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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 γ_L and γ_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. [DOI: 10.1117/1.JNP.8.089996]

Keywords: dispersion; data processing; optical properties

1 The Combination of Drude and Lorentz Models

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

$$\epsilon_{DL}(\omega) = \epsilon_\infty - \frac{\omega_D^2}{\omega(\omega + i\gamma_D)} - \frac{\Delta\epsilon\omega_L^2}{\omega^2 - \omega_L^2 + i\gamma_L\omega}. \tag{1}$$

In the following the angular frequency ω (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 σ_R and σ_I are calculated according formula (8-9) in[1], including the number of data used to compute the fitting equation.

1.1 *Gold (Johnson & Christy[2])*

$$\epsilon_{DL}^{\mathrm{Au}_{JC}}(\omega) = 6.1599 - \frac{1.8160\mathrm{E}32}{\omega^2 + i7.2096\mathrm{E}13\omega} - \frac{4.5011\mathrm{E}31}{\omega^2 - 2.1732\mathrm{E}31 + i1.6694\mathrm{E}15\omega}, \tag{2}$$

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

1.2 *Gold (Palik[3])*

$$\epsilon_{DL}^{\mathrm{Au}_{P}}(\omega) = 0.6888 - \frac{1.5817\mathrm{E}33}{\omega^2 + i7.3731\mathrm{E}15\omega} + \frac{9.3582\mathrm{E}32}{\omega^2 - 5.5354\mathrm{E}30 + i4.9327\mathrm{E}15\omega}, \tag{3}$$

$$C = 0.24646, \quad F = 1.08, \quad \sigma_R = 0.95, \quad \sigma_I = 0.51.$$

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1.3 *Silver (Palik[3])*

$$\epsilon_{DL}^{\mathrm{Ag}_P}(\omega) = 0.0067526 - \frac{1.7584\mathrm{E}32}{\omega^2 + i1.0444\mathrm{E}14\omega} - \frac{9.9267\mathrm{E}32}{\omega^2 - 2.6509\mathrm{E}32 + i7.3068\mathrm{E}15\omega}, \tag{4}$$

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

1.4 *Aluminum (Palik[3])*

$$\epsilon_{DL}^{\mathrm{Al}_P}(\omega) = 0.13313 - \frac{9.0588\mathrm{E}32}{\omega^2 + i3.1083\mathrm{E}15\omega} + \frac{5.6526\mathrm{E}32}{\omega^2 - 1.2718\mathrm{E}31 + i6.4539\mathrm{E}15\omega}, \tag{5}$$

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

1.5 *Chromium (Palik[3])*

$$\epsilon_{DL}^{\mathrm{Cr}}(\omega) = 2.7767 - \frac{2.5306\mathrm{E}32}{\omega^2 + i2.9966\mathrm{E}15\omega} - \frac{1.4736\mathrm{E}32}{\omega^2 - 1.1087\mathrm{E}31 + i2.5764\mathrm{E}15\omega}, \tag{6}$$

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

1.6 *Titanium (Palik[3])*

$$\epsilon_{DL}(\omega) = -5.4742\mathrm{E}7 - \frac{3.4555\mathrm{E}32}{\omega^2 + i5.1502\mathrm{E}15\omega} - \frac{9.3068\mathrm{E}54}{\omega^2 - 1.7001\mathrm{E}47 + i3.2120\mathrm{E}24\omega}, \tag{7}$$

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

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.

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