Errata: Fitting the optical constants of gold, silver, chromium, titanium and aluminum in the visible bandwidth

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Abstract. This paper [J. Nanophoton. 8(1), 083097 (2014)] was published on 6 January 2014. Thanks to a question by Yoann Brûlé from the Fresnel institute (Marseille, France), we found that the values of $\gamma_L$ and $\gamma_D$ were swapped in tables in Ref. 1. The problem comes from a bug in the automatic extraction of data from optimization method. Fortunately the curves in Ref. 1 are correct. This erratum gives a more readily available formulation of fitting for all considered metals and the corresponding criteria. © 2014 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: 10.1117/1.JNP.8.089996]

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1 The Combination of Drude and Lorentz Models

The function of fit $\epsilon_{DL}$ of the relative permittivity of metal is written as the sum of the Drude and the Lorentz models:

$$
\epsilon_{DL}(\omega) = \epsilon_\infty - \frac{\omega_D^2}{\omega(\omega + i\gamma_D)} - \frac{\Delta \epsilon \omega_L^2}{\omega^2 - \omega_L^2 + i\gamma_L \omega},
$$

(1)

In the following the angular frequency $\omega$ (rad/s) that is used in formula falls within the visible domain $[2.354e15; 4.709e15]$ rad/s, corresponding to wavelengths in $[400; 800]$ nm and photon energy in $[1.55, 3.10]$ eV. Outside this domain, the quality of fitting can be impaired. This erratum gives us the opportunity to give better solutions to this hard problem of fitting, by investigating a wider space of search. The values of $\sigma_R$ and $\sigma_I$ are calculated according formula (8-9) in1, including the number of data used to compute the fitting equation.

1.1 Gold (Johnson & Christy2)

$$
\epsilon_{DL}^{JC}(\omega) = 6.1599 - \frac{1.8160E32}{\omega^2 + i7.2096E13 \omega} - \frac{4.5011E31}{\omega^2 - 2.1732E31 + i1.6694E15 \omega},
$$

(2)

$C = 0.99995, \quad F = 0.55, \quad \sigma_R = 0.40, \quad \sigma_I = 0.38.$

1.2 Gold (Palik3)

$$
\epsilon_{DL}^{AP}(\omega) = 0.6888 - \frac{1.5817E33}{\omega^2 + i7.3731E15 \omega} + \frac{9.3582E32}{\omega^2 - 5.5354E30 + i4.9327E15 \omega},
$$

(3)

$C = 0.24646, \quad F = 1.08, \quad \sigma_R = 0.95, \quad \sigma_I = 0.51.$
1.3 Silver (Palik$^3$)

\[ \epsilon_{DL}^{Ag}(\omega) = 0.0067526 - \frac{1.7584 \times 10^{32}}{\omega^2 + i1.0444 \times 10^{14}\omega} - \frac{9.9267 \times 10^{32}}{\omega^2 - 2.6509 \times 10^{32} + i7.3068 \times 10^{15}\omega} , \]

\[ C = 0.80656, \quad F = 0.07154, \quad \sigma_R = 0.053, \quad \sigma_I = 0.048. \]

1.4 Aluminum (Palik$^3$)

\[ \epsilon_{DL}^{Al}(\omega) = 0.13313 - \frac{9.0588 \times 10^{32}}{\omega^2 + i3.1083 \times 10^{15}\omega} + \frac{5.6526 \times 10^{32}}{\omega^2 - 1.2718 \times 10^{31} + i6.4539 \times 10^{15}\omega} , \]

\[ C = 0.996, \quad F = 2.98, \quad \sigma_R = 2.49, \quad \sigma_I = 1.64. \]

1.5 Chromium (Palik$^3$)

\[ \epsilon_{DL}^{Cr}(\omega) = 2.7767 - \frac{2.5306 \times 10^{32}}{\omega^2 + i2.9966 \times 10^{15}\omega} - \frac{1.4736 \times 10^{32}}{\omega^2 - 1.1087 \times 10^{31} + i2.5764 \times 10^{15}\omega} , \]

\[ C = 0.9998, \quad F = 0.947, \quad \sigma_R = 0.63, \quad \sigma_I = 0.71. \]

1.6 Titanium (Palik$^3$)

\[ \epsilon_{DL}(\omega) = -5.4742 \times 10^{7} - \frac{3.4555 \times 10^{32}}{\omega^2 + i5.1502 \times 10^{15}\omega} - \frac{9.3068 \times 10^{54}}{\omega^2 - 1.7001 \times 10^{47} + i3.2120 \times 10^{24}\omega} , \]

\[ C = 0.9665, \quad F = 0.57, \quad \sigma_R = 0.47, \quad \sigma_I = 0.33. \]

2 Conclusion

The proposed results of fitting of relative permittivities of metals are more accurate than those proposed in a previous paper$^4$ and verify the criterion of compatibility with FDTD use. They can be used directly for any spectroscopic simulation$^5,6$ and especially in FDTD codes, and for plasmonics$^7$ and optimization where accurate positions of resonances should be found. The proposed method of fitting under constraint is a combination of PSO and Nelder-mead simplex methods appears to be efficient, even if the solution of the problem of fitting is not unique.

References

