Notes on Metals in `meep`

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1 Material Dispersion

Dielectric materials in `meep` are implemented in terms of a frequency and position dependent μ and ϵ. Specifically, the electric field as a function of angular frequency $\epsilon(\omega)$ is defined according to

$$\epsilon(\omega) = \epsilon_\infty + \sum_n \frac{\sigma_n \omega_n^2}{\omega_n^2 - \omega^2 - \mathrm{i}\omega\Gamma_n} \tag{1}$$

where ϵ_∞ is the instantaneous dielectric response (DC), σ_D is the electric conductivity, ω_n and Γ_n are constants, and σ_n is a function of position specifying the strength of the n^{th} resonance.[1]

In the literature however, metals are commonly specified according to the Lorentz-Drude (LD) model.

$$\epsilon_{LD} = \epsilon_D + \epsilon_L \tag{2}$$

where ϵ_D is contribution from the Drude model, representing the free electron effects

$$\epsilon_D = 1 - \frac{f_1 \omega_p'^2}{\omega(\omega - \mathrm{i}\Gamma_1')} \tag{3}$$

and ϵ_L is the Lorentz contribution, representing the bound electron effects

$$\epsilon_L = \sum_n \frac{f_n \omega_p'^2}{\omega_n'^2 - \omega^2 + \mathrm{i}\omega\Gamma_n'} \tag{4}$$

This particular model and coefficients are obtained from [1]. In this paper, the coefficients are in electron volts. Since `meep` operates in dimensionless units (e.g. $c = \hbar = 1$), the units in [1] must be converted. First a length scale a is chosen. The frequencies are then expressed in c/a, where c is the speed of light. The conversion from joules to electron volts is given by Thus to convert from eV to angular frequency, simply divide the result by $\hbar$. Likewise to convert this angular frequency to dimensionless units, the result must be divided by $2\pi c/a$. Putting this together, given a value X_{eV} in eV, the corresponding value in dimensionless units X_0 is obtained by

$$X_0 = \frac{X_{\text{eV}}}{\hbar} \Big/ (2\pi c/a) \tag{5}$$

$$= X_{\text{eV}} \frac{1}{2\pi\hbar c/a} \tag{6}$$

$$= X_{\text{eV}} \frac{a}{hc} \tag{7}$$

Once normalized, the LD coefficients can be imported into `meep` with the transformations[2]

$$\omega_1 = 1 \times 10^{-20} \tag{8}$$

$$\sigma_n = \frac{f_n \omega_p'^2}{\omega_n^2} \tag{9}$$

$$\epsilon_\infty = 1 \tag{10}$$

$$\Gamma_n = \Gamma_n' \tag{11}$$

[1] `http://ab-initio.mit.edu/wiki/index.php/Dielectric_materials_in_Meep`

[2] Derivation and script by Bala Krishna Juluri `http://juluribk.com/`

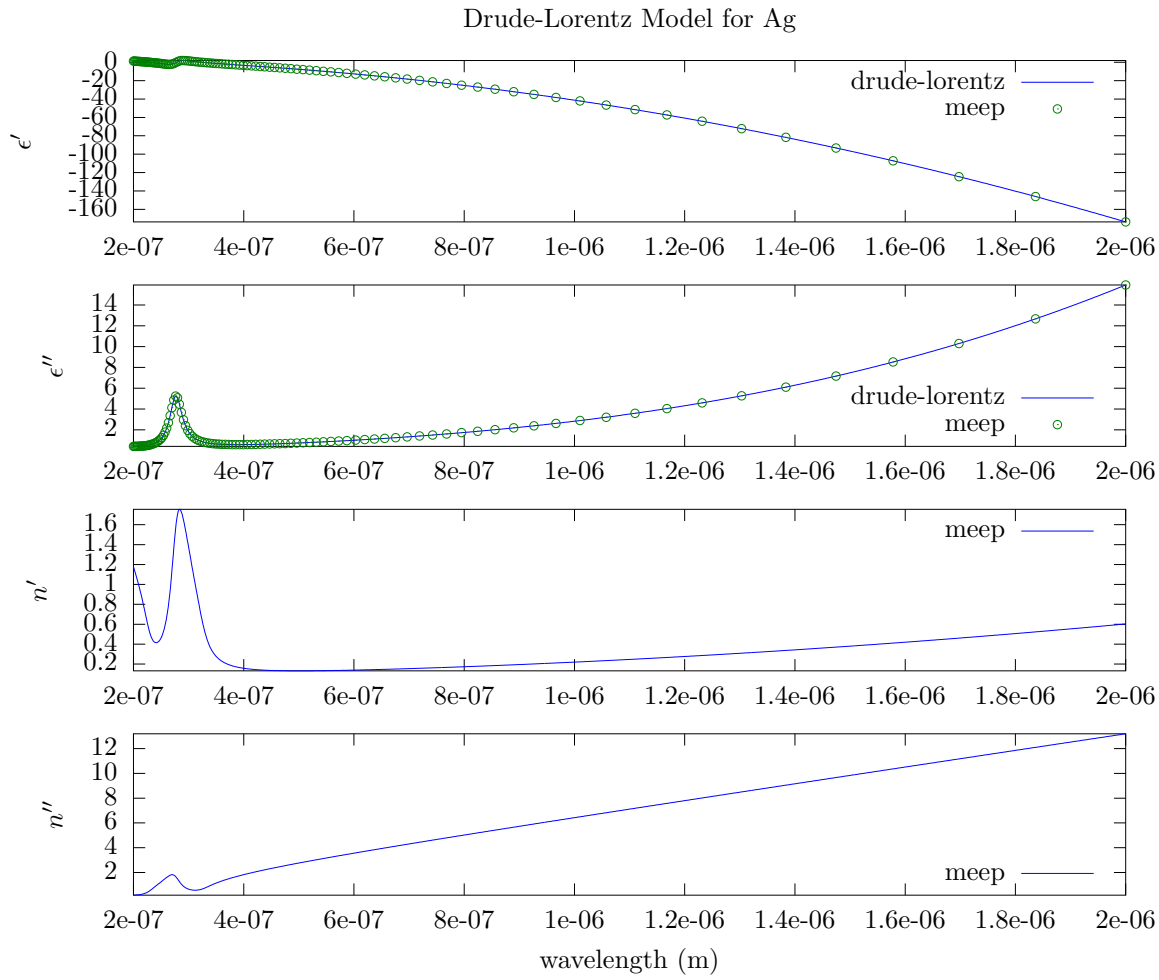
To check these results, a $1 \times 1 \times 1$ pixel region of dielectric was simulated and ϵ was exported with the command `meep-fields-analytic-chi1`. The results, which follow, were then compared to the complex ϵ predicted by the LD model (via `LD.m` courtesy of Bora Ung of Ecole Polytechnique de Montreal)[3].

1.1 `meep` Code for Metals

The following is `meep` code for selected metals with $a = 1\,\mu\text{m}$.

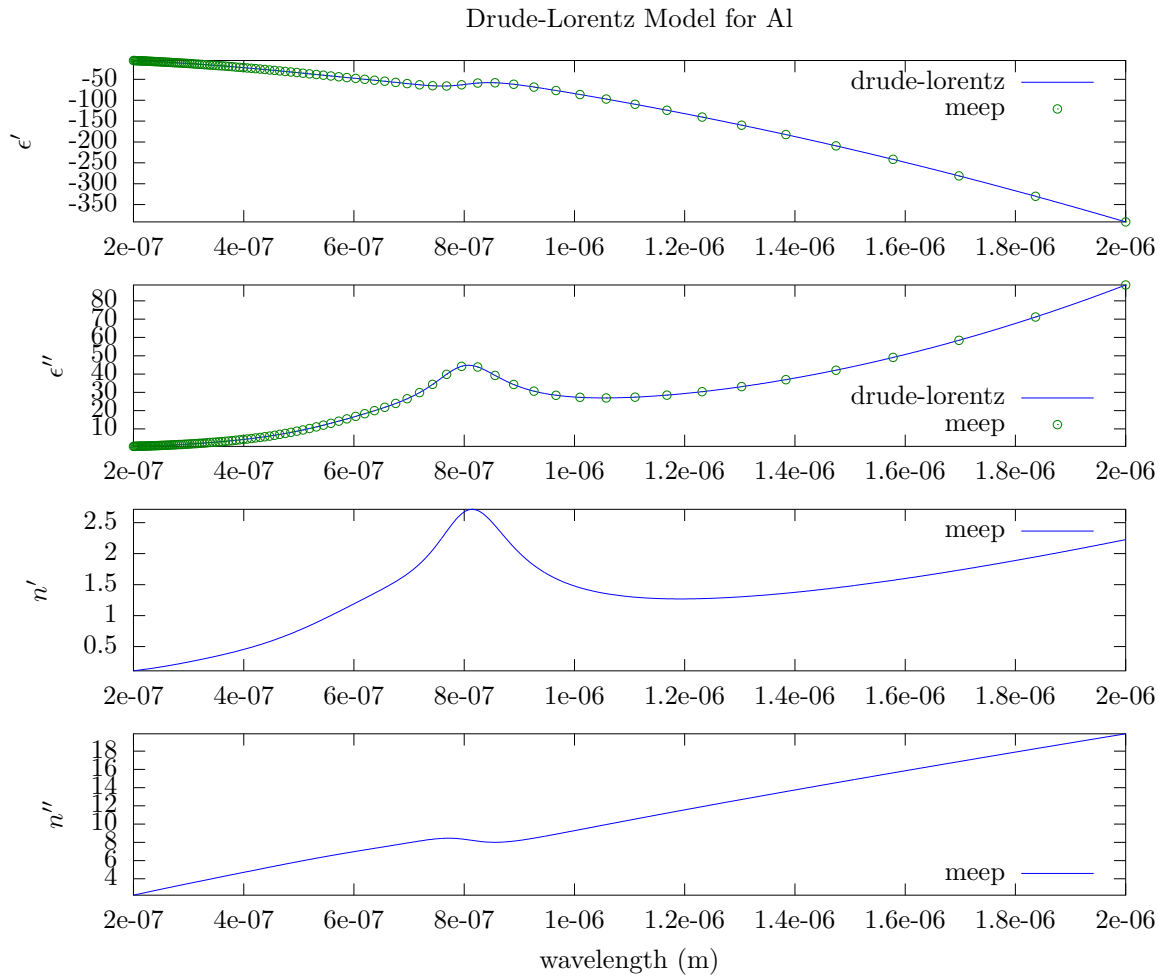
[3] http://falsecolour.com/aw/meep_metals/LD.m

1.1.1 Silver



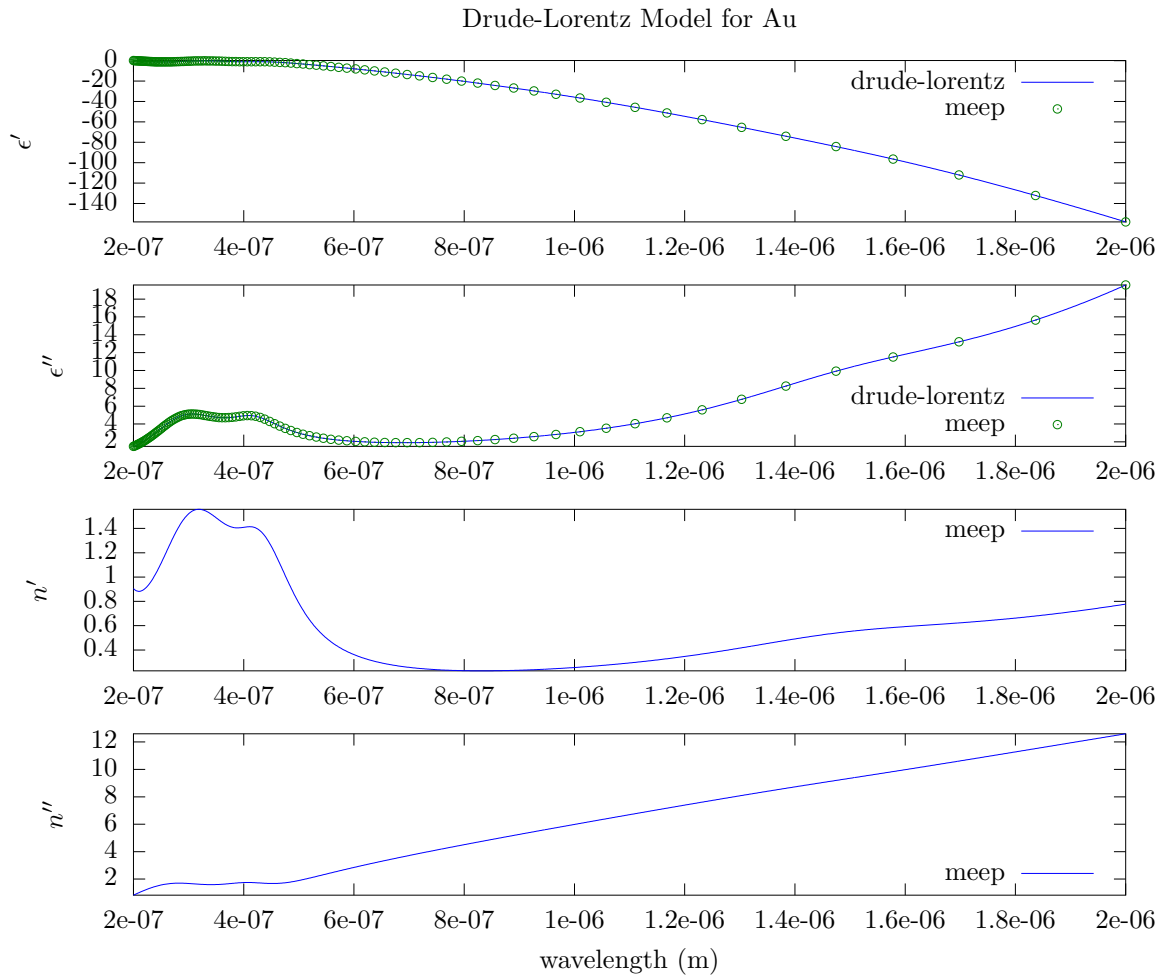

```
(define myAg (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.038715) (sigma 4.4625e+41))
(make polarizability
(omega 0.65815) (gamma 3.1343) (sigma 7.9247))
(make polarizability
(omega 3.6142) (gamma 0.36456) (sigma 0.50133))
(make polarizability
(omega 6.6017) (gamma 0.052426) (sigma 0.013329))
(make polarizability
(omega 7.3259) (gamma 0.7388) (sigma 0.82655))
(make polarizability
(omega 16.365) (gamma 1.9511) (sigma 1.1133))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Agfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=6.6802
```

1.1.2 Aluminum



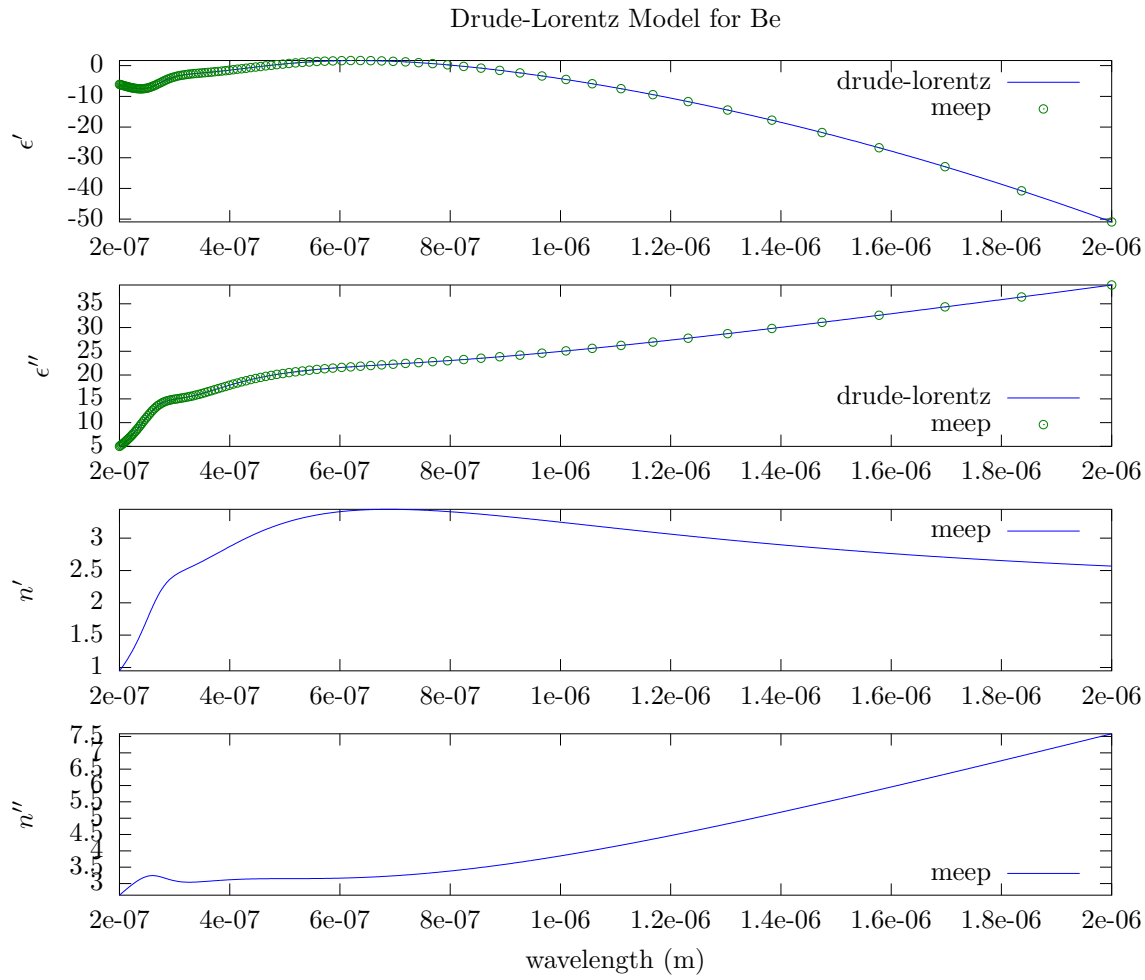

```
(define myAl (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.037908) (sigma 7.6347e+41))
(make polarizability
(omega 0.13066) (gamma 0.26858) (sigma 1941))
(make polarizability
(omega 1.2453) (gamma 0.25165) (sigma 4.7065))
(make polarizability
(omega 1.4583) (gamma 1.0897) (sigma 11.396))
(make polarizability
(omega 2.8012) (gamma 2.7278) (sigma 0.55813))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Alfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=8.7377
```

1.1.3 Gold



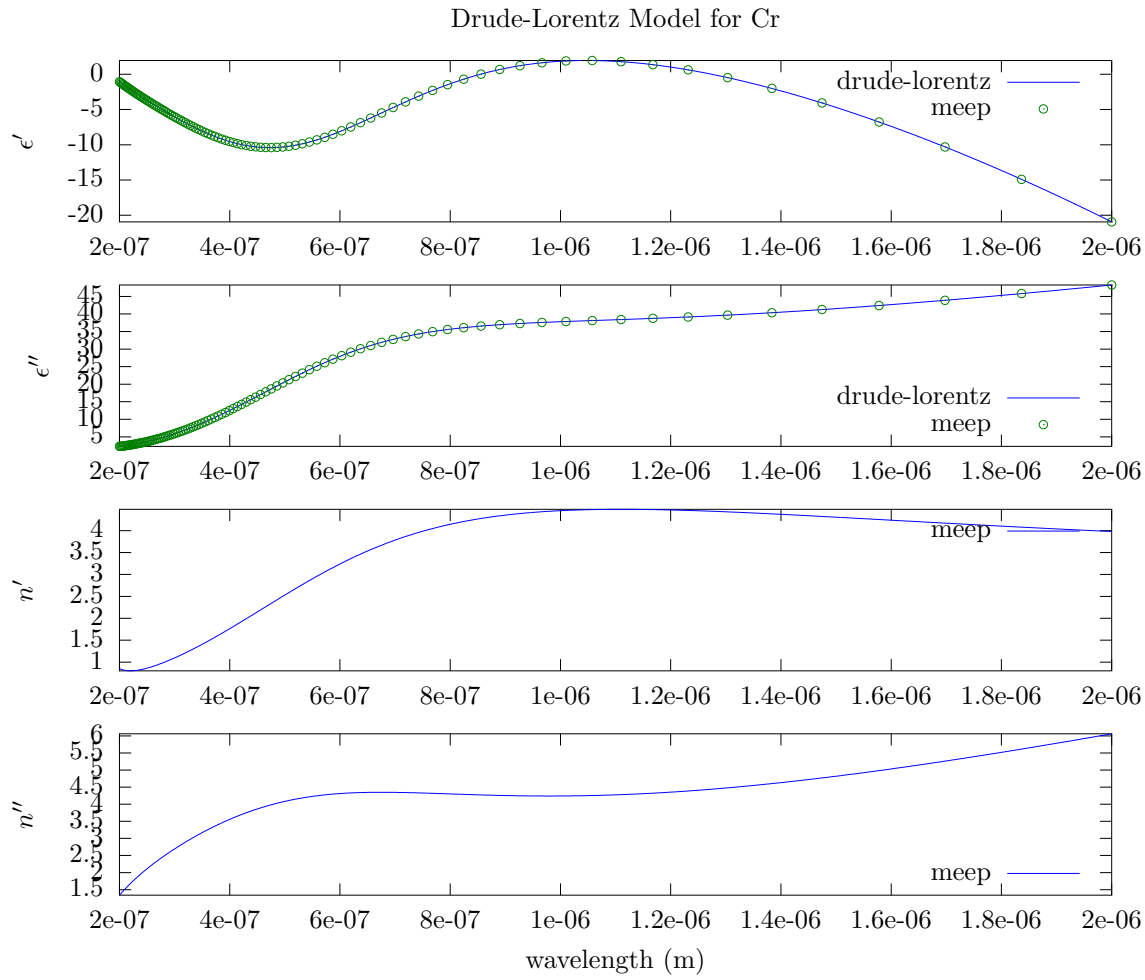

```
(define myAu (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.042747) (sigma 4.0314e+41))
(make polarizability
(omega 0.33472) (gamma 0.19438) (sigma 11.363))
(make polarizability
(omega 0.66944) (gamma 0.27826) (sigma 1.1836))
(make polarizability
(omega 2.3947) (gamma 0.7017) (sigma 0.65677))
(make polarizability
(omega 3.4714) (gamma 2.0115) (sigma 2.6455))
(make polarizability
(omega 10.743) (gamma 1.7857) (sigma 2.0148))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Aufrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=6.3493
```

1.1.4 Beryllium



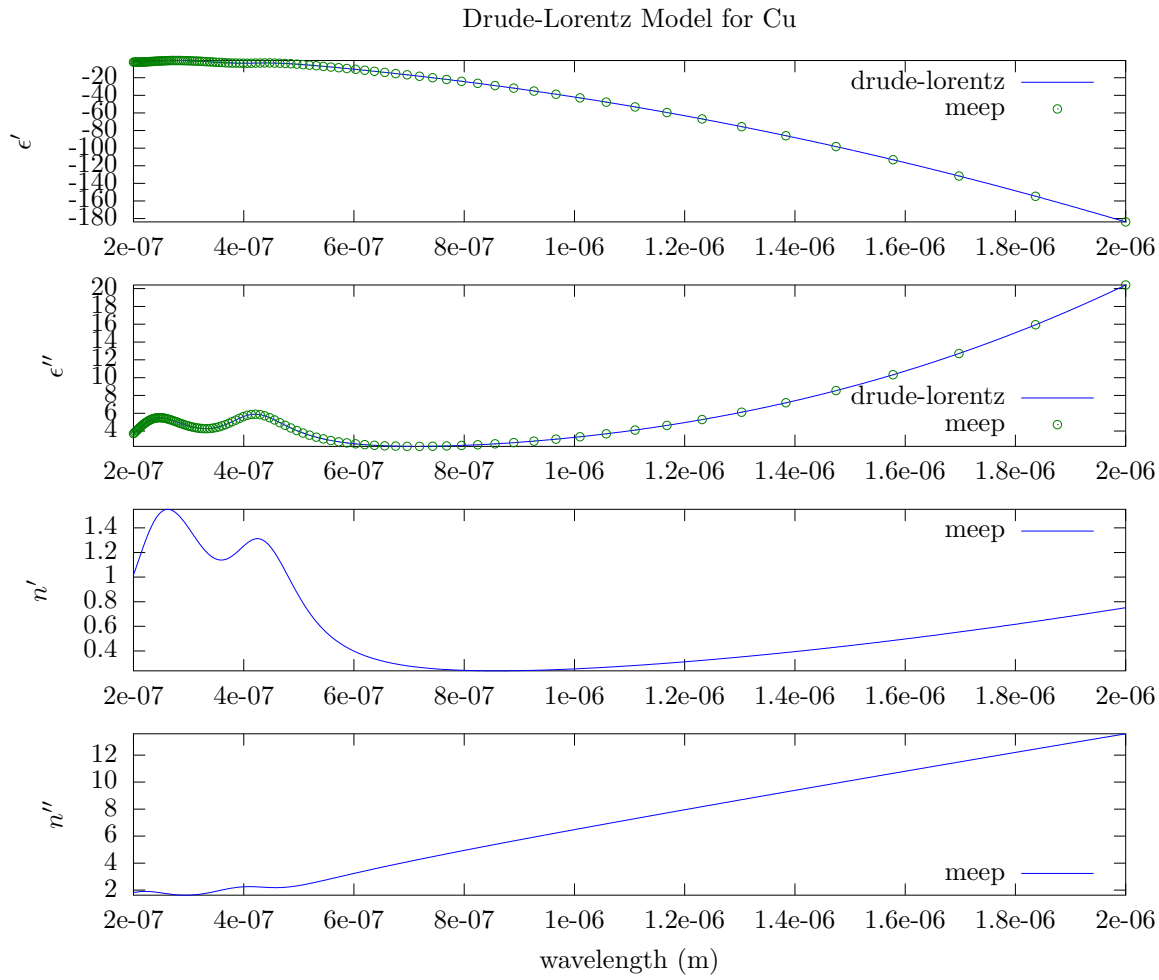

```
(define myBe (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.028229) (sigma 1.8722e+41))
(make polarizability
(omega 0.080655) (gamma 1.3421) (sigma 1062.1))
(make polarizability
(omega 0.83236) (gamma 2.7383) (sigma 45.038))
(make polarizability
(omega 2.5673) (gamma 3.5924) (sigma 17.923))
(make polarizability
(omega 3.7134) (gamma 1.4534) (sigma 2.1013))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Befrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=4.3269
```

1.1.5 Chromium



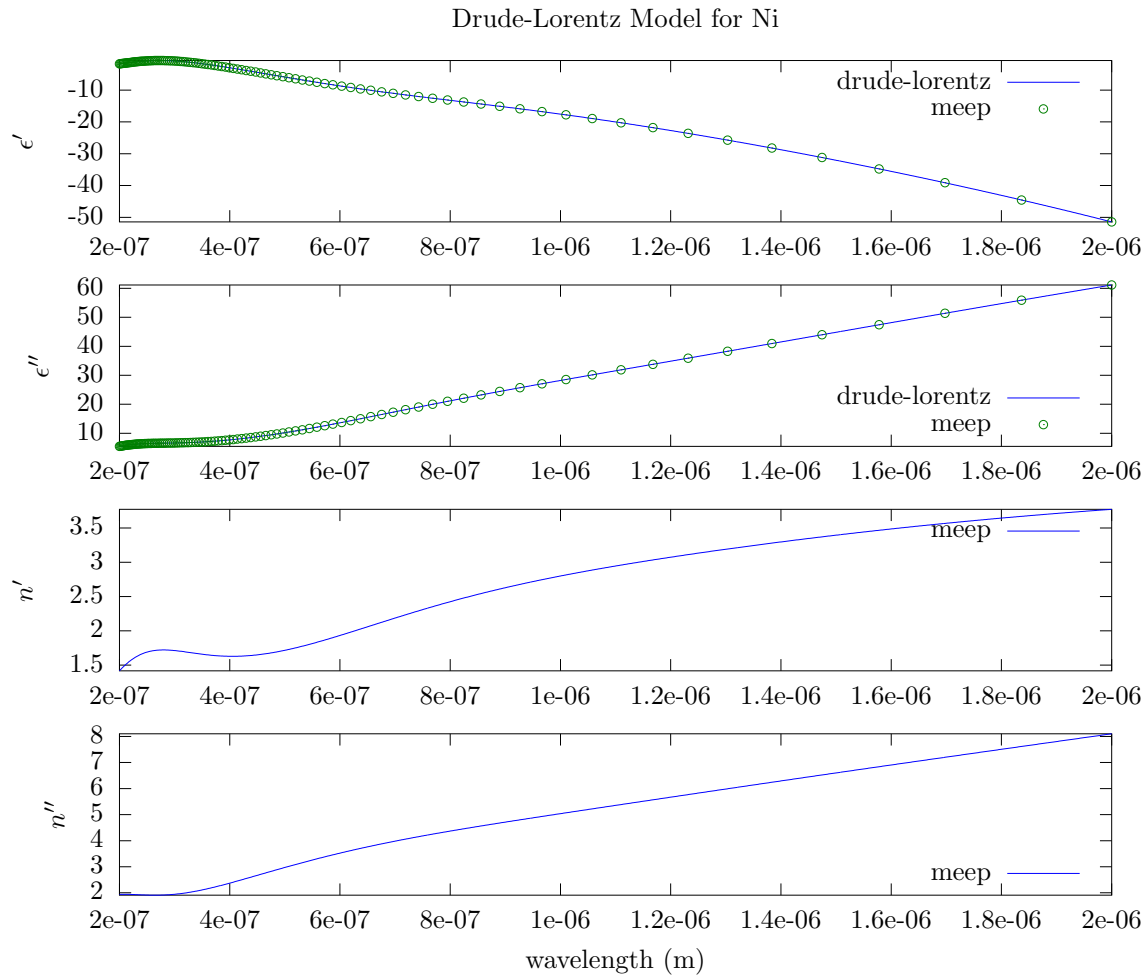

```
(define myCr (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.037908) (sigma 1.263e+41))
(make polarizability
(omega 0.097593) (gamma 2.5608) (sigma 1191.9))
(make polarizability
(omega 0.43796) (gamma 1.0526) (sigma 58.791))
(make polarizability
(omega 1.5889) (gamma 2.1583) (sigma 34.214))
(make polarizability
(omega 7.0775) (gamma 1.0768) (sigma 1.2382))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Crfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=3.5538
```

1.1.6 Copper



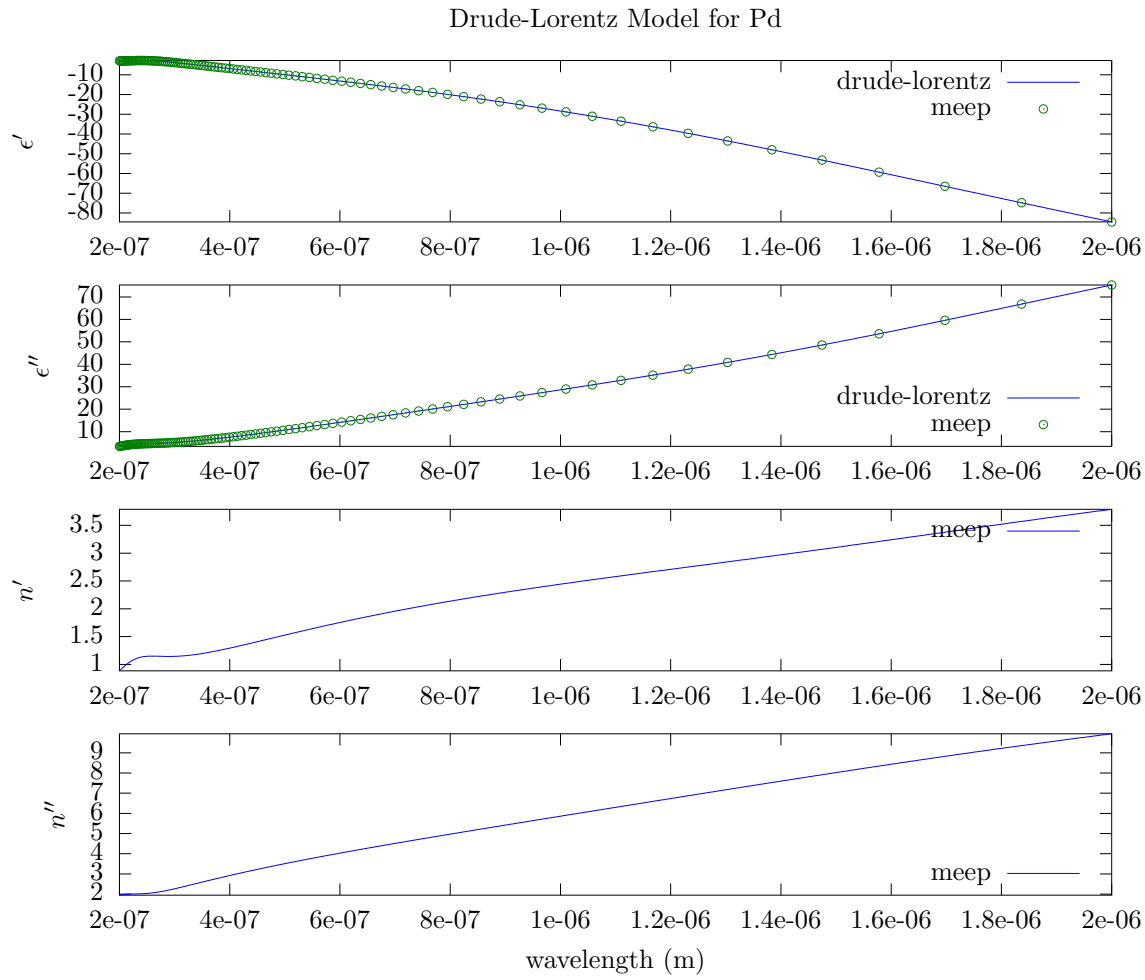

```
(define myCu (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.024197) (sigma 4.3873e+41))
(make polarizability
(omega 0.23471) (gamma 0.30488) (sigma 84.489))
(make polarizability
(omega 2.385) (gamma 0.85172) (sigma 1.395))
(make polarizability
(omega 4.2747) (gamma 2.5915) (sigma 3.0189))
(make polarizability
(omega 9.0173) (gamma 3.4722) (sigma 0.59868))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Cufrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=6.6236
```

1.1.7 Nickel



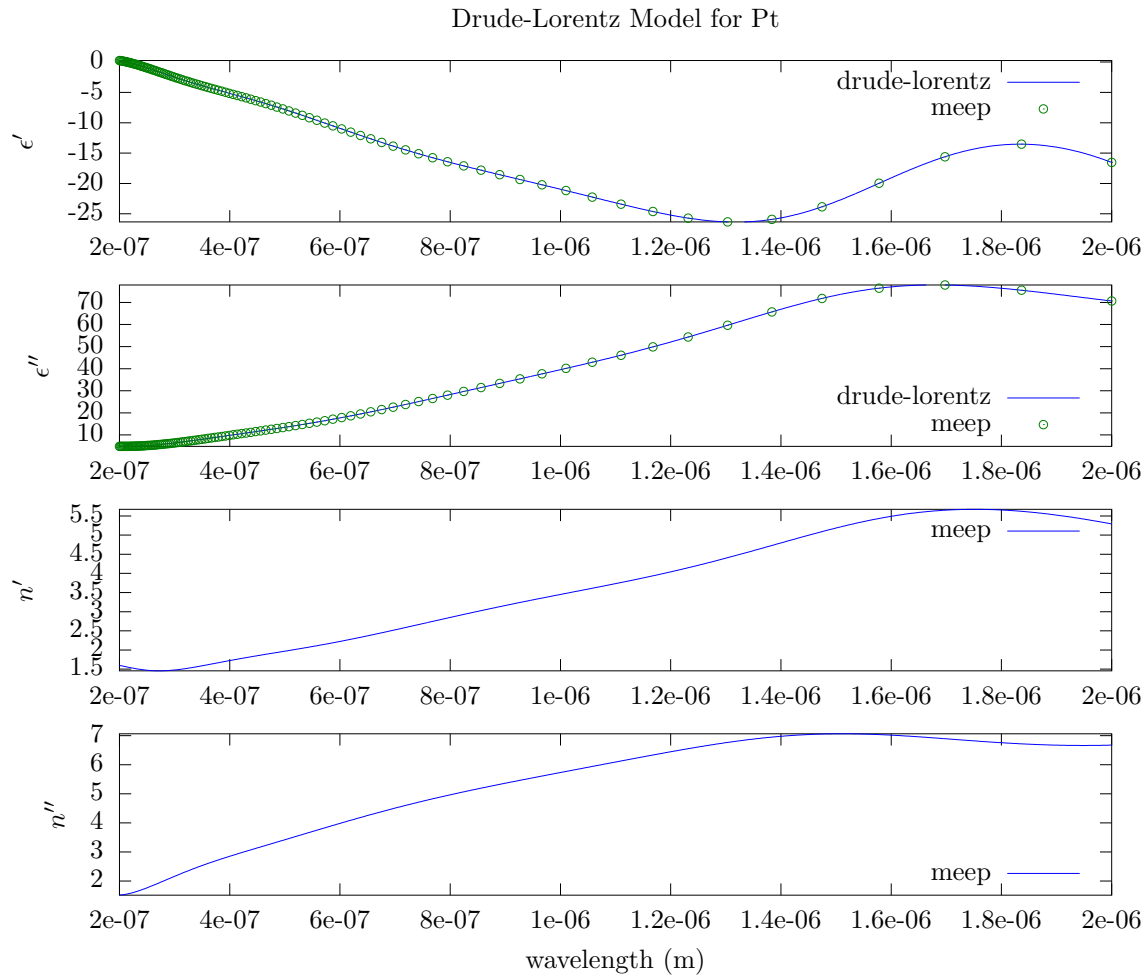

```
(define myNi (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.038715) (sigma 1.5828e+41))
(make polarizability
(omega 0.14034) (gamma 3.6384) (sigma 837.12))
(make polarizability
(omega 0.46941) (gamma 1.0759) (sigma 101.01))
(make polarizability
(omega 1.2881) (gamma 1.7567) (sigma 10.534))
(make polarizability
(omega 4.9111) (gamma 5.0748) (sigma 4.9834))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Nifrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=3.9784
```

1.1.8 Palladium



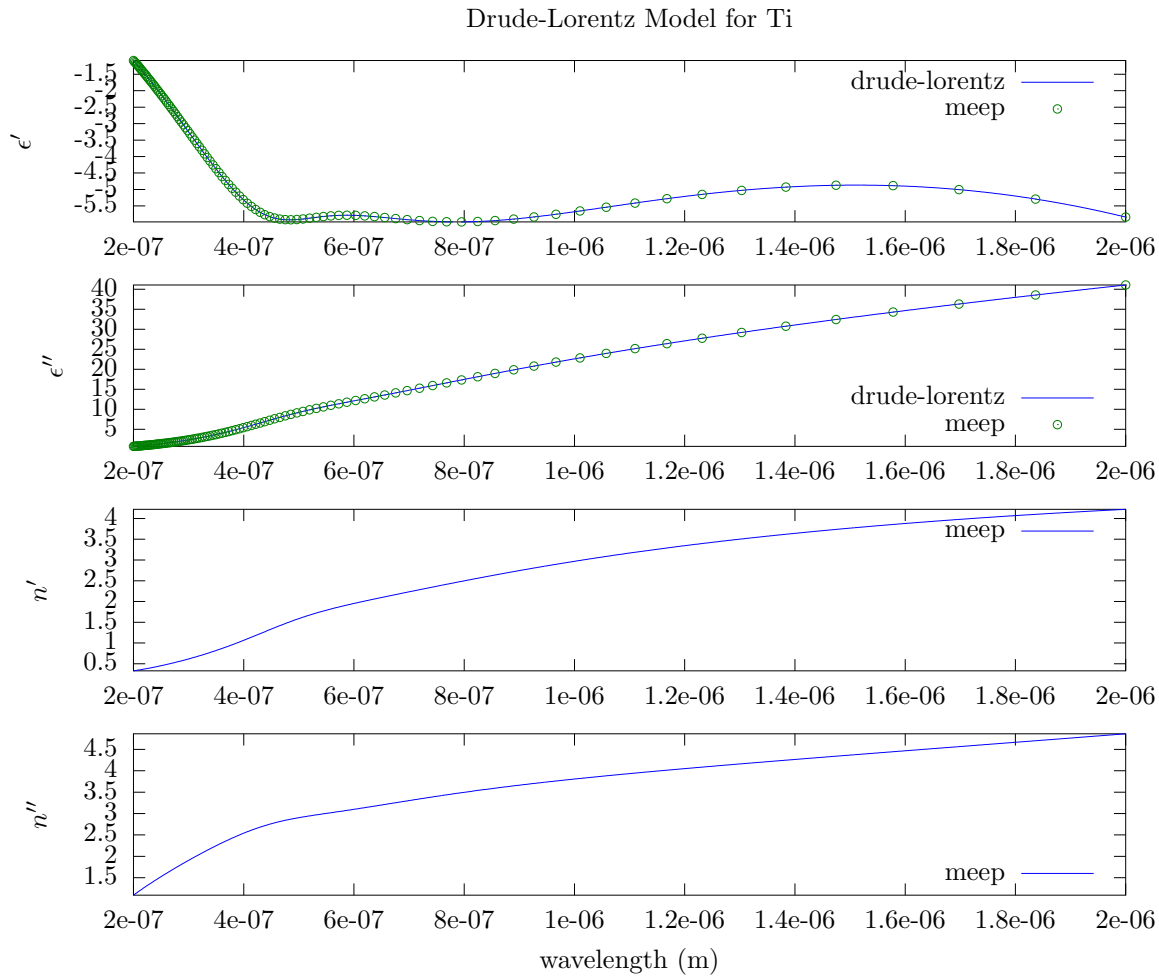

```
(define myPd (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.0064524) (sigma 2.0282e+41))
(make polarizability
(omega 0.271) (gamma 2.3793) (sigma 543.12))
(make polarizability
(omega 0.40408) (gamma 0.44764) (sigma 45.545))
(make polarizability
(omega 1.3381) (gamma 3.7271) (sigma 21.901))
(make polarizability
(omega 4.6095) (gamma 2.61) (sigma 1.3104))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Pdfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=4.5036
```

1.1.9 Platinum



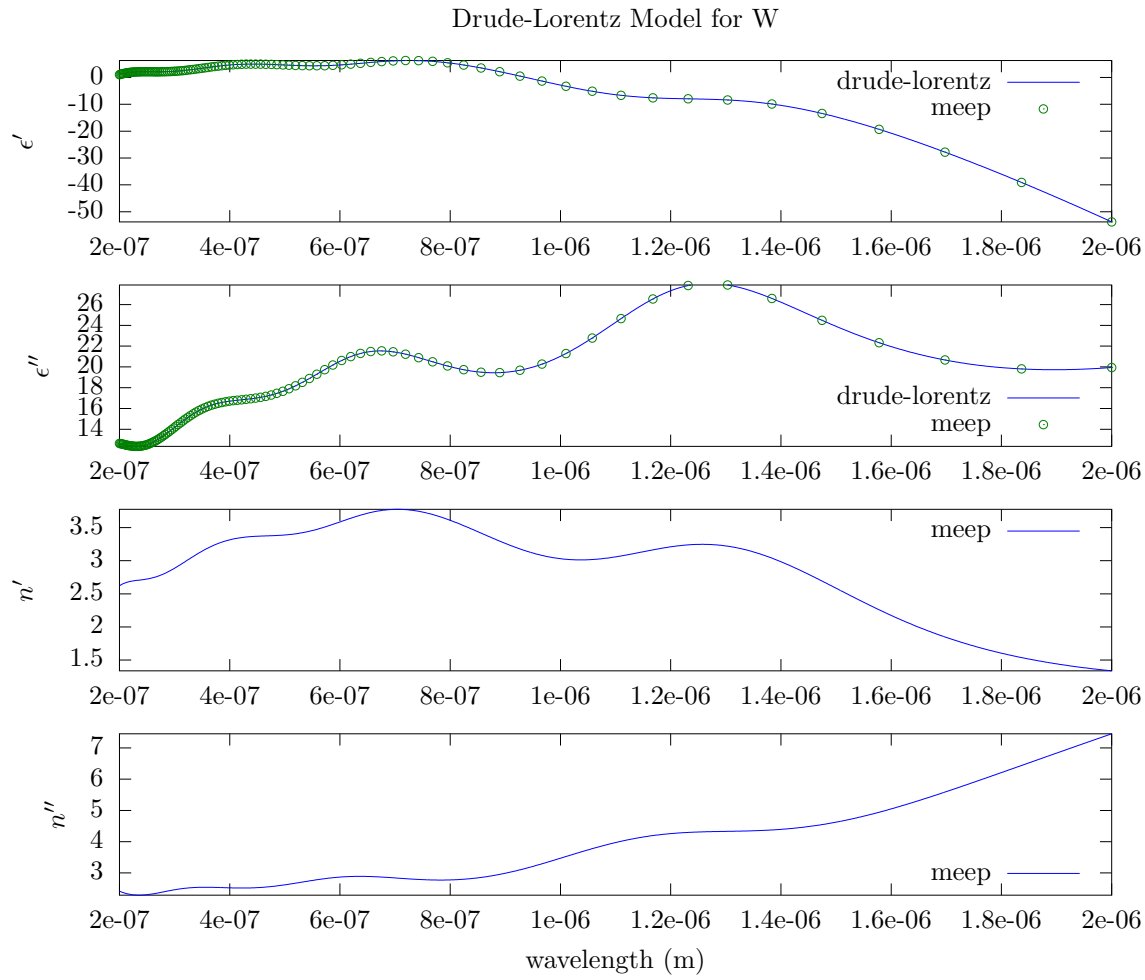

```
(define myPt (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.064524) (sigma 1.9923e+41))
(make polarizability
(omega 0.62911) (gamma 0.41699) (sigma 28.872))
(make polarizability
(omega 1.0598) (gamma 1.4824) (sigma 35.102))
(make polarizability
(omega 2.5334) (gamma 2.9584) (sigma 5.099))
(make polarizability
(omega 7.4598) (gamma 6.8694) (sigma 3.8445))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Ptfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=4.4635
```

1.1.10 Titanium




```
(define myTi (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.066137) (sigma 5.1166e+40))
(make polarizability
(omega 0.62669) (gamma 1.8357) (sigma 79.136))
(make polarizability
(omega 1.2461) (gamma 2.0309) (sigma 8.7496))
(make polarizability
(omega 2.0236) (gamma 1.3413) (sigma 1.5787))
(make polarizability
(omega 1.5671) (gamma 1.4211) (sigma 0.014077))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Tifrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=2.262
```

1.1.11 Tungsten




```
(define myW (make dielectric (epsilon 1)
(polarizations
 (make polarizability
(omega 1e-20) (gamma 0.05162) (sigma 2.3421e+41))
(make polarizability
(omega 0.80978) (gamma 0.42747) (sigma 9.3624))
(make polarizability
(omega 1.5462) (gamma 1.0332) (sigma 7.8945))
(make polarizability
(omega 2.8875) (gamma 2.6874) (sigma 9.6272))
(make polarizability
(omega 6.0475) (gamma 4.7071) (sigma 8.0514))
)))
;Additional Information
;Normalization length=1e-06 in meter
;Material_used_is_Wfrom Rakic et al.,Applied Optics (1998)
;Plasma Angular Frequency (and plasma wave vector,kp) in normalized units=4.8395
```

2 Useful Files

- matlab/octave script to obtain the complex ϵ and n for the above materials.
  (`http://falsecolour.com/aw/meep_metals/LD.m`)
- All of the above material definitions in one file. This can be included in a meep `.ctl` file with the line `(include "meep-metals-inc")`
  (`http://falsecolour.com/aw/meep_metals/meep-metals-inc`)
- Script to plot the above.
  (`http://falsecolour.com/aw/meep_metals/meep_drude_test.tar.gz`)

3 Changes to this Document

1. 03.11.2011 Updated links.
2. 10.10.2011 Fixed incorrect plot units (Georg Wachter).
3. 20.10.2011 Fixed broken links to scripts. (Yasser Khan)

References

[1] Aleksandar D. Rakic, Aleksandra B. Djurišic, Jovan M. Elazar, and Marian L. Majewski. Optical properties of metallic films for vertical-cavity optoelectronic devices. *Appl. Opt.*, 37(22):5271–5283, Aug 1998.