

FreeSnell

Thin-Film Optical Simulator
Version 1c4

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This file documents FreeSnell 1c4 (released January 2024), a simulator for thin-film optics.

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1 Overview

Some wondrous optical technology can result from depositing coatings less than a few micrometers thick on glass, plastic, and other surfaces. These coatings are used to enhance the reflectivity of astronomical mirrors or diminish the reflections from visual displays and lenses; they can improve the efficiency of window glass and solar cells.

FreeSnell computes these effects for parallel layers of dielectric and conductive materials.

1.1 Background

I couldn't find a free implementation of thin-film optical calculations I needed for a project. So I rolled my own.

The first versions were based on webpages [NCSU] and [Nave], but differences in signs and conventions of the complex index of refraction caused havoc with metallic layers. [Sernelius] has a comprehensive treatment with signs consistent from start to finish. The current version is based on that.

The properties of granular films are taken from [Heavens] discussion of *Maxwell Garnett theory*. [Granfilm] computes properties of granular films with great sophistication, but appears to require a PhD in physics in order to use it.

Optics is wavelength based; so this package is also. These routines work out the complex voltages in the forward and reverse directions to find the transmitted and reflected amplitudes. This works only for intensities where the layers act linearly (superposition).

Each layer 0:n has an index of refraction and height. Because the P and S polarizations are independent, they are calculated separately. The square of the absolute value of computed field values expressing power ratios are the returned quantities.

1.2 Theory of Operation

The effects of coatings on light are determined by Snell's law and Fresnel's equations, which model the light's electric and magnetic fields.

Taking the Laplace-transform of the differential equations relating the fields at the surface of each parallel layer of materials yields algebraic equations relating the indexes-of-refraction and the (complex) attenuation and phase as functions of wavelength.

These algebraic equations can be organized into products of 2x2 matrices and 2-vectors. The 2-vectors represent the Laplace transforms of the forward and reverse radiation. Each interface between adjacent materials corresponds to a 2x2 matrix.

The product of the chain of 2x2 matrices produces a single 2x2 matrix expressing the transmittance and reflectance of the layered stack as a whole, solving the system of equations.

This method is not unique to thin-film optics; it is essentially the same as the 2-port method for analysis of linear electrical circuits.

1.3 Wrinkles

Because these optical systems are passive and linear, the attenuation of radiation passing through in one direction must be the same as the attenuation of radiation passing through in the opposite direction.

Radiation that is not transmitted through the stack must be either absorbed or reflected. The absorption at the top is not necessarily the same as the absorption at the bottom.

Rays impinging on the stack with non-normal incidence will leave the stack with non-normal incidence; the angles being identical if the indexes of refraction of the top and bottom materials are identical.

Rays impinging on the stack with non-normal incidence have different attenuation and reflectance depending on the polarization of the impinging radiation. FreeSnell computes outcomes for both polarizations; and can report these separately or averaged.

1.4 Bibliography

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2 Optical Properties of Materials

The salient optical properties of a material are specified by its *complex index of refraction*; which differs from the common index of refraction, n , by incorporating the extinction-coefficient, k/n . There are several conventions for the complex index of refraction. The one employed here follows [Sernelius]: $(n + k*i)$.

Dielectric materials typically have k equal to zero and n which varies little with the wavelength of light being analyzed. They are often computed using a single n value.

Metallic or conductive materials have non-zero k and n which can vary wildly with the wavelength of light being analyzed. These values can be determined through a process called *ellipsometry*.

The Sopra company manufactures spectroscopic ellipsometers. A bundle of spectra for 278 materials available from

<http://www.sopra-sa.com/more/database.asp> (Nov 28, 2000) is included in the FreeSnell distribution database.

The Software Spectra company also distributes the Sopra data, although rewritten into their proprietary format. But their zip file

<http://www.sspectra.com/files/misc/win/SOPRA.EXE>

(Macintosh <http://www.sspectra.com/files/misc/mac/Sopra.sea.hqx>)

contains README.TXT identifying the Sopra files.

Included with FreeSnell are the following metal spectra from the CRC Handbook of Chemistry and Physics:

| | | | |
|-------------|---|---|---|
| ag.nk: eV | n | k | R(th=0) ; Silver |
| al.nk: eV | n | k | R(th=0) ; Aluminium |
| au.nk: eV | n | k | R(th=0) ; Gold, electropolished, Au (110) |
| cr.nk: eV | n | k | R(th=0) ; Chromium |
| cu.nk: eV | n | k | R(th=0) ; Copper |
| fe.nk: eV | n | k | R(th=0) ; Iron |
| ge.nk: eV | n | k | R(th=0) ; Germanium, single crystal |
| li.nk: eV | n | k | R(th=0) ; Lithium |
| ni.nk: eV | n | k | R(th=0) ; Nickel |
| ta.nk: eV | n | k | R(th=0) ; Tantalum |
| ti.nk: eV | n | k | R(th=0) ; Titanium (Polycrystalline) |
| v.nk: eV | n | k | R(th=0) ; Vanadium |
| w.nk: eV | n | k | R(th=0) ; Tungsten |
| zn.nk: eV | n | k | R(th=0) ; Zinc, E _ _ to c^28 |
| zn-e.nk: eV | n | k | R(th=0) ; Zinc, E to c^28 |
| zr.nk: eV | n | k | R(th=0) ; Zirconium (Polycrystalline) |

Many of these materials are included in the Sopra bundle; but the CRC data covers a wider wavelength span than the Sopra spectra. Combining the CRC and Sopra files produces wide bandwidth spectra with finer resolution in the visible and near-infrared bands.

2.1 nk Data Formats

FreeSnell supports SOPRA textual formats with their evenly spaced wavelengths or energies, as well as textual formats where the wavelength or energy of each nk pair is individually specified.

If the first non-whitespace character in the file is a digit, then the file is interpreted as a SOPRA format file. The first number indicates the spectral unit (1 = eV, 2 = μm , 3 = $1/\text{cm}$, 4 = nm). The second and the third numbers indicate the spectral range and the fourth one the number of intervals. The n and k values are then stored in the order N,K,N,K...; each value may be followed by a semicolon, whitespace, or both.

For example, the SOPRA file `a12o3.nk` has 27 values for wavelengths from 0.25. μm to 0.9. μm :

```
2, .25, .9, 26
1.7331,0
1.7163,0
1.7042,0
1.6951,0
1.6881,0
1.6825,0
1.678,0
1.6743,0
1.6713,0
1.6687,0
1.6665,0
1.6646,0
1.6629,0
1.6614,0
1.6601,0
1.659,0
1.6579,0
1.657,0
1.6561,0
1.6553,0
1.6546,0
1.6539,0
1.6532,0
1.6526,0
1.652,0
1.6515,0
1.6509,0
```

The other formats ignore the first line if it begins with a semicolon. The first non-ignored word read indicates the spectral unit, either eV, $1/\text{cm}$, μm , or nm; the rest of that line is discarded. Each line which follows is a triple of the spectral index, the n value, and the k value, separated by whitespace. Extra data on the line (the normal reflectance in some files) is ignored.

This example (`blackbody.nk`) specifies constant n and k values over all wavelengths:

| um | n | k | ; blackbody |
|------|-----|-------|-------------|
| 01.0 | 1.0 | 0.038 | |
| 25.0 | 1.0 | 0.038 | |

3 Material Databases

The FreeSnell package includes a SCM script (program) named *nk* to create, manage, and query a refractive-index spectra database.

Recent versions of the FreeSnell distribution include the relational database (*nk.rwb*) containing the refractive-index spectra. So use of the ‘*nk*’ script is optional.

3.1 The *nk* script

The *nk.scm* file in the distribution functions as a shell script named ‘*nk*’ on Unix systems; under MS-Windows, the *nk* icon invokes *nk.scm* as an interactive command-line shell with the prompt ‘*nk*’.

Use the *nk* program to create, manage, and query a refractive-index spectra database.

The *nk* program can read Sopra format files. These files have a ".nk" suffix. A bundle of spectra for over 275 materials is available from: <http://www.sopra-sa.com/index2.php?goto=dl&rub=4> (2010-06-14). Some metal spectra included with FreeSnell also have a ".nk" suffix, but with a different format.

The zip file <http://www.sspectra.com/files/misc/win/SOPRA.EXE> contains "README.TXT" identifying the Sopra files.

<http://luxpop.com/RefractiveIndexList.html> has 274 refractive-index files, mostly X-ray spectra.

The optional argument [-F path] sets the path to the database file to be accessed or created. If it is not given, then the environment variable "NK_DATABASE_PATH" names the database file if defined, defaulting to "nk.rwb" in the current directory. The name for each spectrum in the database is taken from its filename sans the ".nk" or "ir.nk" suffix.

Usage: *nk* [-F path]

Starts the *nk* shell. Type *nk* commands without the *nk*; ^Z to exit.

Usage: *nk* [-F path] --add FILEGLOB.nk ...

Add spectra matching FILEGLOB to database. Wildcards must be in the leaf directory only.

Usage: *nk* [-F path] --new FILEGLOB.nk ...

Add new or replace spectra matching FILEGLOB to database. Wildcards must be in the leaf directory only.

Usage: *nk* [-F path] --del 'GLOB' ...

Delete spectra of names matching GLOB from database.

Usage: *nk* [-F path] --plot 'GLOB' ...

```

Usage: nk [-F path] --lin-lin 'GLOB' ...
Usage: nk [-F path] --log-log 'GLOB' ...
Usage: nk [-F path] --log-lin 'GLOB' ...
Usage: nk [-F path] --lin-log 'GLOB' ...
Usage: nk [-F path] --lin-eV 'GLOB' ...
Usage: nk [-F path] --log-eV 'GLOB' ...
Usage: nk [-F path] --lin-/cm 'GLOB' ...
Usage: nk [-F path] --log-/cm 'GLOB' ...
    Create encapsulated-PostScript (and view with Ghostview) spectra plots
    from database of names matching GLOB. The first symbol controls the
    y-axis.
Usage: nk [-F path] --list 'GLOB' ...
    List names of spectra matching GLOB in database.
Usage: nk [-F path] --range 'GLOB' ...
    List names and data ranges of spectra matching GLOB in database.
Usage: nk [-F path] --desc 'GLOB' ...
    List names and descriptions of spectra matching GLOB in database.
Usage: nk [-F path] --annotate sopra.txt
    Add chemical-symbol and description annotations to database.
Usage: nk [-F path] NAME NUMBER.UNIT ...
    Prints NAME's n+k*i values at each NUMBER.UNIT from database. The
    NUMBER can be fixed or floating point; the UNIT either "eV"
    (electron-volt) or "m" (meter) with an optional metric prefix or
    "cm^-1" (wave-number).
Usage: nk --help
    Prints this help and exits.

```

3.2 Wedged Databases

Although it tries to be careful, if the 'nk' script encounters an unexpected condition while the database file (default 'nk.rwb') has a table open for writing, then the database file can become unusable from both the 'nk' script and design files. This damage will only result from the 'nk' script; all simulations should be read-only from database files.

To start afresh, delete these files (with all occurrences of 'nk.rwb' replaced by your database name):

- '~\$nk.rwb'
- '#nk.rwb' (isn't created on MS-Windows)
- 'nk.rwb'

If the wedged database was 'nk.rwb' from the distribution, then retrieve 'nk.rwb' from the distribution. Otherwise rebuild your database (using 'nk --add' commands).

3.3 Creating Databases

FreeSnell comes with a database of refractive-index spectra for several hundred materials. If you want to add spectra of your own, it is probably better to create a separate database for them using the '-F' option to the 'nk' script.

```
nk -F mynk.rwb --add *.nk
"sicrir" ==> "sizr"
"sio2ir" ==> "sio2"
ag.nk: ev      n      k      R(th=0) ; Silver
al.nk: ev      n      k      R(th=0) ; Aluminium
au.nk: ev      n      k      R(th=0) ; Gold, electropolished, Au (110)
cr.nk: ev      n      k      R(th=0) ; Chromium
cu.nk: ev      n      k      R(th=0) ; Copper
fe.nk: ev      n      k      R(th=0) ; Iron
ge.nk: ev      n      k      R(th=0) ; Germanium, single crystal
li.nk: ev      n      k      R(th=0) ; Lithium
ni.nk: ev      n      k      R(th=0) ; Nickel
ta.nk: ev      n      k      R(th=0) ; Tantalum
ti.nk: ev      n      k      R(th=0) ; Titanium (Polycrystalline)
v.nk: ev      n      k      R(th=0) ; Vanadium
w.nk: ev      n      k      R(th=0) ; Tungsten
zn-e.nk: ev    n      k      R(th=0) ; Zinc, E || to c^28
zn.nk: ev      n      k      R(th=0) ; Zinc, E |_| to c^28
zr.nk: ev      n      k      R(th=0) ; Zirconium (Polycrystalline)
```

Your new database can be accessed from design files thus:

```
(define mynk (open-database "mynk.rwb" 'rwb-isam))
(define Ag (interpolate-from-table (open-table mynk 'Ag) 2))
```

3.4 Listing the Database

```
nk --list
7059      a-al2o3      a-c      a-sih      ag      againp0
againp1   againp10     againp3   againp6     againp7   al
al2o3     al2o3-e      alas      alas028t    alas052t  alas072t
alas098t  alas125t    alas152t  alas178t    alas204t  alas228t
alas305t  alas331t    alas361t  alas390t    alas421t  alas445t
alas469t  alas499t    alas527t  alas552t    alas578t  alas602t
alas626t  alcu        algaas0   algaas1     algaas10  algaas2
algaas3   algaas4     algaas5   algaas6     algaas7   algaas8
algaas9   alon        alsb      alsi        alsiti     arachi
asi       au          baf2      be          beo        bk7
bk7_abs   caf2        carbam    ccl4        cdse       cdte
co        co_2        cor7059   cosi2-4     cr         cr3si
cr5si3    crsi2el2    csi       cu          cu2o      cuo
d-c      fe          fesi2el1  fesi2el2    fesi2epi  gaas
gaas031t gaas041t    gaas060t  gaas081t    gaas100   gaas103t
gaas111  gaas126t    gaas150t  gaas175t    gaas199t  gaas224t
```

| | | | | | |
|----------|----------|----------|----------|----------|----------|
| gaas249t | gaas273t | gaas297t | gaas320t | gaas344t | gaas367t |
| gaas391t | gaas415t | gaas443t | gaas465t | gaas488t | gaas515t |
| gaas546t | gaas579t | gaas603t | gaas634t | gaaso | gaasox |
| gan-tit | gan01 | gan02 | gan03 | gan60 | gan70 |
| gap | gap100 | gapox | gasb | gasbox | ge |
| ge100 | h2o | h2o-ice | hdpe | hfo2 | hfsi2 |
| hg | hgcdte0 | hgcdte2 | hgcdte3 | hgte | inas |
| inasox | ingaas | ingasb0 | ingasb1 | ingasb10 | ingasb3 |
| ingasb5 | ingasb7 | ingasb9 | inp | inpox | insb |
| insbox | ir | ir3si5e | ir3si5p | ito2 | k |
| kbr | kcl | lasf9 | li | lif | mgf2 |
| mgo | mo | mosi2 | mosi2-e | na | nacl |
| nb | nbsi | nbsi-e | ni | ni2si | ni3si |
| nisi | os | p_sias | p_siud | pbs | pbse |
| pd | pd2si | pd2si-e | pe | pt | resi1-75 |
| resige0 | resige1 | resige22 | resige39 | resige51 | resige64 |
| resige75 | resige83 | resige91 | rh | ringas0 | ringas10 |
| ringas20 | ringas24 | se | se-e | sf11 | si |
| si-t02 | si-t10 | si-t15 | si-t20 | si-t25 | si-t30 |
| si-t35 | si-t40 | si-t45 | si100_2 | si110 | si111 |
| si11ge89 | si20ge80 | si28ge72 | si3n4 | si65ge35 | si85ge15 |
| si98ge02 | siam1 | siam2 | sic | sige_ge | sige_si |
| sin_bf5 | singas0 | singas10 | singas20 | singas24 | sio |
| sio2 | sion0 | sion20 | sion40 | sion60 | sion80 |
| siop | sipoly | sipoly10 | sipoly20 | sipoly30 | sipoly40 |
| sipoly50 | sipoly60 | sipoly70 | sipoly80 | sipoly90 | sipore |
| snte | stsg0 | stsg064 | stsg123 | stsg169 | stsg229 |
| ta | taox1 | taox2 | tasi2 | tasi2-e | te |
| te-e | thf4 | ti | tic | tin | tini |
| tio2 | tio2-e | tisi-e | v | vc | vn |
| vsi2 | vsi2-e | w | ws12 | ws12-e | y2o3 |
| zn | zn-e | zncdte0 | zncdte1 | zncdte10 | zncdte3 |
| zncdte5 | zncdte7 | zncdte9 | zns | znse | znsete0 |
| znsete1 | znsete10 | znsete3 | znsete5 | znsete7 | znsete9 |
| zr | zro2 | zrsi2 | | | |

3.5 Querying the Database

Refractive index data can be retrieved at specified wavelengths, energies and wavenumbers.

```

$ nk co .3.um .5.um 1.3.eV
co: 1.218+2.11i 300.nm (4.13.eV) (33333.3.cm^-1)
co: 2.025+3.72i 500.nm (2.48.eV) (20000.cm^-1)
co: 3.85+4.77i (954.nm) 1.3.eV (10485.2.cm^-1)
$ nk Al 400.cm^-1
al: 75.77+1.7e+02i (25.0.um) (0.0496.eV) 400.cm^-1

```

The ‘--plot’ option creates an encapsulated PostScript graph of n and k/n for the material specified.

```
nk --plot co
```

<http://people.csail.mit.edu/jaffer/FreeSnell/co.png>

4 Specifying Designs

Designs are coded in Scheme language files. More than one design can be specified in a design file, permitting sharing of code. A variety of design examples are contained in the validation suites `dielectric.scm`, `metallic.scm`, and `granular.scm`. The graphs output by these suites are shown and discussed in

<http://people.csail.mit.edu/jaffer/FreeSnell/dielectric.html>,
<http://people.csail.mit.edu/jaffer/FreeSnell/metallic.html>, and
<http://people.csail.mit.edu/jaffer/FreeSnell/granular.html>

4.1 Specifying Materials

The index-of-refraction of dielectric materials often varies little with wavelength. In these cases the index-of-refraction can be a number. It is often convenient to give a symbolic name to numbers. For example:

```
(define ZnS 2.2)
(define Ge 4.2)
```

After these definitions, layers can reference the identifiers:

```
(optical-stack
 (substrate 1)
 (layer ZnS 528.64e-9)
 (layer Ge 178.96e-9)
 (layer ZnS 250.12e-9)
 (layer Ge 123.17e-9)
 ...)
```

Sometimes the index-of-refraction is specified as a formula of wavelength. The *Refractive index database* at <http://refractiveindex.info> gives a formula for the refractive-index of the plastic PMMA over the range 0.4358.um to 1.052.um. We can use its formula as a Scheme function:

```
;; n^2 = C1 + C2*w1^2 + C3*w1^-2 + C4*w1^-4 + C5*w1^-6 + C6*w1^-8
(define PMMA
 (let ((C1 2.399964)
       (C2 -8.308636E-2)
       (C3 -1.919569E-1)
       (C4 8.720608E-2)
       (C5 -1.666411E-2)
       (C6 1.169519E-3))
 (lambda (w) ; wavelength in meters
 ;; wavelength in microns and limited to valid range
 (let* ((w1 (max 0.4358 (min 1.052 (* w 1e6))))
        (w1^-2 (/ 1 w1 w1)))
 (sqrt (+ C1
           (* C2 w1 w1)
           (* (+ C3 (* (+ C4 (* (+ C5 (* C6
                                     w1^-2))
```

```

                                w1^-2))
                                w1^-2))
                                w1^-2))))))

```

For more complicated material properties FreeSnell retrieves the wavelength-dependent index-of-refraction by calling functions which interpolate values from the materials database (see Chapter 3 [Material Databases], page 6).

```

(require 'FreeSnell)
(require 'databases)
(require 'database-interpolate)

(define nk (open-database (or (getenv "NK_DATABASE_PATH") "nk.rwb")
                          'rwb-isam))
(define ge (interpolate-from-table (open-table nk 'ge) 2))
(define zns (interpolate-from-table (open-table nk 'zns) 2))
...

```

In this example *ge* and *zns* can be passed as arguments to *layer* and *substrate*.

For dielectric films embedded with spherical metal granules much smaller than the thickness of the film and the wavelengths under consideration, Maxwell Garnett Theory provides a means to calculate the effective *n* and *k*. The thickness of the granular film must be several times the granule size; otherwise the more complicated machinations of [Granfilm] are required.

granular-IR *ir q ir0* [Function]

The *ir* and *ir0* arguments specify the indexes of refraction for the metallic and matrix materials respectively. Each can be either a (complex) number or function of one real argument returning a (complex) number. The real number *q* is the fractional volume occupied by the metal.

granular-IR returns a complex index-of-refraction (or function returning a complex index-of-refraction) for the composite layer.

If *Au* is a spectral function, the following three definitions are equivalent:

```

(define ruby-glass (granular-IR Au 8.0e-6 1.5))
(define (ruby-glass w) (granular-IR (Au w) 8.0e-6 1.5))
(define ruby-glass (lambda (w) (granular-IR (Au w) 8.0e-6 1.5)))

```

4.2 Optical Stack

optical-stack *layer1* ... [Function]

optical-stack *layer1* ... *bottom-substrate* [Function]

optical-stack *top-substrate layer1* ... *bottom-substrate* [Function]

Returns a data structure combining its *layer* arguments. Each layer is returned from a call to *layer* or *substrate*. Substrate arguments must be first or last and default to having an index-of-refraction of 1. A substrate has arbitrarily large thickness, and is the source or sink of test inputs (radiation).

layer *ir* *thick* *nom* [Function]

layer *ir* *thick* [Function]

Returns a layer having the specified index-of-refraction and thickness.

If *ir* is a number, then the index-of-refraction is *ir* at all wavelengths. If *ir* is a procedure then the index-of-refraction at wavelength *w* is (*ir w*).

If the number *thick* is smaller than 1/50, then it is taken as the actual thickness. Note that the effective optical thickness will be larger than the actual thickness because light is slowed by the index-of-refraction.

If the number *thick* is larger than 1/50, then the thickness is *thick* times *nominal* divided by the real-part of the index-of-refraction at *nominal*, where *nominal* is either the third argument *nom* or the value set by the **nominal** function. This is a convenient notation for the fractional optical wavelengths often used to specify filter elements.

Layers specified by **layer** model the interference effects of reflections of reflections. This is correct for thin layers or if the modeled optical system will be illuminated by coherent light. But layers thicker than several wavelengths have variations extremely sensitive to incident angle.

Incoherent illumination will average over the wiggles. For these layers **FreeSnell** computes the transmitted and reflected power ratios, rather than E-fields.

layer* *ir* *thick* [Function]

Returns an *incoherent* layer having the specified index-of-refraction and thickness.

substrate *ir* [Function]

Returns a substrate having the specified index-of-refraction.

If *ir* is a number then the index-of-refraction is *ir* at all wavelengths. If *ir* is a procedure then the index-of-refraction at wavelength *w* is (*ir w*).

If substrates are not specified, then their index-of-refraction defaults to 1 (vacuum).

To place a substrate between two sets of layers, use **layer*** instead.

nominal *nom* [Function]

Sets the default nominal thickness to *nom*. Multiple **nominal** commands are allowed interspersed with **layer** commands. The arguments to **optical-stack** are considered in order from the first to the last.

repeat *j* *layer1* *layer2* . . . [Function]

Inserts *j* copies of the sequence *layer1*, *layer2*, . . . into the stack.

4.3 Plot-response

plot-response *arg1* *arg2* . . . [Function]

One or more of *arg1*, *arg2*, . . . should be an optical stack returned by **optical-stack**, or a value returned by a call to **IR**. The other arguments should be values returned by the functions in sections Section 4.3.1 [Ranges and Units], page 14, Section 4.3.2 [Traces], page 16, and Section 4.3.3 [Other Outputs], page 18.

`Plot-response` creates a graph, data file, or color patches as directed by its arguments. If more than one optical stack is given, the same quantities are computed for each optical stack; but all are plotted to a single graph.

`stack-colors color1 color2 ...` [Function]

Each *color1*, ... should be a string naming a Resene color, a saturate color, or a number between 0 and 100. If supplied, there should be one color for each optical-stack. *color1*, ... default to black (0). If `stack-colors` is called more than once, then its color arguments are appended together.

`stack-colors` causes the traces from each optical stack to be drawn in its corresponding color.

4.3.1 Ranges and Units

`title str filebase` [Function]

`title str` [Function]

Sets title for the run to *str*. If the string *filebase* is given, then it is used for the output filename root; otherwise *str* is used.

`output-format sym` [Function]

`output-format k1 k2` [Function]

`output-format sym k1 k2` [Function]

According to the symbol *sym*, sets the disposition of plots to be:

| | |
|-------------------|--|
| <code>eps</code> | <i>filebase.eps</i> |
| <code>ps</code> | <i>filebase.ps</i> |
| <code>png</code> | <i>filebase.png</i> |
| <code>jpg</code> | <i>filebase.jpg</i> |
| <code>jpeg</code> | <i>filebase.jpeg</i> |
| <code>pdf</code> | <i>filebase.pdf</i> |
| <code>#t</code> | views <i>filebase.eps</i> using <code>ps:viewer</code> . |

If `output-format` is not used, then the output-format defaults to the value of top-level identifier **output-format**, which defaults to `#t`.

If a pair of nonnegative exact integers, *k1* and *k2* follows *sym*, then the plot will be *k1* pixels horizontally and *k2* pixels vertically.

The `output-format` command does not affect the data written by `output-data`.

`font x` [Function]

`font fnt` [Function]

`font fnt x` [Function]

`font x left-template right-template` [Function]

`font fnt left-template right-template` [Function]

`font fnt x left-template right-template` [Function]

If a string *fnt* is supplied, then it names the PostScript font which will be used. The default value is `Times`.

If a nonnegative real number *x* follows the *fnt*, then *x* is the fontsize.

If two strings follow, then they are used as the templates whose printed representation using *fnt* is used to size the left and right margins respectively. If not specified, the templates default to `'-.0123456789'`.

If *x* is not specified and *k1* is, then the font height will be $k1/33$. If neither is specified, then the font height will be 12.

The `font` command does not affect the data written by `output-data`.

`output-data file` [Function]

`output-data file str1` [Function]

`output-data file str1 str2` [Function]

If the first character of *file* is '|', then lines of data are piped to the stdin of the command line in *file*; otherwise a file of data is written to *file*.

str1 and *str2* are *printf* format strings for the first number and the rest of the numbers printed on one line. If `#f` is passed, then the corresponding numbers are written with full Scheme precision and tab delimited.

`range low high` [Function]

Sets the ordinate range of the plot to *low* to *high*.

`range low high 'db` [Function]

`db low high` [Function]

Sets the ordinate range of the plot to *low* to *high* decibels.

`wavelengths w` [Function]

Sets the abscissa range of the plot to be linear from wavelengths $0.75*w$ to $1.25*w$.

`wavelengths w1 w2` [Function]

Sets the abscissa range of the plot to be linear from wavelengths *w1* to *w2*.

`wavelengths w1 w2 g1 g2` [Function]

Sets the abscissa range of the plot to be linear from wavelengths *w1* to *w2* in a graph rectangle from wavelengths *g1* to *g2*.

`wavenumbers w` [Function]

Sets the abscissa range of the plot to be logarithmic from wavenumbers $0.666*w$ to $1.5*w$.

`wavenumbers w1 w2` [Function]

Sets the abscissa range of the plot to be logarithmic from wavenumbers *w1* to *w2*.

`wavenumbers w1 w2 g1 g2` [Function]

Sets the abscissa range of the plot to be linear from wavenumbers *w1* to *w2* in a graph rectangle from wavenumbers *g1* to *g2*.

`eVs x` [Function]

Sets the abscissa range of the plot to be linear from energy $0.666*x$ to $1.5*x$ electron Volts.

- eVs** *x1 x2* [Function]
Sets the abscissa range of the plot to be linear from energy *x1* to *x2* electron Volts.
- eVs** *x1 x2 g1 g2* [Function]
Sets the abscissa range of the plot to be linear from energy *x1* to *x2* electron Volts in a graph rectangle from energies *g1* to *g2* electron Volts.
- logarithmic** *w* [Function]
Sets the abscissa range of the plot to be logarithmic from wavelengths $0.666*w$ to $1.5*w$.
- logarithmic** *w1 w2* [Function]
Sets the abscissa range of the plot to be logarithmic from wavelengths *w1* to *w2*.
- logarithmic** *w1 w2 g1 g2* [Function]
Sets the abscissa range of the plot to be logarithmic from wavelengths *w1* to *w2* in a graph rectangle from wavelengths *g1* to *g2*.
- angles** *theta* [Function]
Sets the abscissa range of the plot to be linear from angles $0.75*theta$ to $1.25*theta$.
- angles** *theta1 theta2* [Function]
Sets the abscissa range of the plot to be linear from angles *theta1* to *theta2*.
- marker** *w1 w2 . . .* [Function]
Places vertical arrows at abscissa coordinates *w1*, *w2*, The **marker** command does not affect the data written by **output-data**.
- samples** *k* [Function]
Sets the number of abscissa coordinates to *k*. The default value is 200.
- samples** *k spacing* [Function]
Sets the number of abscissa coordinates to *k*. *spacing* is one of the (single-quoted) symbols 'eV', 'ratio', 'wavelength', or 'wavenumber', and determines the spacing of the samples. The default spacing is 'ratio' if the endpoint ratio is between 1.5 and 10000; and 'wavelength' otherwise.
- Note that *spacing* does not need to match the abscissa scale. To generate 10 samples at evenly spaced wavelengths, do:
- (samples 10 'wavelength')
- smooth** *sigma* [Function]
Convolve the traces (before converting values to decibels) with a Gaussian filter having wavelength standard deviation *sigma*.

4.3.2 Traces

These functions specify whether the plot holds angle constant and varies wavelength; holds wavelength constant and varies angle; or plots components of the index-of-refraction of a material. Multiple invocations of any one of these functions puts all those specified traces in one plot. To generate separate plots call **plot-response** multiple times.

The type of a trace appearing in a plot is specified by a symbol. The first ten in this table are for separate polarizations. The rest average the two polarizations.

| | |
|-----|--------------------------------|
| T_s | S-plane transmission |
| R_s | S-plane reflection from top |
| B_s | S-plane reflection from bottom |
| A_s | S-plane absorption from top |
| L_s | S-plane absorption from bottom |
| T_p | P-plane transmission |
| R_p | P-plane reflection from top |
| B_p | P-plane reflection from bottom |
| A_p | P-plane absorption from top |
| L_p | P-plane absorption from bottom |
| T | transmission |
| R | reflection from top |
| B | reflection from bottom |
| A | absorption from top |
| L | absorption from bottom |

A trace can also be a quoted scheme expression combining numbers and the symbols listed above with the operators `+`, `-`, `*`, `/`, `ln`, `log_10`, and `average`. The following example computes the reflectivity relative to a substrate reflectivity of 0.023:

```
(incident 45 '(/ (- R_p .023) .023))
```

incident *angle trace1 trace2* ... [Function]

A plot of *trace1*, *trace2*, ... versus wavelength will be generated for radiation incident at *angle* degrees.

The *angle* argument can also be a list of angles in degrees. In this case the plots of *trace1*, *trace2*, ... will be averaged over the angles given.

This is useful when profiling materials whose thicknesses are several times wavelengths of interest. Plots at a single angle of incidence can oscillate wildly with wavelength as the reflections go in and out of phase, constructively and destructively interfering.

wavelength *w trace1 trace2* ... [Function]

A plot of *trace1*, *trace2*, ... versus incident angle will be generated for radiation at wavelength *w*.

ir *substance comp1 comp2* ... [Function]

Plots characteristics of procedure *substance* versus wavelength. Symbols *comp1*, *comp2*, ... determine the characteristics to be plotted:

```
n
real
real-part
```

n

`k`
`imag`
`imag-part`
`ec`
`extinction-coefficient`

`k`

`k/n` `k/n`

`r0`

`reflect`

`reflectance`

Normal reflectance from a thick layer.

4.3.3 Other Outputs

`color-swatch` *angle trace* [Function]

Computes the color of *trace* at *angle* degrees from normal using CIE illuminant D65.

The following statement will cause `plot-response` to compute the reflected color (average of both polarizations) at 30 degrees from the surface normal.

```
(color-swatch 30 'R)
```

If there are any `color-swatch` statements passed to `plot-response`, then a file named `filebase-color.png` will be written containing 64x64 pixels color squares, one for each color computed. The squares are arrayed horizontally in the order they are passed to `plot-response`. Vertically, one such row is generated for each optical stack.

The `filebase` string is that set by the `title` command.

`solar` *angle token1 token2 . . .* [Function]

For each stack, prints out the results of integrating each trace specified (*token1*, *token2*, . . .) at *angle* with "Key Centre for Photovoltaic Engineering UNSW - Air Mass 1.5 Global Spectrum" solar irradiance.

5 Program Interface

(require 'fresnel-equations)

combine-layers *th-i w layers* [Function]

layers is a list of lists of *index-of-refraction* and *thickness*. The *index-of-refraction* may be a complex number or a procedure of wavelength (*w*) in meters returning a complex number.

Layers with negative *thickness* are modeled as incoherent (with positive thickness); otherwise as coherent (with interference fringing).

The index-of-refraction of the top and bottom media are given by the first and last *layers*, which must have thickness 0. *w* is probe wavelength. *th-i* is the angle of the incident ray in radians.

Combine-layers returns a list of three non-negative real numbers:

- the ratio of transmitted power to incident power;
- the ratio of reflected power (from the top) to incident power; and
- the ratio of reflected power (from the bottom) to incident power.

The transmitted and forward ratios sum to 1.0 if *layers* are all dielectric (lossless). The transmitted and reverse ratios sum to 1.0 if *layers* are all dielectric (lossless).

Negative *w* computes the S-polarization, else the P-polarization.

snell-law *z1 z2 th-i* [Function]

Complex numbers *z1* and *z2* are the indexes of refraction of the incident and opposite side of the boundary plane between two materials. *th-i* is the angle of incidence (from the normal of the boundary plane).

snell-law returns the exit angle (from normal) of an incident ray impinging at *th-i* from normal.

If the ray undergoes total internal reflection, then the returned angle will not be real. If *z1* and *z2* are real, then the real part of the returned value will be $\pi/2$ and represents a quickly decaying evanescent wave. Otherwise, the real part of the return value tends toward $\pi/2$. I don't know a physical interpretation of the imaginary part.

(snell-law 2.8 1.3 .1) \Rightarrow 216.71826868463917e-3

(snell-law 2.8 1.3 .3) \Rightarrow 689.9583515921762e-3

(snell-law 2.8 1.3 .4) \Rightarrow 994.9783891781343e-3

(snell-law 2.8 1.3 .5) \Rightarrow 1.5707963267948965-254.68865153727376e-3i

6 About FreeSnell

```
Free      Software
Fre snel  Equations
      Snell's Law
=====
FreeSnell
```

The author can be reached as 'agj@alum.mit.edu'. The most recent information about FreeSnell can be found on the FreeSnell home page:

<http://people.csail.mit.edu/jaffer/FreeSnell>

6.1 Installation

6.1.1 i386 MS-Windows

- Download and run <http://groups.csail.mit.edu/mac/ftplib/scm/slib-3c1-1.exe>.
- Download and run <http://groups.csail.mit.edu/mac/ftplib/scm/scm-5f4-1.exe>.
- Download and run <http://groups.csail.mit.edu/mac/ftplib/scm/FreeSnell-1c4-1.exe>.

6.1.2 x86_64 GNU/Linux with RPM

```
#!/bin/sh
wget http://groups.csail.mit.edu/mac/ftplib/scm/slib-3c1-1.noarch.rpm
wget http://groups.csail.mit.edu/mac/ftplib/scm/scm-5f4-1.x86_64.rpm
wget http://groups.csail.mit.edu/mac/ftplib/scm/wb-2b4-1.x86_64.rpm
rpm -U slib-3c1-1.noarch.rpm scm-5f4-1.x86_64.rpm wb-2b4-1.x86_64.rpm
wget http://groups.csail.mit.edu/mac/ftplib/scm/FreeSnell-1c4.zip
unzip FreeSnell-1c4.zip
(cd FreeSnell; ./configure --prefix=/usr/local/; make install)
```

6.1.3 Unix (including GNU/Linux)

```
#!/bin/sh
wget http://groups.csail.mit.edu/mac/ftplib/users/jaffer/slib.zip
wget http://groups.csail.mit.edu/mac/ftplib/users/jaffer/scm.zip
wget http://groups.csail.mit.edu/mac/ftplib/users/jaffer/wb.zip
wget http://groups.csail.mit.edu/mac/ftplib/scm/FreeSnell.zip
unzip slib.zip
unzip scm.zip
unzip wb.zip
unzip FreeSnell.zip
(cd slib; ./configure --prefix=/usr/local/; make install)
(cd scm; ./configure --prefix=/usr/local/;
  make scmlit; make scm5; make mydlls; make wbscm.so; make install)
(cd FreeSnell; ./configure --prefix=/usr/local/; make install)
```

6.2 Using FreeSnell

To run FreeSnell from the `C:\Program Files\SCM\FreeSnell` directory, click on the FreeSnell desktop icon. In Unix, from the 'FreeSnell' directory run 'scm'.

You can then type expressions to the SCM interpreter. To run FreeSnell's regression suites type:

```
(load "dielectric.scm")
(dielectric)
(load "metallic.scm")
(metallic)
(load "granular.scm")
(granular)
(load "coherence.scm")
(coherence)
(load "polyethylene.scm")
(polyethylene)
```

I set up design directories as peers of 'FreeSnell'; that is, both are subdirectories of the same directory. I find it useful to put related designs in one directory.

In order to load FreeSnell files, you should create a local SLIB catalog (named `usercat`) within the design directory or your *HOME* directory. This catalog translates symbols to the pathnames of FreeSnell files. Here is the `usercat` included in the FreeSnell distribution, which is suitable to copy to design directories which are peers of FreeSnell:

```
;;; "usercat": SLIB catalog additions for thin-film optics. -*-scheme*-
(
  (fresnel-equations . "fresneleq")
  (optic-compute . "opticompute")
  (optic-plot . "optiplot")
  (optic-color . "opticolr")
  (video-processing . "video")
  (optic-solar . "solar-am15")
  (FreeSnell aggregate optic-compute optic-plot optic-color optic-solar)
)
```

Design files can then load FreeSnell with the expression:

```
(require 'FreeSnell)
```

Realize that this `usercat` file assumes that the FreeSnell directory is named `FreeSnell`. If your FreeSnell directory is named something else, then substitute its name for FreeSnell in the right hand side of lines in `usercat`.

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