1 Data Analysis

1.1 Frequency Scan with Fixed Path Length

The photocurrent in the THz receiver is given by

$$I_{\mathrm{ph}} \propto E_{\mathrm{THz}} \cos\varphi = E_{\mathrm{THz}} \cos(2\pi L\nu/c)$$

where E_{THz} is the amplitude of the THz electric field, L is the deviation from zero path difference at the receiver, i.e. the difference between the length of the receiver arm, and the length of the emitter arm including the terahertz path, ν is the THz frequency and c the speed of light in vacuum.

In the method described here, L is fixed and only ν is varied ("‘scanned"’). Neglecting any dispersive effects of the path length (i.e. $L(\nu) = L = \text{const}$), the frequency dependence of $I_{\mathrm{ph}}(\nu)$ can be expressed

$$I_{\mathrm{ph}}(\nu) = E_{\mathrm{THz}}(\nu) \cos(2\pi L\nu/c) \quad .$$

The receiver photocurrent thus oscillates as a function of the THz frequency ν, with a period $\Delta\nu = c/L$.

For a reliable analysis, $\Delta\nu = c/L$ should, on one hand, be significantly larger than the uncertainty of the frequency $\delta\nu \sim 10\,\mathrm{MHz}$. On the other hand, $\Delta\nu/2$ determines the effective frequency resolution and should thus be smaller than the frequency scale of a feature of interest, e.g. a spectral line. The value of L can be chosen by tailoring the lengths of the optical fibers connecting the transmitter and receiver, and by varying the free-space THz beam path. For many applications, a suitable value is $L \approx 30\,\mathrm{cm}$ and thus $\Delta\nu = c/L \approx 1\,\mathrm{GHz}$. This fulfills the requirement $\Delta\nu \gg \delta\nu$, yet keeping $\Delta\nu$ significantly smaller than the linewidth of typical solid-state samples.

The amplitude values of the photocurrent I_{ph} are easily determined from the envelope of $I_{\mathrm{ph}}(\nu)$, either by a cosine fit around local maxima and minima, or simply by identifying the extrema of the photocurrent oscillations. The phase can equally be determined either by a cosine fit, or by analyzing the positions of the extrema and/or zero crossings of the photocurrent $I_{\mathrm{ph}}(\nu)$.

1.1.1 Amplitude

We assign a counting index $m = 0, 1, 2, ...$ to the extrema of the photocurrent $I_{\mathrm{ph}}(\nu)$, with even values of m corresponding to maxima and odd values corresponding to minima of $I_{\mathrm{ph}}(\nu)$.

Further, we denote the frequency and photocurrent in the m-th extremum by ν_m and I_m, respectively. As indicated above, the extrema I_m may be determined—if appropriate, after smoothing of the raw data—by a search algorithm that either just identifies local maxima and minima or fits low-order polynomials around the maxima and minima. We recommend to combine the information contained in a given maximum and the adjacent minimum, in order to eliminate possible offsets in the photocurrent:

$$\hat{I}_m(\hat{\nu}_m) = |I_m - I_{m+1}|/2, \quad \hat{\nu}_m = (\nu_m + \nu_{m+1})/2 \quad .$$

Thus, one obtains one data point $(\hat{I}_m, \hat{\nu}_m)$ per interval $\Delta\nu/2$, at an interpolated frequency $\hat{\nu}_m$. This confirms the above statement that $\Delta\nu/2$ is the effective frequency resolution of this measurement technique.

The photocurrent amplitude $\hat{I}(\nu)$ can be linearly interpolated to arbitrary frequencies ν, using the two adjacent data points:

$$\hat{I}(\nu) = \frac{\hat{\nu}_{m+1} - \nu}{\hat{\nu}_{m+1} - \hat{\nu}_m}\hat{I}_m + \frac{\nu - \hat{\nu}_m}{\hat{\nu}_{m+1} - \hat{\nu}_m}\hat{I}_{m+1} \quad \text{with} \quad \hat{\nu}_m \leq \nu < \hat{\nu}_{m+1} \quad .$$

The transmittance through a sample, at any frequency ν, is computed by comparing the photocurrent amplitude $\hat{I}_{\mathrm{sam}}$ of the sample to the amplitude $\hat{I}_{\mathrm{ref}}$ of a reference measurement without the sample:

$$T(\nu) = \left(\frac{\hat{I}_{\mathrm{sam}}(\nu)}{\hat{I}_{\mathrm{ref}}(\nu)}\right)^2 \quad ,$$

with $\hat{I}_{\mathrm{sam}}(\nu)$ and $\hat{I}_{\mathrm{ref}}(\nu)$ interpolated to the same frequency ν.

1.1.2 Phase

In addition to the THz amplitude, the phase φ, too, can be determined from the raw data. To do so, one can either use cosine fitting of $I_{\mathrm{ph}}(\nu)$ at the frequency ν of interest. Or, alternatively, one can simply analyze the positions (in frequency) of the extrema and/or zero crossings of I_{ph}. The cosine fit requires more computing power and might be affected by the frequency dependence of $E_{\mathrm{THz}}(\nu)$, whereas the zero crossings are independent of $E_{\mathrm{THz}}(\nu)$.

Analog to the amplitude analysis, we regard the extrema of the photocurrent, to which we once again assign the counting index m. One can approximate (for $E_{\mathrm{THz}}(\nu) \sim \mathrm{const}$)

$$\varphi(\nu_m) = 2\pi L(\nu_m)\nu_m/c = m\pi \quad .$$

Like the amplitude, the phase can be linearly interpolated to arbitrary frequencies:

$$\varphi(\nu) = \frac{\nu_{m+1} - \nu}{\nu_{m+1} - \nu_m}\varphi_m + \frac{\nu - \nu_m}{\nu_{m+1} - \nu_m}\varphi_{m+1} \quad \text{with} \quad \nu_m \leq \nu < \nu_{m+1} \quad .$$

However, in contrast to the amplitude, the correct order m of the extremum has to be used. In the ideal case, when the data acquisition is started at $\nu = 0$ and all extrema are identified unambiguously, the extrema can simply be counted.

Commonly though, no reliable THz data are available below 50 to 100 GHz—due to both the working range of the photomixers, and parasitic interference effects (standing waves) prevalent at low frequencies. However, a broadband measurement allows for extrapolating $\varphi(\nu)$ for $\nu \to 0$, resolving the ambiguity in m. To do so, one exploits the fact that $L(\nu)$ usually exhibits very low dispersion, i.e. one assumes $L(\nu) = L = \text{const}$. Then, one obtains an estimate for L from two extrema (e.g. with a spacing of $m_1 - m_2 \sim 10 \,..\, 100$):

$$L = \frac{c}{2} \frac{m_1 - m_2}{\nu_{m_1} - \nu_{m_2}} \quad .$$

The order m follows from

$$m \approx 2L\nu_m / c$$

by rounding to the nearest integer value (even integer for a maximum, odd integer for a minimum).

The phase shift $\Delta\varphi$ introduced by the sample corresponds to the difference of the phase values of sample and reference measurement, φ_{sam} and φ_{ref}:

$$\Delta\varphi(\nu) = \varphi_{\text{sam}}(\nu) - \varphi_{\text{ref}}(\nu) \quad .$$

Similarly, the change of the optical path length, introduced by the sample, is given by

$$\Delta L(\nu) = L_{\text{sam}}(\nu) - L_{\text{ref}}(\nu) = \frac{\Delta\varphi}{2\pi} \frac{c}{\nu} \quad .$$

Neglecting interference effects within the sample (i.e. multiple reflections between the sample's surfaces), and assuming that the thickness d of the sample is known, the refractive index n of the sample is then calculated from

$$(n-1)d \approx \Delta L \quad .$$

Note! Interpolation errors can be minimized by using extrema of different orders. Let m_{sam} denote the order of a photocurrent extremum of the sample measurement, and m_{ref} the order of a photocurrent extremum of the reference measurement. Ideally, the extrema should be selected so that the frequencies of sample and reference measurement, ν_{sam} and ν_{ref}, are close to each other, i.e. $\nu_{\text{sam},m_{\text{sam}}} \approx \nu_{\text{ref},m_{\text{ref}}}$.

Then, using the frequencies ν_{ref} at extrema m_{ref} and m_{sam},

$$\nu_{\text{ref},m_{\text{ref}}} = m_{\text{ref}} \frac{c}{2L} = (m_{\text{sam}} + (m_{\text{ref}} - m_{\text{sam}})) \frac{c}{2L} = \nu_{\text{ref},m_{\text{sam}}} + (m_{\text{ref}} - m_{\text{sam}}) \frac{c}{2L}$$

which can be rearranged:

$$\nu_{\text{ref},m_{\text{sam}}} = \nu_{\text{ref},m_{\text{ref}}} + (m_{\text{sam}} - m_{\text{ref}}) \frac{c}{2L} \quad .$$

Subtracting the frequency $\nu_{\text{sam},m_{\text{sam}}}$ of the sample measurement on both sides, multiplying with $L/\nu_{\text{sam},m_{\text{sam}}}$ and using Eq. (4) in [Roggenbuck10] yields a final expression for the refractive index n:

$$(n-1)d = \frac{\nu_{\text{ref},m_{\text{ref}}} - \nu_{\text{sam},m_{\text{sam}}}}{\nu_{\text{sam},m_{\text{sam}}}} \cdot L + (m_{\text{sam}} - m_{\text{ref}}) \cdot \frac{c}{2\nu_{\text{sam},m_{\text{sam}}}} \quad .$$