Theory of Tunable Diode Laser Absorption Spectroscopy

Opto Electronic Engineering Laboratory Corporation

http://www.optoelec-engineering.com/index_en.html

The TDLAS (Tunable Diode Laser Absorption Spectroscopy) is based on the Lambert Beer's law, which describes the phenomena of optical power decay passing through the space with the finite length L[m].

$$\frac{I_1[W]}{I_0[W]} = \exp\left(-\alpha[cm^{-1}]\times L[m]\right) = \exp\left(-\sigma[m^2]\times c[{molecule}/{m^3}]\times L[m]\right) \qquad \text{(Eq. A1)}$$

$$\alpha = \sigma[m^2]\times c[{molecule}/{m^3}] \qquad \text{(Eq. A2)}$$

I0 ; Incident Optical Power, I1 ; Output Optical Power, L ; length, α ; Spectral Absorption Coefficient
σ ; Absorption cross section, c ; number density of absorbers per unit volume

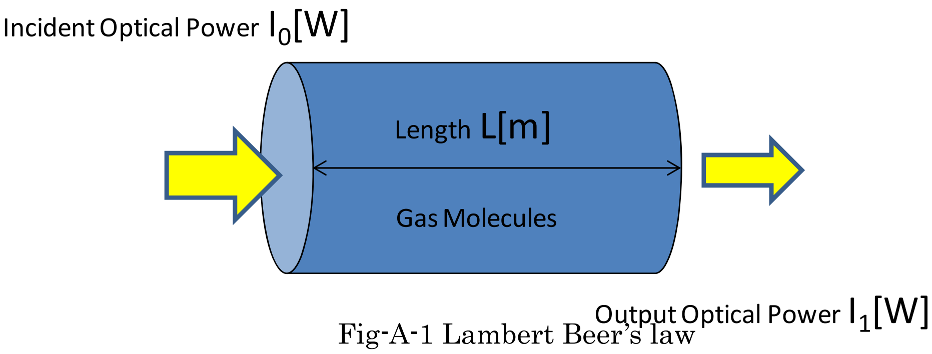

Fig-A-1 Lambert Beer's law

More in detail actually,

$$\frac{I_1[W]}{I_0[W]} = \exp\left(-S(T)[{cm^2\cdot cm^{-1}}/{molecule}]\times g(\lambda-\lambda_0)[{1}/{cm^{-1}}]\times c[{numbers}/{m^3}]\times L[m]\right) \qquad \text{(Eq. A3)}$$

$$\sigma[{m^2}/{molecule}] = S(T)[{cm^2\cdot cm^{-1}}/{molecule}]\times g(\lambda-\lambda_0)[{1}/{cm^{-1}}] \qquad \text{(Eq. A4)}$$

S(T) ; line strength, g(λ-λ0) ; line shape function
Now we can get the line strength value at the database of HITRAN.
Here giving the specific function to σ,

$$\sigma[{m^2}/{molecule}] = \frac{\sigma_0}{1+\left(\frac{\lambda-\lambda_0}{\Delta\lambda}\right)^2} \qquad \text{(Eq. A5)}$$

λ0 ; center wavelength of optical absorption, Δλ ; Full Width Half Maximum of wavelength,
σ0 ; cross section at central wavelength λ0

Here we use the techniques of Frequency Modulation Spectroscopy (FM Spectroscopy) as to Laser frequency with modulation frequency around fm=10 kHz. The Fig-A-2 shows the transform FM to AM (Amplitude Modulation) through absorption spectrum of Gas. It is apparent that the phase of modulation signal is shifted with π [rad] between positive slope region and negative slope region. It shows the characteristic of the 1st derivative of absorption spectrum with availability of slope to feedback control of auto Laser frequency control (AFC). So we use the feed-forward control technique with tuning the Laser temperature and Laser current in order to lock the state of Laser into available region of AFC.

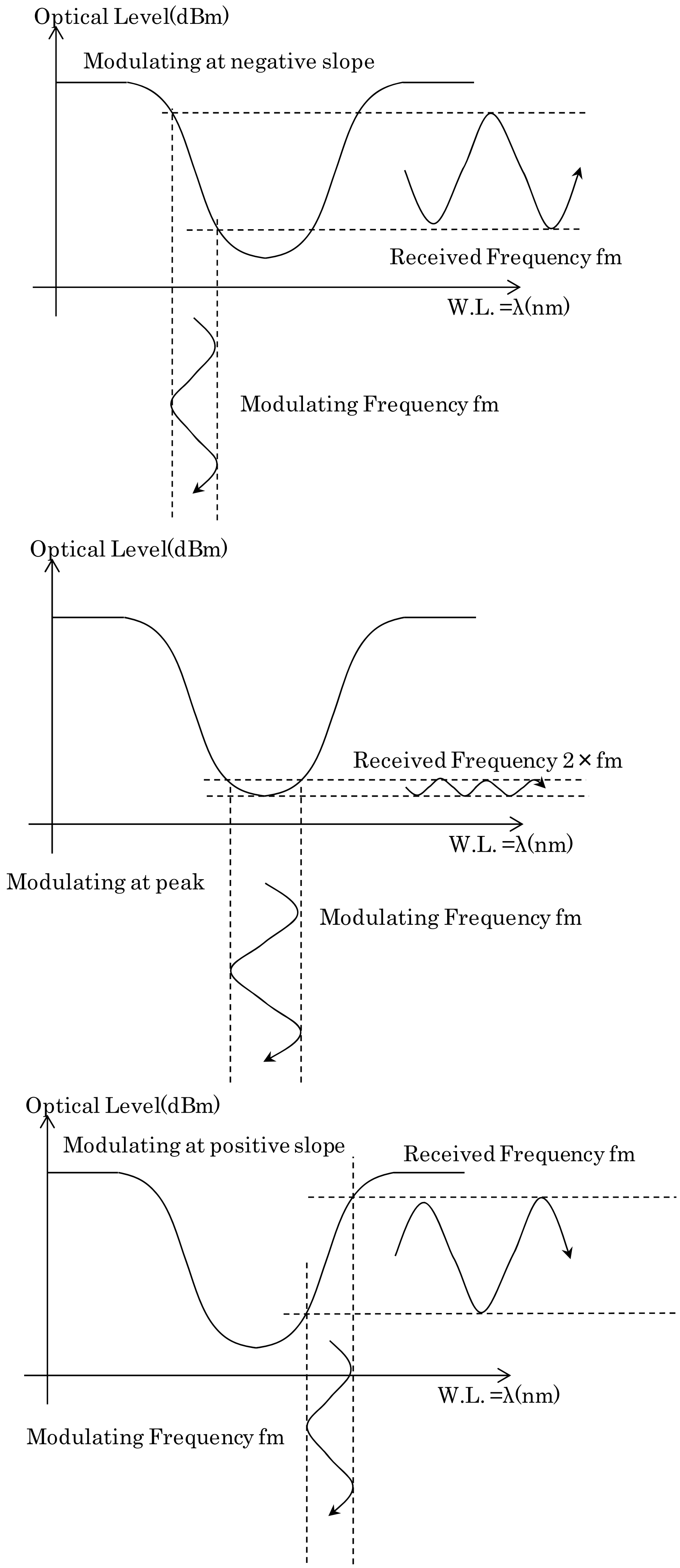

Fig-A-2 Frequency Modulation Spectroscopy (FM Spectroscopy)

The FM Spectroscopy shows the several equations as to modulation of optical frequency as noted below, The transmitted intensity I1 through Gas is noted for the function of optical frequency ω=2πf with modulation frequency ωm, (m ; modulation depth)

$$I_1(f) = I_1(f + m\cdot\sin(\omega_m\cdot t)) \qquad \text{(Eq. A6)}$$

Here we take m, ωm =2πf <ΔΓ = line-width of the absorption. Now we can expand I1 as a Taylor series

$$I_1(f + m\cdot\sin(\omega_m\cdot t))$$
$$= I_1(f) + (m\cdot\sin(\omega_m\cdot t))\times\frac{dI_1(f)}{df} + \frac{m^2\cdot\sin^2(\omega_m\cdot t)}{2!}\times\frac{d^2I_1(f)}{df^2} + \frac{m^3\cdot\sin^3(\omega_m\cdot t)}{3!}\times\frac{d^3I_1(f)}{df^3} + \cdots$$

(Eq. A7)

We use the formula of a trigonometric identity,

$$I_1(f + m\cdot\sin(\omega_m\cdot t))$$
$$= \left\{I_1(f) + \frac{m^2}{4}\cdot\frac{d^2I_1(f)}{df^2} + \cdots\right\} +$$
$$\sin(\omega_m\cdot t)\times\left\{m\cdot\frac{dI_1(f)}{df} + \frac{m^3}{12}\times\frac{d^3I_1(f)}{df^3} + \cdots\right\} +$$
$$\cos(2\omega_m\cdot t)\times\left\{-\frac{m^2}{4}\cdot\frac{d^2I_1(f)}{df^2} + \cdots\right\} + \cdots \qquad \text{(Eq. A8)}$$

So, the transmitted intensity I1 contains a DC term, a term oscillating at ωm, a term oscillating at 2ωm, and so on. If phase-sensitive detection is performed at ωm, 2ωm, the coefficient of the sin(ωm*t) term and of cos(2ωm*t) term can be extracted. In particular, since we have assumed that *m* is small, the coefficient of the sin(ωm*t) term is essentially *m* multiplied by the first derivative of the transmitted intensity I1. And more we have *m*^2 multiplied by the second derivative of the absorption at the cos(2ωm*t) term.

$$I_1(f + m\cdot\sin(\omega_m\cdot t)) \approx I_1(f) + \frac{m^2}{4}\cdot\frac{d^2I_1(f)}{df^2} + \sin(\omega_m\cdot t)\times m\cdot\frac{dI_1(f)}{df} - \cos(2\omega_m\cdot t)\times\frac{m^2}{4}\cdot\frac{d^2I_1(f)}{df^2}$$

(Eq. A9)

Then we calculate the first derivative and the second derivative of the transmitted intensity I1 as to optical wavelength. From (Eq. A3), (Eq. A5), we have obtained

$$\frac{d}{d\lambda}I_1(\lambda) = \frac{d}{d\lambda}\left\{I_0 \cdot K \cdot \exp\left(-S \times g(\lambda-\lambda_0) \times c \times L\right)\right\}$$

$$= \frac{d}{d\lambda}\left\{I_0 \cdot K \cdot \exp\left(-\sigma \times c \times L\right)\right\}$$

$$= \frac{d}{d\lambda}\left\{I_0 \cdot K \cdot \exp\left(-\frac{\sigma_0}{1+\left(\frac{\lambda-\lambda_0}{\Delta\lambda}\right)^2} \times c \times L\right)\right\} \qquad \text{(Eq. A9)}$$

Here, K is loss factor via Dust particles. By the way we should know about the relation between the deviation fragment df and dλ. The relation between the frequency and the wavelength is noted below, (υ is the light velocity)

$$\upsilon[m/s] = f[Hz] \times \lambda[m] \qquad \text{(Eq. A10)}$$

We differentiate the equation (Eq. A10) by df,

$$0 = f \times \frac{d\lambda}{df} + \frac{df}{df} \times \lambda = f \times \frac{d\lambda}{df} + \lambda$$

$$\frac{d\lambda}{\lambda} = -\frac{df}{f} \qquad \text{(Eq. A11)}$$

Now we are able to assume 1/f□1/f0=const., 1/λ□1/λ0=const. cause of slightly small variation of 1/f and of 1/λ around 1/f0,1/λ0 compared with df, dλ. So we get the equation

$$df = -\frac{f_0}{\lambda_0} \cdot d\lambda \qquad \text{(Eq. A12)}$$

Then the constant term –f0/λ0 is should be included into factor K. And we are continuing the calculations of (Eq. A9),

$$\frac{d}{d\lambda}\exp\left(-\frac{\sigma_0}{1+\left(\frac{\lambda-\lambda_0}{\Delta\lambda}\right)^2} \times c \times L\right) = \frac{d}{d\lambda}\exp\left[\frac{F}{1+X^2}\right] = \frac{d}{d\lambda}\exp(Y) \qquad \text{(Eq. A13-1)}$$

$$\frac{d}{d\lambda}I_1(\lambda) = I_0 \cdot K \cdot \frac{d}{d\lambda}\exp\left(-\frac{\sigma_0}{1+\left(\frac{\lambda-\lambda_0}{\Delta\lambda}\right)^2} \times c \times L\right) = I_0 \cdot K \cdot \frac{d}{d\lambda}\exp\left[\frac{F}{1+X^2}\right] = I_0 \cdot K \cdot \frac{d}{d\lambda}\exp(Y)$$

(Eq. A13-2)

Here,

$$F = -\sigma_0 \times c \times L, X = \frac{\lambda-\lambda_0}{\Delta\lambda} \qquad \text{(Eq. A14)}$$

Setting the parameter Y as,

$$Y = \frac{F}{1+X^2} \qquad \text{(Eq. A15)}$$

We get the relations about each deviation

$$\frac{dX}{d\lambda}=\frac{1}{\Delta\lambda},\frac{dY}{dX}=\frac{-2FX}{\left(1+X^2\right)^2}=\frac{-2FX}{\varsigma^2},\frac{d}{dY}\exp(Y)=\exp(Y) \qquad \text{(Eq. A15)}$$

Here,

$$\varsigma=1+X^2 \qquad \text{(Eq. A16)}$$

So we are continuing the calculations from (Eq. A13)

$$\frac{d}{d\lambda}\exp(Y)=\frac{d}{d\lambda}\exp\left[\frac{F}{1+X^2}\right]=\frac{dX}{d\lambda}\cdot\frac{dY}{dX}\cdot\frac{d}{dY}\exp(Y)$$

$$=\frac{1}{\Delta\lambda}\cdot\frac{-2FX}{\left(1+X^2\right)^2}\cdot\exp(Y)=\frac{1}{\Delta\lambda}\cdot\frac{-2FX}{\varsigma^2}\cdot\exp(Y) \qquad \text{(Eq. A17)}$$

Next we calculate the second derivative of the transmitted intensity I1 as to optical wavelength.

$$\frac{d^2}{d\lambda^2}\exp(Y)=\frac{d^2}{d\lambda^2}\exp\left[\frac{F}{1+X^2}\right]=\frac{1}{\Delta\lambda}\cdot\frac{d}{d\lambda}\left\{\frac{-2FX}{\varsigma^2}\right\}\cdot\exp(Y)+\frac{1}{\Delta\lambda}\cdot\frac{-2FX}{\varsigma^2}\cdot\frac{d}{d\lambda}\exp(Y) \qquad \text{(Eq. A18)}$$

Here we obtain

$$\frac{d}{dX}\varsigma=2X,\frac{d}{dX}\varsigma^2=4X\cdot(1+X^2)=4X\cdot\varsigma \qquad \text{(Eq. A19)}$$

And then

$$\frac{d}{d\lambda}\left\{\frac{-2FX}{\varsigma^2}\right\}=(2F)\cdot\frac{4X^2-\varsigma}{\varsigma^3} \qquad \text{(Eq. A20)}$$

So (Eq. A18) becomes

$$\frac{d^2}{d\lambda^2}\exp(Y)=\frac{2F}{\Delta\lambda}\cdot\frac{\exp(Y)}{\varsigma^3}\cdot\left\{\left(4X^2-\varsigma\right)+\frac{2FX^2}{\Delta\lambda\cdot\varsigma}\right\} \qquad \text{(Eq. A21)}$$

We are going to apply the AFC in which the optical wavelengthλ is nearly equal to the central absorption wavelength λ0, so the X is very small (X<<1), the ζ is nearly equal to value 1 (ζ□1). Then we obtain

$$\frac{d^2}{d\lambda^2}\exp(Y)\approx\frac{-2F}{\Delta\lambda}\cdot\frac{\exp(Y)}{\varsigma^2}=\frac{2\times\sigma_0\times c\times L}{\Delta\lambda}\cdot\frac{\exp\left[-\dfrac{\sigma_0\times c\times L}{1+\left(\dfrac{\lambda-\lambda_0}{\Delta\lambda}\right)^2}\right]}{\left(1+\left(\dfrac{\lambda-\lambda_0}{\Delta\lambda}\right)^2\right)^2}\approx\frac{2\sigma_0 cL}{\Delta\lambda}\cdot\exp\left[-\sigma_0 cL\right]$$

(Eq. A22)

$$\frac{d^2I_1(\lambda)}{d\lambda^2}=I_0\cdot K\cdot\frac{d^2}{d\lambda^2}\exp(Y)=I_0\cdot K\cdot\frac{2\sigma_0 cL}{\Delta\lambda}\cdot\exp\left[-\sigma_0 cL\right] \qquad \text{(Eq. A23)}$$

Substituting the (Eq. A23) into the (Eq. A9) as to 2*ωm term

$$I_1(2\omega_m\cdot t)=\cos(2\omega_m\cdot t)\times\frac{m'^2}{4}\cdot\frac{d^2I_1(\lambda)}{d\lambda^2}=\cos(2\omega_m\cdot t)\times\frac{m'^2}{4}\cdot I_0\cdot K\cdot\frac{2\sigma_0 cL}{\Delta\lambda}\cdot\exp\left[-\sigma_0 cL\right]$$

(Eq. A24)

The (Eq. A24) is indicating that we are able to obtain directly the concentration c [ppm / ℓ] of Gas by measuring the received signal modulated in the frequency 2*ωm via the phase sensitive detection method.

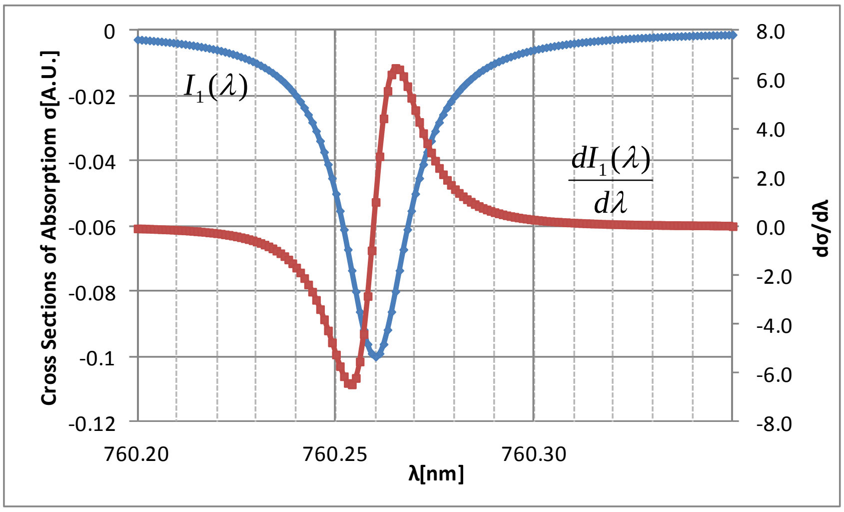

Fig-A-3 the simulation result of absorption spectrum and its first derivative

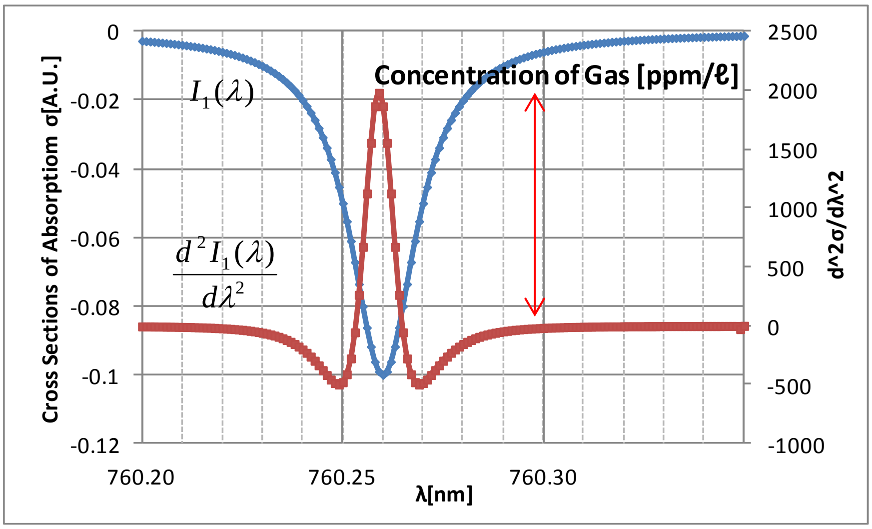

Fig-A-4 the simulation result of absorption spectrum and its second derivative

■the phase sensitive detection method

There are two signals Is, I0 with each frequency ωs and ω0. The expressions of Is, I0 are noted below,

$$I_s(t) = A\cdot\sin(\omega_s t + \varphi_0) = A\cdot\sin(2\pi\cdot f_s t + \varphi_0) \qquad \text{(Eq. A25)}$$

$$I_{o1}(t) = B\cdot\sin(\omega_0 t) = B\cdot\sin(2\pi\cdot f_0 t) \qquad \text{(Eq. A26)}$$

Here A, B are the constant amplitude of signals, φ0 is the phase difference. The Is is the sensed signal, the Io1 is the local oscillator signal (modulator signal). The strength of the local oscillator signal B is larger than the value of A.

More we prepare the local oscillator signal Io2 with the phase delay π/2 to Io1.

$$I_{o2}(t) = B\cdot\sin(\omega_0 t + \pi/2) = B\cdot\sin(2\pi\cdot f_0 t + \pi/2) \qquad \text{(Eq. A27)}$$

We are multiplying the (Eq. A25) by (Eq. A26) and by (Eq. A27), and extracting the amplitude term and the phase term with the assumptions that ω0=ωs as the homodyne detection, it is obtained through the LPF that

$$\overline{I_s(t)\times I_{o1}(t)} = A\cdot B\cdot\cos(\varphi_0) \qquad \text{(Eq. A28)}$$

$$\overline{I_s(t)\times I_{o2}(t)} = A\cdot B\cdot\sin(\varphi_0) \qquad \text{(Eq. A29)}$$

Amplitude term

$$A = \frac{2}{B}\cdot\sqrt{\left(\overline{I_s(t)\times I_{o1}(t)}\right)^2 + \left(\overline{I_s(t)\times I_{o2}(t)}\right)^2} \qquad \text{(Eq. A30)}$$

Phase term

$$\varphi = \tan^{-1}\left\{\frac{\left(\overline{I_s(t)\times I_{o2}(t)}\right)}{\left(\overline{I_s(t)\times I_{o1}(t)}\right)}\right\} \qquad \text{(Eq. A31)}$$