Determination of size and concentration of gold and silica nanoparticles from absorption and turbidity spectra

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The average size and concentration of plasmonic and dielectric nanoparticles can be evaluated from absorption (A) and turbidity (τ) spectra, respectively. Here, these approaches are exemplified by colloidal gold and Stöber silica nanoparticles. For spherical gold nanoparticles, the average size is determined by the spectral position of plasmonic peak (510-580 nm), independently on the particle concentration. And *vice versa*, the particle concentration can be determined from the absorption in the short wavelength part of spectrum (e.g., at 450 nm) independently on the particle size. It is generally believed that such correlations between the size/concentration and the absorption spectrum can be derived from Mie theory. Here, we discuss this point in the context of a long-term collection of published experimental data and T-matrix simulations, which account for the particle shape and size polydispersity.[1] In principle, the concentration of silica particles can be evaluated by combining the TEM particle size, the optical density measurements, and Mie calculations of the particle extinction cross section, which equals the scattering cross section in this case. However, such an approach uses two independent methods, and, what is more important, one needs to know the refractive index of silica particles. Here, we discuss a spectroturbidimetry (STT) approach[2] based on two experimental parameters: (1) the wavelength exponent $w = -d\log(\tau)/d\log(\lambda)$, which is nothing but the average slope of spectrum $\tau \sim \lambda^{-w}$ in logarithmic coordinates ($400 \leq \lambda \leq 600$ nm); and (2) the average turbidity (extinction) at 500 nm. Given the average refractive index of silica nanoparticles $n = 1.475$,[2] we have calculated calibration plots for simple and convenient determination of the average particle size and concentration, with the measured values of the wavelength exponent and turbidity (extinction) at the average wavelength 500 nm. TEM measurements for several experimental samples are shown to be in excellent agreement with the STT average diameters, whereas the dynamic light scattering (DLS) gives somewhat worse values with unrealistic dispersions. Our estimation of the refractive index n=1.475 seems to be a best-fitting compromise ensuring fairly accurate determination of both the particle size and the concentration, in comparison with benchmark TEM and material balance data, respectively.

1. "Determination of size and concentration of gold nanoparticles from extinction spectra", Nikolai G. Khlebtsov, *Anal. Chem*, 80, 6620 (2008).

2. "Determination of the size, concentration, and refractive index of silica nanoparticles from turbidity spectra" Boris N. Khlebtsov, Vitaly A. Khanadeev, Nikolai G. Khlebtsov, *Langmuir*, 24, 8964 (2008).