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Technical Note
UV-VIS as a Tool to Determine Size and Concentration

TN801

Using UV-VIS as a tool to determine size and concentration of Spherical Gold Nanoparticles (SGNPs) from 5 to 100 nm[1]

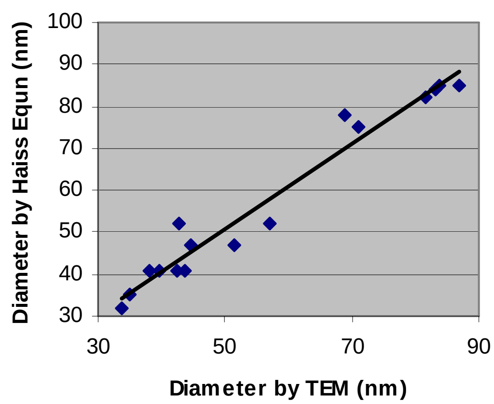
In this technical note, we describe the use of a UV-VIS as a QA/QC instrument for sizing and concentration determination of spherical gold nanoparticles (SGNPs). Up until now, Transmission Electron Microscopy (TEM) has been used. However, electron microscopy does not lend itself to being a good QA/QC instrument due to its limitations in sample size, invitation to the potential increase in operator error, and low throughput.

Calculating SGNP size from SPR Peak location

Two equations were provided from the reference. One equation applied to nanoparticles greater than 35 nm in diameter, the other for gold nanoparticles 5 to 30 nm in diameter. The different equation for the smaller gold nanoparticles can be attributed to a pronounced increase of the ratio of surface atoms to bulk atoms. From his publication, for nanoparticles 35-100 nm in size, Haiss uses:

$$d = \frac{\ln\left(\frac{\lambda_{spr} - \lambda_0}{L_1}\right)}{L_2} \qquad (1)$$

where d is the diameter of the SGNP, λ_{spr} is the wavelength at the peak of the surface plasmon resonance (SPR), $\lambda_0 = 512$, $L_1 = 6.53$, and $L_2 = 0.0216$. Utilizing over 50 data points in his paper, Haiss finds an absolute error of 3%. Applying the equation to our



[1] W. Haiss et al., Determination of Size and Concentration of Gold Nanoparticles from UV-VIS Spectra, Anal. Chem. 2007, 79, 4215-4221

gold nanoparticles determined by TEM, we find an error of 4%.

To calculate the diameter of our SGNPs for sizes 5 to 30 nm, we use another Haiss equation:

$$d = \left(\frac{A_{spr}\left(5.89 X 10^{-6}\right)}{c_{Au} \exp\left(C_1\right)} \right)^{\frac{1}{C_2}} \quad (2)$$

Where A_{spr} is the absorption (AU) at the peak SPR, c_{Au} (moles/L) is the amount of gold used in the synthesis, C_1 = -4.75, and C_2 = 0.314. The error calculated by Haiss is ~ 6%.

Calculating SGNP concentration

Concentration is determined by using the diameter of the gold nanoparticles calculated in (1) and (2) with the known absorption at 450 nm. This equation is given by:

$$N = \frac{A_{450} X 10^{14}}{d^2 \left[-0.295 + 1.36 \exp\left(-\left(\frac{d - 96.8}{78.2} \right)^2 \right) \right]} \quad (3)$$

where N is the number density of SGNPs in nps/ml, A_{450} is the absorption (AU) at 450 nm, and d is the diameter of the SGNP. Haiss finds this equation to be accurate to ~6%. From this equation, we can find a host of other concentration measurements. This includes Wt. conc., Wt. %, ppm, molarity, and molar extinction.

$$Wt.conc\left(\frac{\mu g}{ml}\right) = \frac{nps}{ml} x \frac{\frac{4}{3}\pi r^3 cm^3 x \frac{19.28 x 10^{-21} g}{cm^3}}{nps} x \frac{10^6 \mu g}{g} \quad (4)$$

where r is the radius of the gold nanoparticle, and nps refers to the number of particles.

$$\text{Wt. \%} = \text{Wt. conc. x } 10^{-6} \quad (5)$$

$$\text{ppm} = \text{wt. conc.} \quad (6)$$

$$\text{molarity (pM)} = \text{nps/ml} \times 1.67\text{x}10^{-9} \quad (7)$$

$$\text{Molar Ext. } (M^{-1}cm^{-1}) = \text{OD} \times 10^{12}/\text{molarity} \quad (8)$$

To determine the percentage attributed to absorption and scattering of the total extinction, we use Jain et. al[2] where we curve fit their data points for sizes 20-80 nm with the equation:

$$\%\ \text{scattering} = 0.0001d^2 - 0.0054d + 0.0589 \quad (9)$$

$$\%\ \text{absorption} = 1 - \%\text{scattering} \quad (10)$$

where *d* is the diameter of the gold nanoparticle.

[2] Jain, Lee, El-Sayed, and El-Sayed M., "Calculated Absorption and Scattering Properties of Gold Nanoparticles of Different Size, Shape, and Composition: Applications in Biological Imaging and Biomedicine," J. Phys. Chem. B 2006, 110, 7238-7248