COMMENTS

Comment on "Simulation of the Optical Absorption Spectra of Gold Nanorods as a Function of Their Aspect Ratio and the Effect of the Medium Dielectric Constant"

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A few years ago,[1] Link and co-workers modeled the optical absorption spectra of gold nanorods and derived a simple relationship equation between the absorption maximum of the longitudinal plasmon resonance, λ_{max}, and the aspect ratio, R, and the medium dielectric constant, ϵ_m. Such an equation would be indeed desirable because it allows us to predict the maximum of the longitudinal mode, λ_{max}, for a certain aspect ratio R and medium dielectric constant ϵ_m. However, we find that their equation is erroneous because there is a mistake in their linear fit. We've derived a new equation by the same method.

Gans' theory[2] is employed by Link et al. to model the absorption spectra of gold nanorods treated as elongated ellipsoids. By considering that the resonance condition for the longitudinal resonance is roughly fulfilled if

$$\epsilon_1 = -\frac{(1 - P_A)\epsilon_m}{P_A} \tag{1}$$

an equation is derived to express the relationship between λ_{max} and R and ϵ_m. The real part of the gold dielectric function, ϵ_1, is wavelength-dependent. P_A is the depolarization factor for the axis A of the rod. Plotting ϵ_1 as a function of the wavelength of the interacting light in the range between 500 and 800 nm and linearizing yield

$$\epsilon_1 = -0.071\lambda + 33.05 \tag{2}$$

with a regression coefficient of 0.9999. This equation is close to the result of Link et al. Similarly, plotting $(1 - P_A)/P_A$ as a function of the aspect ratio R between 2 and 4 leads to another equation with a regression coefficient of 0.9991:

$$\frac{1 - P_A}{P_A} = -2.95 + 3.75R \tag{3}$$

However, this equation is quite different from that of Link et al., which is as follows:

$$\frac{1 - P_A}{P_A} = -3.40 + 2.45R \tag{4}$$

Combining eqs 1−3 then gives our new equation:

$$\lambda_{max} = (52.95R - 41.68)\epsilon_m + 466.38 \tag{5}$$

Because there are errors in their calculation, especially in eq 4, eq 5 is quite different from the result of Link et al., which is as follows:

$$\lambda_{max} = (33.34R - 46.31)\epsilon_m + 472.31 \tag{6}$$

Together with the experimental values for λ_{max} and R, the medium dielectric constants ϵ_m calculated by eq 5 are around 2, as listed in Table 1. In contrast, those ϵ_m derived from eq 6 are between 3.9 and 6.9.

TABLE 1: Absorption Maximum of the Longitudinal Plasmon Resonance, λ_{max}, and Average Aspect Ratio, R, of the Gold Nanorod Samples and Respective Medium Dielectric Constants, ϵ_m, Obtained by Calculation

R^a	$\lambda_{max}{}^a$ (nm)	$\epsilon_m{}^b$	$\epsilon_m{}^c$
3.3	740	2.06	4.2
2.9	722	2.28	5.0
2.6	700	2.43	5.6
2.3	682	2.69	6.9

[a] λ_{max} and R are obtained by thermal reshaping in experiment by Link et al. [b] ϵ_m was calculated via eq 5. [c] ϵ_m was calculated via eq 6 by Link et al.

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References and Notes

(1) Link, S.; Mohamed, M. B.; El-Sayed, M. A. *J. Phys. Chem. B* **1999**, *103*, 3073.
(2) Papavassiliou, G. C. *Prog. Solid State Chem.* **1980**, *12*, 185.

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