# Engineering Aspects of Terahertz Time-Domain Spectroscopy

by

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Thesis submitted for the degree of

**Doctor of Philosophy**

in

School of Electrical & Electronic Engineering
Faculty of Engineering, Computer & Mathematical Sciences
The University of Adelaide, Australia

December, 2009

# Appendix A

# Miscellaneous Relations

MISCELLANEOUS relations have been used throughout the thesis. This appendix summarises some important relations for the sake of reference. These include the relation between optical and dielectric constants, and the Kramers-Kronig relations.

## A.1 Relation between optical and dielectric constants

If $\hat{n}(\omega)$ is the complex index of refraction and $\hat{\epsilon}(\omega)$ is the complex relative permittivity, for dielectrics the relation between the two is given by

$$\hat{\epsilon}(\omega) = \hat{n}^2(\omega) \; . \tag{A.1}$$

Expanding the relative complex permittivity into the dielectric constants gives

$$\hat{\epsilon} = \epsilon' - j\epsilon'' \; , \tag{A.2}$$

and expanding the complex index of refraction into the optical constants gives

$$\hat{n} = n - j\kappa \; . \tag{A.3}$$

The dielectric constants can be expressed in terms of the optical constants as

$$\epsilon' = n^2 - \kappa^2 \; , \tag{A.4a}$$

$$\epsilon'' = 2n\kappa \; , \tag{A.4b}$$

and vice versa, the optical constants can be expressed in terms of the dielectric constants as

$$n = \left\{ \frac{\sqrt{\epsilon'^2 + \epsilon''^2} + \epsilon'}{2} \right\}^{1/2} \; , \tag{A.5a}$$

$$\kappa = \left\{ \frac{\sqrt{\epsilon'^2 + \epsilon''^2} - \epsilon'}{2} \right\}^{1/2} \; . \tag{A.5b}$$

Note that the absorption coefficient $\alpha$ and the extinction coefficient $\kappa$ are used interchangeably. The relation between the two is

$$\alpha = 2\frac{\omega\kappa}{c} \; . \tag{A.6}$$

Also note that the loss tangent, $\tan\delta$, is defined as the ratio of the imaginary part of the permittivity to the real part of the permittivity, or

$$\tan\delta = \frac{\epsilon''}{\epsilon'} \; . \tag{A.7}$$

## A.2 Kramers-Kronig relations

The index of refraction and extinction coefficient are related via the Kramers-Kronig relations. Given that a medium has a complex refractive index $n(\omega) - j\kappa(\omega)$ and a propagation length $l$, the transfer function of the medium relative to free space is given by

$$H(\omega) = \exp\left\{-j[n(\omega) - j\kappa(\omega) - 1]\frac{\omega l}{c}\right\} . \tag{A.8}$$

Take the logarithm to find

$$-\frac{c}{\omega l}\ln[H(\omega)] = \kappa(\omega) + j[n(\omega) - 1] . \tag{A.9}$$

Because of the causality of the transfer function, the index of refraction and extinction coefficient can be related through the Kramers-Kronig relations, or

$$n(\omega) = 1 + \frac{2\omega}{\pi}\mathcal{P}\int_0^\infty \frac{\kappa(\omega')}{\omega'^2 - \omega^2} d\omega' , \tag{A.10}$$

$$\kappa(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\omega'[n(\omega') - 1]}{\omega'^2 - \omega^2} d\omega' , \tag{A.11}$$

where $\mathcal{P}$ is the Cauchy principal value.

# Appendix B

# Analytical Models for T-ray Signals

ANALYTICAL models for T-ray signals have been used in the simulations in this thesis. The models that can closely reproduce the experiments are of great importance, since they strongly influence the simulation outcomes. This section briefly covers the employed signal and spectrum models, based on the generation and detection processes in PCAs. The original work was reported by Duvillaret *et al.* (2001). For further discussion of T-ray generation and detection using PCAs, please refer to Chapter 2.

## B.1 Modelling for transmitting photoconductive antenna

The apparent photocurrent density in a transmitting PCA, $J_{\mathrm{tx}}(t)$, equals the convolution between the profile of the optical pump pulse and the impulse response of the PCA, or

$$J_{\mathrm{tx}}(t) \quad = \quad P_{\mathrm{opt}}(t) * [q n_{\mathrm{tx}}(t) v_{\mathrm{tx}}(t)] \, , \tag{B.1}$$

where $*$ denotes the convolution operator; $P_{\mathrm{opt}}(t)$ is the optical pump pulse; $q$ is the carrier charge, equal to $1.602 \times 10^{-19}$C; $n_{\mathrm{tx}}(t)$ is the free-carrier density; and $v_{\mathrm{tx}}(t)$ is the free-carrier average velocity. The subscript 'tx' represents the transmitter.

The optical pump pulse from a laser assumes a Gaussian temporal profile with a duration $\tau_{\mathrm{las}}$, or mathematically

$$P_{\mathrm{opt}}(t) \quad \propto \quad \frac{P_{\mathrm{tx}}}{\tau_{\mathrm{las}}} \exp\left(-\frac{4t^2 \ln 2}{\tau_{\mathrm{las}}^2}\right) \, , \tag{B.2}$$

where $P_{\mathrm{tx}}$ is the average laser power. The density of carriers generated via photoexcitation exponentially decays as a result of carrier recombination and trapping. Thus, the carrier density is described as

$$n_{\mathrm{tx}}(t) \quad \propto \quad \exp\left(-\frac{t}{\tau_{\mathrm{tx}}}\right) \, , \tag{B.3}$$

where $\tau_{\mathrm{tx}}$ is the free-carrier recombination time. The free-carrier average velocity, $v_{\mathrm{tx}}(t)$, is related to the applied electric field, $E_{\mathrm{DC}}$, by

$$\frac{dv_{\mathrm{tx}}(t)}{dt} = -\frac{v_{\mathrm{tx}}(t)}{\delta\tau_{\mathrm{tx}}} + \frac{q}{m^*} E_{\mathrm{DC}} \, , \tag{B.4}$$

where $\delta\tau_{\mathrm{tx}}$ is the carrier collision time and $m^*$ is the carrier effective mass.

Performing the convolution in Equation B.1 using the relations in Equations B.2, B.3, and B.4 gives the photocurrent density in the transmitting antenna,

$$\begin{aligned} J_{\mathrm{tx}}(t) \quad \propto \quad & \frac{P_{\mathrm{tx}} E_{\mathrm{DC}} \delta\tau_{\mathrm{tx}}}{m_{\mathrm{tx}}^*} \left\{ \exp\left(\frac{\tilde{\tau}_{\mathrm{las}}^2}{4\tau_{\mathrm{tx}}^2} - \frac{t}{\tau_{\mathrm{tx}}}\right) \mathrm{erfc}\left(\frac{\tilde{\tau}_{\mathrm{las}}}{2\tau_{\mathrm{tx}}} - \frac{t}{\tilde{\tau}_{\mathrm{las}}}\right) \right. \\ & \left. - \exp\left(\frac{\tilde{\tau}_{\mathrm{las}}^2}{4\tilde{\tau}_{\mathrm{tx}}^2} - \frac{t}{\tilde{\tau}_{\mathrm{tx}}}\right) \mathrm{erfc}\left(\frac{\tilde{\tau}_{\mathrm{las}}}{2\tilde{\tau}_{\mathrm{tx}}} - \frac{t}{\tilde{\tau}_{\mathrm{las}}}\right) \right\} \, . \end{aligned} \tag{B.5}$$

Here, $\tilde{\tau}_{\mathrm{las}} = \tau_{\mathrm{las}}/(2\sqrt{\ln 2})$ and $1/\tilde{\tau}_{\mathrm{tx}} = 1/\tau_{\mathrm{tx}} + 1/\delta\tau_{\mathrm{tx}}$.

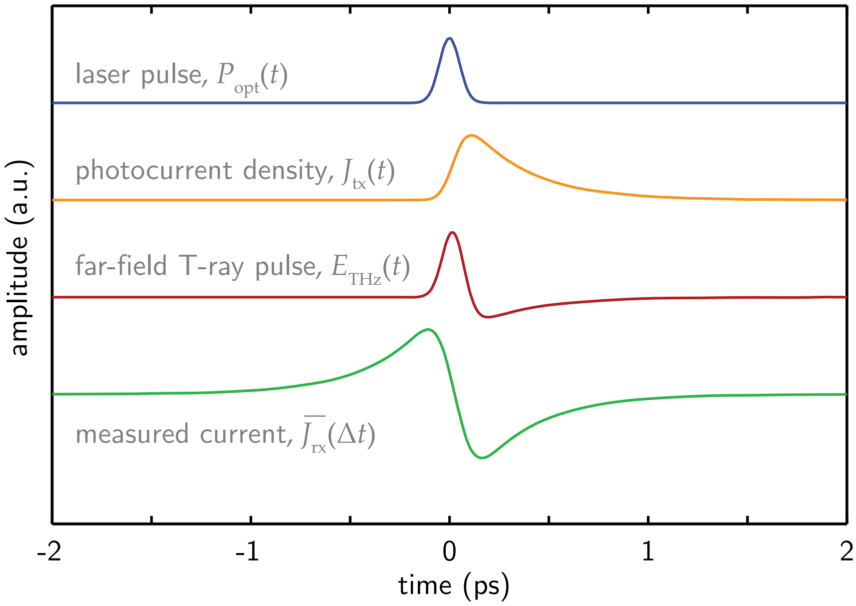

**Figure B.1. Normalised pulse profiles in PCAs.** The parameters used in the calculation are as follows: the laser pulse duration $\tau_{\mathrm{las}}$=120 fs; the carrier recombination times in the transmitter and receiver, $\tau_{\mathrm{tx}} = \tau_{\mathrm{rx}}$ =300 fs; and the carrier collision times in the transmitter and receiver, $\delta\tau_{\mathrm{tx}} = \delta\tau_{\mathrm{rx}}$ =30 fs.

A rapid change in the current density results in T-ray radiation from the transmitter. The far-field T-ray signal is proportional to the first derivative of the photocurrent density, or

$$E_{\mathrm{THz}}(t) \propto \frac{dJ_{\mathrm{tx}}(t)}{dt}, \tag{B.6}$$

which corresponds to the spectrum of

$$E_{\mathrm{THz}}(\omega) \propto \frac{P_{\mathrm{tx}}E_{\mathrm{DC}}\delta\tau_{\mathrm{tx}}(\tau_{\mathrm{tx}} - \tilde{\tau}_{\mathrm{tx}})}{2\pi m^*_{\mathrm{tx}}} \times \frac{\omega \exp(-\omega^2\tilde{\tau}^2_{\mathrm{las}}/4)}{(1 - j\omega\tau_{\mathrm{tx}})(1 - j\omega\tilde{\tau}_{\mathrm{tx}})}\,. \tag{B.7}$$

The example profiles of the laser pulse, photocurrent density, and far-field T-ray pulse are demonstrated in Figure B.1. Figure B.2 shows the far-field T-ray spectrum.

## B.2 Modelling for receiving photoconductive antenna

Similar to the photocurrent density in the transmitting antenna, the photocurrent density in the receiving antenna, which is gated by the optical probe pulse, is given by the convolution between the profile of the optical probe pulse and the PCA impulse

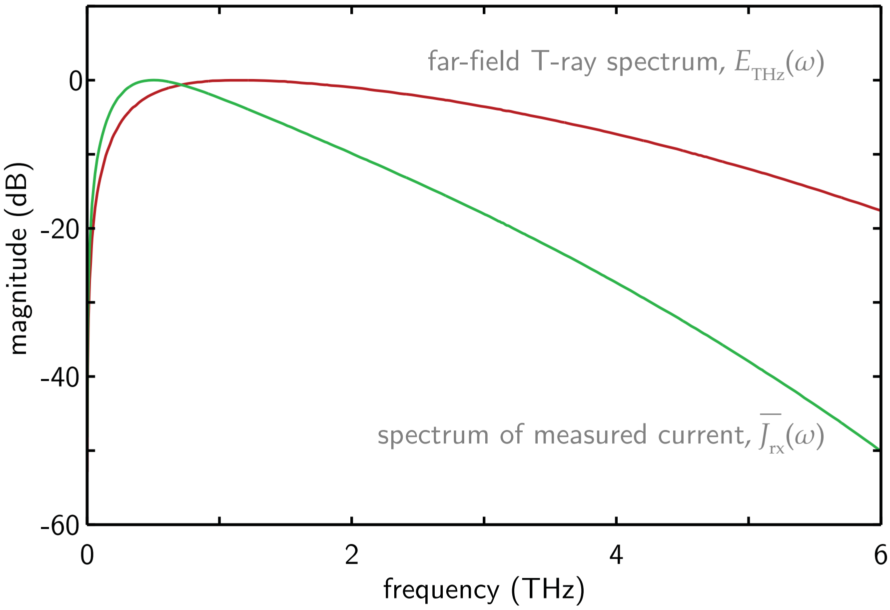

**Figure B.2. Normalised spectra of T-ray pulse and photocurrent density.** The parameters used in the calculation are identical to those used for Figure B.1.

response, or

$$J_{\mathrm{rx}}(t;\Delta t) \quad = \quad P_{\mathrm{opt}}(t) * [q n_{\mathrm{rx}}(t) v_{\mathrm{rx}}(t;\Delta t)]\ , \tag{B.8}$$

where the subscript 'rx' represents the receiver, and the expressions for $P_{\mathrm{opt}}(t)$ and $n_{\mathrm{rx}}(t)$ are equivalent to those for the transmitting antenna. For the receiving antenna the current density $J_{\mathrm{rx}}(t;\Delta t)$ is a function of the delay time $\Delta t$ between the optical pump and probe pulses, since the carrier average velocity $v_{\mathrm{rx}}(t;\Delta t)$ in this case is tied to the dynamic bias or the incoming T-ray electric field $E_{\mathrm{THz}}(t+\Delta t)$. That is

$$\frac{dv_{\mathrm{rx}}(t;\Delta t)}{dt} \quad = \quad -\frac{v_{\mathrm{rx}}(t;\Delta t)}{\delta\tau_{\mathrm{rx}}} + \frac{q}{m^*_{\mathrm{rx}}} E_{\mathrm{THz}}(t+\Delta t)\ . \tag{B.9}$$

Due to a slower response of an electronic measurement system, the measurable current at the output ports of the receiving antenna is proportional to the average of the photocurrent. Hence,

$$\begin{aligned}
\overline{J_{\mathrm{rx}}}(\Delta t) &\propto \int_{-\infty}^{+\infty} J_{\mathrm{rx}}(t;\Delta t)dt \\
&\propto \frac{P_{\mathrm{tx}}P_{\mathrm{rx}}E_{\mathrm{DC}}\delta\tau_{\mathrm{tx}}\tau_{\mathrm{rx}}\tilde{\tau}_{\mathrm{rx}}}{m_{\mathrm{tx}}^{*}m_{\mathrm{rx}}^{*}(\tau_{\mathrm{tx}}+\tau_{\mathrm{rx}})(\tilde{\tau}_{\mathrm{tx}}+\tau_{\mathrm{rx}})} \\
&\quad \times \left\{(\tau_{\mathrm{tx}}+\tau_{\mathrm{rx}})\exp\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}}{2\tilde{\tau}_{\mathrm{tx}}^{2}}-\frac{\Delta t}{\tilde{\tau}_{\mathrm{tx}}}\right)\mathrm{erfc}\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}-\Delta t\tilde{\tau}_{\mathrm{tx}}}{\sqrt{2}\tilde{\tau}_{\mathrm{tx}}\tilde{\tau}_{\mathrm{las}}}\right)\right. \\
&\quad +(\tau_{\mathrm{tx}}-\tilde{\tau}_{\mathrm{tx}})\exp\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}}{2\tau_{\mathrm{rx}}^{2}}+\frac{\Delta t}{\tau_{\mathrm{rx}}}\right)\mathrm{erfc}\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}+\Delta t\tau_{\mathrm{rx}}}{\sqrt{2}\tau_{\mathrm{rx}}\tilde{\tau}_{\mathrm{las}}}\right) \\
&\quad \left. -(\tau_{\mathrm{rx}}+\tilde{\tau}_{\mathrm{tx}})\exp\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}}{2\tau_{\mathrm{tx}}^{2}}-\frac{\Delta t}{\tau_{\mathrm{tx}}}\right)\mathrm{erfc}\left(\frac{\tilde{\tau}_{\mathrm{las}}^{2}-\Delta t\tau_{\mathrm{tx}}}{\sqrt{2}\tau_{\mathrm{tx}}\tilde{\tau}_{\mathrm{las}}}\right)\right\}. \qquad \text{(B.10)}
\end{aligned}$$

Fourier transform of the measured current $\overline{J_{\mathrm{rx}}}(\Delta t)$ with respect to the time axis $\Delta t$ gives a detectable spectrum,

$$\overline{J_{\mathrm{rx}}}(\omega) \propto \frac{P_{\mathrm{tx}}P_{\mathrm{rx}}E_{\mathrm{DC}}\tau_{\mathrm{tx}}\tau_{\mathrm{rx}}\tilde{\tau}_{\mathrm{tx}}\tilde{\tau}_{\mathrm{rx}}}{2\pi m_{\mathrm{tx}}^{*}m_{\mathrm{rx}}^{*}} \times \frac{\omega\exp(-\omega^{2}\tilde{\tau}_{\mathrm{las}}^{2}/2)}{(1-j\omega\tau_{\mathrm{tx}})(1+j\omega\tau_{\mathrm{rx}})(1-j\omega\tilde{\tau}_{\mathrm{tx}})}. \qquad \text{(B.11)}$$

Profiles for the measured current and its spectrum are depicted in Figure B.1 and B.2, respectively.

# Appendix C

# Uncertainty Propagation

EVALUATION of the uncertainty in THz-TDS measurements, developed in Chapter 7, correlates the uncertainty in sources to the uncertainty in measurands. A law of propagation of uncertainty, which is required in the evaluation, is elucidated in this appendix, together with a derivation for the propagation of the variance from the amplitude to optical constants.

## C.1 Law of propagation of uncertainty

This appendix, referred to by Section 7.4.3, derives the formulae that are vital in determining the variance (and covariance) of a measurand, which is influenced by the variance and covariance of input quantities through a measurement function.

Typically, a measurand, $\Phi$, is expressed by a measurement function containing input quantities $X_1, X_2, \ldots, X_M$, or $\Phi(X_1, X_2, \ldots, X_M)$. If variances and covariances appear at the inputs, they will propagate to the measurand through this function. For $\phi_l$ determined from $x_{1l}, x_{2l}, \ldots, x_{Ml}$, the first-order Taylor series expansion around the arithmetic means $\overline{x}_1, \overline{x}_2, \ldots, \overline{x}_M$ is

$$\phi(x_{1l}, x_{2l}, \ldots, x_{Ml}) = \phi(\overline{x}_1, \overline{x}_2, \ldots, \overline{x}_M) + \sum_{i=1}^{M} \left.\frac{\partial \phi}{\partial x_i}\right|_{x_i=\overline{x}_i} (x_{il} - \overline{x}_i) \ . \tag{C.1}$$

Rearranging the equation yields

$$\phi_l - \overline{\phi} = \sum_{i=1}^{M} \left.\frac{\partial \phi}{\partial x_i}\right|_{x_i=\overline{x}_i} (x_{il} - \overline{x}_i) \ . \tag{C.2}$$

For the sake of conciseness, from now on, $\partial\phi/\partial x_i|_{x_i=\overline{x}_i}$ will be represented by $\partial\phi/\partial\overline{x}_i$. The empirical variance of $\phi$ calculated over $N$ observations is defined as

$$s_\phi^2 = \frac{1}{N-1}\sum_{l=1}^{N}(\phi_l - \overline{\phi})^2 \ . \tag{C.3}$$

By substituting Equation C.2 into Equation C.3, it follows that

$$\begin{aligned} s_\phi^2 &= \frac{1}{N-1}\sum_{l=1}^{N}\left[\sum_{i=1}^{M}\frac{\partial\phi}{\partial\overline{x}_i}(x_{il}-\overline{x}_i)\right]^2 \\ &= \frac{1}{N-1}\sum_{l=1}^{N}\left[\sum_{i=1}^{M}\left(\frac{\partial\phi}{\partial\overline{x}_i}\right)^2(x_{il}-\overline{x}_i)^2 + 2\sum_{i=1}^{M-1}\sum_{j=i+1}^{M}\frac{\partial\phi}{\partial\overline{x}_i}\frac{\partial\phi}{\partial\overline{x}_j}(x_{il}-\overline{x}_i)(x_{jl}-\overline{x}_j)\right] \end{aligned} \tag{C.4}$$

where the above equation can be rewritten in terms of empirical variances and covariances of the inputs,

$$s_\phi^2 = \sum_{i=1}^{M}\left(\frac{\partial\phi}{\partial\overline{x}_i}\right)^2 s_{x_i}^2 + 2\sum_{i=1}^{M-1}\sum_{j=i+1}^{M}\frac{\partial\phi}{\partial\overline{x}_i}\frac{\partial\phi}{\partial\overline{x}_j}s_{x_ix_j} \ , \tag{C.5}$$

where

$$s_{x_i}^2 = \frac{1}{N-1}\sum_{l=1}^{N}(x_{il}-\overline{x}_i)^2 \ , \tag{C.6a}$$

$$s_{x_ix_j} = \frac{1}{N-1}\sum_{l=1}^{N}(x_{il}-\overline{x}_i)(x_{jl}-\overline{x}_j) \ . \tag{C.6b}$$

If the input parameters are uncorrelated, Equation C.5 simplifies to

$$s_\phi^2 = \sum_{i=1}^{M} \left( \frac{\partial \phi}{\partial \overline{x}_i} \right)^2 s_{x_i}^2 \,. \tag{C.7}$$

The above equation shows that, based on the first-order approximation, the variances of the inputs propagate to the measurand through the sensitivity coefficients $\partial\phi/\partial\overline{x}_i$.

Now consider two measurement functions, $\Phi_1$ and $\Phi_2$, sharing the same set of input parameters, $X_1, X_2, \ldots, X_M$. Similar to Equation C.2, the first-order Taylor series expansions of these two functions around the arithmetic means are

$$\phi_{1l} - \overline{\phi}_1 = \sum_{i=1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} (x_{il} - \overline{x}_i) \,, \tag{C.8a}$$

$$\phi_{2l} - \overline{\phi}_2 = \sum_{j=1}^{M} \frac{\partial \phi_2}{\partial \overline{x}_j} (x_{jl} - \overline{x}_j) \,. \tag{C.8b}$$

By defining the empirical covariance between $\Phi_1$ and $\Phi_2$ calculated over $N$ observations,

$$s_{\phi_1\phi_2} = \frac{1}{N-1} \sum_{l=1}^{N} (\phi_{1l} - \overline{\phi}_1)(\phi_{2l} - \overline{\phi}_2) \,, \tag{C.9}$$

it turns out that

$$\begin{aligned} s_{\phi_1\phi_2} &= \frac{1}{N-1} \sum_{l=1}^{N} \left[ \sum_{i=1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} (x_{il} - \overline{x}_i) \sum_{j=1}^{M} \frac{\partial \phi_2}{\partial \overline{x}_j} (x_{jl} - \overline{x}_j) \right] \\ &= \frac{1}{N-1} \sum_{l=1}^{N} \left[ \sum_{i=1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} \frac{\partial \phi_2}{\partial \overline{x}_i} (x_{il} - \overline{x}_i)^2 + 2 \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} \frac{\partial \phi_2}{\partial \overline{x}_j} (x_{il} - \overline{x}_i)(x_{jl} - \overline{x}_j) \right] \\ &= \sum_{i=1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} \frac{\partial \phi_2}{\partial \overline{x}_i} s_{x_i}^2 + 2 \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} \frac{\partial \phi_2}{\partial \overline{x}_j} s_{x_i,x_j} \,. \end{aligned} \tag{C.10}$$

In case that no correlation among the input parameters, the above equation reduces to

$$s_{\phi_1\phi_2} = \sum_{i=1}^{M} \frac{\partial \phi_1}{\partial \overline{x}_i} \frac{\partial \phi_2}{\partial \overline{x}_i} s_{x_i}^2 \,. \tag{C.11}$$

It shows that a covariance between two functions is a result from the two functions sharing one or more input variables.

## C.2 Propagation of variance from the amplitude

This appendix, referred to by Sections 7.5.1 and 8.3, shows a derivation of the variance in the optical constants that propagates from the variance in the T-ray amplitude. From the amplitude in the time domain, the variance is transferred to the variance of the magnitude and phase spectra in the frequency domain via Fourier transform. Then the combination between the variances of sample and reference measurements produces the variance in the transfer function of a sample. The variance eventually appears at the optical constants. For general details about the propagation of variance and covariance, please consult Appendix C.1.

The discrete Fourier transform of a time-resolved signal, $E(k)$, is (Press *et al.* 1992)

$$E(\omega) = \sum_k E(k)\exp(-j\omega k\tau)\ , \tag{C.12}$$

where $k$ is the temporal index and $\tau$ is the sampling interval. If $E(\omega) = E_\mathrm{r}(\omega) + jE_\mathrm{i}(\omega)$, where $E_\mathrm{r}(\omega)$ and $E_\mathrm{i}(\omega)$ are real, then

$$E_\mathrm{r}(\omega) = \sum_k E(k)\cos(\omega k\tau)\ , \tag{C.13a}$$

$$E_\mathrm{i}(\omega) = -\sum_k E(k)\sin(\omega k\tau)\ . \tag{C.13b}$$

Assuming that the amplitude at each time sample is statistically independent from the amplitude at other time samples, the variances of the real and imaginary parts of the spectrum are, respectively (Forniés-Marquina *et al.* 1997),

$$s^2_{E_\mathrm{r}}(\omega) = \sum_k \cos^2(\omega k\tau)s^2_E(k)\ , \tag{C.14a}$$

$$s^2_{E_\mathrm{i}}(\omega) = \sum_k \sin^2(\omega k\tau)s^2_E(k)\ , \tag{C.14b}$$

where $s^2_E(k)$ is the variance of the time-domain signal $E(k)$. Since the real and imaginary parts of the spectrum share the same set of inputs, their covariance is then (Bich 1996, Forniés-Marquina *et al.* 1997)

$$s_{E_\mathrm{r}E_\mathrm{i}}(\omega) = -\sum_k \sin(\omega k\tau)\cos(\omega k\tau)s^2_E(k) = -\frac{1}{2}\sum_k \sin(2\omega k\tau)s^2_E(k)\ . \tag{C.15}$$

The magnitude and phase of the signal, determined from the real and imaginary parts of the complex spectrum, are

$$|E(\omega)| = \sqrt{E^2_\mathrm{r}(\omega) + E^2_\mathrm{i}(\omega)}\ , \tag{C.16a}$$

$$\angle E(\omega) = \arctan(E_\mathrm{i}(\omega)/E_\mathrm{r}(\omega))\ . \tag{C.16b}$$

Correspondingly, the variances of the magnitude and phase are

$$s^2_{|E|}(\omega) = \frac{1}{|E(\omega)|^2}\left[E_\mathrm{r}^2(\omega)s^2_{E_\mathrm{r}}(\omega) + E_\mathrm{i}^2(\omega)s^2_{E_\mathrm{i}}(\omega) + 2E_\mathrm{r}(\omega)E_\mathrm{i}(\omega)s_{E_\mathrm{r}E_\mathrm{i}}(\omega)\right], \tag{C.17a}$$

$$s^2_{\angle E}(\omega) = \frac{1}{|E(\omega)|^4}\left[E_\mathrm{i}^2(\omega)s^2_{E_\mathrm{r}}(\omega) + E_\mathrm{r}^2(\omega)s^2_{E_\mathrm{i}}(\omega) - 2E_\mathrm{r}(\omega)E_\mathrm{i}(\omega)s_{E_\mathrm{r}E_\mathrm{i}}(\omega)\right]. \tag{C.17b}$$

Substituting the variances and covariance of the real and imaginary parts from Equations C.14 and C.15 simplifies Equations C.17a and C.17b to, respectively,

$$s^2_{|E|}(\omega) = \frac{1}{|E(\omega)|^2}\sum_k \left[E_\mathrm{r}(\omega)\cos(\omega k\tau) - E_\mathrm{i}(\omega)\sin(\omega k\tau)\right]^2 s^2_E(k)\,, \tag{C.18a}$$

$$s^2_{\angle E}(\omega) = \frac{1}{|E(\omega)|^4}\sum_k \left[E_\mathrm{i}(\omega)\cos(\omega k\tau) + E_\mathrm{r}(\omega)\sin(\omega k\tau)\right]^2 s^2_E(k)\,. \tag{C.18b}$$

Some mathematical manipulations reduce the above pair of equations to

$$s^2_{|E|}(\omega) = \frac{1}{|E(\omega)|^2}\sum_k \Re^2[E(\omega)\exp(j\omega k\tau)]s^2_E(k)\,, \tag{C.19a}$$

$$s^2_{\angle E}(\omega) = \frac{1}{|E(\omega)|^4}\sum_k \Im^2[E(\omega)\exp(j\omega k\tau)]s^2_E(k)\,, \tag{C.19b}$$

where $\Re^2$ and $\Im^2$ denote the square of the real and of imaginary parts, respectively. According to Equation C.19a the amplitude variances of the sample and reference spectra are given by, respectively,

$$s^2_{|E_\mathrm{sam}|}(\omega) = \frac{1}{|E_\mathrm{sam}(\omega)|^2}\sum_k \Re^2[E_\mathrm{sam}(\omega)\exp(j\omega k\tau)]s^2_{E_\mathrm{sam}}(k)\,, \tag{C.20a}$$

$$s^2_{|E_\mathrm{ref}|}(\omega) = \frac{1}{|E_\mathrm{ref}(\omega)|^2}\sum_k \Re^2[E_\mathrm{ref}(\omega)\exp(j\omega k\tau)]s^2_{E_\mathrm{ref}}(k)\,, \tag{C.20b}$$

and according to Equation C.19b the phase variances of the sample and reference spectra are given by, respectively,

$$s^2_{\angle E_\mathrm{sam}}(\omega) = \frac{1}{|E_\mathrm{sam}(\omega)|^4}\sum_k \Im^2[E_\mathrm{sam}(\omega)\exp(j\omega k\tau)]s^2_{E_\mathrm{sam}}(k)\,, \tag{C.21a}$$

$$s^2_{\angle E_\mathrm{ref}}(\omega) = \frac{1}{|E_\mathrm{ref}(\omega)|^4}\sum_k \Im^2[E_\mathrm{ref}(\omega)\exp(j\omega k\tau)]s^2_{E_\mathrm{ref}}(k)\,. \tag{C.21b}$$

The sample and reference fields are independent from each other, resulting in the absence of a covariance term. The transfer function of a sample is calculated by dividing the sample spectrum by the reference. In terms of the magnitude and phase, this operation is given by

$$|H(\omega)| = |E_\mathrm{sam}(\omega)|/|E_\mathrm{ref}(\omega)|\,, \tag{C.22a}$$

$$\angle H(\omega) = \angle E_\mathrm{sam}(\omega) - \angle E_\mathrm{ref}(\omega)\,. \tag{C.22b}$$

The variances of Equation C.22a and C.22b are, respectively,

$$\begin{aligned} s^2_{|H|}(\omega) &= \frac{1}{|E_{\text{ref}}(\omega)|^2} s^2_{|E_{\text{sam}}|}(\omega) + \frac{|E_{\text{sam}}(\omega)|^2}{|E_{\text{ref}}(\omega)|^4} s^2_{|E_{\text{ref}}|}(\omega) \,, && \text{(C.23a)} \\ s^2_{\angle H}(\omega) &= s^2_{\angle E_{\text{sam}}}(\omega) + s^2_{\angle E_{\text{ref}}}(\omega) \,. && \text{(C.23b)} \end{aligned}$$

The magnitude and phase of the signals are presumably treated as independent input parameters, and consequently there is no covariance between the magnitude and phase. Substituting Equations C.20 and C.21 into Equations C.23a and C.23b gives

$$\begin{aligned} s^2_{|H|}(\omega) &= \frac{1}{|E_{\text{ref}}(\omega)E_{\text{sam}}(\omega)|^2} \sum_k \Re^2[E_{\text{sam}}(\omega)\exp(j\omega k\tau)] s^2_{E_{\text{sam}}}(k) \\ &\quad + \frac{|E_{\text{sam}}(\omega)|^2}{|E_{\text{ref}}(\omega)|^6} \sum_k \Re^2[E_{\text{ref}}(\omega)\exp(j\omega k\tau)] s^2_{E_{\text{ref}}}(k) \,, && \text{(C.24a)} \\ s^2_{\angle H}(\omega) &= \frac{1}{|E_{\text{sam}}(\omega)|^4} \sum_k \Im^2[E_{\text{sam}}(\omega)\exp(j\omega k\tau)] s^2_{E_{\text{sam}}}(k) \\ &\quad + \frac{1}{|E_{\text{ref}}(\omega)|^4} \sum_k \Im^2[E_{\text{ref}}(\omega)\exp(j\omega k\tau)] s^2_{E_{\text{ref}}}(k) \,. && \text{(C.24b)} \end{aligned}$$

From the measurement function, the refractive index and the extinction coefficient are evaluated from the magnitude and phase of the transfer function via

$$\begin{aligned} n(\omega) &= n_0 - \frac{c}{\omega l} \angle H(\omega) \,, && \text{(C.25a)} \\ \kappa(\omega) &= \frac{c}{\omega l} \left\{ \ln\left[\frac{4n(\omega)n_0}{(n(\omega)+n_0)^2}\right] - \ln|H(\omega)| \right\} \,. && \text{(C.25b)} \end{aligned}$$

Thus, the variances of the refractive index and the extinction coefficient due to the magnitude and phase variances are

$$\begin{aligned} s^2_n(\omega) &= \left(\frac{c}{\omega l}\right)^2 s^2_{\angle H}(\omega) \,. && \text{(C.26a)} \\ s^2_\kappa(\omega) &= \left[\frac{c}{\omega l|H(\omega)|}\right]^2 s^2_{|H|}(\omega) + \left[\frac{c}{\omega l}\left(\frac{n(\omega)-n_0}{n(\omega)+n_0}\right)\right]^2 \frac{s^2_n(\omega)}{n^2(\omega)} \,. && \text{(C.26b)} \end{aligned}$$

Equations C.24a and C.24b are then combined with Equation C.26a or C.26b to produce

$$\begin{aligned} s^2_{n,E}(\omega) &= \left(\frac{c}{\omega l}\right)^2 \left\{ \frac{1}{|E_{\mathrm{sam}}(\omega)|^4} \sum_k \Im^2[E_{\mathrm{sam}}(\omega) \exp(j\omega k\tau)] s^2_{E_{\mathrm{sam}}}(k) \right. \\ &\quad \left. + \frac{1}{|E_{\mathrm{ref}}(\omega)|^4} \sum_k \Im^2[E_{\mathrm{ref}}(\omega) \exp(j\omega k\tau)] s^2_{E_{\mathrm{ref}}}(k) \right\} , \qquad \text{(C.27a)} \\ s^2_{\kappa,E}(\omega) &= \left(\frac{c}{\omega l}\right)^2 \left\{ \frac{1}{|E_{\mathrm{sam}}(\omega)|^4} \sum_k \Re^2[E_{\mathrm{sam}}(\omega) \exp(j\omega k\tau)] s^2_{E_{\mathrm{sam}}}(k) \right. \\ &\quad + \frac{1}{|E_{\mathrm{ref}}(\omega)|^4} \sum_k \Re^2[E_{\mathrm{ref}}(\omega) \exp(j\omega k\tau)] s^2_{E_{\mathrm{ref}}}(k) \\ &\quad \left. + \left(\frac{n(\omega) - n_0}{n(\omega) + n_0}\right)^2 \frac{s^2_{n,E}(\omega)}{n^2(\omega)} \right\} . \qquad \text{(C.27b)} \end{aligned}$$

The models above explicitly express the variances of the optical constants in terms of the variance in the signal amplitude.

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# Glossary

The physical constants used in this thesis are in accordance with a recommendation of the Committee on Data for Science and Technology (Mohr and Taylor 2005).

| Quantity | Symbol | Value |
|---|---|---|
| Avogadro constant | $N_A$ | $6.022\,1415(10)\times10^{23}$ mol$^{-1}$ |
| Boltzmann constant | $k_\mathrm{B}$ | $1.380\,6505(24)\times10^{-23}$ J/K |
|  |  | $8.617\,343(15)\times10^{-5}$ eV/K |
| electron volt | eV | $1.602\,176\,53(14)\times10^{-19}$ J |
| Planck constant | h | $6.626\,0693(11)\times10^{-34}$ J·s |
|  |  | $4.135\,667\,43(35)\times10^{-15}$ eV·s |
| speed of light in vacuum | $c, c_0$ | 299 792 458 m/s |
| vacuum permeability (magnetic constant) | $\mu_0$ | $4\pi\times10^{-7}$ N/A$^2$ |
| vacuum permittivity (electric constant) | $\epsilon_0$ | $8.854\,187\,817\ldots\times10^{-12}$ F/m |

# Acronyms

| | |
|---|---|
| BIPM | International Bureau of Weight and Measures, 181 |
| CDMS | Cologne database for molecular spectroscopy, 129 |
| COC | cyclic olefin copolymer, 59 |
| CT | computed tomography, 49 |
| CVD | chemical vapour deposition, 265 |
| CW | continuous wave, 83 |
| DFG | difference frequency generation, 17 |
| DSP | digital signal processing, 118 |
| DTDS | differential time-domain spectroscopy, 45 |
| EHF | extremely high frequency, 3 |
| EO | electrooptical, 21 |
| FDTD | finite-difference time-domain, 77 |
| FEL | free electron laser, 15 |
| FIR | far infrared, 3 |
| FTIR | Fourier transform infrared spectrometer, spectroscopy, 15 |
| FWHM | full width at half maximum, 131 |
| GEISA | Gestion et Etude des Informations Spectroscopiques Atmosphériques, 130 |
| GUM | guide to the expression of uncertainty in measurement, 181 |
| HDPE | high-density polyethylene, 58 |
| HITRAN | high-resolution transmission molecular absorption database, 129 |

| | |
|---|---|
| HOS | human osteosarcoma, 166 |
| HWHM | half width at half maximum, 131 |
| IEC | International Electrotechnical Commission, 181 |
| IFCC | International Federation of Clinical Chemistry, 181 |
| ISO | International Organization for Standardization, 9 |
| IUPAC | International Union of Pure and Applied Chemistry, 181 |
| IUPAP | International Union of Pure and Applied Physics, 181 |
| JPL | Jet Propulsion Laboratory, 129 |
| LDPE | low-density polyethylene, 250 |
| LOO | leave-one-out, 167 |
| LPC | linear predictive coding, 74 |
| LTEM | laser terahertz-emission microscopy, 48 |
| MCS | Monte Carlo simulation, 180 |
| MSE | mean-square error, 153 |
| NHB | normal human bone, 166 |
| NIR | near infrared, 59 |
| OIML | International Organization of Legal Metrology, 181 |
| PCA | photoconductive antenna, 20 |
| PE | polyethylene, 82 |
| PMMA | poly(methyl methacrylate), 60 |
| PP | polypropylene, 57 |
| PTFE | polytetrafluoroethylene, 57 |
| QCL | quantum cascade laser, 17 |
| QWP | quantum well photodetector, 17 |

| | |
|---|---|
| SMO | sequential minimal optimisation, 165 |
| SNR | signal-to-noise ratio, 154 |
| SOS | silicon on sapphire, 23 |
| SVM | support vector machine, 157 |
| SVMAF | spatially variant moving average filter, 118 |
| TE | transverse electric, 255 |
| THz-TDS | terahertz time-domain spectroscopy, 1 |
| TM | transverse magnetic, 256 |
| UHMWPE | ultra-high molecular weight polyethylene, 57 |
| VIM | International Vocabulary of Basic and General Terms in Metrology, 181 |
| WBCAF | wide-band cross ambiguity function, 161 |

# Index

# Biography

**Withawat Withayachumnankul** was born in Bangkok, Thailand in 1980. From 1996 to 2000, he was educated at King Mongkut's Institute of Technology at Ladkrabang (KMITL), in his hometown, where he obtained a Bachelor's Degree in Electronic Engineering with honours. Working at the Biomedical Signal & Image Processing Laboratory at KMITL in 2000 as a postgraduate student, he performed a research involving digital signal/image processing and computer graphics. After receiving a Master's degree in Electronic Engineering in 2002, he served at his *alma mater* as a lecturer, a position that he currently retains. In this role, he conducted the computer programming and computer graphics courses in the Department of Information Engineering.

In 2005, he was a visiting scholar at the University of Adelaide, under Prof Derek Abbott, with research interest in T-ray signal processing. In 2006, he was granted an Australian Endeavour International Postgraduate Research Scholarship (EIPRS) and University of Adelaide Scholarship for Postgraduate Research to study toward his PhD under Prof Derek Abbott, Dr Bernd Fischer, and Dr Samuel Mickan, within the Adelaide T-ray group, the School of Electrical & Electronic Engineering, The University of Adelaide. During his candidature, Mr Withayachumnankul has received an IEEE LEOS Graduate Student Fellowship (now IEEE Photonics Society Graduate Student Fellowship), 2008, SPIE Scholarship in Optical Science and Engineering, 2008, award for the poster presentation at the SPIE Symposium on Microelectronics, MEMS, and Nanotechnology, Canberra, Australia, 2007, and contingency travel grant for the SPIE conference, 2007. He won a prestigious Australian Postdoctoral (APD) Fellowship awarded by the Australian Research Council (ARC), and he will take up this position in 2010.

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## Scientific Genealogy of
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