



# Analytical Model for Determination of Size-Distribution of Colloidal Silver Nanoparticles from Surface Plasmon Resonance Wavelength and Dielectric Functions

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Through use of shift functions  $f_2(D)$  and  $f_3(D)$  on concentration  $c_j(D)$  given by (6) and conservation of total concentration, characteristic diameters of log-normal size distribution are obtained. Namely, those are mode (most frequent) diameter  $D_m$ , volume average diameter  $\langle D \rangle = D_m e^{\frac{s^2}{2}}$  and model diameter  $D_M = D_m e^{\frac{3s^2}{2}}$ . Concretely, from conservation of total concentration volume average diameter  $\langle D \rangle$  is obtained, by multiplying concentration with shift function  $f_2(D)$  mode diameter  $D_m$  is obtained and by multiplying concentration with shift function  $f_3(D)$  model diameter  $D_M$  is obtained. From that, we start with following system of equations:

$$K_2 \frac{D_m^2}{D_m^2 + (\Delta\lambda)^2} = e^{\frac{3}{2}s^2} \quad (S1)$$

$$K_3 \frac{1}{(D_M)^2 + (\Delta\lambda)^2} = \frac{1}{(\langle D \rangle)^3} \quad (S2)$$

Combining the two equations (S1) and (S2), relation between redshift constants is obtained:

$$K_3 = K_2 \frac{1}{D_m} \frac{\left(D_m e^{\frac{s^2}{2}}\right)^2 + (\Delta\lambda)^2}{D_m^2 + (\Delta\lambda)^2} \quad (S3)$$

In order to calculate shift of concentration by function  $f_3(D)$ , (S3) is used and following must be satisfied:

$$K_3 \frac{\left(D_m e^{\frac{s^2}{2}}\right)^3}{\left(D_m e^{\frac{s^2}{2}}\right)^2 + (\Delta\lambda)^2} = K_2 \frac{D_m^2 e^{\frac{3}{2}s^2}}{D_m^2 + (\Delta\lambda)^2} \quad (S4)$$

Expression (S4) must be by definition equal to:

$$K_2 \frac{D_m^2 e^{\frac{3}{2}s^2}}{D_m^2 + (\Delta\lambda)^2} = \left(\frac{D_M}{\langle D \rangle}\right)^3 \quad (S5)$$

Before continuing derivation, one can show that (S1) can be rewritten as:

$$e^{\frac{1}{2}s^2} = K_2 \cdot \left(\frac{\lambda_0}{\lambda_{SPR}}\right)^3 \quad (S6)$$

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Rewriting equation (S5), one obtains:

$$D_M^3 = K_2 \frac{D_m^5}{D_m^2 + (\Delta\lambda)^2} \quad (S7)$$

If now all diameters in equation (S7) are shifted for  $e^{-\frac{s^2}{2}}$ , we obtain:

$$D_m^3 = K_2 \frac{\left(D_m e^{-\frac{s^2}{2}}\right)^5}{\left(D_m e^{-\frac{s^2}{2}}\right)^2 + (\Delta\lambda)^2} \quad (S8)$$

Using (S6) in (S8) in order to eliminate factors  $e^{-\frac{s^2}{2}}$  we obtain:

$$D_m^3 = \frac{K_2^{-\frac{2}{3}} D_m^5 \left(\frac{\lambda_{SPR}}{\lambda_0}\right)^{15}}{K_2^{-\frac{2}{3}} D_m^2 \left(\frac{\lambda_{SPR}}{\lambda_0}\right)^6 + (\Delta\lambda)^2} \quad (S9)$$

Solving (S9) by variable  $D_m$ , analytical expression is obtained:

$$D_m = K^{\frac{1}{3}} \left(\frac{\lambda_0}{\lambda_{SPR}}\right)^3 \frac{\Delta\lambda}{\sqrt{\left(\frac{\lambda_{SPR}}{\lambda_0}\right)^9 - 1}} \quad (S10)$$

Final formula is shifted from (S10) by  $\left(\frac{\lambda_{SPR}}{\lambda_0}\right)^2$  so finally it writes:

$$D_m^* = K^{\frac{1}{3}} \left(\frac{\lambda_0}{\lambda_{SPR}}\right) \frac{\Delta\lambda}{\sqrt{\left(\frac{\lambda_{SPR}}{\lambda_0}\right)^9 - 1}} \quad (S11)$$