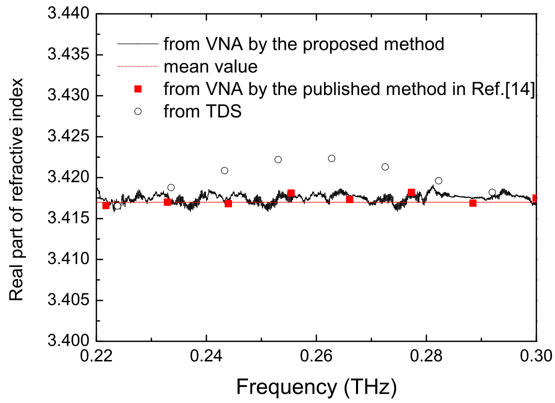

Fig. 3. The refractive index of silicon wafer obtained from VNA and TDS by the proposed and published method.

Another limitation in the published method is that for dispersive materials, their asymmetrical transmission spectra are unlike those distributions in Fig. 2. The proposed method is not restricted by assumptions that are required for analysis by Yang et al. For example, when a polymethlmethacrylate (PMMA) with the thickness of 5.728mm wafer is measured via VNA, amplitude and phase curves are shown with cross symbols and solid line in Fig. 4(a). By using our method, the complex refractive index of the PMMA sample is accurately obtained, shown in Fig.4(b). Its values of n and k are plotted with a solid line and cross symbols, respectively. To demonstrate this dispersive property, we magnify the extinction coefficient k of PMMA in Fig. 4(b) and compare with that of silicon wafer, as shown in the inset of Fig.4(b). The extinction coefficient curves of silicon wafer and PMMA are shown with solid line and cross symbols respectively. It is clear that the coefficient of PMMA is increasing with frequency while that of silicon stays level. The noises in the k curve of PMMA are due to the uniform internal distribution of material when it was manufactured, similar to the amplitudes curve in Fig.4(a). The refractive index of PMMA in Fig.4 corresponds with the reported value of 1.6 at 0.2 THz, which was obtained by TDS method [20]. The result of the method proposed here, however, is taken to be the more accurate for estimating n and k, given that its analysis proceeds without making physical assumptions. The assumptions used in the TDS method by Jin et al [20] are n and k expressions. This case proves that the method in this paper can work well in dispersive materials as well, which makes it more general.

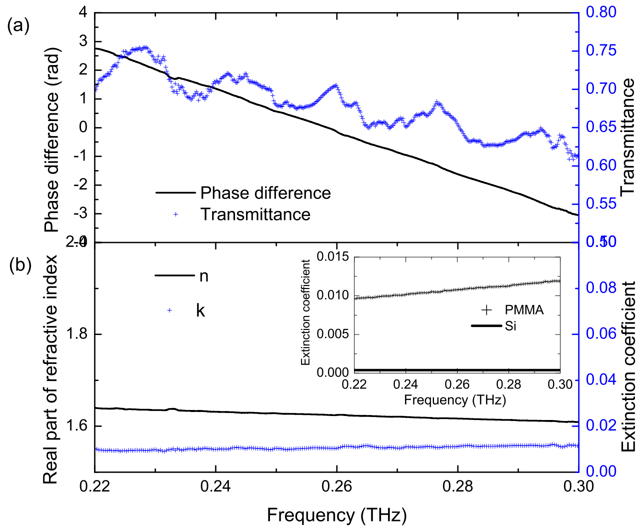

Fig. 4. The measured transmittance and phase difference of PMMA wafer (a) and its complex refractive index n and k(b).

In conclusion, we present a Fabry-Perot model to calculate the optical constants through measured complex transmission by VNA at THz range. The method has been compared with conventional method based on TDS system and VNA. Compared with those published methods, this method can not only provide accurate continuous results over the instrument spectral domain, but also overcome the limitation of calculation algorithm only for non-dispersive materials. The applicability of this method will be coextensive with the development and availability of high-frequency extender 'heads' beyond 1 THz for use by VNAs.

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