El problema inverso

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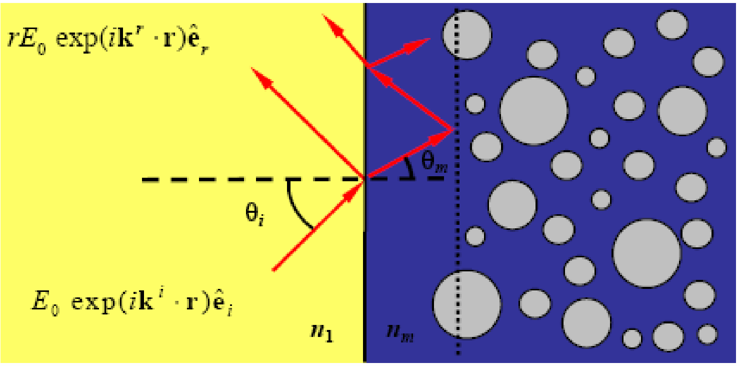


* Asesor del Centro de Investigación en Polímeros, Grupo Comex



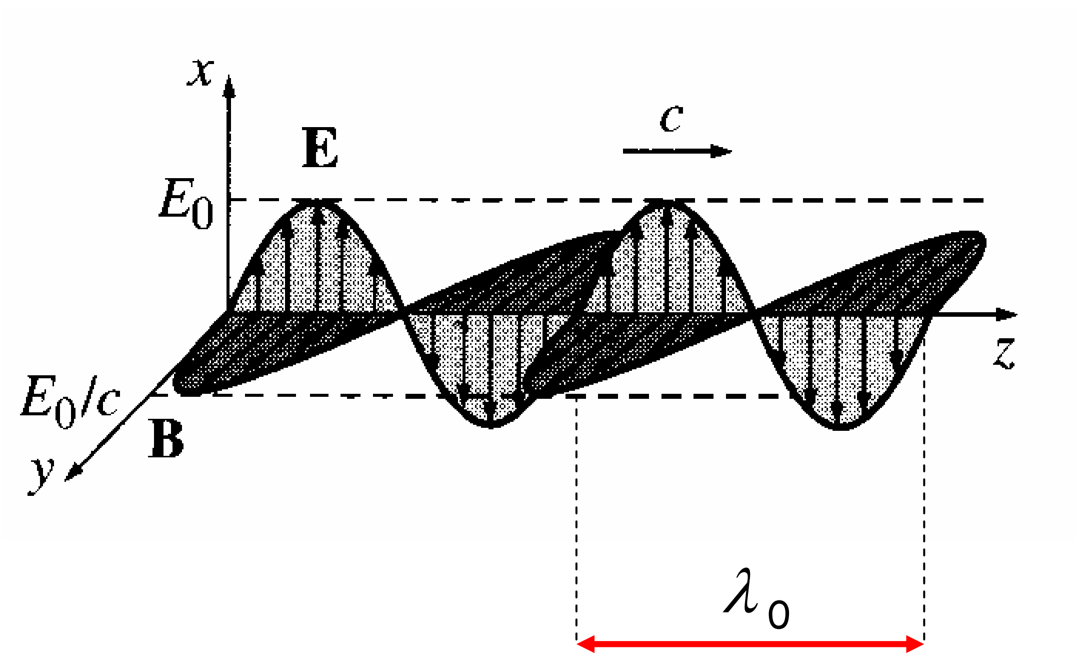



+ Carolina Keiman

Conceptos básicos

ondas

$$\vec{E} = \mathrm{Re}\left[\vec{E}_0 e^{i(k_0 z - \omega t)}\right] = \vec{E}_0 \cos(k_0 z - \omega t)$$



vector de onda

$$k_0 = \frac{\omega}{c} = \frac{2\pi}{\lambda_0}$$

$$k_0 z = 2\pi \frac{z}{\lambda_0}$$

en materiales

$$k = \frac{2\pi}{\lambda_0} n = \frac{2\pi}{\underbrace{\lambda_0 / n}}$$

índice de refracción

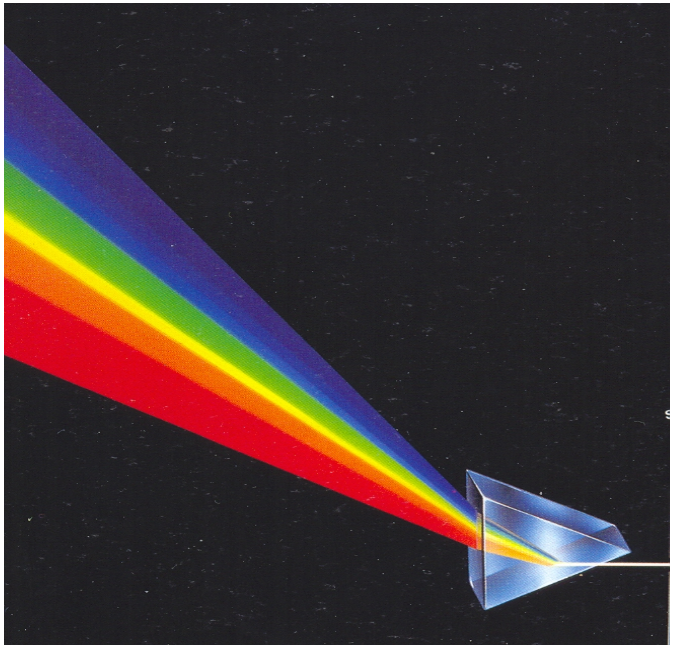
$$n = \frac{c}{v}$$

$$v_{agua} = \frac{3}{4}c \qquad v_{vidrio} = \frac{2}{3}c$$

$$n_{agua} = 1.33 \qquad n_{vidrio} = 1.5$$

dispersión

$$n(\omega)$$



blanca

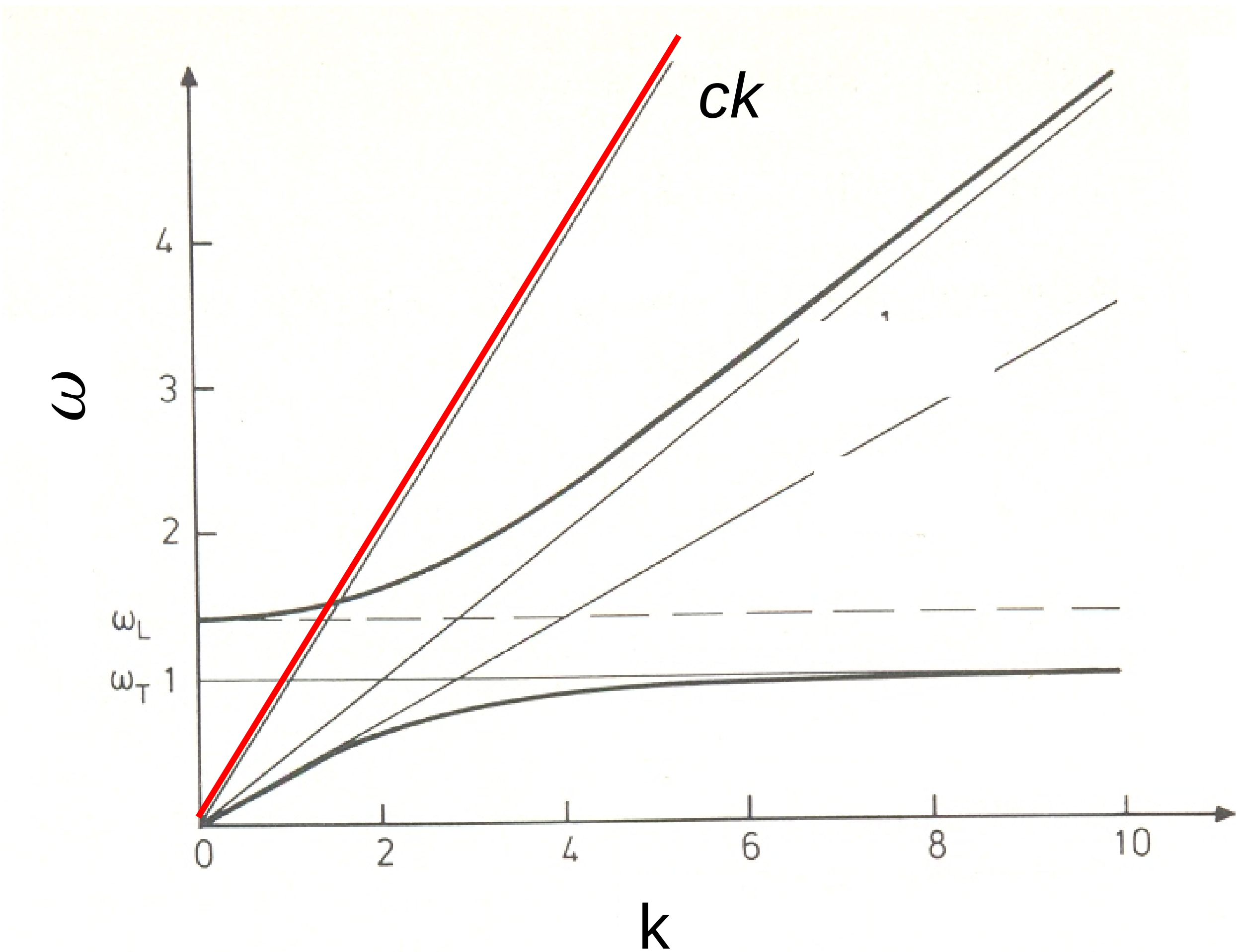
ondas en medios materiales

$$k = \frac{\omega}{c} n(\omega)$$

relación de dispersión

$$\omega(k)$$

$\omega(k)$



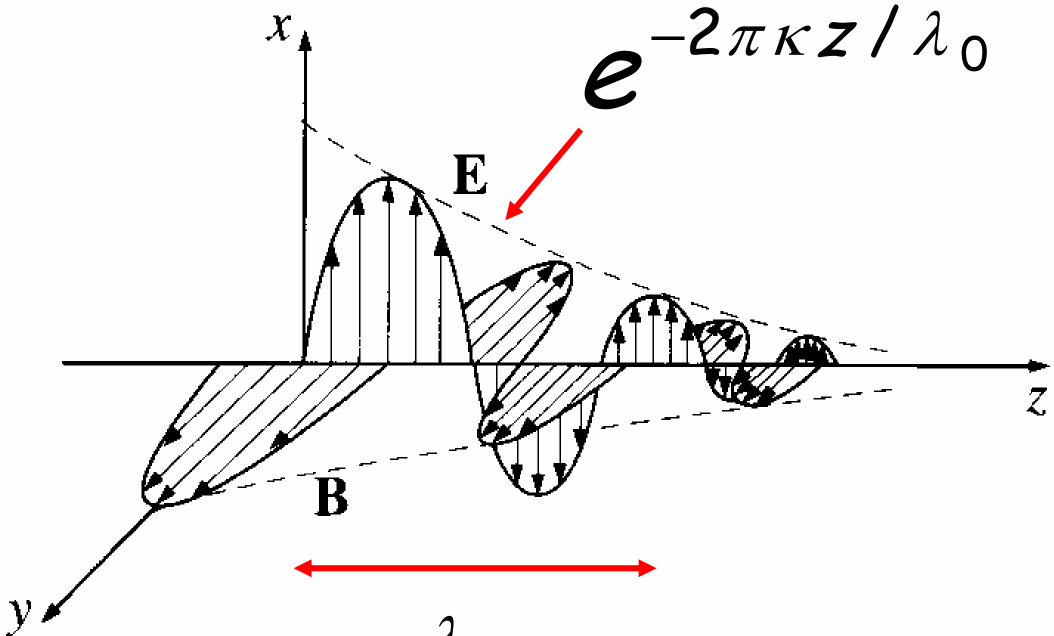
absorción

$$\tilde{n}(\omega) = n(\omega) + i\underline{\kappa(\omega)}$$

"absorción"

$$l_p = \frac{\lambda_0}{4\pi\kappa}$$

$$e^{-2\pi\kappa z/\lambda_0}$$



$$\frac{\lambda_0}{2\pi\kappa}$$

$$\lambda_0 \approx 0.5\,\mu m$$

κ	l_p
10	4.0 nm
1	0.04 μm
10^{-2}	4.0 μm
10^{-4}	0.40 mm
10^{-6}	4.0 cm
10^{-8}	4.0 m

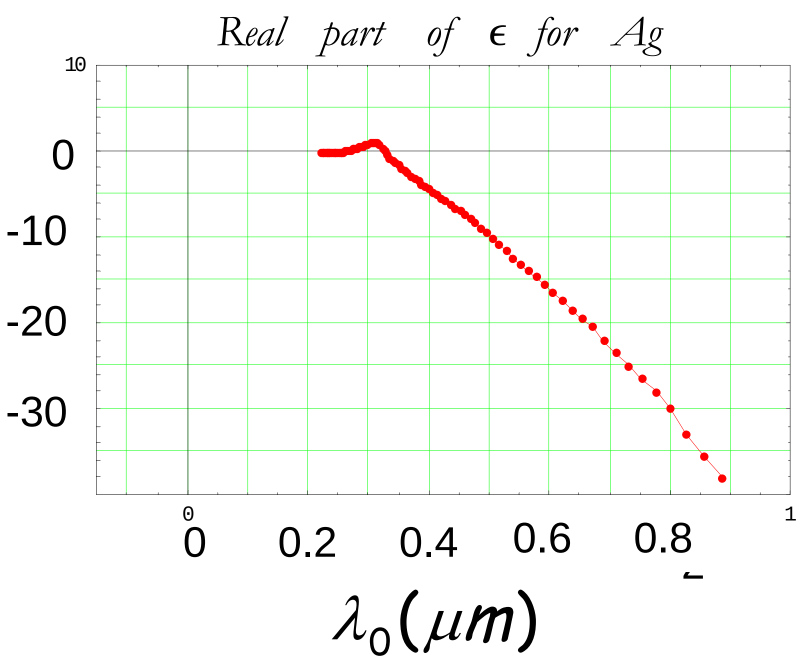
metales

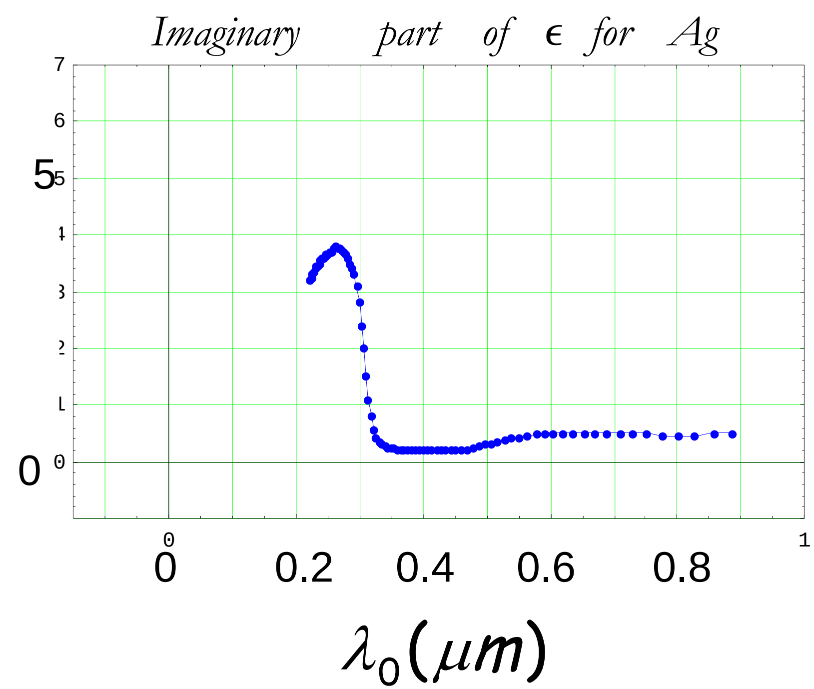
$$n(\omega) = \sqrt{\varepsilon(\omega)\,\mu(\omega)}$$

no magnético

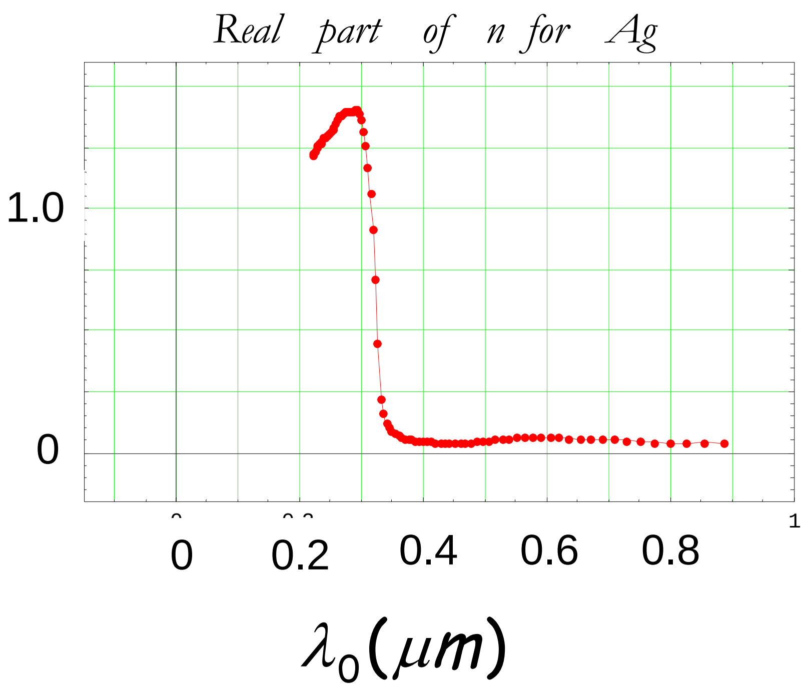
$$n(\omega) = \sqrt{\varepsilon(\omega)} = \sqrt{\varepsilon' + i\,\varepsilon''}$$

absorción

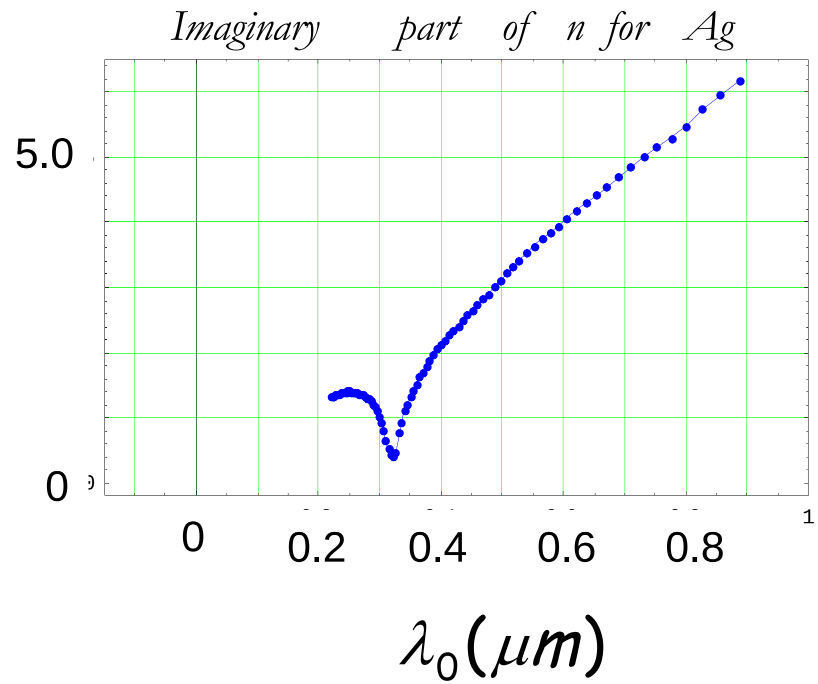




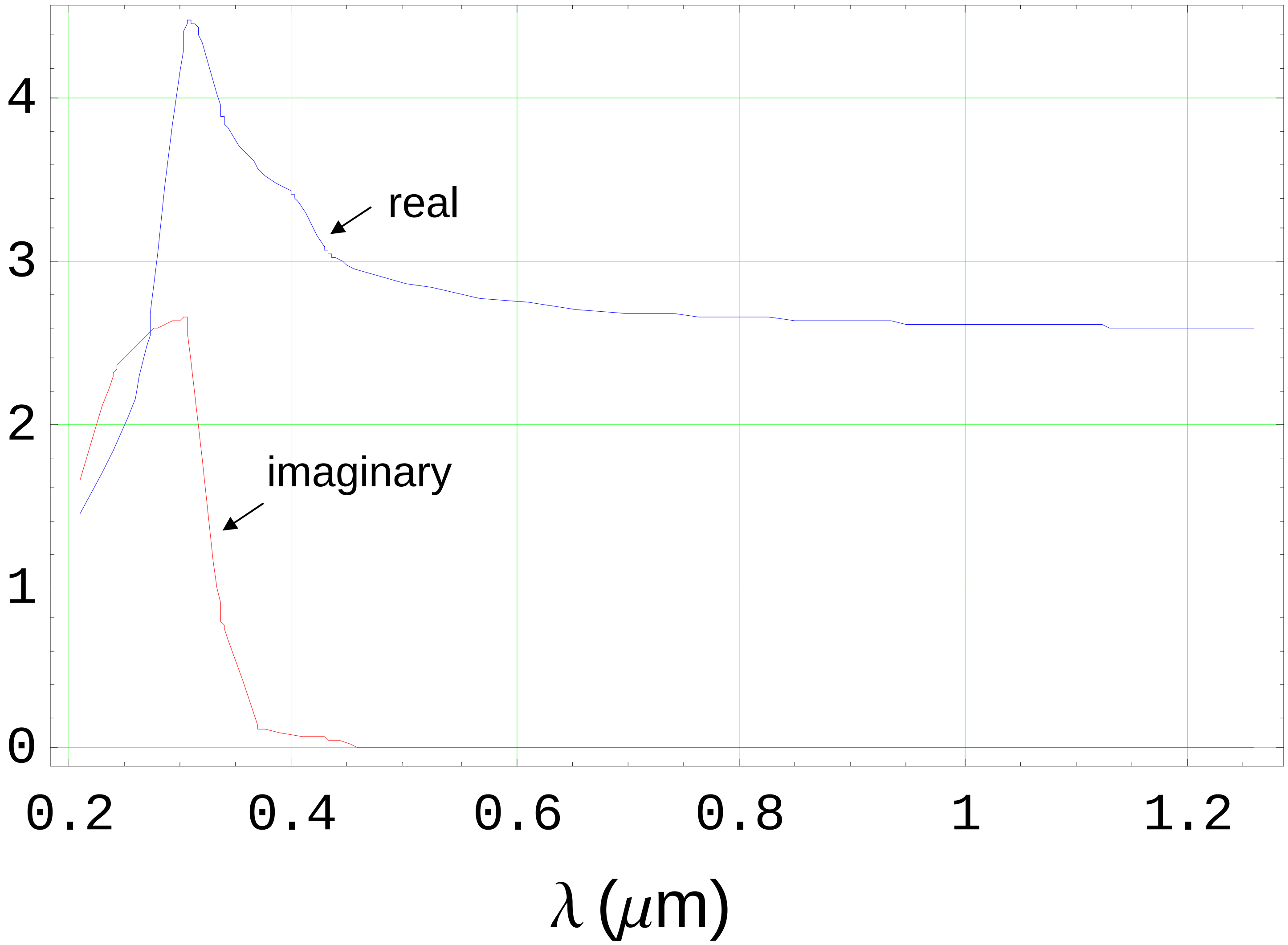
Ag



$$\tilde{n} \approx i\kappa$$



Refractive index TiO_2

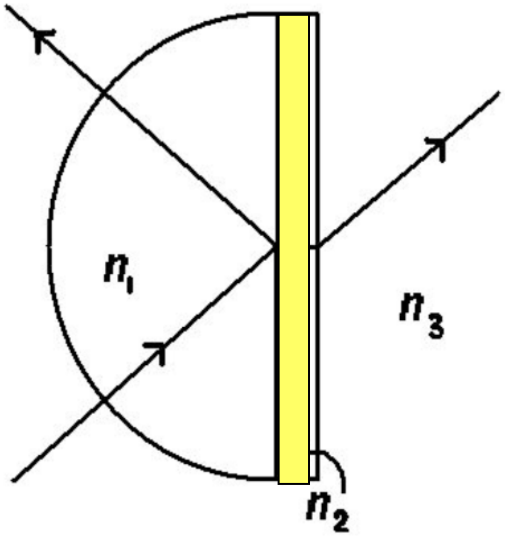


Problema

Determinar la parte real y la parte imaginaria del índice de refracción de una resina, utilizada en pinturas blancas base agua

$$n_2 \sim 1.5$$

$$\kappa_2 \sim \underline{10^{-5} - 10^{-6}}$$

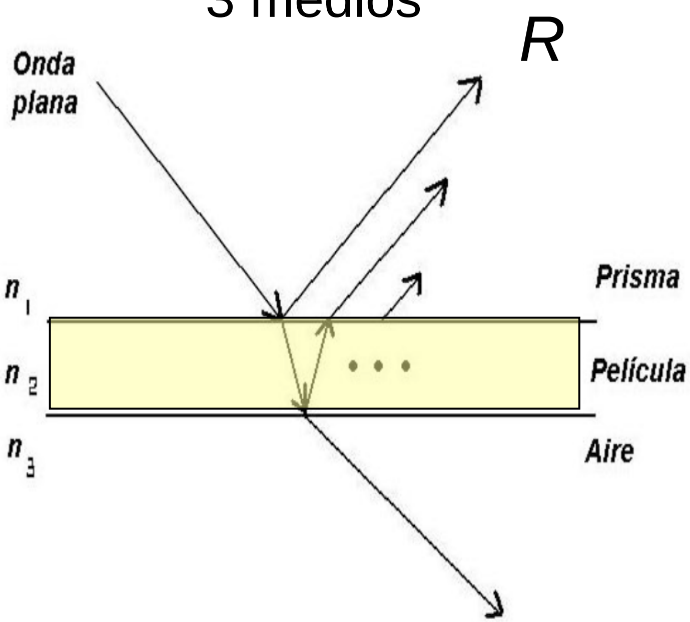


$$R_S(\theta_i; \lambda_0; n_2, \kappa_2)$$

El problema directo

Algoritmo de cálculo

3 medios



$$R\left[\theta_i, d; \lambda_0, n_1, \tilde{n}_2, n_3\right]$$

7 parámetros ⟶ 3 ⟶ 2

$$R = \left| \frac{r_{12} + r_{23}\, e^{2i\alpha}}{1 + r_{12} r_{23}\, e^{2i\alpha}} \right|^2$$

$$r_{ij} = \frac{Z_i - Z_j}{Z_i + Z_j}$$

$$Z_{s,i} = \frac{1}{\tilde{n}_i \cos\theta_i}$$

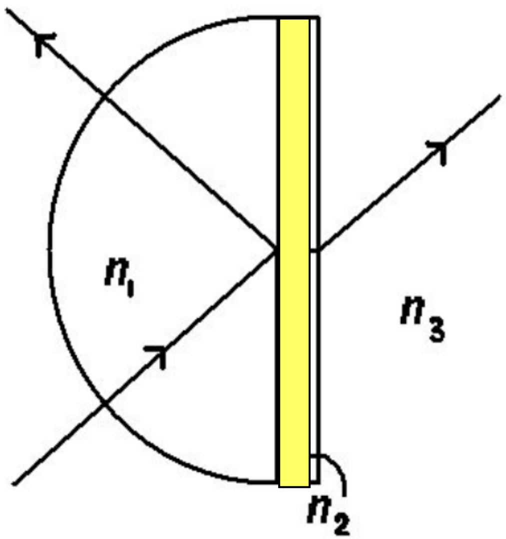
S,P

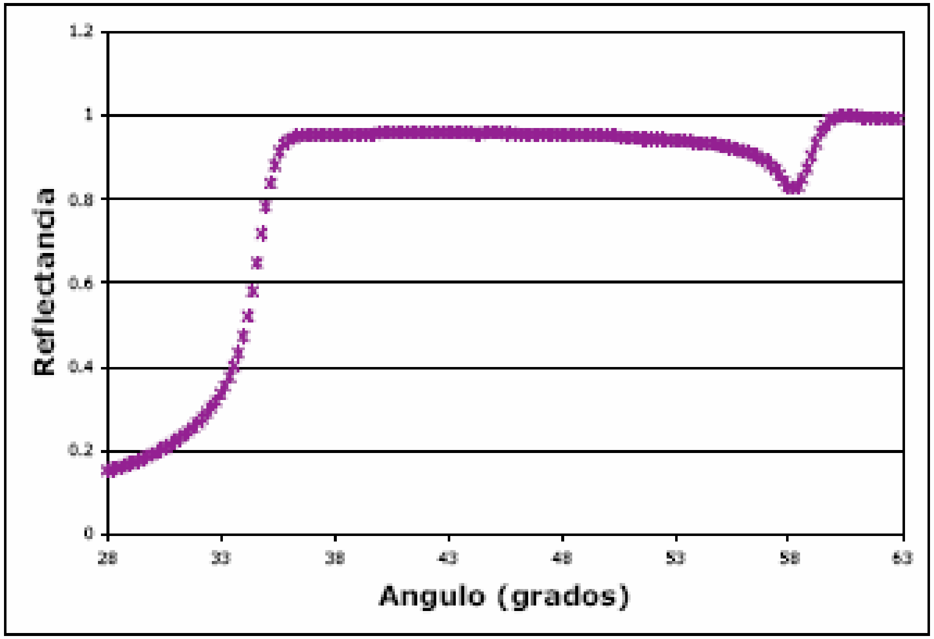
$$\alpha = \frac{2\pi}{\lambda_0} \tilde{n}_2\, d \cos\theta_2$$

$$n_i sen\theta_i = n_{i+1} sen\theta_{i+1}$$

El problema inverso

$$R_s(\theta_i;\lambda_0)$$



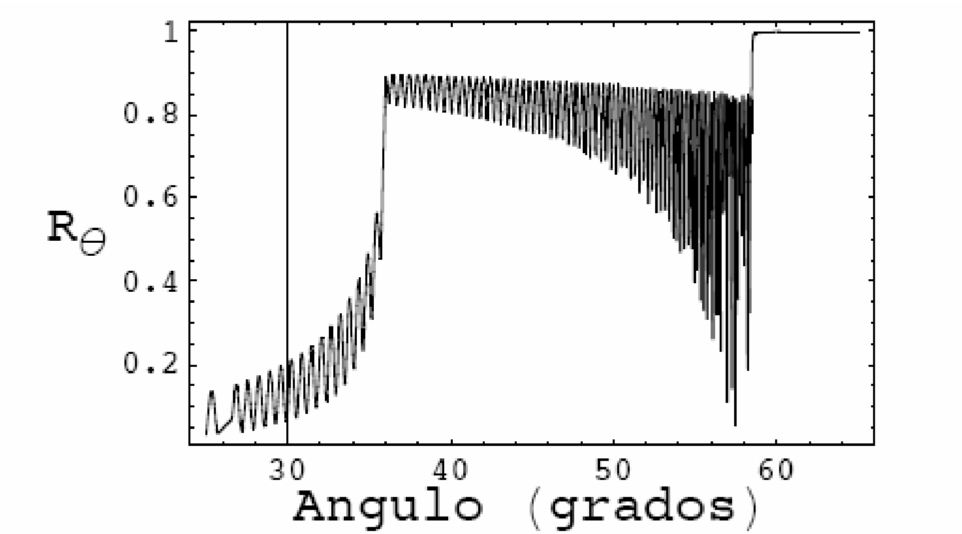


$$R_s(\theta_i;\lambda_0;n_2,\kappa_2) \quad \longrightarrow \quad \tilde{n}_2 = n_2 + i\kappa_2$$

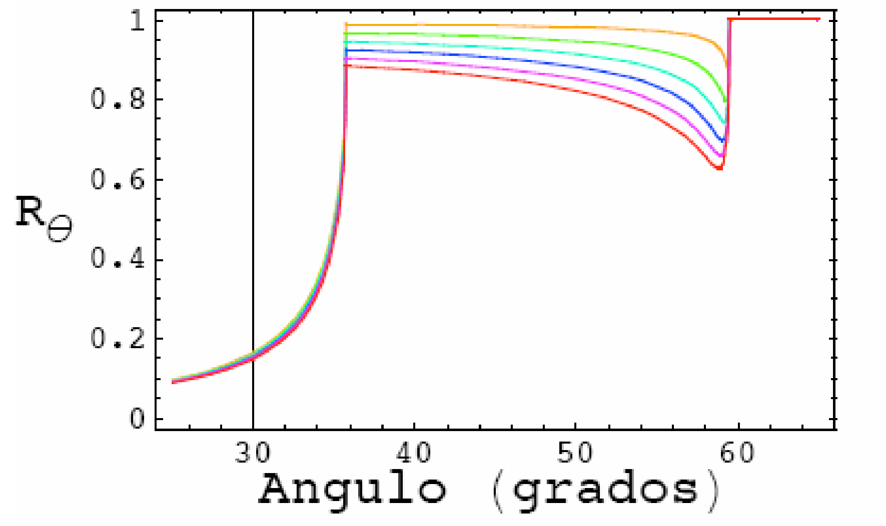
Imposible depejar

Ajuste

coherente



incoherente

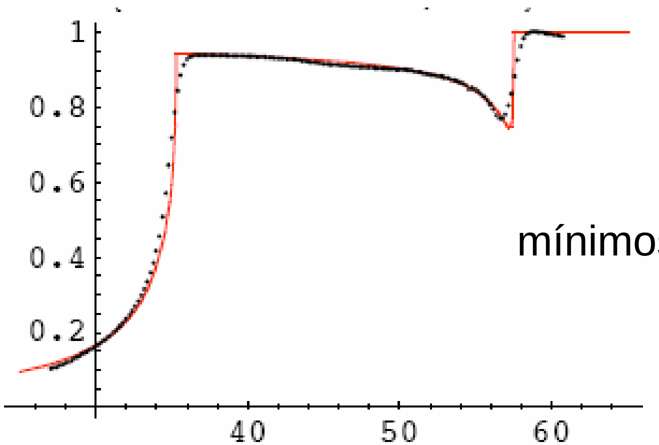


ajuste “a mano”

$$n_2 \sim 1.5$$

$$\kappa_2 \sim 10^{-5} - 10^{-6}$$

La solución NO es única



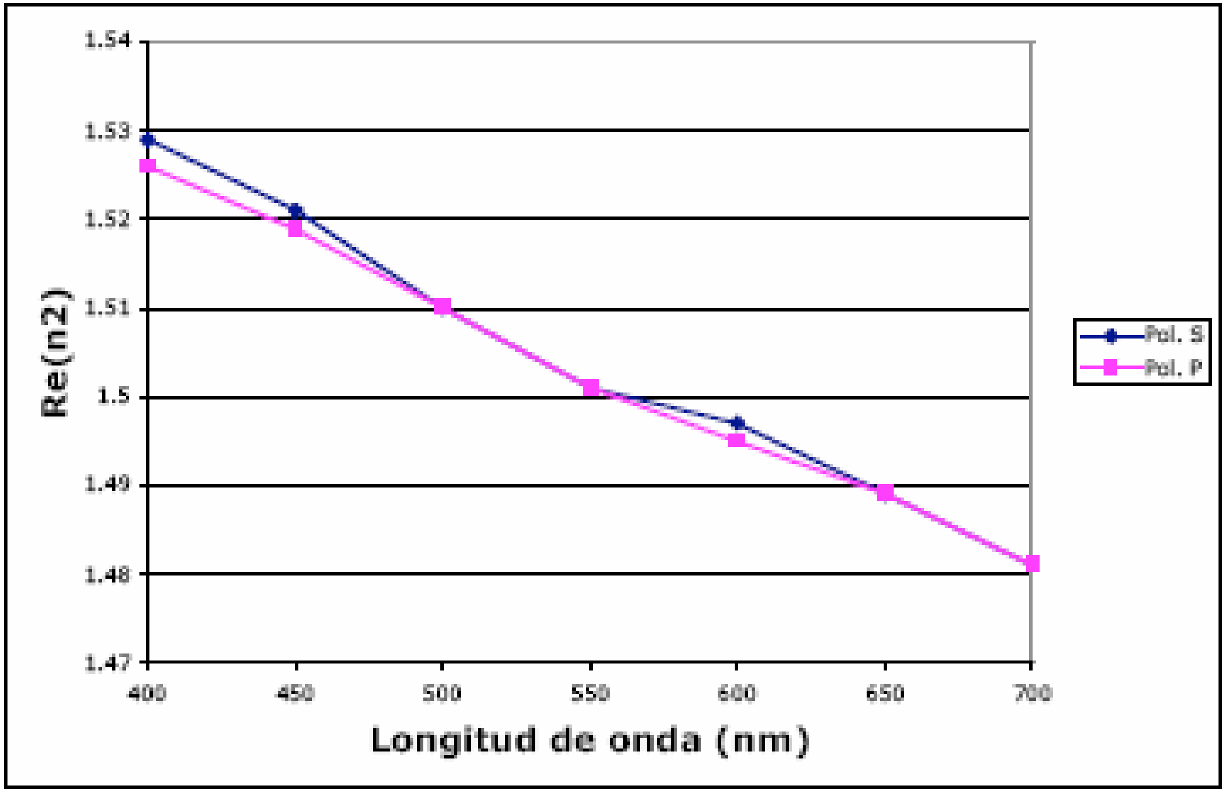
mínimos cuadrados

Gajes del oficio

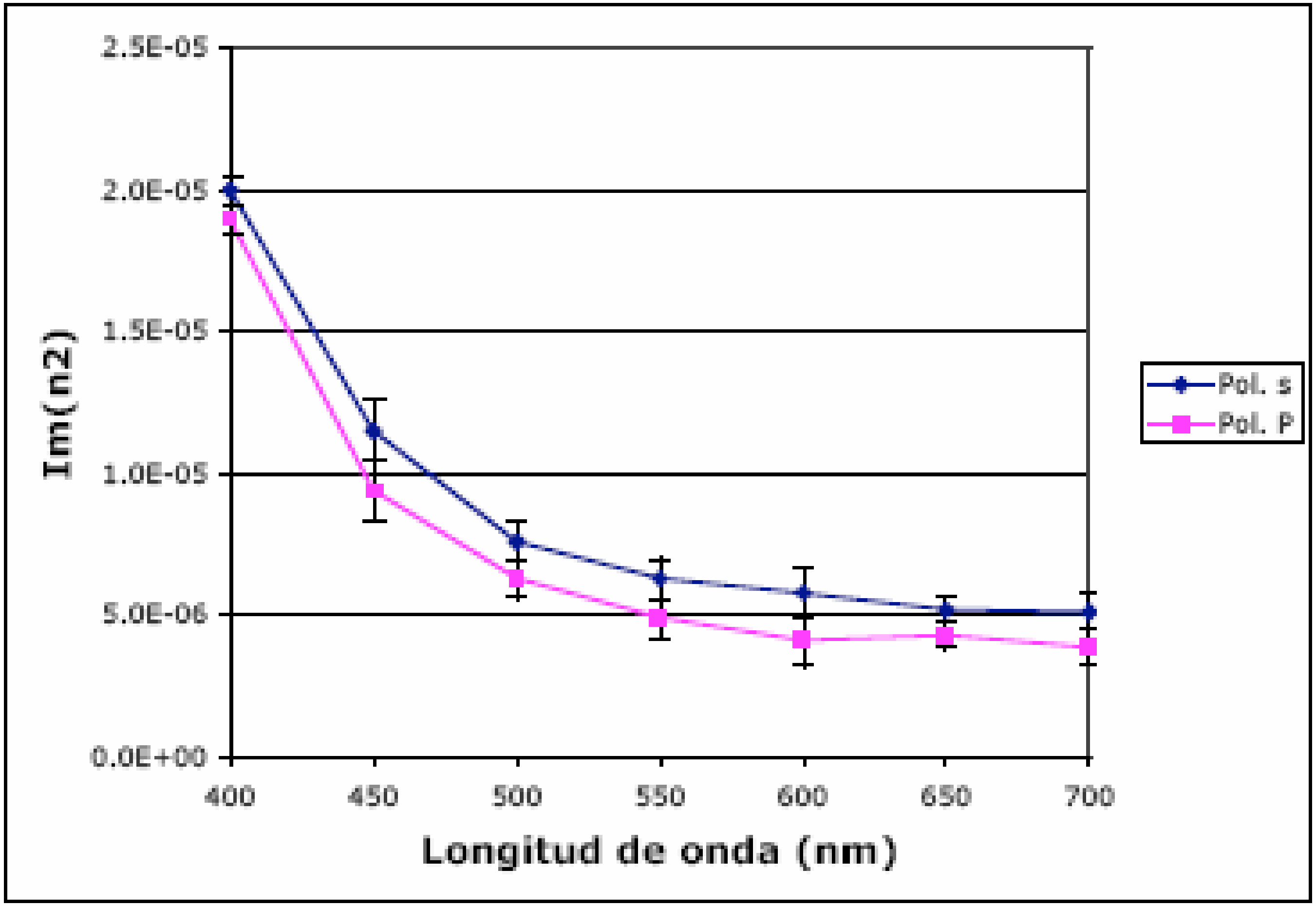
Pruebas de consistencia $R_S(\theta_i;\lambda_0;n_2,\kappa_2) \longleftrightarrow R_P(\theta_i;\lambda_0;n_2,\kappa_2)$

Relajación de parámetros $R_S(\theta_i;\lambda_0;n_2,\kappa_2;\, d_0 \pm \Delta d)$

Resultados



$\kappa_2(\lambda_0)$



Pinturas blancas

Transferencia radiativa

balance de flujo

$$\frac{dI(\vec{r},\hat{s})}{ds} = -\rho\sigma_T I(\vec{r},\hat{s}) + \rho\frac{\sigma_T}{4\pi}\int_{4\pi} p(\hat{s},\hat{s}')I(\vec{r},\hat{s}')d\Omega'$$

$$\rho = \frac{N}{V}$$

independiente

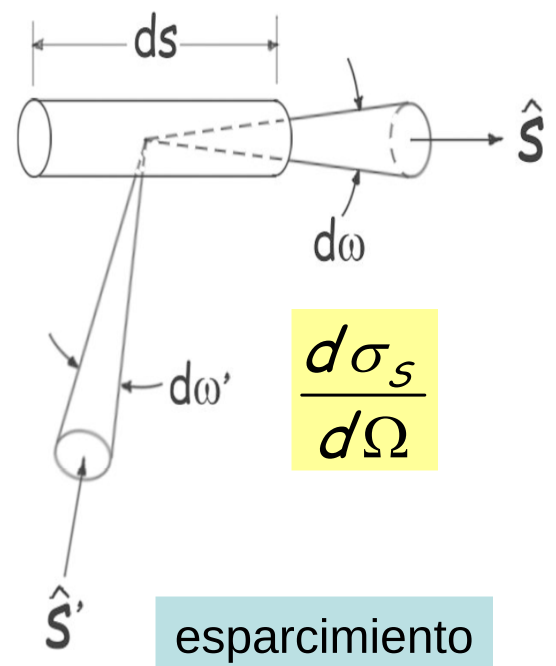
$$\sigma_T = \sigma_A + \sigma_S$$

tamaño

forma

$$\frac{d\sigma_S}{d\Omega}(\lambda_0,\tilde{n}_p,\tilde{n}_M;a,\hat{a})$$

$$\sigma_S = \int_{4\pi}\frac{d\sigma_S}{d\Omega}d\Omega$$



$$\frac{d\sigma_S}{d\Omega}$$

esparcimiento múltiple

Solución numérica

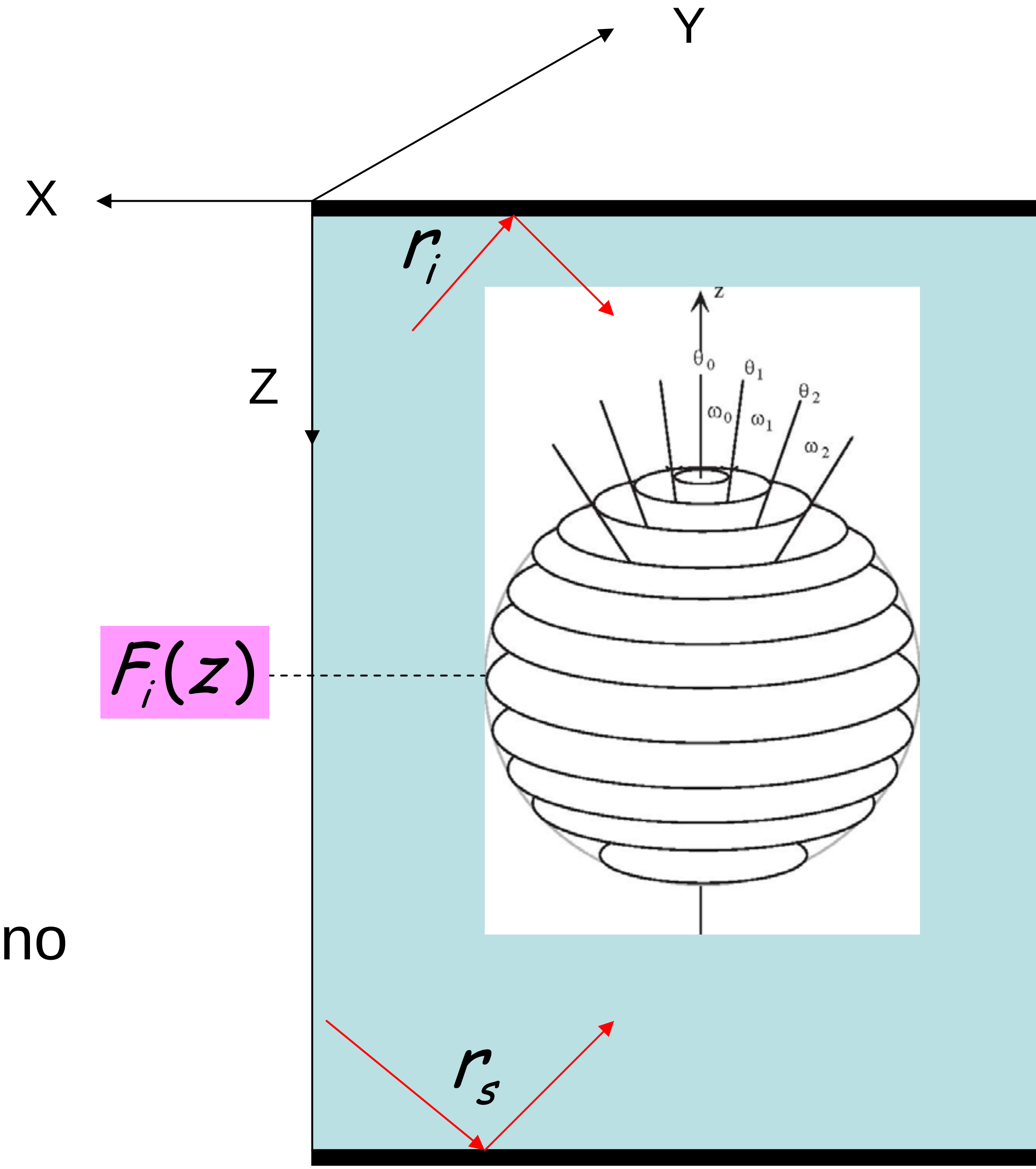
$$\int_{4\pi} \rightarrow \sum_j$$

$$\frac{dF_i}{dz} = \sum_j S_{ij} F_j$$

$$S_{ij}(\lambda_0, \tilde{n}_p, \tilde{n}_M; a, \hat{a})$$

\+ condiciones de contorno

$$r_i\underbrace{(\tilde{n}_M, \tilde{n}_p, \rho, a, \hat{a})}_{\text{Modelo de medio efectivo}},\ r_s,\ d$$



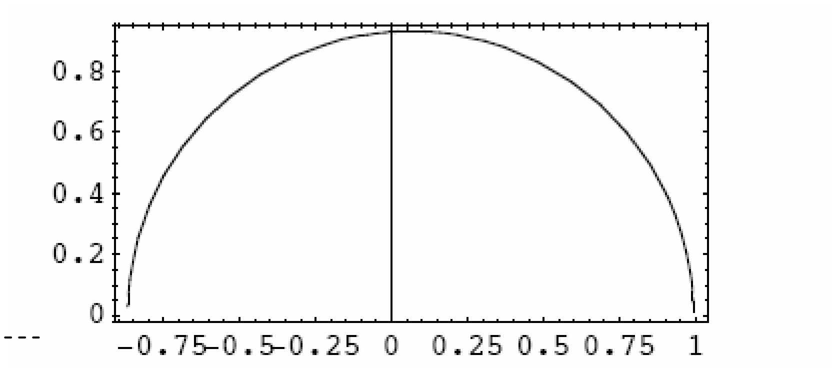
N-flujos

Resultados

$$F_i(z;\lambda_0,\tilde{n}_p,\tilde{n}_M,r_i,r_s;a,\hat{a};\rho,d)$$

F_0

$z = z_0$

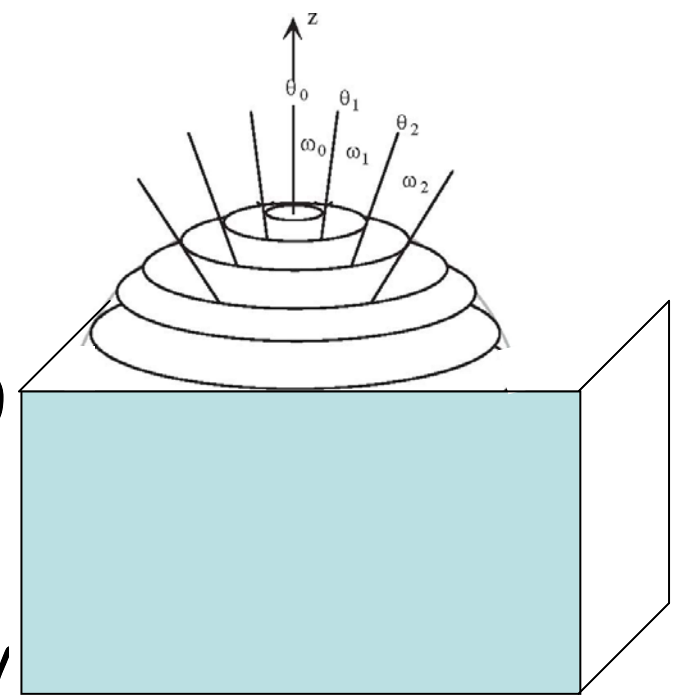


Reflectancia difusa

$$R_{difusa} = \frac{1}{F_0}\sum_{i(arriba)} F_i(z=0)$$

$$R_{difusa}(\lambda_0,\tilde{n}_p,\tilde{n}_M,r_i,r_s;a,\hat{a};\rho,d)$$

$z=0$

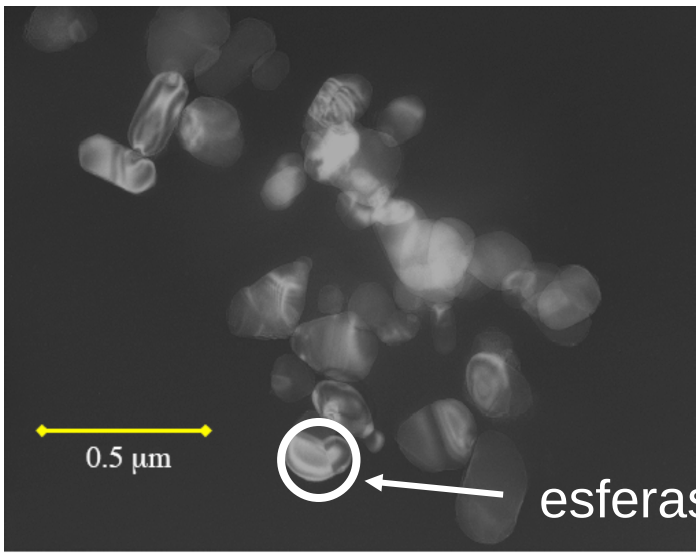


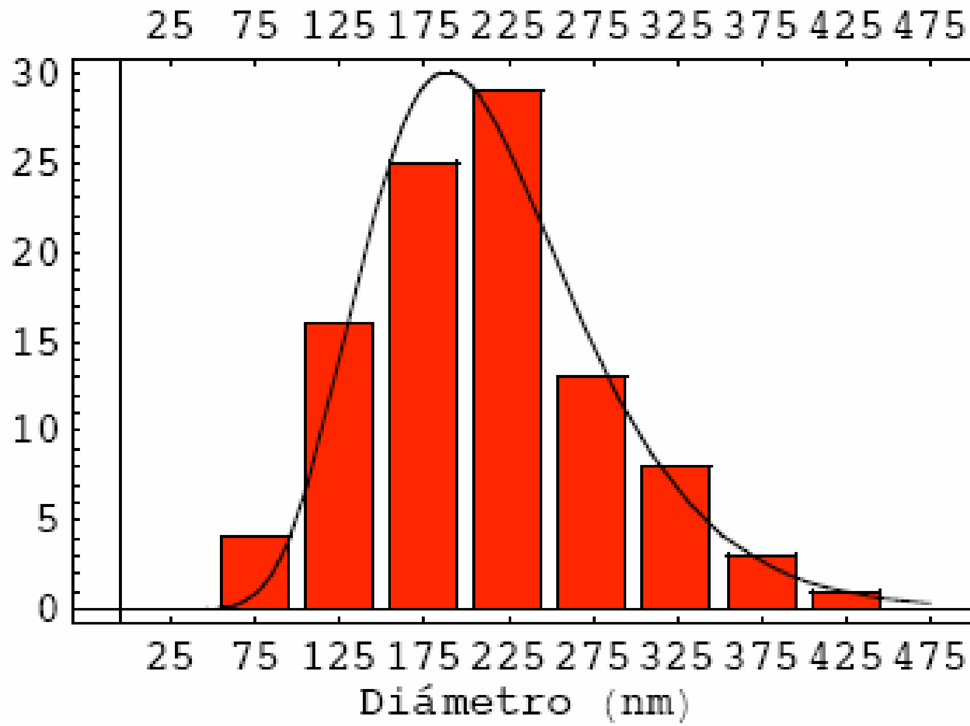
$z=d$

Experimento

Distribución de tamaños

SIMPLEX





TiO_2

$$D(a_0,\sigma)$$

Partículas no-esféricas

J. Phys. Chem. B **2003,** *107,* 6269−6275 **6269**

ARTICLES

Optical Properties of Metal Nanoparticles with Arbitrary Shapes

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Received: November 7, 2002; In Final Form: May 5, 2003

We have studied the optical properties of metallic nanoparticles with arbitrary shape. We performed theoretical calculations of the absorption, extinction, and scattering efficiencies, which can be directly compared with experiments, using the discrete dipole approximation (DDA). In this work, the main features in the optical spectra have been investigated depending of the geometry and size of the nanoparticles. The origin of the optical spectra are discussed in terms of the size, shape, and material properties of each nanoparticle, showing that a nanoparticle can be distinguish by its optical signature.

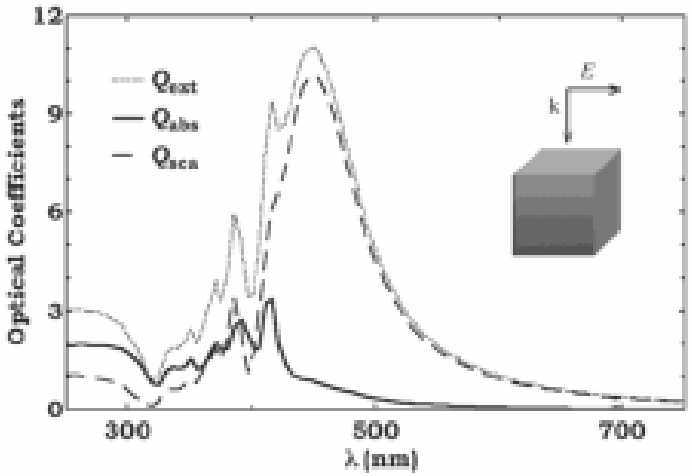


Figure 2. Optical coefficients for a silver nanocube.

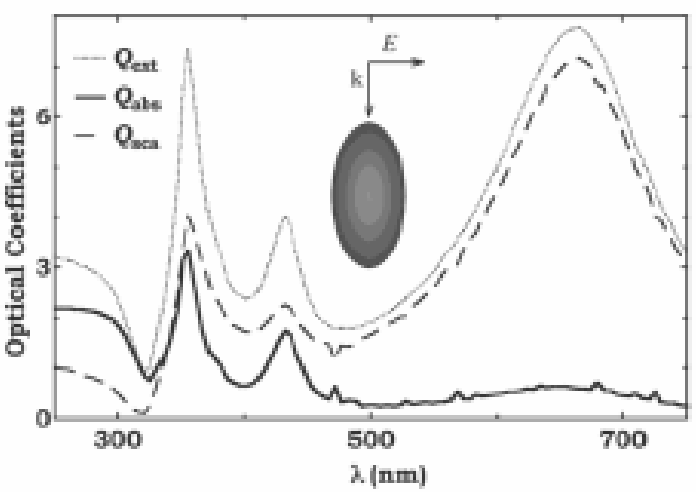


Figure 3. Optical coefficients for a silver nanospheroid for an electric field polarized along the minor axis.

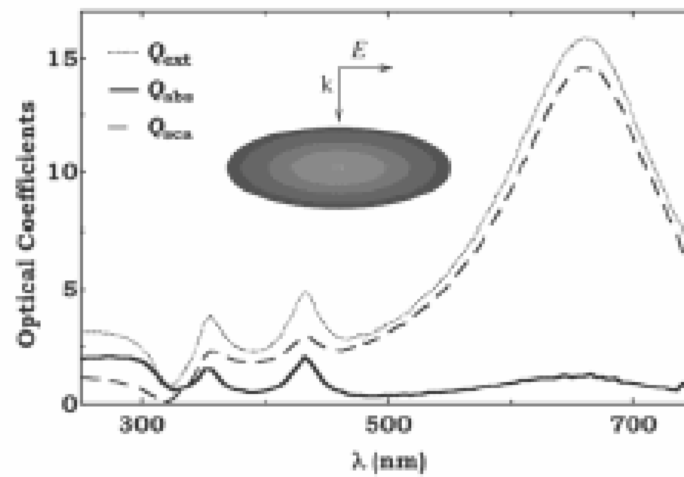


Figure 4. Optical coefficients for a silver nanospheroid for an electric field polarized along the major axis.

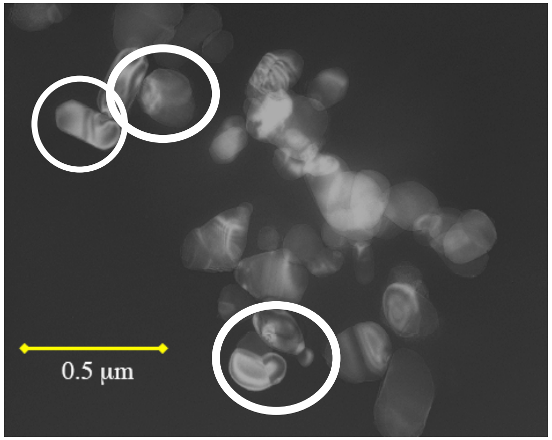
elucidate the problem. For example, it is known that scattering effects of smaller particles have a maximum at smaller wavelengths; therefore, it is possible to hide the multipolar effects if they appear at the same wavelength as scattering effects do. In such a case, a detailed study of the absorption and extinction efficiencies is necessary. We have also calculated the optical efficiencies for smaller ellipsoidal nanoparticles with a major semiaxis of 12 nm. In this case, the main contribution to Q_{ext} comes from light absorption processes due to the excitation of one surface plasmon (dipolar excitation) whose location depends on the particular geometry of each nanoparticle and on its material properties. From 475 to 750 nm, the main contribution to Q_{ext} come from light-scattering effects, although we also observed a tail in Q_{abs}. Although this tail shows also a few peaks, they are washed out as the number of dipoles in the calculation is increased dramatically,[20] so they should come from lack of convergence in the calculations. It is interesting to note

Problema directo

SIMPLEX

$$\frac{Nv_p}{V}$$

$$R_{difusa}\underbrace{(\lambda_0,\tilde{n}_p,\tilde{n}_M,r_i,r_s;\overbrace{a_0,\sigma};f,d)}_{\text{11 parámetros}}$$



No todos los parámetros son iguales….

más precisos...	λ_0, f
más accesibles…	d
accesibles…	n_p, n_M
problemáticos…	a_0, σ, r_i
más sensibles…	κ_M, a_0, σ, κ_p (*f* alta)
inaccesibles…	r_s

Ajustes

r_s → negro
blanco (en aire)

r_i → medio
efectivo

Use and abuse of the effective refractive index in colloidal systems

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Abstract

laboratorio

$\kappa_M \longrightarrow$ Medición utilizando ATR

$\kappa_p \longrightarrow$ Medición utilizando técnicas fototérmicas

$\left\{ \begin{array}{l} 10^{-5} - \kappa_p - 10^{-6} \\ \text{coloide} \end{array} \right.$

J. Phys. IV France **125** (2005) 153-156

DOI: 10.1051/jp4:2005125035

Measurement of low optical absorption in highly scattering media using the thermal lens effect

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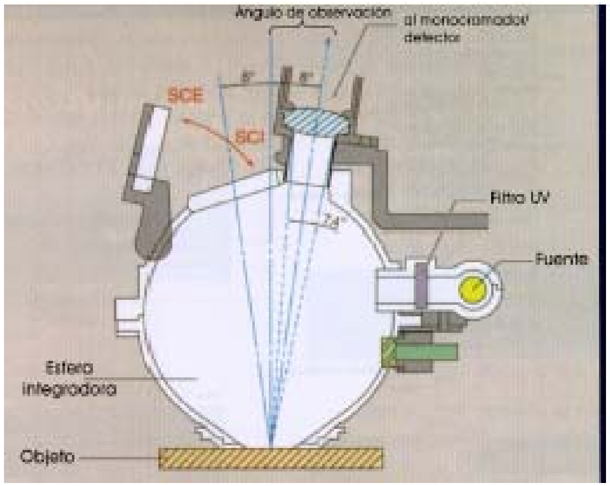
Abstract. In this work we show that the thermal lens effect can be applied to highly scattering and weakly absorbing materials. We apply the thermal lens effect and the z-scan technique to estimate the effective absorption coefficient of a suspension of TiO_2 particles with a mean diameter of 220 nm at two wavelengths: 488 nm and 514 nm. From the effective absorption coefficient we estimate the absorption cross section of the particles.

Comparación con el experimento

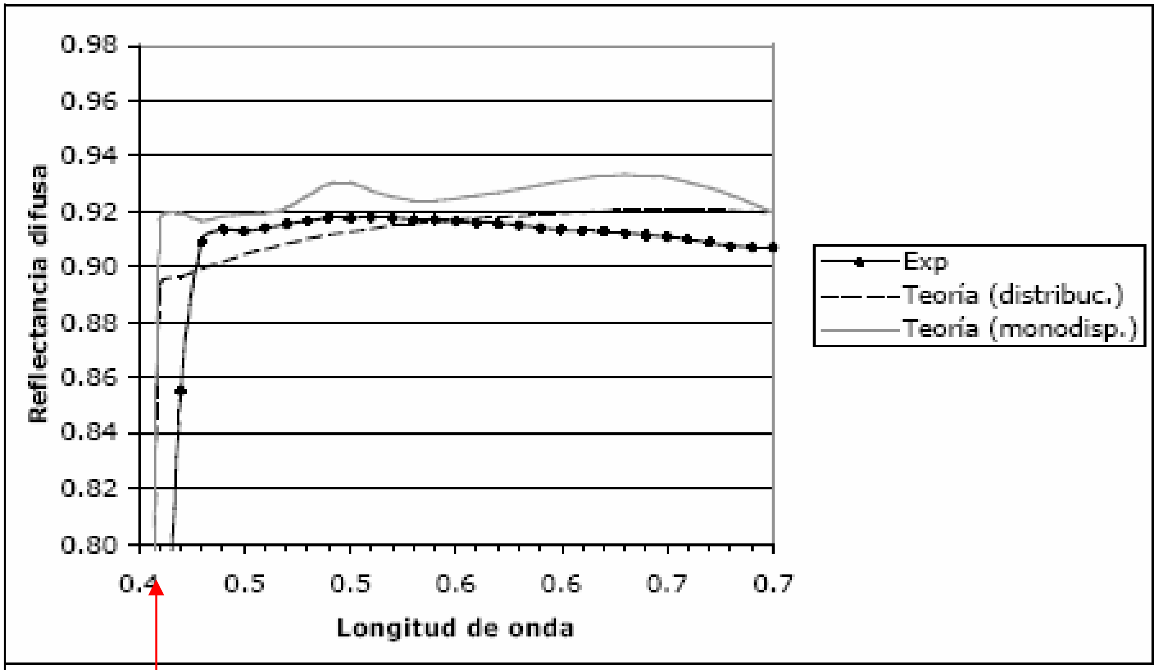
$$R_{difusa}(\lambda_0, \tilde{n}_p, \tilde{n}_M, r_i, r_s; \underbrace{a_0, \sigma}_{\text{“cota”}}; f, d)$$



espectrofotómetro

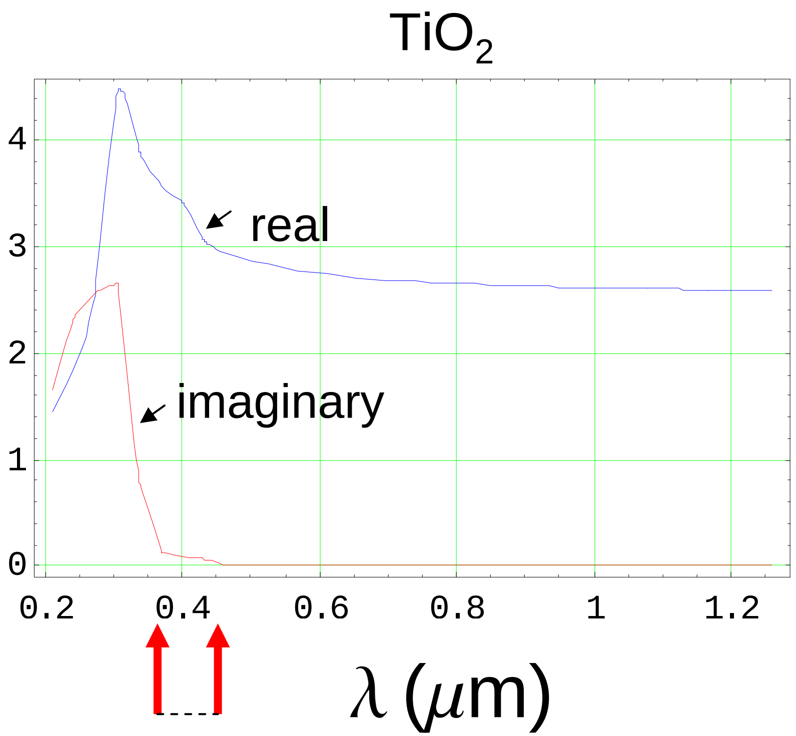
$$R^{exp}_{difusa}$$

simplex



“ajustes”

ajustes



Ajuste sistemático ⇐ Algoritmo de ajuste multiparamétrico

CIMAT

Pintura blanca

Pintura = simplex + cargas + dispersantes

EXP : R_d más sensible a (a_0 , σ)

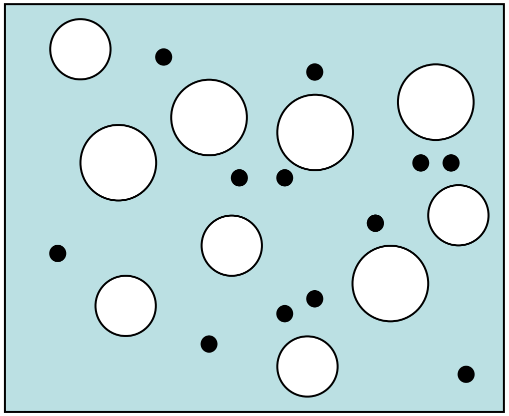
Estudios con distintos grados de dispersión del pigmento

Tesis

Las cargas absorben menos que la resina, por lo que la absorción total disminuye, y eso afecta las propieades ópticas…

→ nueva línea de investigación

…se tomaban como “ópticamente pasivas”..



CONTINUARLA…

Bases

Bases = simplex + negro + cargas + dipersantes

Problema directo

(i) $\tilde{n}_B = n_B + i\kappa_B \longrightarrow S_{ij}^B$

(ii) distribución de tamaños $\longrightarrow \langle S_{ij}^B \rangle$

$\Big\}$ 4 parámetros

(iii) distribución de aire (estructura de la película) $\longrightarrow \langle S_{ij}^{aire} \rangle$

$$S_{ij} = f_p \langle S_{ij}^p \rangle + f_B \langle S_{ij}^B \rangle + f_{aire} \langle S_{ij}^{aire} \rangle \longrightarrow \boxed{R_{difusa}^{exp}(\lambda_0)}$$

Problema inverso

$$R_{difusa}^{medido}(\lambda_0) \xrightarrow{\hspace{2cm}} (f_p, f_B)$$

ALGORITMO

PRECISION

$$\left| R_{difusa}^{medido}(\lambda_0) - R_{difusa}^{exp}(\lambda_0) \right|^2 \leq \delta$$

TRI-ESTIMULO

$$R_y = \int_{\lambda_1}^{\lambda_2} w(\lambda_0)\, R_{difusa}^{exp}(\lambda_0)$$

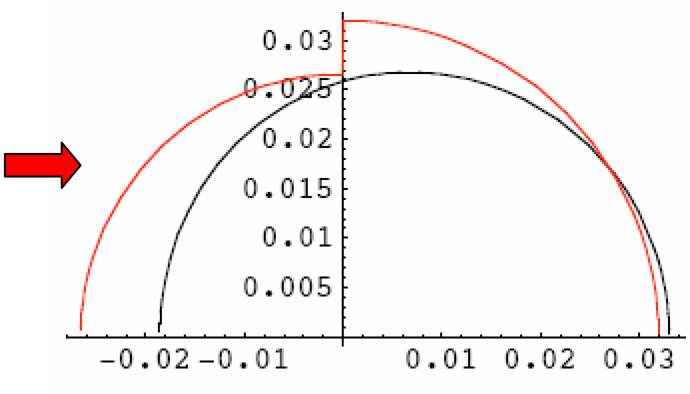
$$\left| R_y - R_y^{medido} \right|^2 \leq \delta$$

Kubelka-Munk

N flujos → 2 flujos (KM)

$S_{ij} \rightarrow S, K$

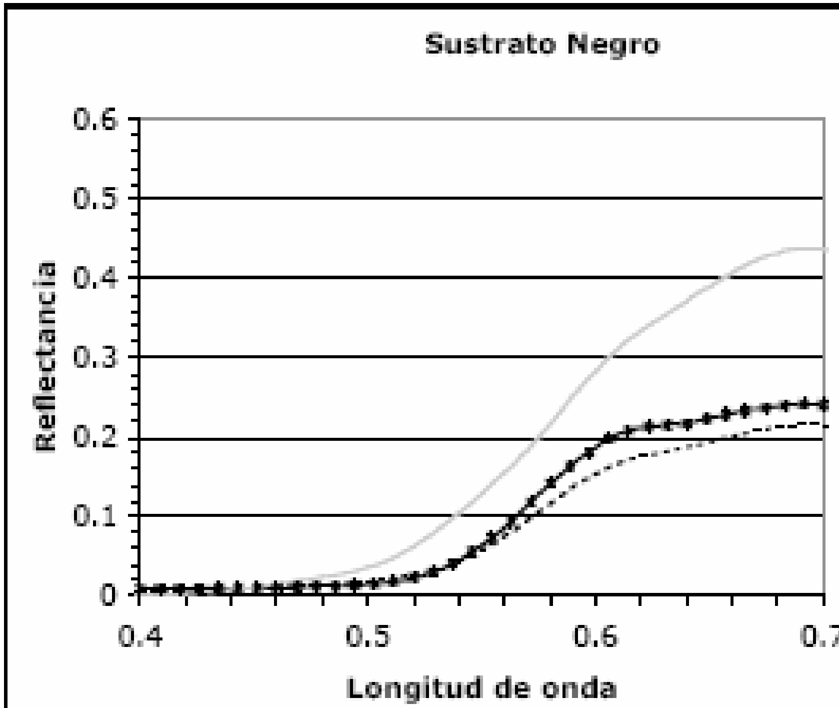
$\frac{K}{S} \ll 1$



F_- F_+

N flujos = 2 flujos

TiO_2 *alto PVC*



Fe_2O_3

$PVC = 5\%$
$d = 25\mu m$

Ventajas

$$\tilde{n}_B = n_B + i\kappa_B \longrightarrow \left(s_B = \frac{S_B}{f}, k_B = \frac{K_B}{f} \right)$$

$$R^{\exp}_{difusa}(\lambda_0, d, s_p, k_p, s_B, k_B, r_i, r_s; a_0^p, \sigma^p; a_0^B, \sigma^B, f_p, f_B)$$

$$\left.\begin{aligned} S &= f_p \langle s_p \rangle + f_B \langle s_B \rangle \\ K &= f_p \langle k_p \rangle + f_B \langle k_B \rangle \end{aligned}\right\} \quad R^{\exp}_{difusa}(\lambda_0, d, S, K, r_i, r_s)$$

$$R^{\exp}_{difusa}(\lambda_0) \longrightarrow (f_p, f_B)$$

ALGORITMO

Parámetros

$$R_{B,difuso}^{medido}(\lambda_0) \longrightarrow (s_B, k_B)$$

$$R_{p,difuso}^{medido}(\lambda_0) \longrightarrow (s_p, k_p)$$

Cubriente total

$$R_\infty^{KM} = 1 + \frac{K}{S} - \sqrt{\left(1 + \frac{K}{S}\right)^2 - 1}$$

$$\frac{K}{S} = f_p \left\langle \frac{k_p}{s_p} \right\rangle + f_B \left\langle \frac{k_B}{s_B} \right\rangle$$

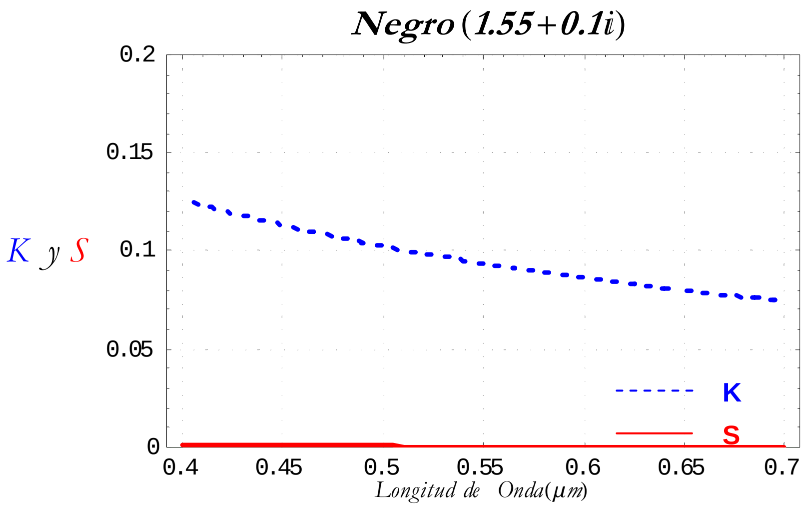
$$R_{difusa}^{\exp}(R_\infty^{KM}, d, r_i, r_s)$$

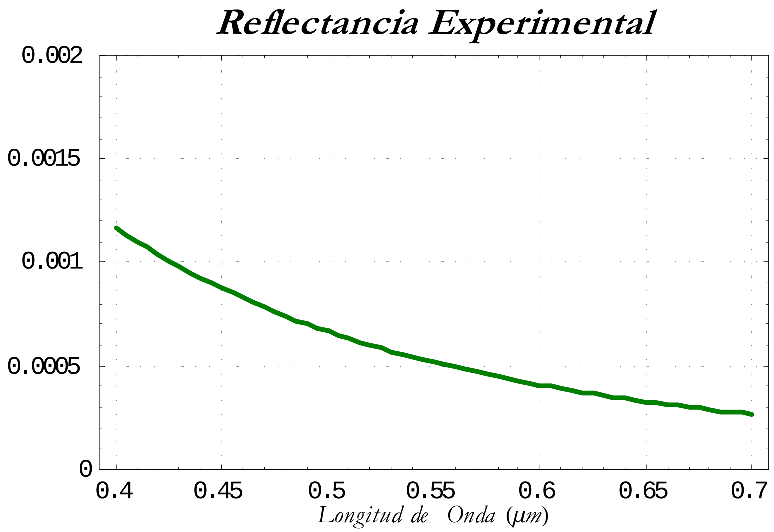
el negro

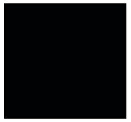
$$\tilde{n}_B = n_B + i\kappa_B$$

<u>Caso 1:</u> nP= 1.55+0.1*i*

COEFICIENTES DE ABSORCIÓN Y ESPARCIMIENTO DE KUBELKA-MUNK Y REFLECTANCIA



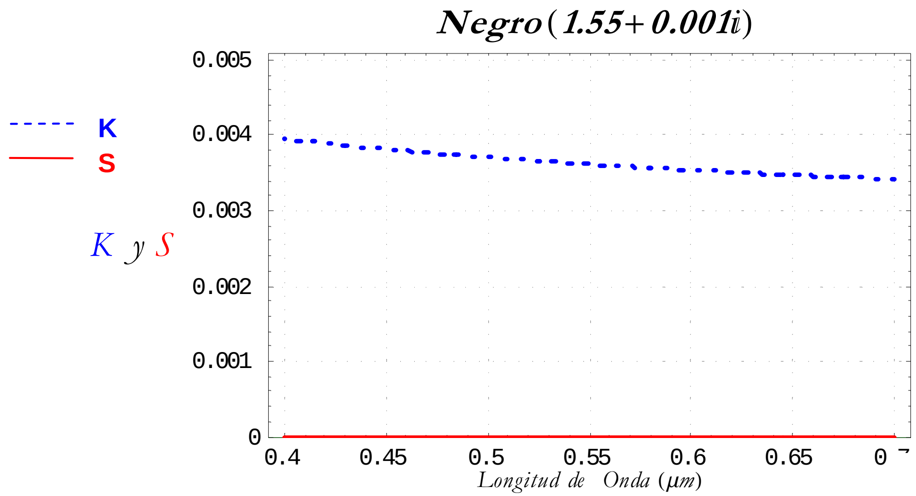


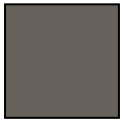


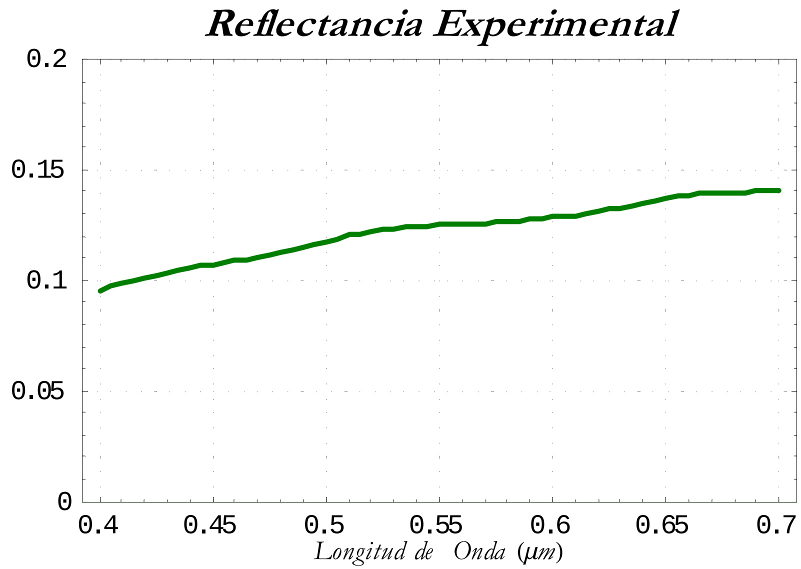
Negros con distintos Índices de refracción sobre sustrato blanco, (CREELL), f = 4%, r = 0.03μm, X=150

Caso 2: nP= *1.55+0.001i*

COEFICIENTES DE ABSORCIÓN Y ESPARCIMIENTO DE KUBELKA-MUNK Y REFLECTANCIA



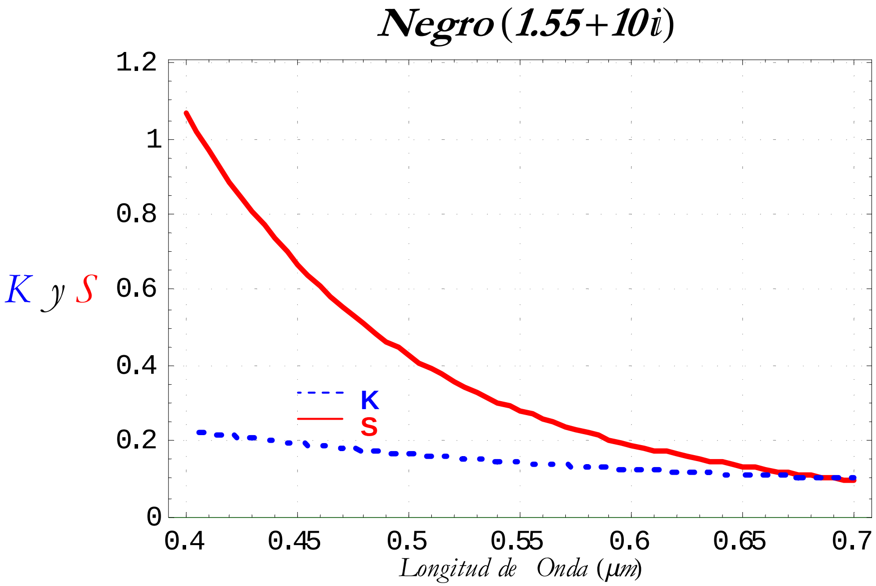


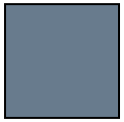


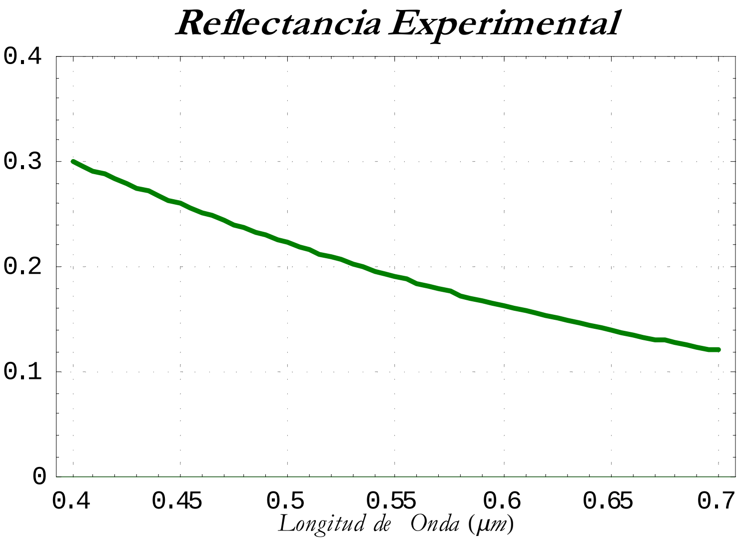
Negros con distintos Índices de refracción sobre sustrato blanco, (CREELL), f = 4%, r = 0.03μm, X=150

<u>Caso 3:</u> nP= *1.55+10i*

COEFICIENTES DE ABSORCIÓN Y ESPARCIMIENTO DE KUBELKA-MUNK Y REFLECTANCIA



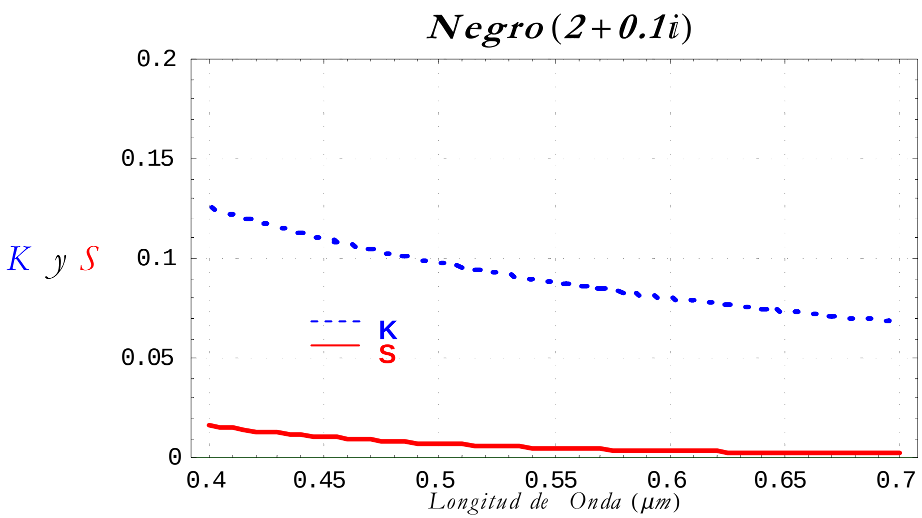


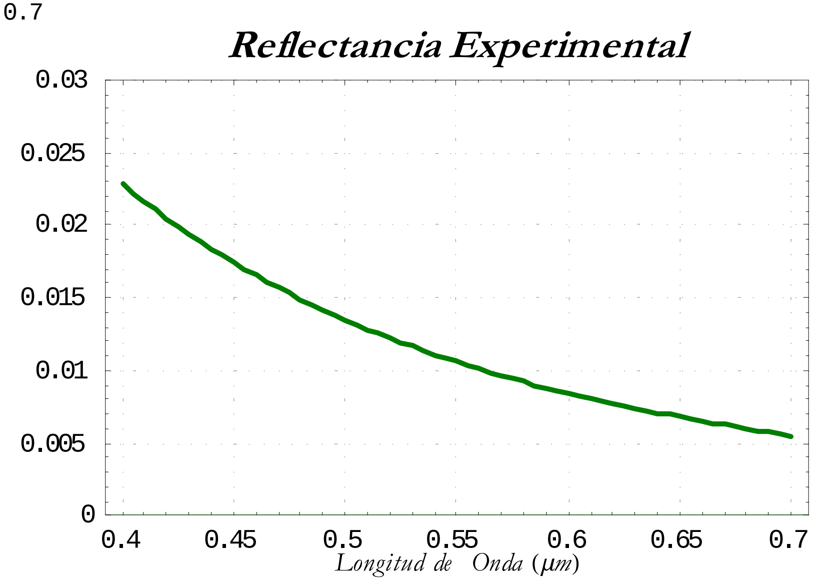


Negros con distintos Índices de refracción sobre sustrato blanco, (CREELL), f = 4%, r = 0.03μm, X=150

Caso 5: nP= *2+0.1i*

COEFICIENTES DE ABSORCIÓN Y ESPARCIMIENTO DE KUBELKA-MUNK Y REFLECTANCIA





Negros con distintos Índices de refracción sobre sustrato blanco, (CREELL), f = 4%, r = 0.03μm, X=150