Describing the optical properties of astronomical dust analogs through numerical techniques

Giuseppe Cataldo[1,2] S. Rinehart[1] D. Benford[1] E. Dwek[1]
R. Kinzer[1,3] J. Nuth[1] E. Wollack[1]

[1]NASA Goddard Space Flight Center

[2]Universities Space Research Association

[3]Oak Ridge Associated Universities

From Dust to Galaxies, Paris, 06/30/2011

Outline

1. Introduction
   - The interstellar medium in the infrared
   - The quest for the optical constants
2.
   - Previous work
   - Methodology
3.
   - Experimental data and apparatus
   - Analytical outputs
4.
   - Conclusions
   - Future perspectives

Outline

1. Introduction
   - The interstellar medium in the infrared
   - The quest for the optical constants
2. Modeling
   - Previous work
   - Methodology

- Experimental data and apparatus
- Analytical outputs

- Conclusions
- Future perspectives

Outline

1. Introduction
   - The interstellar medium in the infrared
   - The quest for the optical constants
2. Modeling
   - Previous work
   - Methodology
3. Results
   - Experimental data and apparatus
   - Analytical outputs
4. Summary
   - Conclusions
   - Future perspectives

Outline

1. Introduction
   - The interstellar medium in the infrared
   - The quest for the optical constants
2. Modeling
   - Previous work
   - Methodology
3. Results
   - Experimental data and apparatus
   - Analytical outputs
4. Summary
   - Conclusions
   - Future perspectives

The relation between dust and the infrared

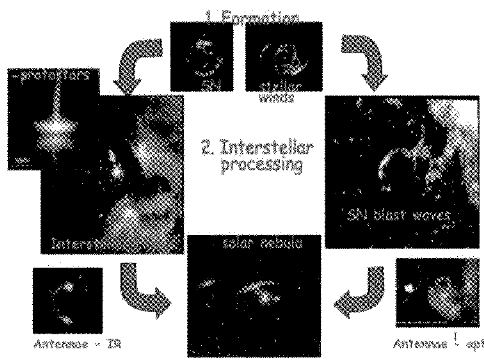


Figure: Formation, processing, and evolution of interstellar dust (Rinehart et al., 2008)

Interstellar dust:

- plays a role in the birth of stars
- precursor material for the formation of planets
- hides astronomical objects from our view

The relation between dust and the infrared

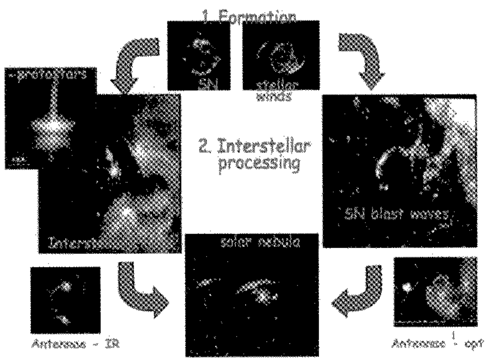


Figure: Formation, processing, and evolution of interstellar dust (Rinehart et al., 2008)

Interstellar dust:

- plays a role in the birth of stars
- precursor material for the formation of planets
- hides astronomical objects from our view

Infrared observations are crucial to understanding the origins of the universe.

The importance of studying silicates

Spectral features attributed to:

- silicates
- carbonaceous grains
- PAHs

[illegible] on chemical and physical structure

Their spectra need be analyzed through laboratory experiments reproducing astrophysical environments (See Henning & Mutschke 2010)

The importance of studying silicates

Spectral features attributed to:

- silicates
- carbonaceous grains
- PAHs

Constraints on chemical and physical structure

Their spectra need be analyzed through laboratory experiments reproducing astrophysical environments. (See Henning & Mutschke, 2010)

The importance of studying silicates

Spectral features attributed to:

- silicates
- carbonaceous grains
- PAHs

Constraints on chemical and physical structure

Their spectra need be analyzed through laboratory experiments reproducing astrophysical environments. (See Henning & Mutschke, 2010)

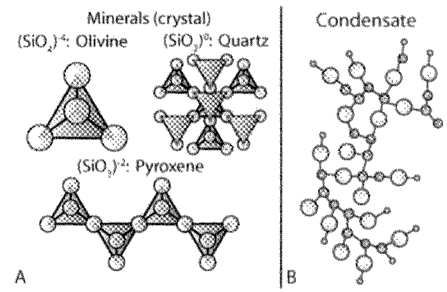


Figure: A) Silicates on Earth are ordered solids. B) In space their structure is chaotic. (Adapted from Rinehart et al., 2008)

The optical constants as primary parameters

Definition

Complex refractive index $m = n + ik$

- The refractive index n determines the velocity of constant-phase waves.
- The extinction index k determines the attenuation of the wave as it propagates through the medium.

Dielectric constant [illegible] $(n + ik)$ [illegible]

[illegible] the optical constants are not directly [illegible]

The optical constants as primary parameters

Definition

Complex refractive index $m = n + ik$

- The refractive index n determines the velocity of constant-phase waves.
- The extinction index k determines the attenuation of the wave as it propagates through the medium.

Definition

Dielectric constant $\varepsilon = (n + ik)^2 = \varepsilon' + i\varepsilon''$

However, the optical constants are not directly measurable

The optical constants as primary parameters

Definition

Complex refractive index $m = n + ik$

- The refractive index n determines the velocity of constant-phase waves.
- The extinction index k determines the attenuation of the wave as it propagates through the medium.

Definition

Dielectric constant $\varepsilon = (n + ik)^2 = \varepsilon' + i\varepsilon''$

Problem: the optical constants are not directly measurable.

Objectives of the OPASI-T program

- Experimental apparatus and measurements
- Development of [illegible] for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to [illegible]
- Analysis and interpretation of post-processed data
- Population of a [illegible] of optical properties in the far infrared regime

Objectives of the OPASI-T program

- Experimental apparatus and measurements
- Development of numerical algorithms for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to [illegible]
- Analysis and interpretation of post-processed data
- Population of a [illegible] of optical properties in the far infrared regime

Objectives of the OPASI-T program

- Experimental apparatus and measurements
- Development of numerical algorithms for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to laboratory data
- Analysis and interpretation of post processed data
- Population of a [illegible] of optical properties in the far infrared regime

Objectives of the OPASI-T program

- Experimental apparatus and measurements
- Development of numerical algorithms for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to laboratory data
- Analysis and interpretation of post-processed data
- Population of a [illegible] of optical properties in the far infrared regime

Objectives of the OPASI-T program

- Experimental apparatus and measurements
- Development of numerical algorithms for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to laboratory data
- Analysis and interpretation of post-processed data
- Population of a library of optical properties in the far-infrared regime

Hypotheses and mathematical models

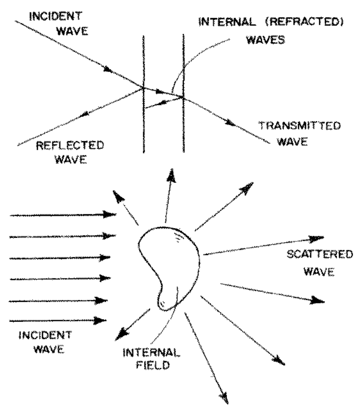


Figure: Analogy between scattering by a particle and transmission-reflection-absorption by a slab (Bohren and Huffman, 1983)

Transmission-line approximation

- One-layer slab model (Bohren and Huffman 1983)
- Beer's law (Halpern et al 1986)

Transition modes

- Lorentz model

Mixtures

- Maxwell Garnett formul. (Maxwell Garnett 1904)

Hypotheses and mathematical models

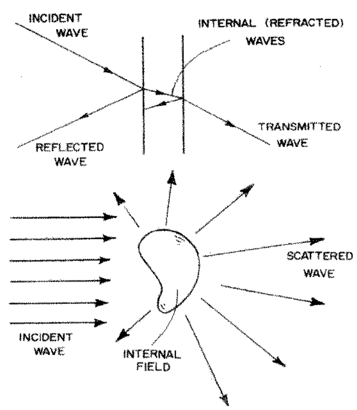


Figure: Analogy between scattering by a particle and transmission-reflection-absorption by a slab (Bohren and Huffman, 1983)

Transmission-line approximation

- One-layer slab model (Bohren and Huffman, 1983)
- Beer's law (Halpern et al., 1986)

Transition modes

- Lorentz model

Mixtures

- Maxwell-Garnett formula (Maxwell Garnett, 1904)

Hypotheses and mathematical models

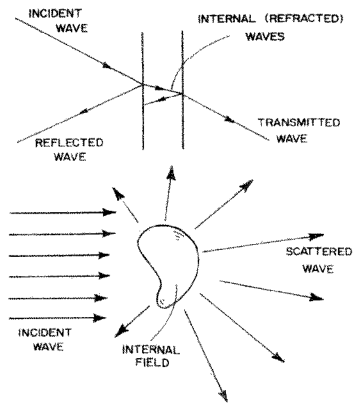


Figure: Analogy between scattering by a particle and transmission-reflection-absorption by a slab (Bohren and Huffman, 1983)

Transmission-line approximation

- One-layer slab model (Bohren and Huffman, 1983)
- Beer's law (Halpern et al., 1986)

Transition modes

- Lorentz model

Mixtures

- Maxwell-Garnett formula (Maxwell Garnett, 1904)

Hypotheses and mathematical models

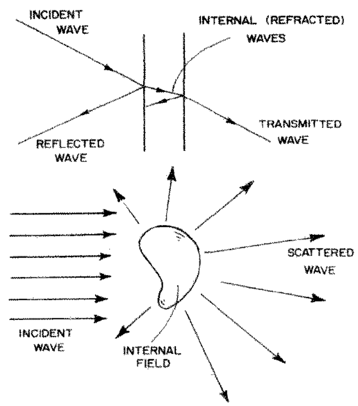


Figure: Analogy between scattering by a particle and transmission-reflection-absorption by a slab (Bohren and Huffman, 1983)

Transmission-line approximation

- One-layer slab model (Bohren and Huffman, 1983)
- Beer's law (Halpern et al., 1986)

Transition modes

- Lorentz model

Mixtures

- Maxwell-Garnett formula (Maxwell Garnett, 1904)

Constrained minimization as main working tool

Definition (Least-Squares Nonlinear Fit)

$$\min_{DOFs}\chi_m^2 = \min_{DOFs}\frac{1}{N}\sum_{j=1}^{N}\left[T\left(DOFs,\lambda_j\right) - T_{measured}\right]^2$$

$$DOF_{min} \leq DOF \leq DOF_{max}$$

N = number of data points
λ = wavelength

Initial condition → Fit → DOFs → $\begin{cases} T, R, A \\ n, k \end{cases}$

Constrained minimization as main working tool

Definition (Least-Squares Nonlinear Fit)

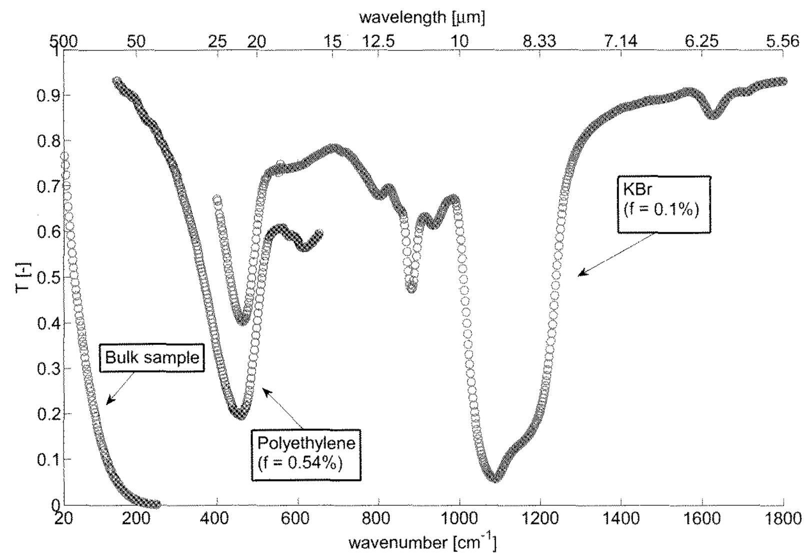
$$\min_{DOFs}\chi_m^2 = \min_{DOFs}\frac{1}{N}\sum_{j=1}^{N}\left[T\left(DOFs,\lambda_j\right) - T_{measured}\right]^2$$

$$DOF_{min} \leq DOF \leq DOF_{max}$$

$$\begin{aligned} N &= \text{number of data points} \\ \lambda &= \text{wavelength} \end{aligned}$$

$$\text{Initial condition} \longrightarrow \text{Fit} \longrightarrow DOFs \longrightarrow \begin{cases} T, R, A \\ n, k, \varepsilon \end{cases} \forall\lambda_j$$

SiO_x: Measured transmission spectrum at room temperature



SiO_x: Sample characterization

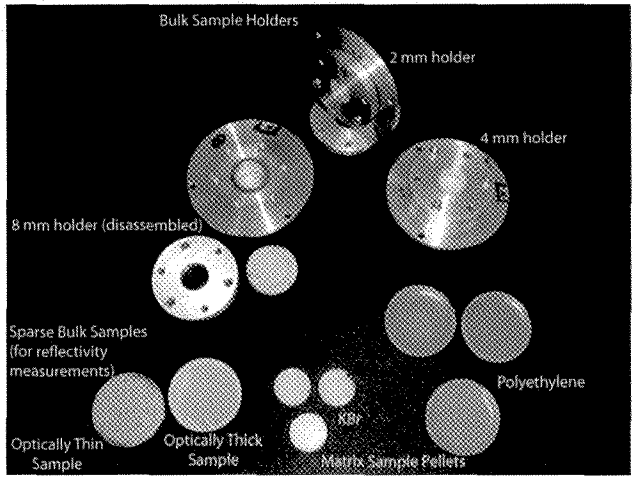


Figure: Various sample preparations are needed to cover the wide frequency range (Rinehart, Cataldo, et al., *Applied Optics*, in press).

SiO_x: Sample characterization

Each sample preparation has a different optical depth, which allows us to obtain transmission values in the range of 0.2-0.8 as needed to determine the optical constants to high accuracy.

Sample type	Spectral coverage [μm]
8-mm	300 – 1000
4-mm	100 – 500
2-mm	100 – 350
Polyethylene	15 – 100
KBr	1 – 25

SiO_x: How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$\alpha = a \left(\frac{\omega}{2\pi}\right)^b$$

h = sample thickness

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega} \left(\frac{\omega}{2\pi}\right)^{b-1}$$

$$T = T(n, a, b)$$

SiO_x: How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega}\left(\frac{\omega}{2\pi}\right)^{b-1}$$

$$\alpha = a\left(\frac{\omega}{2\pi}\right)^b$$

h = sample thickness

$$T = T(n, a, b)$$

SiO_x: How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$\alpha = a \left(\frac{\omega}{2\pi}\right)^b$$

h = sample thickness

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega}\left(\frac{\omega}{2\pi}\right)^{b-1}$$

$$T = T(n, a, b)$$

SiO_x: How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega}\left(\frac{\omega}{2\pi}\right)^{b-1}$$

$$\alpha = a\left(\frac{\omega}{2\pi}\right)^{b}$$

h = sample thickness

$$T = T(n, a, b)$$

SiO_x: How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega}\left(\frac{\omega}{2\pi}\right)^{b-1}$$

$$\alpha = a\left(\frac{\omega}{2\pi}\right)^{b}$$

h = sample thickness

$$T = T(n, a, b)$$

SiO_x: How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, \varepsilon_i\right)$$

SiO_x: How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, \varepsilon_i\right)$$

Lorentz model

$$\varepsilon_i = (n + ik)^2 = \varepsilon_{i,\infty} + \sum_{j=1}^{M} b_m \frac{\omega_{p,j}^2}{\omega_{0,j}^2 - \omega^2 - i\omega\nu_j} = \varepsilon_i(DOFs, \omega)$$

SiO_x: How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, \varepsilon_i\right)$$

Lorentz model

$$\varepsilon_i = (n + ik)^2 = \varepsilon_{i,\infty} + \sum_{j=1}^{M} b_m \frac{\omega_{p,j}^2}{\omega_{0,j}^2 - \omega^2 - i\omega\nu_j} = \varepsilon_i\left(DOFs_i, \omega\right)$$

SiO_x: How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, \varepsilon_i\right)$$

Lorentz model

$$\varepsilon_i = (n + ik)^2 = \varepsilon_{i,\infty} + \sum_{j=1}^{M} b_m \frac{\omega_{p,j}^2}{\omega_{0,j}^2 - \omega^2 - i\omega\nu_j} = \varepsilon_i\left(DOFs_i, \omega\right)$$

Modified Lorentz model (Sihvola, 1999)

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, DOFs_i, \omega\right)$$

SiO_x: How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, \varepsilon_i\right)$$

Lorentz model

$$\varepsilon_i = (n + ik)^2 = \varepsilon_{i,\infty} + \sum_{j=1}^{M} b_m \frac{\omega_{p,j}^2}{\omega_{0,j}^2 - \omega^2 - i\omega\nu_j} = \varepsilon_i\left(DOFs_i, \omega\right)$$

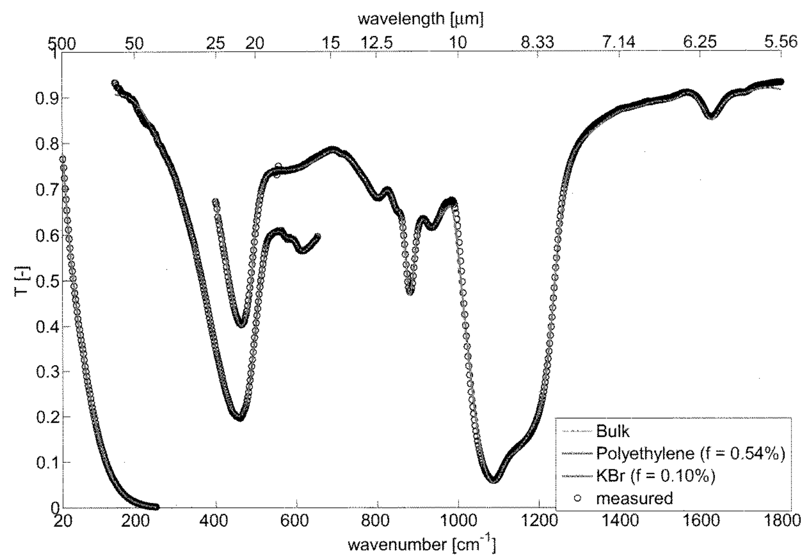
Modified Lorentz model (Sihvola, 1999)

$$\varepsilon_{eff} = \varepsilon_{eff}\left(f, \varepsilon_b, DOFs_i, \omega\right)$$

One-layer slab model (averaged)

$$T = T\left[f, \varepsilon_b, (4M+1)DOFs_i, \omega\right]$$

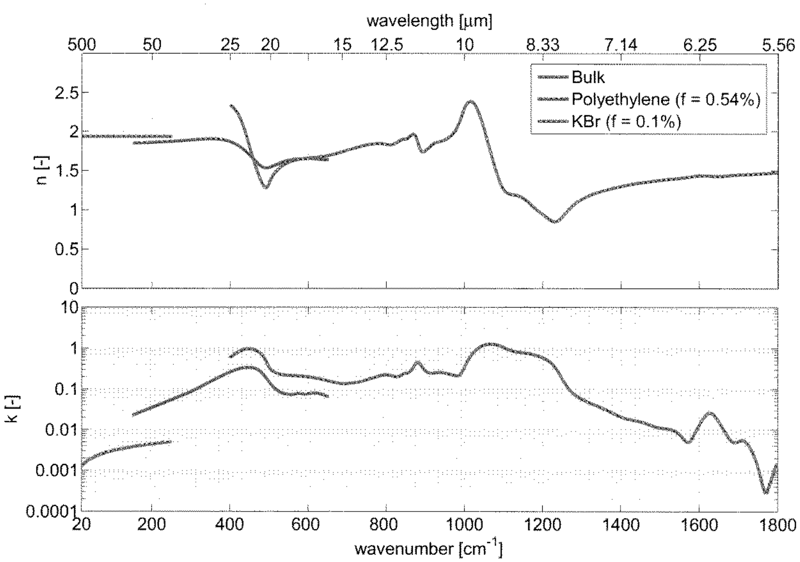
SiO_x: Fit and output parameters (Cataldo et al., in prep.)



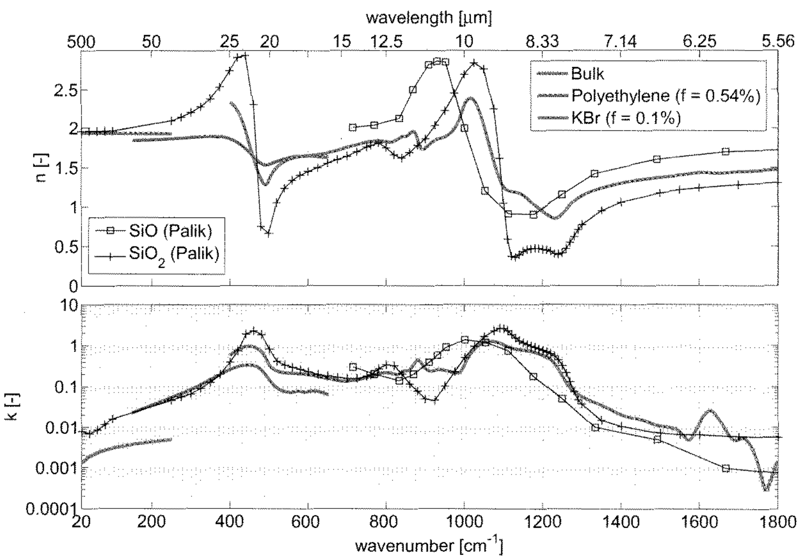
SiO_x: Fit and output parameters

		Bulk (4-mm)	Polyethylene	KBr
DOFs		3	53 (13 LOs)	153 (38 LOs)
Residual	average	0.32	0.62	0.25
ΔT [%]	maximum	2.68	3.93	1.47
χ^2_m		$2.55 \cdot 10^{-5}$	$11.12 \cdot 10^{-5}$	$1.29 \cdot 10^{-5}$
σ		0.005	0.012	0.008
χ^2		109.89	239.81	146.26
χ^2_ν		0.93	1.15	0.25

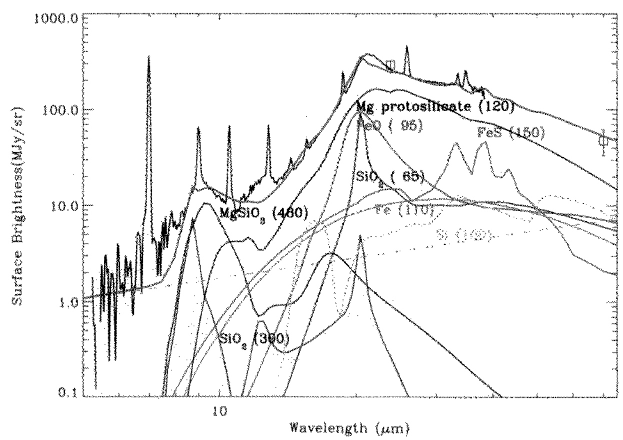
SiO_x: The optical constants in the FIR and MIR



SiO_x: The optical constants in the FIR and MIR



SiO_x: The optical constants in the FIR and MIR



(Adapted from Rho et al., 2008)

Our sample description

	Advantages	Disadvantages
Bulk sample	n consistent with other measurements	n not well constrained
	$a = 0.003$, $b = 1.552$ (Agladze et al., 95;...)	Need for data at longer wavelengths
Mixture	$n - k$ independent from filling fraction	$n - k$ dependent on matrix
	$x \approx 1.5$	Fine-tuning of starting guess
	DOFs well constrained	
	Outputs for mix and particles	Uncertainty in measurements

Next steps

- Measured reflectance data (TOP PRIORITY)
- [illegible] dependence (Cataldo et al., in prep.)
- Development of more sophisticated models
  - [illegible] powders: Fe- and Mg-rich silicates (Kinzer, Cataldo, et al., in prep.)
  - [illegible]
  - Multiple-layered structures
  - Unparalleled faces and roughness
- Application to [illegible] upcoming laboratory data and observations

Next steps

- Measured reflectance data (TOP PRIORITY)
- Temperature dependence (Cataldo et al., in prep.)
- Development of more sophisticated models
  - [illegible] powders: Fe- and Mg-rich silicates (Kinzer, Cataldo et al., in prep.)
  - [illegible]
  - Multiple layered structures
  - Unparallel faces and roughness
- Application to new upcoming laboratory data and observations

Next steps

- Measured reflectance data (TOP PRIORITY)
- Temperature dependence (Cataldo et al., in prep.)
- Development of more sophisticated models
  - Metal-enriched powders: Fe- and Mg-rich silicates (Kinzer, Cataldo, et al., in prep.)
  - Scattering
  - Multiple-layered structures
  - Unparalleled faces and roughness
- Application to the upcoming laboratory data and observations

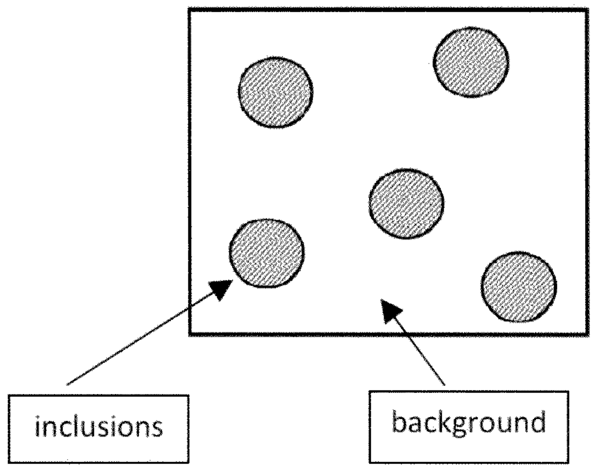
Next steps

- Measured reflectance data (TOP PRIORITY)
- Temperature dependence (Cataldo et al., in prep.)
- Development of more sophisticated models
  - Metal-enriched powders: Fe- and Mg-rich silicates (Kinzer, Cataldo, et al., in prep.)
  - Scattering
  - Multiple-layered structures
  - Unparalleled faces and roughness
- Application to new upcoming laboratory data and observations

Thanks!
Questions?

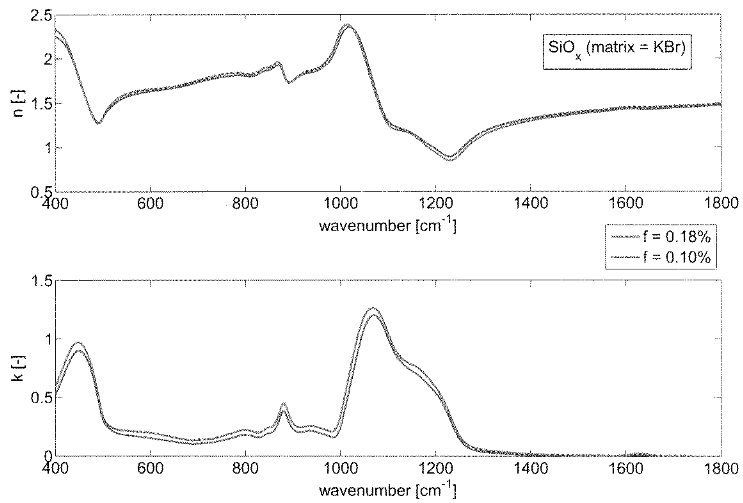
The effective medium structure

Back

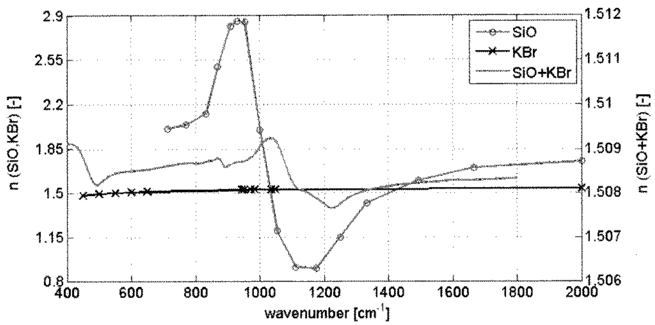


The optical constants as a function of filling fraction

◄ Back

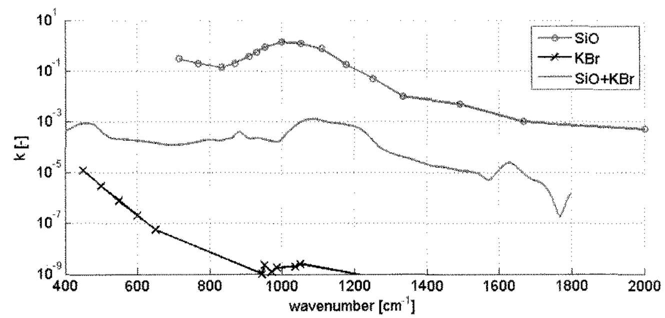


The optical constants for the $SiO_x - KBr$ mixture



(Rinehart, Cataldo, et al., *Applied Optics*, in press)

The optical constants for the $SiO_x - KBr$ mixture



(Rinehart, Cataldo, et al., *Applied Optics*, in press)